Interplay of Magnetism and Superconductivity in Strongly Correlated Electron Systems

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Abstract

This thesis considers various aspects of the interplay between superconductivity and magnetism in strongly correlated electron systems.

Chapter 2 studies the effects of weak translational symmetry breaking on the quasiparticle spectrum of a \(d\)-wave superconductor. A general formalism is developed to discuss periodic charge order, as well as quasiparticle scattering off localized defects. I argue that STM experiments on \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}\) cannot be explained using a simple charge density wave order parameter, but are consistent with the presence of a periodic modulation in the electron hopping or pairing amplitude. I also discuss the effects of randomness and pinning of the charge order and compare it to the impurity scattering of quasiparticles.

Chapter 3 explores the possibility of direct detection of spin nematic order: a state which breaks spin SU(2) symmetry while preserving translational and time reversal symmetries. Spin nematic order can arise naturally from charge fluctuations of a spin stripe state. The nematic is a spin-two operator, and therefore does not couple directly to neutrons. However, I show that neutron scattering and Knight shift experiments can detect the spin anisotropy of electrons moving in a nematic background. I build a nematic wave function starting from a \(t-J\) type model, and analyze the mean field phase diagram for the nematic taking into account spin-orbit effects.

Finally, in Chapters 4 and 5, I investigate the competition between antiferromagnetism and triplet superconductivity in quasi one-dimensional Bechgaard salts, unifying the two orders in an SO(4) symmetric framework. I demonstrate the existence of such symmetry in one-dimensional Luttinger liquids, and argue that approximate SO(4) symmetry remains valid even when interchain hopping is strong enough to turn the system into a strongly anisotropic Fermi liquid. SO(4) symmetry, which strongly constrains the phase diagram, can explain coexistence regions between antiferromagnetic, superconducting, and normal phases, as observed in \((\text{TMTSF})_2\text{PF}_6\). I discuss experimental tests of the SO(4) symmetry, including the prediction of a sharp resonance in neutron scattering experiments on superconducting samples.
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Chapter 1

Introduction

1.1 General outlook

This work deals primarily with the interplay between magnetism and superconductivity in low dimensional systems. These are materials with highly anisotropic band structures, such as the quasi-two dimensional high temperature cuprates and heavy-fermion superconductors, and the quasi-one dimensional organic superconductors. Despite having drastically different lattice structures and microscopic interactions, these systems have a number of properties in common which distinguish them from conventional superconductors, such as strong Coulomb interactions, the formation of superconducting pairs with non-zero angular momentum, and strong fluctuations due to reduced dimensionality. Perhaps most importantly, the normal state in these materials shows strong deviations from Fermi liquid behavior, which precludes a conventional description of the onset of superconductivity in terms of the Bardeen-Cooper-Schrieffer (BCS) mechanism. In this sense, these materials are “strongly correlated”. In addition, these materials generically display a wealth of magnetic phases that lie close to and sometimes even overlap with the superconductivity. While the nature of the interaction between superconductivity and magnetism in these materials is not well-established, such an understanding is likely to shed light into many of their properties, including possibly the nature of the normal state and the mechanism by which the superconductivity is attained in these compounds. This is in sharp contrast to conventional superconductors, which are good metals at high temperatures. The low energy excitations in the metallic state are well-defined fermionic quasiparticles, as prescribed by Landau’s theory of Fermi liquids[109, 108, 110]. At low temperatures, for arbitrarily weak attraction, these quasiparticles are unstable to the formation of Cooper pairs, which condense to form a superconductor according to the BCS theory[10]. The combination of these two theories provides a paradigm by which most of the low energy electronic properties in metals are quantitatively understood. Unlike the unconventional case, no low energy instabilities other than superconductivity are observed.
Among the themes treated in this work are: i) The interaction between magnetic order and fermionic quasiparticles within a superconductor. In particular, in Chapter 2, I will look at the effect of various types of translational symmetry breaking order parameters on the electronic local density of states. Comparing these results to STM measurements carried out on Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$[72, 73, 74, 75] will place constrains on the possible nature of the order involved. In addition, I will study the experimental signatures of non-magnetic impurities on electronic inhomogeneity[151]. Chapter 3 will discuss the effects of a spin nematic state on electron dynamics. I will show that nematic order induces anisotropy in the electronic spin response which can be detected in Knight shift and neutron scattering experiments[150]. ii) The interplay in low dimensional systems between nesting of the Fermi surface, which favors spontaneous breaking of symmetry, and strong thermal and quantum fluctuations, which tend to restore this symmetry. This leads to the Luttinger liquid picture for one dimensional electronic systems which is used, in Chapters 4 and 5, to study the quasi-one dimensional Bechgaard salts. iii) The possible existence of a higher symmetry group uniting superconducting and magnetic orders. Such symmetry can sometimes be found in microscopic models, and can be an important guiding principle in understanding regions in the phase diagram where these phases coexist or are in close proximity. This principle is applied, in the analysis of Chapters 4 and 5, to constrain the phase diagram and low energy excitations of Bechgaard salts in the proximity of the antiferromagnetic/superconducting phase transition.

In the remainder of the Introduction I will give an overview of some of the phenomenology of the high temperature cuprates and of the quasi one-dimensional superconductors, with an emphasis on the themes outlined above. This will be preceded by a brief discussion of Fermi liquid theory, which will help highlight some of the unusual properties of the materials discussed in this work.

### 1.1.1 Fermi liquid theory and BCS superconductivity

Many-body Coulomb interactions provide a serious challenge in condensed matter systems, as they are typically of the same order of magnitude as the electronic kinetic energy[63]. This prevents us from taking the Fermi gas as a viable starting point and using perturbation theory to systematically take the effects of interactions into account (or, conversely, from starting with a strongly interacting ground state and treating the kinetic energy as a perturbation). However, as shown by Landau, the description of the low energy properties of these systems can often be made in terms of weakly interacting fermionic excitations.

In a Fermi liquid, close to the Fermi surface, well-defined fermionic quasiparticles, with the same charge and spin quantum numbers as individual electrons, survive the electron-electron interactions. In particular, just as in a non-interacting Fermi gas, there is a step discontinuity in the Fermi occupation number at zero temperature, which allows to define a Fermi surface, although the discontinuity is smaller than one
due to interactions (on the other hand, the volume enclosed by the Fermi surface is left invariant by the interactions, as proved non-perturbatively in Luttinger’s theorem). The interactions renormalize the quasiparticle mass and introduce a finite quasiparticle lifetime $\tau$ due to scattering. However, the Pauli exclusion principle constrains strongly the available phase space for this scattering, limiting the scattering rate at low energies $1/\tau \sim \epsilon^2$ for three dimensional systems. Thus, for small enough energy $\epsilon$, these quasiparticles are well-defined (underdamped) as their energy is larger than their scattering rate. This description is particularly well-suited for a conventional metal, where the Fermi energy is of the order of $1eV \approx 10000K$, whereas typical experiments are carried out at much smaller temperatures, of the order of $1$ to $300 K$. The Fermi liquid theory predicts universal low temperature dependencies for many measurable quantities. For instance, the scattering rate $1/\tau$ affects various transport properties and leads naturally to a low temperature dependence of the resistivity $\rho \sim T^2$.

Note that Landau’s derivation of the Fermi liquid relies on a self-consistency argument, and is valid even when the Coulomb interactions are strong. In fact, for an instability to a different state to occur, one needs either extremely strong interactions or interactions of a special form. For instance, for very strong repulsion, Mott insulator and Wigner crystal behaviors can be stabilized, depending on the presence or absence of a lattice. On the other hand, due to Fermi surface nesting, arbitrarily weak repulsion is sufficient to destroy the Fermi liquid for one dimensional systems and for higher-dimensional systems with special Fermi surfaces. These cases will be discussed in more detail in Sections 1.2.2 and 1.4.

Finally, as shown by BCS, quasiparticles are unstable to the formation of Cooper pairs in the case of arbitrarily weak effective attraction between quasiparticles, leading to superconductivity. In a sense, this can be viewed as nesting in the particle-hole channel, since a particle at wave vector $k$ and a hole at $-k$ are automatically degenerate at the Fermi surface, leading to a logarithmic divergence in the pairing susceptibility $\chi_{\text{pair}}(T)$ at low temperatures. On a mean-field level, the onset of superconductivity then occurs when the BCS condition is satisfied, $1 = -U\chi_{\text{pair}}(T)$ (note that this is the analogue in the particle-particle channel of the Stoner criterion in the particle-hole channel). Hence, for attractive interactions $U < 0$, for low enough temperature superconductivity is established.

Implicit in the discussion above is the fact that the main effect of the Coulomb interaction is taken into account by the formation of a Fermi liquid, and that weak residual attractive interactions are then responsible for the superconductivity. In other words, we assume that Cooper pairs are formed as bound states of well-defined quasiparticles. This is the paradigm by which conventional superconductors are understood. Hence, the existence of superconductivity in systems where the normal state exhibits non-Fermi liquid behavior presents a serious challenge. From the theoretical point of view, one-dimensional Luttinger liquids provide the only well-understood case where superconductivity emerges from non-Fermi liquid behavior. Luttinger liq-
uid physics may be responsible for superconductivity in the quasi-one dimensional Bechgaard salts and will be discussed in more detail in Section 1.4, as well as Chapters 4 and 5. We begin, however, by looking at another family of strongly correlated materials, the high temperature cuprates.

1.2 High temperature superconductivity

The superconducting state of the high-$T_c$ cuprates is remarkably BCS-like, formed by the condensation of charge $2e$ Cooper pairs in a spin-singlet state, and displays well-defined Bogolons (the fermionic excitations of a BCS superconductor), at least in the region of the Fermi surface surrounding the nodal points [87]. Unlike conventional superconductors, Cooper pairing occurs with $d$-wave symmetry, and the pairing may be mediated by non-phononic excitations. However, these are not important limitations, since the BCS theory can be easily adapted to treat these cases so long as well-defined fermionic excitations exist in the normal state. However, for the underdoped and optimally doped samples, the normal state displays important deviations from Fermi liquid behavior. For instance, for optimal doping, raising the temperature above $T_c$ yields a linear, rather than quadratic, increase in resistivity [177]. Other examples of non-Fermi liquid behavior are found in Raman scattering [176], NMR [199], Hall effect [209], optical conductivity [182], and thermal conductivity [175] measurements. Furthermore, for underdoped samples, even at temperatures below $T_c$, local suppression of superconductivity by the formation of vortices in an applied magnetic field leads to exposure of local antiferromagnetic or charge density wave order instead of a metallic state, as seen with neutron scattering [105, 106, 96, 95] and STM [72]. Hence, in order to analyze low energy properties, as well as the onset of superconductivity, in underdoped samples, it may be natural to think of these systems as doped Mott insulators, rather than Fermi liquids undergoing a BCS transition [163].

1.2.1 Chemical structure of the high $T_c$ compounds

Superconductivity in the high temperature cuprates was discovered by Bendorz and Müller in 1986 [15]. Figure 1.1 shows some of the main features of the phase diagram of a high $T_c$ cuprate as a function of temperature and hole doping $x$. At low temperatures and in the absence of doping, the parent compound is an antiferromagnetic Mott insulator [190]. As the number of carriers is increased, the system becomes superconducting until, for very large values of $x$, metallic behavior is observed down to the lowest temperatures. The superconducting critical temperature $T_c(x)$ as a function of $x$ traces a dome; samples with the maximum $T_c$ are called optimally doped ($x \sim 0.15$ for La$_x$Sr$_{1-x}$CuO$_4$), while samples on either side of this are either underdoped or overdoped. Figure 1.1 also contains a “pseudogap” region for underdoped samples at high temperatures, which displays a partial gapping of
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Figure 1.1: Schematic phase diagram for a hole doped high-temperature superconductor. Only phases that have been well-established to appear across different materials are shown. In addition, other magnetic phases that are present in some materials include spin glass\cite{94}, spin stripes\cite{189}, CDW order\cite{135}, and possibly other, more exotic, phases.

the Fermi surface and evidence of superconducting pairing fluctuations\cite{127, 48, 202}, but no long-range superconducting order. A similar phase diagram is observed for electron-doped systems, although the antiferromagnetic phase is then stable up to a much larger doping of about 0.15, and the superconducting phase is less robust than in hole-doped compounds.

The high $T_c$ cuprates are layered materials, including hole doped La$_x$Sr$_{1-x}$CuO$_4$ (LSCO), YBa$_2$Cu$_3$O$_{6.35}$ (YBCO), Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO), and electron doped Nd$_{2-x}$Ce$_x$CuO$_4$ (NCCO). The low energy electronic carriers reside on CuO$_2$ planes, separated by insulating layers of interstitial rare-earth and oxygen atoms that act as a reservoir of carriers. The chemical structure of La$_2$CuO$_{4+x}$, the parent compound of LSCO, is shown in Figure 1.2. Stoichiometrically, trivalent La$^{3+}$ donates three electrons per atom, while each O$^{2-}$ atom absorbs two electrons in order to fill its $p$-shell. Therefore, at half-filling, in order to preserve charge neutrality, the copper atoms are in the Cu$^{2+}$ state, where the 4$s$ electron and one of the 3$d$ electrons are stripped away. Due to crystal field effects, the hole left in the 3$d$ shell occupies the $d_{x^2-y^2}$ orbital. Although this orbital is higher in energy than the $p_x$ and $p_y$ orbitals of the planar oxygens, the difference is comparable to their overlap energy\cite{142}. This

\footnote{Except in YBCO, where some of the layers contain metallic CuO chains.}
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La$_2$CuO$_{4+x}$[124]. The superconductivity and magnetic properties are assumed to occur on the CuO$_2$ planes, shown at right, while the atoms between the planes serve as a charge reservoir. The d$_{x^2-y^2}$ orbital of Cu and the p$_x$ and p$_y$ orbitals of O are shown. La$_x$Sr$_{1-x}$CuO$_4$ is obtained by chemical substitution of trivalent La$^{3+}$ with divalent Sr$^{2+}$, thus introducing one hole per Sr atom.

leads to strong hybridization of d$_{x^2-y^2}$, p$_x$, and p$_y$ orbitals and the formation of completely full bonding and non-bonding bands, and a half-filled anti-bonding band. Doping the system by substituting divalent Sr$^{2+}$ atoms for trivalent La$^{3+}$ introduces extra holes, moving the conduction band away from half-filling.

The one-band Hubbard model captures many of the electronic properties of the CuO$_2$ planes. In this model, the system is represented by a lattice in which a single Wannier state is kept for each CuO$_2$ basis, corresponding to the anti-bonding combination described above$^2$. The model includes a tunnelling amplitude $t_{ij}$ for an electron to hop from site to site, and a local Coulomb repulsion $U$ when two electrons of opposite spin occupy the same site,

$$\mathcal{H}_{\text{Hubbard}} = -t \sum_{(ij)\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1.1)$$

Here, $c_{i\sigma}^\dagger$ creates an electron with spin $\sigma$ on site $i$, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ counts the number of such electrons. The use of a tight-binding model is justified, since electrons cannot hop directly from one copper site to the next, but must instead hybridize with oxygen first. This leads to a smaller overlap between Wannier states than observed, for example, in the alkali metals. A more serious assumption of the model is the restriction to on-site interactions only. While Coulomb interactions are exponentially

$^2$Some important effects may be lost by the reduction of three bands, corresponding to d$_{x^2-y^2}$, p$_x$, and p$_y$ orbitals, to one. For instance, non-trivial phase factors between the three bands may lead to an orbital current state, which has been proposed to explain the pseudogap[192].
Figure 1.3: Nesting in the half-filled Hubbard model with nearest neighbor hopping only. Electrons on opposite sides of the Fermi surface are connected by a single wave vector $Q = (\pi, \pi)$.

small at large distances due to screening, neglect of short-range intersite interactions can result in failure to reproduce some important features, such as the charge-ordering of spin stripes observed in $\text{La}_{1.6-x}\text{Nd}_{0.4}\text{Sr}_x\text{CuO}_4$\cite{189}. Finally, the Hubbard model in its simplest form does not incorporate potentially important effects such as lattice vibrations and disorder. Despite these limitations, the model’s simplicity makes it a good starting point to understand many of the magnetic properties, and perhaps even superconductivity, in these systems.

1.2.2 Mott insulators

From the point of view of band theory, it is surprising at first that the cuprates at half-filling are insulators. From lattice translational invariance, Bloch’s theorem predicts the electronic spectrum to be composed of a single half-filled band, resulting in metallic behavior. However, N. Mott proposed that for systems on a lattice with strong enough Coulomb repulsion, electrons prefer localized wave functions to the extended Bloch states in order to minimize their overlap \cite{137}.

The Hubbard model at half-filling, with nearest neighbor hopping only, is a special case in which the insulating state is preferred over the metallic state, even when the repulsion $U$ is arbitrarily weak. This is due to nesting: The Fermi surface is highly symmetric, see Fig. 1.3, so that the wave vector $Q = (\pi, \pi)$ always connects two points on the Fermi surface. This leads to a divergence $\chi_0(Q, T) \sim (\log T)^2$ in the spin susceptibility of the non-interacting ($U = 0$) model (the square in the logarithm comes from a diverging density of states due to van Hove singularities at the Fermi surface). Hence, by the Stoner criterion, an arbitrarily weak repulsion
$U > 0$ is sufficient to stabilize the antiferromagnetic state. Due to hybridization between states with momenta $k$ and $k + Q$, the onset of antiferromagnetism leads to a splitting of the conduction band into an upper Hubbard band and a lower Hubbard band. These are separated by a gap that straddles the chemical potential, resulting in insulating behavior. However, due to the onset of Néel order, the lattice unit cell is doubled. Hence, the insulating antiferromagnet can also be viewed as a regular band insulator, where application of Bloch’s theorem yields a completely full lower band, and an empty upper band. The value of the Hubbard gap for charge transport is proportional to the antiferromagnetic moment in this case.

In the strong coupling regime, on the other hand, the charge gap is much larger than expected from a band insulator picture. To see this, let us consider the large-$U$ limit of the Hubbard model (1.1). Sites with double electron occupancy cost a lot of energy, and these states can be projected out of the Hilbert space. Residual interaction between spins arise due to virtual processes, in which an electron temporarily hops onto an adjacent site that is occupied (by an electron with the opposite spin, as required by Pauli exclusion). Such kinetic energy-driven process is suppressed by a factor of $U$, and leads to the $t - J$ model, where electron spins interact through an antiferromagnetic exchange $J = 4t^2/U$,

$$
\mathcal{H}_{t-J} = -t \sum_{\langle i,j \rangle, \sigma} \mathcal{P}_{i,\sigma} c_i^{\dagger} c_{j\sigma} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,
$$

(1.2)

where the Gutzwiller projector $\mathcal{P}_{i,\sigma} = 1 - n_{i,\sigma}$ forbids hopping into an already occupied site. Thus, at half-filling, the Hamiltonian reduces to an antiferromagnetic spin-1/2 Heisenberg model. In two dimensions, this model allows Néel order, with a staggered magnetization that is reduced from its maximal value by a factor of about 1/3 due to quantum fluctuations [27], in good agreement with experiment [188]. The spectrum of magnetic excitations of the insulating antiferromagnetic phase is consistent with such a model, with antiferromagnetic exchange constant of the order of $J \approx 135 \text{ meV}$[181, 147]. The energy scale for spin excitations is set by $J$, whereas charge excitations are suppressed by a much larger gap of order $U$, a few electron volts. Thus, this state differs in a strongly quantitative way from a band insulator, despite the fact that the two states have the same symmetries and can be adiabatically continued to one another.

In dimensions greater than $d = 1$, very few models are known to display a true Mott transition without spontaneous translational symmetry breaking. A review of Mott insulators with an emphasis on experimental systems is given in Ref. [77].

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3Model (1.2) does not include a three-site interaction term of the form $\mathcal{P}_{i,\sigma} c_i^{\dagger} S_j c_k$, which also arises from second-order virtual processes of the Hubbard model. This term vanishes at half-filling, and is usually neglected for simplicity.
1.2.3 Stripes

As carriers are introduced into the Mott insulating state through doping, the Néel temperature decreases rapidly until it reaches zero at a material-dependent doping of between 2 and 5%. At higher doping, stripe order may appear. A stripe is a unidirectional collinear spin density wave that combines both spin and charge order, see Fig. 1.4. The carriers organize into one dimensional rivers of charge, which act as anti-phase domain walls separating antiferromagnetic domains: the staggered magnetization flips sign between adjacent domains.

In the cuprates, stripes were first observed through elastic neutron scattering experiments on La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$[189]. Near 1/8 doping, LSCO has a tendency to distort from its usual low temperature orthorhombic (LTO) structure to a low temperature tetragonal (LTT) phase. Doping of LSCO with neodymium stabilizes the LTT phase, which is accompanied by the onset of the Bragg peaks shown in Fig. 1.5. There are four peaks near the $(\pi, \pi)$ point, instead of two as required for a unidirectional SDW. However, the data is consistent with the presence of domains with different stripe orientations. Subsequent transport[141] and photoemission[214] experiments support the one-dimensional character of the order. Khaykovich et al. have argued for the microscopic coexistence of SDW order and superconductivity in neutron scattering experiments on La$_{2}$CuO$_{4+y}$[96].

Theoretical motivation for the onset of stripe order has been given both for weak and strong correlations [121, 152, 168, 206, 201, 128]. In the weak coupling limit, a Hartree-Fock analysis of the two-dimensional Hubbard model with nearest neighbor hopping only shows that SDW order is preferred over Néel order for arbitrarily small doping, and that the periodicity of the SDW grows linearly with doping[168]: the perfect nesting of Fig. 1.3 is destroyed upon doping, shifting the maximum of the magnetic susceptibility away from $(\pi, \pi)$. Furthermore, it is found that the magnetic

![Figure 1.4: Spin stripe.](image-url)
modulation is not sinusoidal but solitonic in nature, where the staggered magnetization is approximately constant (and commensurate with the lattice) on each half of the period of modulation, changing sign abruptly across a narrow domain wall. Holes occupy bound states that are localized along the domain wall, and whose energy lies below the magnetic gap, thus stabilizing the solitonic behavior of the stripe.

In the strong coupling limit, electrons on nearest neighbor sites feel an antiferromagnetic spin exchange, as derived in the $t - J$ model (1.2) above. Figure 1.6 shows the effects of adding a single hole to an antiferromagnetic background. As the hole hops from site to site, it forms a string of broken antiferromagnetic bonds along its path. This is contrasted with the stripe configuration shown in Fig. 1.4, where holes are free to move in directions perpendicular to the stripe without generating any broken bonds. Thus stripe order arises as a phase with microscopic phase separation which balances the tendency of holes to group together, due to the antiferromagnetic coupling $J$, with the tendency for holes to delocalize due to the hopping $t$.

Note that in both the strong and weak coupling descriptions of stripes, the onset of collinear spin order is always accompanied by charge order. This feature is generic, and follows from symmetry considerations, as seen from a Ginzburg-Landau (GL) treatment [208]. Incommensurate collinear SDW order can be described by a complex vector $\vec{\Phi}$, in terms of which the magnetization is given by

$$\vec{S}(r) = Re(\vec{\Phi}e^{ir\cdot\vec{K}_s}),$$

where $\vec{K}_s$ is the wave vector of the SDW. Similarly, the order parameter of a unidirectional CDW is a complex scalar $\varphi$,

$$\delta\rho(r) = Re(\varphi e^{ir\cdot\vec{K}_c}),$$
Figure 1.6: A hole moving in an antiferromagnetic background. As the hole moves from A to B following the dotted path, a string of broken antiferromagnetic bonds (jagged lines) is left behind [191].

where $K_c$ is the wave vector of the CDW, and $\delta \rho$ is the modulation in charge or, more generically, some other spin-invariant quantity such as the hopping amplitude. Then, so long as the two wave vectors satisfy the constrain $K_c = 2K_s$, the GL free energy contains an interaction term between the two orders,

$$F = a\varphi^*\Phi^2 + a^*\varphi(\Phi^*)^2 + \ldots$$

Hence, the onset of SDW order $\Phi \neq 0$ induces a contribution to the free energy that is linear in $\varphi$, thus forcing $\varphi$ to be non-zero at the minimum of $F$. Hence, a collinear SDW always induces a CDW with twice the modulation wave vector. This accounts for the extra set of Bragg peaks observed in the neutron scattering data of Fig. 1.5 surrounding $q = 0$. Note that the converse is not true: CDW order does not automatically induce SDW order. A complete treatment of the interaction between SDW and CDW orders at the mean-field GL level is given in [208].

Although Nd-free La$_x$Sr$_{1-x}$CuO$_4$ does not display static spin stripe order, there are indications that fluctuating stripes may exist as low energy collective excitations in underdoped samples. Inelastic neutron scattering experiments find low energy peaks near $(\pi, \pi)$ at a doping-dependent wave vector that grows linearly with doping[60]. This doping dependence, usually referred to as the Yamada plot, agrees with that expected from the stripe picture. As doping grows to $x \geq 1/8$, the wave vector saturates to $K_s = (\pi \pm \pi/8, \pi)$ due to commensurability effects. This value matches the wave vector of static stripes in La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ near $x = 1/8$.

### 1.2.4 Spin Nematic Order

The spin stripe state breaks many of the symmetries of the Hamiltonian: lattice translational and rotational symmetries, time reversal invariance, and SU(2) spin
symmetry. As fluctuations are increased for example, by increasing the temperature or the doping, the system eventually becomes a paramagnet, in which all of the above symmetries are restored. The transition between these two phases could be direct. However, by allowing independent fluctuations in the spin and charge degrees of freedom of a spin stripe, many more possibilities are available. For example, in strongly underdoped YBa$_2$Cu$_3$O$_{6.35}$, the onset of static CDW order occurs without static SDW order [135], although fluctuating SDW order is seen. In this case, fluctuations of the spin component of the stripes randomizes their staggered magnetization, thus restoring SU(2) spin symmetry and time reversal invariance. However, the charge degrees of freedom remain ordered, leaving behind a CDW with half the periodicity of the original SDW. This CDW breaks lattice translational and rotational symmetries, see Fig. 1.7(b).

Another possibility, suggested in [207, 143], involves fluctuations of the charge component of the spin stripes. Here, the anti-phase domain walls fluctuate strongly while, at the same time, the staggered magnetization within each domain remains well-defined. The situation is illustrated in Figs. 1.7 (a) and (c). The ground state of the system is a linear combination of many fluctuating configurations such as the one shown in Fig. 1.7(c), so that translational symmetry has been restored to the system. Note that the expectation value of the magnetization at any given point is zero, $\langle S(r) \rangle = 0$, so that time reversal symmetry has also been restored. However, the staggered magnetization at any given point still has a preferred direction, modulo a sign. Thus, the square of the coarse-grained magnetization along different directions will in general be different, $\langle (S^x)^2 \rangle \neq \langle (S^y)^2 \rangle \neq \langle (S^z)^2 \rangle$. This is nematic order, where the order parameter is a vector with its head and tail identified.

Implicit in the mechanism for the onset of nematic order described above is that the domain walls maintain their integrity even after fluctuations set in. If we consider the topological defects of a stripe in two dimensions, this is equivalent to the requirement that, while loop defects proliferate, disclinations do not, see Fig. 1.8. In addition, for the magnetization within each domain to remain well-defined, topological excitations of the spin (e.g. vortices for XY spins) cannot proliferate. Krieger and Scheidl studied the phase diagram for classical XY spin stripes in two dimensions based on a Kosterlitz-Thouless analysis of the topological defects shown in Fig. 1.8 [102]. They found a phase diagram displaying the four phases shown in Fig. 1.7, with non-universal scaling properties at the transitions.

The nematic state was originally proposed to explain the experiments of Lake et al., in which antiferromagnetic order is induced in underdoped superconducting La$_x$Sr$_{1-x}$CuO$_4$ when an applied magnetic field creates vortices[105, 106]. If, in addition to superconductivity, the system has long-range spin nematic order, vortices will pin the charge fluctuations locally, thus exposing the underlying antiferromagnetic order around each vortex[207]. Furthermore, in a picture of stripe fractionalization, charge fluctuations pin the Néel order on distant vortices in phase, leading to long range antiferromagnetic correlations across the sample. This may account for the
Figure 1.7: Two different pathways for restoration of symmetry, starting from a spin stripe state (a), and ending with a paramagnet (d). (a) In the spin stripe state, translational, rotational, spin, and time-reversal symmetries are all broken. The arrows indicate the staggered magnetization on each domain, and the lines represent anti-phase domain walls. (b) The CDW phase is formed when fluctuations of the spin degrees of freedom average over the magnetization axis of a spin stripe. Spin and time reversal symmetries are restored, but carriers may still have a tendency to accumulate in the location of the old anti-phase domains, leading to modulation of the charge density. (c) The nematic phase forms when anti-phase domain walls fluctuate as shown. The staggered magnetization on each fluctuating domain is well-defined, although the ground state is a linear combination of many such configurations, so that the expectation value of the local magnetization at any given point is zero. However, spin symmetry is still broken by this state, since $\langle (S_x)^2 \rangle \neq \langle (S_y)^2 \rangle \neq \langle (S_z)^2 \rangle$. The spin nematic is translationally invariant.
fact that the onset temperature of the field-induced antiferromagnetic order is field-independent. In this picture, this is just the onset temperature for nematic order[207].

The order parameter of the nematic is a spin-two (i.e. tensor) operator:

$$\hat{Q}_{ab} = \frac{1}{2} \left( \hat{S}^a \hat{S}^b + \hat{S}^b \hat{S}^a \right) - \frac{\delta_{ab}}{3} \mathbf{S} \cdot \mathbf{S}. $$

Note that, for spin-1/2 fermions, the Dirac algebra of the Pauli spin matrices, $\{\sigma^a, \sigma^b\} = 2\delta^{ab}$, insures that $Q_{ab}$ written as above vanishes identically. In this case, $Q_{ab}$ can be defined by choosing spins on neighboring sites. Since the spin nematic order parameter is a spin-two operator, it does not couple directly to many of the conventional probes at linear order. For instance, neutron scattering with momentum transfer $\mathbf{q}$ detects long range correlations between pairs of spins,

$$\lim_{r \to \infty} e^{i\mathbf{q} \cdot \mathbf{r}} \langle \hat{S}^a(\mathbf{r}, t) \hat{S}^b(0, 0) \rangle,$$

whereas in order to couple to the nematic order parameter one would need a probe that measures long range correlations between four spins,

$$\lim_{r \to \infty} e^{i\mathbf{q} \cdot \mathbf{r}} \langle Q^{ab}(\mathbf{r}, t) Q^{cd}(0, 0) \rangle.$$

The Wilson line of a $\mathbb{Z}_2$ gauge theory has been proposed as an alternate order parameter for the nematic state in cases where the nematic arises from stripe fractionalization [207]. However, this is a highly non-local quantity and is unlikely to be directly accessible to experiments. Chapter 3 addresses the problem of detection of nematic order. There, it is shown that electrons moving in a nematic background experience a spin anisotropic interaction that can be measured directly by Knight shift and neutron scattering experiments. Chapter 3 also addresses the possibility of observing director density waves, the Goldstone modes corresponding to spin nematic order, through neutron scattering.
Figure 1.9: (a) STM setup: A metallic tip is brought in close proximity to a sample, and the tunneling current $I$ is measured as a function of sample bias $V$. Due to exponential dependence of tunneling amplitude on distance, very high resolution is attainable. (b) STM measures the local density of electronic states. Assuming a metallic tip with constant density of states $\rho_T$, the current $I$ is proportional the density of states of the sample $\rho_S$ integrated from the chemical potential up to the bias energy $eV$.

Other quantum liquid crystal phases that arise from fluctuating spin stripe order have been considered in the literature. A review of some of these states is found in Ref. [99], including proposals for their detection. Note that the nematic state discussed there is not a spin nematic. Instead, it is a state that arises from fluctuations of a unidirectional CDW phase, such that translational invariance is restored, but memory of the orientation of the CDW is maintained, so that (discrete) lattice rotational invariance is broken. This type of “charge nematic” can be easily detected by measuring the anisotropy of various quantities along perpendicular directions in the CuO$_2$ planes[99].

1.2.5 Scanning Tunneling Microscopy

Scanning Tunneling Microscopy (STM) has emerged over the past few years as one of the most powerful experimental methods to study spatial inhomogeneity in the high $T_c$ cuprates. The setup of an STM experiment is shown schematically in Fig. 1.9(a). A very sharp tip is brought in close proximity to the sample, and the tunneling current $I$ is measured as a bias voltage $V$ is applied. Due to the exponential dependence of tunneling matrix elements on distance, only electrons on the surface of the sample near the point closest to the tip contribute significantly to the tunneling, so that measurements with spatial resolution that is higher than the interatomic distance of the sample can be achieved. Then, the differential conductance of the
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sample, \( g \equiv \frac{dI}{dV} \), is proportional to the local density of states (LDOS) \( \rho \):

\[
\rho(\mathbf{r}, eV) = \sum_n \left\{ \left| \langle 0 | \psi(\mathbf{r}) | n \rangle \right|^2 \delta(\epsilon_n - eV) + \left| \langle 0 | \psi^\dagger(\mathbf{r}) | n \rangle \right|^2 \delta(\epsilon_n + eV) \right\}
\]

This expression holds for zero temperature, \( \psi^\dagger (\psi) \) is an electron creation (annihilation) operator at position \( \mathbf{r} \), \( |0\rangle \) is the ground state, and the sum runs over all excited states \( n \). A heuristic argument for the proportionality between \( g \) and \( \rho \) is given in Fig. 1.9(b). The metal tip is assumed to be a good metal, with a constant density of states \( N_T \) over the energy range of interest. Thus, so long as the tunneling matrix element does not depend on bias over this range, the zero temperature tunneling current at \( V \) is proportional to the number of occupied states above the chemical potential in the sample, \( I(V) \propto \int_{\mu}^{\mu+eV} \rho_s(\mathbf{r}, eV) \). Taking the derivative with respect to \( V \), we find

\[
g(\mathbf{r}, z, eV) = f(\mathbf{r}, z) \rho(\mathbf{r}, eV).
\]

Here, \( \mathbf{r} \) is the position along the surface of the sample, \( z \) is the vertical distance between tip and sample, and the energy is measured relative to the chemical potential. Since we have assumed that the tunneling matrix element does not depend on bias, the proportionality constant \( f \) depends on geometry only. One is often interested in the shape of the LDOS at a single point, in which case the value of \( f \) is unimportant. However, experiments that compare the LDOS at different points, such as the Fourier-transformed LDOS analysis described below, require detailed knowledge of the variation of \( f \) to obtain reliable results for some of their predictions. In Chapter 2, I discuss sum rules that may be used to remove errors due to the space dependent normalization from measurements.

Most STM experiments on the high-T\(_c\) cuprates are carried out on Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\), which has weakly coupled layers that cleave cleanly to provide surfaces that are flat at the atomic level. STM has been used to study the local electronic environment surrounding impurity sites [145, 76] and vortices in a magnetic field [159, 72]. In particular, in Ref. [72], the LDOS shows period-four modulations on halos surrounding the vortex cores. This has been interpreted in terms of proximity to a magnetic phase [45, 213], where low energy SDW modes can be locally pinned by vortices. Only the charge modulations of the SDW are actually pinned in this process – long range order would be necessary for the local spin to get an expectation value, but charge order can be locally established by the vortices, which break translational symmetry. Additional evidence for proximity to a magnetic phase been found in the elastic neutron scattering experiments of B. Lake et al. [105, 106] and B. Khaykovich et al. [96, 95], where incommensurate magnetic order is stabilized in superconducting LSCO samples by application of an external magnetic field.

A very powerful technique that has emerged over the last two years to study spatial inhomogeneity in the cuprates is the Fourier-transformed local density of states (F-LDOS) analysis. This consists of taking STM spectra \( \rho(\mathbf{r}, eV) \) for a large field of view...
at a lattice of points separated by the interatomic distance, or less. The F-LDOS is then simply the Fourier series of the STM data as a function of sample bias and wave vector,

\[ \rho_{q}(eV) = \frac{1}{N} \sum_{i} \rho(r_{i}, eV)e^{ir_{i} \cdot q}. \]

The momentum resolution of the F-LDOS is given by the size of the field of view, whereas the maximum wave vector accessible to this technique is limited by the spatial separation between measurement locations.

F-LDOS has been used to study inhomogeneity in the superconducting state of slightly-overdoped \( \text{Bi}_{2}\text{Sr}_{2}\text{CaCu}_{2}\text{O}_{8+\delta} \)[72, 73, 74, 75, 130]. Strong intensity peaks are found at various different wave vectors, whose location disperses with sample bias. This has been interpreted in terms of Friedel oscillations due to quasiparticle scattering off impurities[200, 73]. In the presence of impurities, momentum is not a good quantum number, and hybridization between different wave vector states can occur, leading to spatial inhomogeneity. In the superconducting state, the quasiparticle dispersion is \( E_{k} = \sqrt{\epsilon_{k}^{2} + |\Delta_{k}|^{2}} \), where \( \Delta_{k} \) is the \( d \)-wave superconducting gap. Hence, at low energies, the contours of constant energy are elongated curved ellipses shown in Fig. 1.10. Along a given contour, the gradient of energy with respect to wave vector is smallest at the end points of the ellipse. These points contribute the most to the density of states. The arrows shown in Fig. 1.10 connect these points in pairs and give the wave vectors at which spatial inhomogeneity due to impurity scattering appears in the F-LDOS. With this model, the dispersion of the F-LDOS peaks gives a measurement of the gap function and of the shape of the Fermi surface that are in good agreement with those found in photoemission experiments[200, 73].

In addition to the dispersing peaks discussed above, there are indications that non-dispersing peaks may also be present in slightly overdoped samples[74, 75, 99], and in the pseudogap regime in underdoped samples[194]. These non-dispersing peaks are consistent with period-four CDW order. In Chapter 2, I will discuss how the energy profile of the F-LDOS can be used to distinguish different types of static spin-invariant modulations, including modulations in the charge density, hopping strength, and superconducting pairing amplitude. These non-dispersing peaks have also been interpreted as dynamic SDW modes pinned by impurities[153, 155].

1.3 Enhanced symmetry in strongly correlated electron systems

Symmetry is a powerful principle in elucidating the properties of a complex system. The symmetry group of a quantum mechanical Hamiltonian contains information regarding the degeneracy of states, and provides a scheme by which to organize the
Figure 1.10: Origin of dispersing peaks in F-LDOS experiments on slightly overdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [73]. A contour of constant energy is shown for the quasiparticles of a $d$-wave superconductor (dashed curved ellipses). Along the contour, the maximal density of states is attained at the intersections with the Fermi surface of the normal state (solid curve). States at these points hybridize when impurities are present, leading to Friedel oscillations at the seven distinct wave vectors shown.
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spectrum of excitations. In situations where the symmetry of the Hamiltonian is spontaneously broken with the onset of long range order, the pattern of symmetry breaking determines the spectrum of gapless Goldstone modes uniquely[42].

Although the symmetry of the Hamiltonian is explicit in most cases, there are situations in strongly correlated electron systems where, for special values of parameters, the Hamiltonian displays a higher symmetry than manifest. This typically occurs at the phase boundary between two seemingly unrelated orders, where the extra symmetry generators rotate the degenerate order parameters into one another. The addition of new Goldstone modes leads to a suppression of the critical temperature. In addition, the enhanced symmetry group constrains the form of the Ginzburg-Landau free energy for the competing orders, leading to strong constrains on the topology of the phase diagram near the phase transition.

To illustrate these ideas, I will concentrate on the Hubbard model on a bipartite lattice at half filling[204, 210]. The Hamiltonian (1.1) can be rewritten after a shift of the chemical potential $\mu$, and including a Zeeman field $h$ along the $z$-axis:

$$
\mathcal{H} = -t \sum_{\langle ij \rangle} c_i^\dagger \sigma c_j \sigma + U \sum_i (n_i^\uparrow - \frac{1}{2}) (n_i^\downarrow - \frac{1}{2}) - \mu \sum_i (n_i^\sigma - \frac{1}{2}) - h \sum_i (n_i^\uparrow - n_i^\downarrow).
$$

This system is always invariant under the U(1) group of phase rotations, $[\mathcal{H}, Q] = 0$, which are generated by the total charge operator $Q = \frac{1}{2} \sum_\sigma (n_i^\sigma - \frac{1}{2})$. Also, in the absence of a magnetic field, the model is explicitly invariant under spin SU(2) rotations, $[\mathcal{H}, S^\alpha] = 0$, generated by the total spin operators,

$$
S^z = \frac{1}{2} \sum_i \left( c_i^\dagger c_i^\downarrow c_i c_i^\dagger \right)
$$

$$
S^+ = \sum_i c_i^\dagger c_i^\uparrow
$$

$$
S^- = \sum_i c_i^\dagger c_i^\downarrow
$$

In addition, the model on a bipartite lattice possesses discrete particle-hole symmetry (the notation $(-1)^i$ is shorthand for +1 on one sublattice, $-1$ on the other),

$$
P_{p-h} : c_i \sigma \rightarrow (-1)^i c_i^\dagger \sigma.
$$

Under this transformation, the kinetic and potential energy terms remain invariant, while the magnetic field and the chemical potential change signs, $h \rightarrow -h$, $\mu \rightarrow -\mu$. This demonstrates that the physics is the same for electron-doped and hole-doped systems. A second particle-hole transformation is possible, in which only one spin species is transformed,

$$
P^\dagger_{p-h} : \left\{ \begin{array}{c} c_i^\dagger \\ c_i \end{array} \right\} \rightarrow \left\{ \begin{array}{c} c_i^\dagger \\ (-1)^i c_i \end{array} \right\}
$$
This leads to a new Hubbard model with the sign of the interaction flipped, $U \rightarrow -U$, and with the roles of the charge and $z$-magnetization exchanged, $\mu \rightarrow h, h \rightarrow \mu$.

An important consequence of the transformation $P_{p-h}^\dagger$ is that, for a system at half-filling in the absence of a magnetic field, the Hubbard model has a continuous symmetry group that is larger than $U(1)_{\text{charge}} \times SU(2)_{\text{spin}}$. To see this, note that the spin generators are transformed under $P_{p-h}^\dagger$ into a new set of operators $P_{p-h}^\dagger : S^\alpha \rightarrow \eta^\alpha$, where

$$
\eta^- = \frac{1}{2} \sum_i \left( c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow} - 1 \right) = Q
$$

$$
\eta^+ = \sum_i (-1)^i c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger
$$

$$
\eta^- = \sum_i (-1)^i c_{i\uparrow} c_{i\downarrow}.
$$

Since the spin operators commute with the $-U$ Hubbard model Hamiltonian, the “pseudospin” operators $\eta^\alpha$ must commute with the $+U$ Hubbard model Hamiltonian. This can be verified through explicit calculation,

$$
[H, \eta^\pm] = \mp 2\mu \eta^\pm,
$$

which vanishes at half-filling ($\mu = 0$). Thus, spin and particle-hole symmetries together imply pseudospin symmetry. The pseudospin generators are spin-singlet operators, and therefore commute with the total spin $[S^\alpha, \eta^\alpha] = 0$. Hence, the total symmetry group is $SO(4) \approx SU(2)_{\text{spin}} \times SU(2)_{\text{pseudospin}} / \mathbb{Z}_2$.

Let us now examine how do the order parameters of the theory transform under the symmetry group. Here we will concentrate on the negative-$U$ case, where particles in the ground state like to form on-site spin-singlet pairs. These pairs may condense to form a superconductor, or they may instead prefer to arrange themselves in a periodic pattern to form a checkerboard CDW. In fact, these two types of order are connected by the pseudospin group,

$$
[\eta^a, \Delta^b] = i\epsilon^{abc} \Delta^c
$$

where,

$$
\Delta^+ = \sum_i c_{i\downarrow}^\dagger c_{i\uparrow}.
$$

In Chapters 4 and 5, where this relation appears for a different group $SO(4)$, I am a little sloppy regarding the difference between the groups $SO(3)$ and $SU(2)$, and the presence of the quotient group $\mathbb{Z}_2$. However, these are differences in the global topology of these groups; at the level of Lie algebras, the difference is not important. Hence, for instance, the Goldstone modes are unaffected by this change, whereas an analysis of topological excitations could depend critically on this difference.
\[ \Delta^- = \sum_i c_i^\dagger c_i \]
\[ \Delta^z = \frac{1}{2} \sum_{i\sigma} (-1)^i n_{i\sigma}. \]

Thus, by symmetry, the two types of order are actually degenerate.

Since the two types of order are degenerate, it is possible to construct a new class of low energy states by alternating regions with local SC and CDW orders that slowly twist into one another. For short-ranged interactions (as is the case for the Hubbard model), the energy of such states is made arbitrarily small by making the twist arbitrarily slow. Thus, enhanced symmetry leads to gapless Goldstone modes associated with the pseudospin operators, \( \eta \), which generate the rotations between the two orders. In the quantum system, such low energy modes are created by acting with \( \eta \) on the ground state, as seen in equation (1.3). Away from \( \mu = 0 \), the excited state is a massive pseudo-Goldstone mode whose gap softens as the SO(4) symmetric point \( \mu = 0 \) is approached to yield a true Goldstone mode.

The dynamics of these low energy modes can be captured by a quantum rotor model [46], which is obtained by coarse-graining the lattice into small clusters, and then projecting onto the low energy Hilbert space on each cluster. By symmetry, the remaining degrees of freedom must decompose into well-defined representations of SO(4). In this case, they are mapped into a local three dimensional vector order parameter \( \vec{\Delta}_i \) on cluster \( i \), subject to the local constraint \( |\vec{\Delta}_i|^2 = 1 \). The quantum rotor model then consists of a kinetic energy term for each rotor, in addition to a ferromagnetic coupling for rotors on adjacent clusters. Quantum rotor models are applied to study collective modes, in a spin nematic state in Chapter 3, and for quasi one-dimensional Bechgaard salts in Chapter 5.

The presence of new low energy modes at a transition between two states leads to enhanced fluctuations of the order parameters, and to a reduced critical temperature \( T_c \) at the transition. A dramatic demonstration of this effect is provided by the anisotropic Heisenberg model in two dimensions,

\[ \mathcal{H} = \sum_{\langle i,j \rangle} \left( J_{\perp} (S_i^x S_j^x + S_i^y S_j^y) + J_z S_i^z S_j^z \right), \]

where AF couplings are chosen, \( J_{\perp}, J_z > 0 \). At low temperatures, the system is an Ising antiferromagnet for \( J_z/J_{\perp} > 1 \), with critical temperature \( T_{\text{Ising}} \), whereas for \( J_z/J_{\perp} < 1 \) an algebraically-ordered XY antiferromagnet forms with critical temperature \( T_{\text{XY}} \). Exactly at the point \( J_z = J_{\perp} \), the Hamiltonian becomes an isotropic Heisenberg model, with explicit SO(3) symmetry. By the Mermin-Wagner theorem, no finite temperature ordered phases can exist at this point. Hence, enhanced symmetry leads to enhanced fluctuations, suppressing \( T_{\text{Ising}} \) and \( T_{\text{XY}} \) all the way down to zero at the transition between Ising and XY phases [42]. Similarly, the negative-\( U \) Hubbard model in two dimensions at half-filling remains disordered at all finite temperatures.
Symmetry principles have been introduced to study the competition of order parameters in a variety of experimental systems. In S.C. Zhang’s SO(5) theory of high $T_c$ superconductivity\[211\], antiferromagnetism and $d$-wave superconductivity are treated as components of a five dimensional vector order parameter. In addition to the generators of the usual charge SO(2) and spin SO(3) symmetries, new $\pi$-operators are introduced, which rotate superconductivity and antiferromagnetism into each other. A combination of analytical approximations and numerical results can be used to argue an approximate SO(5) theory of a class of two dimensional lattice models, such as the Hubbard and the $t$-$J$ model \[131, 53\]. The SO(5) symmetry has also been used to discuss quasi two-dimensional organic $\kappa$-BEDT-TTF salts\[138\]. The unification approach based on higher symmetries has been generalized to several other types of competing states. SO(5) and SO(8) symmetries have been used to classify possible many-body ground states in electronic ladders \[166, 116\]. SO(6) symmetry has been introduced to discuss competing striped phases and superconductivity in the cuprates\[126\]. SO(4) symmetry has been used to combine $d$-wave superconductivity and $d$-density wave phases \[113, 140\]. It has also been suggested that the SO(5) algebra can be used to combine ferromagnetism and triplet superconductivity in quasi two-dimensional Sr$_2$RuO$_4$ \[139\], although the existence of microscopic models with such symmetry has not been demonstrated.

Note that there are situations where the classical Ginzburg-Landau free energy for interacting order parameters has a renormalization group (RG) flow that leads, at low energies and long wavelengths, towards a point of higher symmetry than contained in the microscopic Hamiltonian. However, the notion of enhanced symmetry in the RG sense is weaker than the one considered above, since typically only the static properties of the system become symmetric under the flow, and not the full dynamics.

1.4 Quasi-one dimensional superconductors

1.4.1 Materials

The discovery of quasi-one dimensional organic Bechgaard salts in 1980 opened a new direction in the study of superconductivity in strongly correlated systems \[83\]. These are materials with highly anisotropic band structures such that, at high temperatures, transport in two of the three principal directions is incoherent due to thermal fluctuations. Hence, rather than being a Fermi liquid, the high temperature normal state is better described as a set of weakly coupled one dimensional Luttinger liquids. Figure 1.11 shows the chemical structure of $(\text{TMTSF})_2\text{PF}_6$, the first quasi one-dimensional compound to display superconductivity. The TMTSF molecules are flat and elongated, stacking on top of each other to form a salt of weakly coupled chains. The overlap integral of low energy $\pi$ orbitals on adjacent molecules within a stack is much larger than among molecules belonging to different stacks, leading to a hopping
anisotropy along the three principal directions of $t_a : t_b : t_c = 250 : 25 : 1$. The family of compounds (TMTTF)$_2$X, in which the selenium atoms in TMTSF are replaced by sulfur, have an even more one-dimensional character, with $t_a : t_b : t_c = 250 : 10 : 1$. The anion X=PF$_6$ donates one hole for every two TMTSF molecules, leading to a nominally quarter-filled band. However, weak structural dimerization observed in these compounds leads to a doubling of the unit cell, and to splitting of the conduction band into a completely full lower band and a half-filled upper band [183].

At ambient pressure, (TMTSF)$_2$PF$_6$ is an antiferromagnetic insulator as seen, for instance, in the jump in resistivity below $T_N \sim 12$ K [82], and in the divergence of the NMR spin lattice relaxation rate $1/T_1$ due to softening of low-lying magnetic excitation modes at $T_N$ [20]. Then, as pressure is increased above 9 kbar, a superconducting phase is stabilized. Evidence for spin-triplet Cooper pairing includes strong suppression of superconductivity through disorder ($10^{-5}$ non-magnetic impurities per TMTSF molecule are sufficient to destroy the superconductivity entirely [32, 36, 185]), an electron spin susceptibility that does not decrease below $T_c$ [111], and a critical magnetic field $H_{c2}$ in the interchain direction that exceeds the paramagnetic (Clogston-Chandrasekhar) limit [112]. Insulator to superconductor transitions as a function of pressure have also been observed in other materials of the same family, including (TMTSF)$_2$AsF$_6$ [23] and (TMTTF)$_2$PF$_6$ [80]. In addition, in (TMTSF)$_2$ClO$_4$, superconductivity is stable under ambient pressure and also shows signatures of triplet pairing [179, 69, 84, 144]. Fig. 1.12 combines various members of the (TMTSF)$_2$X and (TMTTF)$_2$X families into a single generalized phase diagram.
Figure 1.12: Generalized temperature-pressure phase diagram of Bechgaard salts. SP denotes spin-Peierls order, AF is antiferromagnetic (or SDW) order, and TSC triplet superconductivity. The dashed line gives a crossover temperature between metallic (Normal) and charge-localized (CL) behaviors. The zero-pressure position of each material is marked beneath the figure. Adapted from [83].
Enhanced control of the applied hydrostatic pressure has allowed researchers to zero in on the neighborhood of the AF/TSC transition in (TMTSF)$_2$PF$_6$. Here, transport experiments give indications of a first order transition between the AF and TSC phases, as well as a first order transition over a section of the boundary between the AF and Normal phases. The evidence includes hysteresis in the resistivity as temperature is cycled, as well as indications that the onset of macroscopic superconductivity occurs along a percolating cluster due to phase separation [198, 100]. Strictly speaking, phase separation should not be observed when the phase diagram is tuned by intrinsic variables, such as pressure. However, the pressure-transmitting medium inside the pressure cells in these experiments solidifies at the pressures and temperatures considered, leading to significant inhomogeneity in the applied pressure across different regions of the sample\(^5\). Near a first order transition, a weakly inhomogeneous pressure distribution surrounding the critical pressure is sufficient to give phase separation. Figure 1.13 shows the phase diagram as a function of temperature and experimentally controlled pressure.

In the next few subsections I will introduce some of the unusual properties of one-dimensional electron systems. Then, at the end of this section, I will return to the problem of quasi-one dimensional superconductivity.

### 1.4.2 Luttinger liquids in one dimension

In a strictly one dimensional electron system, arbitrarily weak interactions are sufficient to destroy Fermi liquid behavior. On the one hand, the Fermi surface in one dimension consists of just two points, $\pm k_f$. Hence, the wave vector $2k_f$ always satisfies a perfect nesting condition, leading to a divergent low temperature spin and charge susceptibility at $k = 2k_f$, and to either SDW or CDW instabilities for repulsive interactions. On the other hand, the pairing susceptibility always diverges in a time reversal invariant system, leading to a superconducting instability for attractive interactions. Thus, at zero temperature, there is always a tendency towards the formation of an ordered state, the nature of which is determined by the particular form of the electronic interactions, independently of how weak these may be.

This intrinsic tendency of 1D systems towards spontaneous symmetry breaking, and towards the formation of long range order, is countered by strong quantum fluctuations of the order parameter. These fluctuations occur in two space-time dimensions and, by the Mermin-Wagner theorem, they prevent the formation of long-range order (to be precise, fluctuations prevent the breaking of \textit{continuous} symmetry only; as we’ll see below, formation of spin and charge gaps is possible in one dimension due to spontaneous breaking of a \textit{discrete} group). The interplay of the intrinsic tendency towards the formation of long range order with the strong effects of fluctuations in suppressing

\(^5\)Current efforts are underway to study this transition using different pressure-transferring media, which may allow to tune pressure directly across the transition, as well as reduce the pressure inhomogeneity across the sample (M. Naughton, private communication).
Figure 1.13: Phase diagram of (TMTSF)$_2$PF$_6$ near the transition between antiferromagnetic (AF) and triplet superconducting (TSC) phases, obtained from transport measurements [198, 100]. Inhomogeneous coexistence regions between AF/Normal and AF/TSC phases are observed. Adapted from [198].
that order lead, at zero temperature, to a system that is always critical: for any form of the interaction, the correlator between local observables decays algebraically with distance. The decay exponents, and therefore the dominant correlations at long distances, are determined by the form of the interaction. Such critical behavior defines a new universality class, called a Luttinger liquid, which differs markedly from a Fermi liquid\(^6\).

Recall that the operational definition of a Fermi liquid was given in terms of the existence of well-defined low energy fermionic quasiparticles, whose scattering rate \(1/\tau \propto (\epsilon - \epsilon_F)^2\) goes to zero faster than their energy near the Fermi surface. How do quasiparticles behave in one dimension? In this case, due to collinearity of all the momenta, \(1/\tau \propto |\epsilon - \epsilon_F|\), which does not decay fast enough. In fact, the quasiparticle density of states vanishes at the Fermi surface as a power law in \(|\epsilon - \epsilon_F|\), as observed in tunneling experiments on carbon nanotubes\(^{17}\). But then, if fermionic quasiparticles are not well-defined, what are the fundamental excitations of a Luttinger liquid?

### 1.4.3 Bosonization

A hint to the question above is given in Fig. 1.14. There, one sees that in two dimensions or more, an electron can move through a cloud of other electrons more or less freely. As the electron moves along, the cloud rearranges itself slightly due to interactions, leading to screening of charge at long distance, to a renormalization of the electron mass, and to the possibility of collective motion. However, the electron itself maintains its fundamental properties, including its spin, charge, and its fermionic character. On the other hand, in one dimension, dynamics is very restricted, whereupon an electron attempting to move past another experiences very strong interactions (in the case of spinless fermions, this is strictly forbidden by Pauli exclusion). Motion in this case is reminiscent of sound waves and is purely collective. Hence, it may be natural to look for bosonic modes as the fundamental excitations of Luttinger liquids.

\(^6\)Excellent reviews of Luttinger liquid physics are given, for example, in Refs. [63, 169, 174, 196].

---

**Figure 1.14**: Qualitative difference between interactions in one dimension and higher dimensions.
To be specific, for now let us consider non-interacting fermions without spin. The band structure of a one dimensional electron gas is shown in Fig. 1.15(a). Low energy excitations surround the two Fermi points $\pm k_f$. Figure 1.15(c) shows the corresponding spectrum for particle-hole excitations with center-of-mass momentum $q$, created by acting on the vacuum by the density operator $\rho(q) = \frac{1}{L} \sum_k c_{k}^{\dagger}c_{k-q}$. While, for any finite value of $q$ there is a continuum of energies available to the particle-hole pairs, as $q$ approaches zero this continuum collapses to a line with slope equal to the Fermi velocity $v_f$. Thus, the low momentum particle-hole pairs are a candidate for a fundamental bosonic excitation with a well-defined linear dispersion at low energies.

Considerable simplification occurs by approximating the single particle excitations by a linearized spectrum, with slope $v_f$ (see the dotted lines in Fig. 1.15(a)). As far as the low energy properties of the system are concerned, one may ignore deviations from this linear dispersion, and instead work with the band structure shown in Fig. 1.15. The price paid for linearization is the introduction of two separate branches instead of one, for left and right moving electrons. Two sets of creation operators are necessary, $a_{\pm,k}^{\dagger}$, where the upper sign applies to right moving states, and where we follow the convention that momentum is measured relative to the Fermi points $\pm k_f$, so that the dispersion in these bands is given by $\epsilon_k = \pm v_f k$. On the other hand, linearization leads to considerable simplification in the particle-hole spectrum, Fig. 1.15(d): the continuum of low energy states at small momenta has been replaced by a line of excitations with a well-defined spectrum, generated by the two bosonic operators $\rho_{\pm}(q) = \frac{1}{L} \sum_k a_{\pm,k}^{\dagger}a_{\pm,k-q}$. The linearized model is called the Luttinger model, and it can be solved exactly at low energies in the presence of short range interactions, as I will discuss below. The curvature of the band structure at the Fermi points has been shown to be an irrelevant perturbation [70].

The fact that the operators $\rho_{\pm}(q)$ create excitations with well-defined energy implies that they are eigenoperators of the free Hamiltonian $H_0$, $[H_0, \rho_{\pm}(q)] = \pm v_f q \rho_{\pm}(q)$. This, together with the fact that the operators $\rho_{\pm}(q)$ form a complete basis for the Hilbert space [70], can be used to write $H_0$ as a quadratic function of $\rho_{\pm}$. This is a highly non-trivial statement: $H_0$, a quadratic function of Fermi operators in its original form, has been rewritten as a quartic function of fermions! Furthermore, it is now trivial to introduce interactions, as these are explicitly quadratic in the density operators. Thus, the entire Hamiltonian is a quadratic function of the bosonic densities, and it can be solved exactly in a trivial manner.

Instead of working with the densities $\rho_{\pm}$ directly, it is customary to introduce two new variables $\phi$ and $\theta$, defined by (using the conventions in Ref. [63]):

$$\phi(x), \theta(x) = \mp (N_+ \pm N_-) \frac{\pi x}{L} \mp \frac{i \pi}{L} \sum_{p \neq 0} \frac{1}{p} e^{-\alpha|p|/2} e^{-ipx} \left( \rho_{+}^{\dagger}(p) \pm \rho_{-}^{\dagger}(p) \right).$$

Here, the upper signs are for $\phi$; $\alpha$ is a short distance cutoff; and $N_{\pm} \equiv \rho_{\pm}(0) - \langle 0 | \rho_{\pm}(0) | 0 \rangle$ is the density of right or left movers relative to the ground state. In terms
Figure 1.15: (a) Single electron dispersion band in the absence of interactions. (b) In the Luttinger model, the band is linearized about the two Fermi points $\pm 2k_f$ with slope given by the Fermi velocity $v_f$. In order to maintain a linear dispersion up to high energies, two bands are necessary, for right and left moving electrons. The Fermi sea has been substituted by a Dirac sea, in which electronic states with arbitrarily negative energies are filled. (c) Particle-hole excitations of the original band. For small center-of-mass momentum $q$, the continuum of excitations becomes narrower, approaching a linear dispersion. (d) In the Luttinger model, all low energy particle-hole excitations near $q = 0$ have a well-defined linear dispersion [63].
of these, the electron creation operators become,
\[ \psi^\dagger_\pm(x) = \eta_\pm \lim_{\alpha \to 0} \frac{1}{\sqrt{2\pi \alpha}} e^{\mp i(k_F - \pi/L)x} e^{i(\phi(x) - \theta(x))}, \]
where \( \eta_\pm \) is a Klein factor, an operator that changes the fermion number by one, as necessary for both sides of the equation to have matching statistics. Similarly, the interacting Hamiltonian can be written in terms of \( \phi \) and \( \theta \) as
\[ H_{\text{spinless}} = \frac{1}{2\pi} \int dx \left[ uK(\pi\Pi(x))^2 + \frac{u}{K} (\nabla \phi(x))^2 \right], \]
where \( \Pi(x) = \frac{1}{\pi} \nabla \theta(x) \) is the momentum conjugate to the field \( \phi \). The dimensionless parameter \( K \) acts as the strength of the interaction (\( K = 1 \) for the non-interacting Fermi gas) and \( u \) is the velocity of excitations (\( u = v_f \) in the absence of interactions).

Let us now consider the situation of spin-1/2 fermions. In the absence of interactions, we can classify all possible short-range interactions between low energy spin-1/2 electrons in terms of three numbers only, the backward scattering amplitude \( g_1 \), and the two forward scattering amplitudes \( g_2 \) and \( g_4 \).

\[ H = H_0 + H_1 + H_2 + H_4 \]
\[ H_0 = \sum_{rks} (\epsilon_{r,ks} - \mu) a^\dagger_{r,ks} a_{r,ks} \]
\[ H_1 = \frac{g_1}{L} \sum_{a} a^\dagger_{+,ks} a^\dagger_{-,pt} a_{+p} a_{-q} a_{+} a_{-q} \]
\[ H_2 = \frac{g_2}{L} \sum_{a} a^\dagger_{+,ks} a^\dagger_{-,p} a_{+} a_{-q} a_{+} a_{-q} \]
\[ H_4 = \frac{g_4}{L} \sum_{a} a^\dagger_{+,ks} a^\dagger_{-,p} a_{+} a_{-q} a_{+,ks} + \frac{g_4}{L} \sum_{a} a^\dagger_{-,ks} a^\dagger_{-,p} a_{-q} a_{+,ks} \]

Furthermore, the transformations described above can be repeated, but this time introducing two sets of variables, one for each spin: \( \theta_1 \), \( \theta_4 \), \( \phi_1 \), and \( \phi_4 \). These can be decomposed into “charge” variables, \( \phi_\rho = \frac{1}{\sqrt{2}} (\phi_1 + \phi_4) \) and \( \theta_\rho = \frac{1}{\sqrt{2}} (\theta_1 + \theta_4) \); and “spin” variables, \( \phi_\sigma = \frac{1}{\sqrt{2}} (\phi_1 - \phi_4) \) and \( \theta_\sigma = \frac{1}{\sqrt{2}} (\theta_1 - \theta_4) \). Then the Hamiltonian for the full spin-1/2 system becomes,

\[ H = H_\rho + H_\sigma \]
\[ H_\rho = \frac{1}{2\pi} \int dx \left[ u_\rho K_\rho (\pi\Pi_\rho(x))^2 + \frac{u_\rho}{K_\rho} (\nabla \phi_\rho(x))^2 \right], \]
\[ H_\sigma = \frac{1}{2\pi} \int dx \left[ u_\sigma K_\sigma (\pi\Pi_\sigma(x))^2 + \frac{u_\sigma}{K_\sigma} (\nabla \phi_\sigma(x))^2 + \frac{g_1}{\pi \alpha^2} \cos(\sqrt{8} \phi_\sigma(x)) \right]. \]

\(^7\)Ignoring, for now, lattice effects at commensurate densities.

\(^8\)Implicit in the definition of spin variables is a choice of axis of quantization of spin along \( \hat{z} \). This form of bosonization, called Abelian, is the simplest to implement, but the formalism is not explicitly spin invariant, often making it difficult to show spin invariance at the end of a calculation. Alternative, non-Abelian realizations exist, which are more complex but manifestly spin invariant.
Figure 1.16: Spin charge separation: (a) a hole introduced into the system, e.g. by knocking out an electron at point A in a photoemission experiment, (b) quickly separates into a charge-carrying excitation (holon) at point B, and a spin-carrying excitation (spinon), marked by a broken antiferromagnetic bond.

The interaction strengths $K_\rho = \sqrt{\frac{2\pi v_f + g_1 - 2g_2 + g_4}{2\pi v_f - g_1 + 2g_2 + g_4}}$, $K_\sigma = \sqrt{\frac{2\pi v_f + g_1}{2\pi v_f - g_1}}$, and the velocities $u_\rho = \sqrt{(v_f + \frac{g_1}{\pi})^2 - (\frac{g_1 - 2g_2}{2\pi})^2}$, $u_\sigma = \sqrt{v_f^2 + (\frac{g_1}{2\pi})^2}$ are all given by the interaction parameters.

Perhaps the most surprising feature of Eq. (1.4) is the complete separation between the dynamics of spin and charge degrees of freedom. Hence, the onset of quasi-long range order occurs independently in the spin and charge sectors. Furthermore, spin and charge excitations in general move with distinct velocities, $u_\rho \neq u_\sigma$. The origin of spin-charge separation is shown heuristically in Fig. 1.16. There, a single particle excitation evolves with time into two separate excitations, a spinon carrying only spin degrees of freedom and a holon, carrying only charge. This should be contrasted with the analogue situation in two dimensions, Fig. 1.6, where a string of broken bonds is created as the hole moves away from its original location. There, the energy cost grows linearly with distance, binding the holon and spinon to each other. Experimental evidence for spin-charge separation in quasi-one dimensional organic conductors, from optical, transport, and magnetic measurements, is discussed in Ref. [50]; photoemission experiments on the compound TTF-TCNQ are discussed in Ref. [33].

As before, the charge component of the Hamiltonian (1.4) is non-interacting in the bosonized representation. On the other hand, the spin component is a sine-Gordon Hamiltonian, due to the appearance of the cosine term proportional to $g_1$ in (1.4). The phase diagram of the sine-Gordon Hamiltonian is known through renormalization group (RG) calculations. One finds that, for $g_1 > 0$, the cosine term is an irrelevant perturbation whereas, for $g_1 < 0$, it is relevant and leads to the opening of a spin gap. The cosine acts as a potential for the field $\phi_\sigma(x)$, which has a discrete set of minima

\footnote{However, models of spin-charge separation exist in two-dimensional strongly-correlated systems. For instance, the excitations of a resonating valence bond state split into spinons and holons[160, 3].}
to choose from. As $g_1$ grows in the RG flow, $\phi_\sigma$ is frozen at one of these minima, thus gapping out the sliding degree of freedom of the spin. Since the symmetry group that is broken is discrete (it is isomorphic to the group of integers), the Mermin-Wagner theorem does not prevent the formation of such gap.

Figure 1.17 shows the phase diagram of a Luttinger liquid at zero temperature, obtained by comparing correlation function exponents for CDW, SDW, singlet (SSC) and triplet (TSC) superconducting orders through bosonization and RG methods[64]. As discussed above, for $g_1 > 0$ there is no spin gap, so that SDW and TSC are favored over CDW and SSC phases; for $g_1 < 0$ the converse it true. In addition, the case $K_\rho > 1$ ($K_\rho < 1$) corresponds to attractive (repulsive) interactions between electrons: Hence, superconductivity is preferred above $K_\rho = 1$, whereas spin and charge density waves are preferred below $K_\rho = 1$. The line $K_\rho = 1$ is special: the Hamiltonian along that line displays an enhanced symmetry group that will be introduced in Section 1.4.5 and is the topic of Chapters 4 and 5.

1.4.4 Mott insulators in one dimension

In the absence of a lattice, or when the electron filling is incommensurate with the lattice, even the phases labelled as SDW and CDW in Figure 1.17 are superconducting rather than insulating\textsuperscript{10}. This is due to the fact that the phase in the charge sector $\phi_\rho$ is not pinned, allowing the CDW and SDW to slide freely along the chain to obtain the so-called Froehlich superconductivity. Another way to view this is that all

\textsuperscript{10}This is, of course, assuming that no disorder is present to pin these states.
the interaction terms conserve momentum, and therefore there is no mechanism by which to damp a current. Things are different for systems at commensurate filling. The simplest case is half-filling, where the Fermi vector satisfies $4k_f = 2\pi$. Thus, one can include low energy scattering events where two right-movers turn into two left-movers, or vice versa, while conserving the total crystal momentum,

$$\mathcal{H}_3 = \frac{g_3}{2L} \sum a_{+,k+qs}^\dagger a_{+,p-qt}^\dagger a_{-,p} - a_{-,k+qs}^\dagger a_{-,p} + \frac{g_3}{2L} \sum a_{-,k+qs}^\dagger a_{-,p} - a_{+,p} a_{+,k+qs}.$$

Such umklapp scattering does not conserve total momentum, potentially leading to finite conductivity in the SDW and CDW phases.

Bosonization of the umklapp term $\mathcal{H}_3$ leaves the spin Hamiltonian unchanged while introducing an extra contribution to the charge Hamiltonian,

$$\mathcal{H}_\rho = \ldots + \frac{2g_3}{(2\pi\alpha)^2} \int dx \cos(\sqrt{8}\phi_\rho(x)).$$

This, once again, is a sine-Gordon term. The charge and spin Hamiltonians now have the same form, with the roles of charge and spin exchanged, as well as those of backscattering $g_1$ and umklapp $g_3$. The expression for the Luttinger parameter in the charge sector $K_\rho$ as a function of the interaction coefficients $g_i$ changes when umklapp is introduced, but there still is a direct transition at $K_\rho = 1$ between SDW and TSC phases, and between CDW and SSC phases. For $K_\rho > 1$, $g_3$ is irrelevant, there is no charge gap, and the system is superconducting whereas, for $K_\rho < 1$, $g_3$ is relevant and a charge gap appears. The phase $\phi_\rho$ of the charge degrees of freedom is then frozen at one of the minima of the umklapp potential, thus making the SDW and CDW phases insulating.

For commensurate fillings other than half-filling, it is also possible to get insulating behavior. For instance, for a quarter-filled lattice, there are processes at third order in perturbation theory in which four right-movers turn into four left movers, and vice versa. For example, starting with four right-moving electrons with momentum $+\pi/4$,

\[
\{ \frac{\pi}{4} \uparrow \frac{\pi}{4} \downarrow \frac{\pi}{4} \downarrow \frac{\pi}{4} \downarrow \} \xrightarrow{g_4} \{ -\frac{\pi}{4} \uparrow \frac{3\pi}{4} \uparrow \} \xrightarrow{g_4} \{ -\frac{\pi}{4} \uparrow \frac{3\pi}{4} \uparrow \} \xrightarrow{g_3} \{ -\frac{\pi}{4} \uparrow -\frac{\pi}{4} \uparrow \}
\]

where the first two steps conserve total momentum, and the third step is an umklapp scattering event. The amplitude for such process, $g' \sim (\frac{g_4}{D})^2 g_3$, is suppressed by the square in the band-width $D$. However, although the bare value of $g'$ is small, it is a relevant perturbation for strong enough repulsion, leading to insulating behavior. In particular, $n^{th}$ order umklapp ($n = 1$ for half-filling, $n = 2$ for quarter-filling, etc) is relevant for $K_\rho < 1/n^2$ [62]. Note that the Luttinger parameter in the charge sector $K_\rho$ is a monotonically decreasing function of electron-electron repulsion strength. However, for short-range repulsion of range $m$, $K_\rho$ is constrained from below, $K_\rho \geq \ldots$
1/2m^2, regardless of the strength of the interaction. For instance, for the Hubbard model, no matter how strong the on-site \((m = 1)\) repulsion is, \(K_p \geq 1/2\). This means that 2nd order umklapp is irrelevant in this case. This is, in fact, very sensible, since it is impossible to create an insulator for a quarter filled band with only on-site repulsion.

### 1.4.5 Competition of orders in Bechgaard salts

As discussed in Section 1.4.1, in the Bechgaard salt \((TMTSF)_2PF_6\) there is experimental evidence of a direct transition, tuned by pressure, between an antiferromagnetic insulator and a triplet superconductor. This is reminiscent of the phase diagram of a strictly one-dimensional Luttinger liquid, Fig. 1.17, where such a direct transition exists across \(K_p = 1\), whenever the backscattering amplitude \(g_1\) is positive. Assume, for the moment, that the normal state of Bechgaard salts can be treated as a collection of weakly coupled Luttinger liquids down to low temperatures. In that case, above (below) the critical pressure \(p_c\), one would expect the main divergence in the correlation length of the intrachain Hamiltonian to occur in the TSC (SDW) channel. As temperature decreases and the correlation length in that channel grows, interchain coupling kicks in to stabilize true long-range order. In this picture, the region surrounding \(p_c\) corresponds to the neighborhood of the half-line \(K_p = 1, g_1 > 0\) in the intrachain Hamiltonian, and pressure tunes the intrachain Luttinger parameter \(K_p\) across the transition.

This prompts us to look more closely at the symmetry generators of the Luttinger liquid near the line \(K_p = 1\). Bechgaard salts have very weak spin-orbit coupling: microwave absorption experiments in \((TMTSF)_2AsF_6\) find the relative anisotropy in the exchange couplings to be \(10^{-6}\) [186], while NMR experiments in \((TMTSF)_2PF_6\) find a divergence of \(T_1^{-1}\) at the Néel temperature that is well-described by the O(3) isotropic Heisenberg model [20]. Thus, the total charge \(Q\) and total spin \(S\) of the system are good symmetry generators. In addition, as discussed in Chapters 4 and 5, there is extra symmetry on the line \(K_p = 1\) [25, 161], generated by the operators,

\[
\Theta^\dagger_\pm = \pm \sum_k a^\dagger_{\pm, k} a^\dagger_{\pm, -k},
\]

where \(r = \pm\). These operators create spin-singlet electron pairs with total momentum \(\pm 2k_f\). For a linearized single-particle spectrum, the particle pairs have zero total kinetic energy. Therefore, \(\Theta^\dagger_\pm\) commutes with the kinetic energy operator \(H_0\). On the other hand, upon bosonization, \(\Theta^\dagger_\pm\) which is a spin-singlet operator, can be expressed in terms of charge variables only. However, \(K_p = 1\) corresponds to a system of non-interacting fermions as far as the charge sector is concerned. This implies that, for systems at incommensurate filling, \(\Theta^\dagger_\pm\) commutes with the entire Hamiltonian at \(K_p = 1\), as shown explicitly in Appendix B.1.
Chapter 1: Introduction

The Θ operators can be combined with the total charge operators for right and left movers, \( Q_\pm \), to form two separate “isospin” algebras \( (r, r' = \pm) \),

\[
\begin{align*}
J_r^x &= \frac{1}{2} (\Theta^\dagger_r + \Theta_r), \\
J_r^y &= \frac{1}{2i} (\Theta^\dagger_r - \Theta_r), \\
J_r^z &= Q_r, \\
\left[ J_a^r, J_b^{r'} \right] &= i \delta_{r,r'} \epsilon^{abc} J_c^{r'}. 
\end{align*}
\]

In this case, the total symmetry group at \( K_\rho = 1 \) is \( \text{SO}(3) \text{_{right}} \times \text{SO}(3) \text{_{left}} \times \text{SO}(3) \text{_{spin}} \). However, Bechgaard salts have commensurate band filling (they are half-filled due to dimerization), and therefore umklapp scattering must be taken into account. Umklapp changes the total number of right or left movers, so that the charge operators \( Q_\pm \) are not conserved separately. In fact, one can show that only the sum of the two isospin algebras, \( I_a = J_a^+ + J_a^- \), is conserved in this case\[25, 161\]. Thus, the symmetry of the system at half-filling is reduced to \( \text{SO}(4) \sim \text{SO}(3) \text{_{isospin}} \times \text{SO}(3) \text{_{spin}} \).

As discussed above, from the bosonization point of view, the system with umklapp maps to a sine-Gordon Hamiltonian in both the spin and charge sectors. The charge sector is \( \text{SO}(3) \) isospin symmetric, just as the spin sector has an exact \( \text{SO}(3) \) spin symmetry that is not manifest in the Abelian bosonized form. Indeed, starting from the bosonized expression for \( \Theta^\dagger \) in Appendix B.1, and replacing the charge variables \( \phi_\rho \) and \( \theta_\rho \) by spin variables \( \phi_\sigma \) and \( \theta_\sigma \), one obtains the bosonized expression for the spin raising operator \( S^+ \).

The \( \text{SO}(4) \) symmetry allows us to treat the complex vector triplet superconducting order parameter, \( \vec{\Psi} \), and the real Néel vector, \( \vec{N} \), as degenerate components of a unified matrix order parameter,

\[
\hat{Q} = \begin{pmatrix}
(\text{Re} \vec{\Psi})_x & (\text{Im} \vec{\Psi})_x & N_x \\
(\text{Re} \vec{\Psi})_y & (\text{Im} \vec{\Psi})_y & N_y \\
(\text{Re} \vec{\Psi})_z & (\text{Im} \vec{\Psi})_z & N_z
\end{pmatrix}.
\]

The group \( \text{SO}(3) \text{_{spin}} \) rotates the columns of the matrix, whereas \( \text{SO}(3) \text{_{isospin}} \) rotates the rows. The consequences of enhanced symmetry, outlined in Section 1.3, can be used in the case at hand, for instance to reduce the number of free parameters in the GL free energy near the AF/TSC transition from five to only two. This leads to a strongly constrained phase diagram, computed in Chapter 5, which agrees with many of the qualitative features of the experimental phase diagram, Fig. 1.13. Furthermore, enhanced dynamic symmetry leads to new low energy collective modes, corresponding to rotations between the order parameters \( \vec{\Psi} \) and \( \vec{N} \) due to the isospin generators. These “Θ-modes”, which soften at the AF/TSC phase boundary, can be detected in tunneling and neutron scattering experiments on superconducting samples. Softening
of modes does not generally occur at a first order transition. Here, pseudo-Goldstone modes become true Goldstone modes at the transition as a direct consequence of enhanced symmetry.

Despite the fact that the isospin $\Theta$ operators are reminiscent of the pseudospin $\eta$ operators of the half-filled Hubbard model, note the important differences between the two. First of all, $\eta$ is a symmetry for arbitrary values of the interaction $U$, but only at half-filling, whereas $\Theta$ is a symmetry only at a fixed value of the interaction strength in the charge sector, $K_\rho = 1$, but for arbitrary band filling (in fact, away from half-filling it generates an even larger symmetry group). Furthermore, as shown in Chapter 5, the two symmetries connect different sets of order parameters.

Finally, although the above analysis relied on modelling Bechgaard salts as a collection of weakly coupled Luttinger liquids, the results outlined above hold even in the limit when interchain hopping is large enough that electron hopping is coherent in two directions rather than one. Indeed, there are indications that, at high pressures and low temperatures, it may be necessary to model the normal phase of Bechgaard salts in terms of a highly anisotropic Fermi liquid in two dimensions [195, 19, 51]. For instance, field-induced SDW experiments, in which SDW order is stabilized by a large external magnetic field, have been interpreted as a crossover from two dimensional to one dimensional behavior with applied field [104, 9, 22, 66, 52, 203]. In Section 5.8, I will show that for a highly anisotropic Fermi liquid with weak interactions, the GL free energy remains approximately SO(4) symmetric despite the fact that interchain coupling deteriorates nesting, thus affecting the Néel order much more profoundly than the superconductivity. In terms of dynamic properties, the low energy $\Theta$ modes of the one dimensional Hamiltonian are likely to be weakly gapped, and to be broadened, due to the interchain hopping. However, they should still be present as low energy excitations in inelastic neutron scattering that soften as the AF/TSC transition is approached, providing a strong signature of enhanced symmetry.
Chapter 2

Translational Symmetry Breaking in the Superconducting State of the Cuprates: Analysis of the Quasiparticle Density of States

2.1 Introduction

Puzzling properties of the high-$T_c$ cuprates have often been attributed to the existence of competing instabilities, and proximity (or even coexistence) of several ordered states. Possible instabilities that have been discussed in this context include charge density wave (CDW) order, non-two-sublattice spin density wave (SDW) order [206, 55, 211, 154], spin Peierls order [197], and orbital magnetism [28, 193]. Neutron scattering experiments on La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ [187], La$_x$Sr$_{1-x}$CuO$_4$ [89, 106], and La$_2$CuO$_{4+x}$ [96] demonstrated the coexistence of magnetism and superconductivity, while recent experiments on strongly underdoped YBa$_2$Cu$_3$O$_{6.35}$ [135] have seen evidence of CDW order coexisting with superconductivity. Particularly striking in this context are recent STM experiments on Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [72, 75, 74] which see spatial structure in the tunneling density of states with a period of four lattice constants. This structure was originally observed in the experiments in a magnetic field by J.E. Hoffman et al. [72], and later also seen in zero field by C. Howald et al. [75, 74]. Modulo certain experimental subtleties, these experiments can be thought of as measurements of the spatial Fourier component (at the ordering wave vector $\mathbf{Q}$) of the energy dependent local density of states (LDOS) $\rho_{\mathbf{Q}}(\epsilon)$.

In this paper, we demonstrate that the energy dependence of $\rho_{\mathbf{Q}}(\epsilon)$ provides important information about the nature of charge ordering in these materials. It allows us to separate simple charge density wave order, that has only the Hartree-Fock potential modulation, from the more unusual charge orders that involve modulation
of the electron kinetic energy (dimerization) or the pairing amplitude (anomalous dimerization). For example, when \( \mathbf{Q} = (2\pi/4, 0) \) (as observed in slightly overdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$), there is a change of sign in \( \rho_{\mathbf{Q}}(\epsilon) \) for energies around 40 meV when dimerizations are present, but not in the case of a simple CDW. When several of the simple distortions are present simultaneously, we can understand the resulting \( \rho_{\mathbf{Q}}(\epsilon) \) as (roughly) a superposition of the corresponding simple cases, since the induced \( \rho_{\mathbf{Q}}(\epsilon) \) is approximately linear in the order parameter for small distortions. Such a superposition is necessary to understand the experiments of [75, 74].

This superposition principle also applies when we have potential modulation at several wavevectors, and \( \rho_{\mathbf{q}}(\epsilon) \) can be analyzed separately for each wavevector \( \mathbf{q} \). This is necessary, for example, when we have randomness that pins the charge order, so that the single particle potential is not a delta function in momentum space but has a narrow distribution centered at the ordering wavevector \( \mathbf{Q} \). This leads to a finite \( \rho_{\mathbf{q}}(\epsilon) \) for a range of wavevectors around \( \mathbf{Q} \) and, as we discuss below, taking a reasonable value of the CDW correlation length reproduces well the “weak dispersion” of the CDW peak observed in [74]. Our analysis can be extended to systems with no charge order but, instead, with localized defects, e.g. impurities. In this case we have a potential that is essentially momentum independent and we find strongly dispersing peaks in \( \rho_{\mathbf{q}}(\epsilon) \) for a wide range of wavevectors. Such peaks have been observed in the STM experiments in [73, 130] and discussed theoretically in [200, 153]. We provide a qualitative comparison of the STM spectra for systems with disordered CDW and impurity scattering.

It is common to discuss spin density wave (SDW) order as the primary competitor to superconductivity in the underdoped cuprates [206, 211, 168, 157, 213]. An order parameter for non-two-sublattice magnetism is

\[
\tilde{S}(\mathbf{r}) = \tilde{\phi} e^{i \mathbf{Q}_s \mathbf{r}} + \tilde{\phi}^* e^{-i \mathbf{Q}_s \mathbf{r}},
\]

where the complex-valued vector \( \tilde{\phi} \) acquires an expectation value in a state with broken spin symmetry. When the SDW order in (2.1) is collinear, it has an associated spin singlet order parameter that only breaks translational symmetry and can be described as a generalized charge density wave [213]

\[
\delta \rho(\mathbf{r}) = \varphi e^{i \mathbf{Q}_c \mathbf{r}} + \varphi^* e^{-i \mathbf{Q}_c \mathbf{r}}.
\]

Symmetry arguments determine the wavevector \( \mathbf{Q}_c = 2 \mathbf{Q}_s \) of such generalized CDW, but they do not clarify its internal structure. For example, modulation of the local Hartree-Fock potential of the electrons and modulation of the electron kinetic energy (hopping) are both spin singlet order parameters that can be defined at the same wavevector and described by (2.2). Modulation of the electron pairing amplitude also belongs to the same class of translational symmetry breaking since, in the superconducting state with condensed Cooper pairs, order parameters with charge two and zero are not orthogonal. It is important to note, however, that a long range SDW
order is not a prerequisite for translational symmetry breaking. One can have a situation where quantum or thermal fluctuations destroy the spin order but preserve a long range order in the charge sector [208]. This was observed, for example, in underdoped YBa$_2$Cu$_3$O$_{6.35}$ [135], where neutron scattering found period eight CDW but no static spin order. For slightly overdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, on which most of the tunneling experiments have been performed, neutron scattering experiments suggest dynamic spin fluctuations [57]. In our analysis we then assume that there is no SDW order and concentrate on the effects of spin singlet translational symmetry breaking. Another possible origin of a generalized CDW with no spin symmetry breaking comes from pinning of SDW by disorder [153, 155] or vortices [213, 30].

We restrict our analysis to the case of weak translational symmetry breaking, when the new order parameter can be treated as a small perturbation to the superconducting mean-field Hamiltonian. This limit clearly applies to the experimental situation in [72, 75, 73, 130, 74, 35], where the measured modulation is weak, and allows us to obtain explicit approximate expressions for $\rho_Q(\epsilon)$. [This circumvents solving a complicated set of equations numerically, as for instance carried out in [155].] Furthermore, we do not address the issue of the origin of charge order, but introduce it phenomenologically and study its consequences for the STM experiments. Our basic motivation is that a comparison of the energy dependence of $\rho_Q$ with experimental data can, in principle, be used to identify the correct order parameter(s) which, in turn, is crucial for understanding their origin.

This paper is organized as follows. In Section II we introduce mean-field Hamiltonians that describe several kinds of translational symmetry breaking in a lattice system. For these generalized CDWs we derive an explicit formula for the Fourier component of the tunneling density of states at the ordering wavevector. Section III displays numerical results of this expression in the case of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ type band structure and period four charge order. We show that recent STM experiments by [75, 74] are consistent with a generalized CDW that has modulation of either the electron hopping or the pairing amplitude. We also consider period eight structure that may be relevant to YBa$_2$Cu$_3$O$_{6.35}$. In Section IV we extend our analysis to phases with randomness and show that a realistic value of the CDW correlation length $\langle 20a_0 \rangle$, with $a_0$ the unit cell size) provides good agreement with the “weak dispersion” of the CDW peak observed in [74]. As a different application of our formalism we also consider localized perturbations in the crystal, such as impurity potentials, and demonstrate that these can account for the strongly dispersing peaks observed in [73, 130] at wavevectors not corresponding to the CDW order. In Section V we review how to include a more realistic model of the atomic wavefunctions, whose main effect is to introduce a momentum dependent structure factor. An important implication of this result is that the signal at wavevectors differing only by a reciprocal lattice vector should have peaks at the same energies, although their amplitudes may differ. We also discuss complications in the analysis of the STM data introduced by the normalization procedure used in the experiments. Finally, in Section VI we
discuss several sum rules for the Fourier components of the density of states that may be useful for analyzing experiments.

2.2 Order parameters and Mean-Field Hamiltonians for generalized charge density wave phases

Our starting point is a two dimensional one-band mean-field Hamiltonian that is commonly believed to be a good model for the physics of the \(d_{x^2-y^2}\) superconducting state of the cuprates:

\[
\mathcal{H} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_k \Delta_k (c_{k\uparrow}^\dagger c_{-k\downarrow} + c_{-k\uparrow} c_{k\downarrow}) \tag{2.3}
\]

Here \(\epsilon_k = -2t(\cos(k_x) + \cos(k_y)) - 4t_1 \cos(k_x) \cos(k_y) - \mu\), \(\Delta_k = \frac{\Delta_0}{2} (\cos k_x - \cos k_y)\) (from now on the unit cell size is set to unity), \(c_{r\sigma} = N^{-1/2} \sum_k c_{k\sigma} e^{ikr}\), and \(N\) is the number of sites in the lattice. The Hamiltonian (2.3) can be diagonalized using the Bogoliubov transformation \(c_{k\uparrow} = u_k \gamma_{k\uparrow} + v_k \gamma_{-k\downarrow}\), \(c_{-k\downarrow} = u_k \gamma_{-k\downarrow} - v_k \gamma_{k\uparrow}\) with \(u_k^2 + v_k^2 = 1\), \(u_k v_k = \frac{\Delta_k}{2E_k}\), \(c_{r\sigma} = \frac{1}{N} \sum_k c_{k\sigma} e^{ikr}\), and \(E_k = \left(\epsilon_k^2 + \Delta_k^2\right)^{1/2}\).

Weak charge order may be introduced into the state (2.3) by assuming the appearance of one or more of the additional order parameters listed below. We note that distinction between site and bond centered orders discussed below is only defined for CDW with integer periods.

**Site-centered charge density wave.** The local Hartree-Fock potential is modulated along \(x\) with potential extrema on the lattice sites (see Fig. 1a):

\[
\Delta H_1 = V_0 \sum_{\sigma, k} \left( c_{k+Q\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{k+Q\sigma} \right)
\]

**Bond-centered charge density wave.** The local Hartree-Fock potential is modulated along \(x\) with the extrema of the modulation at midpoints of the horizontal bonds (see Fig. 1b):

\[
\Delta H_2 = V_0 \sum_{\sigma, k} \left( \alpha^* c_{k+Q\sigma}^\dagger c_{k\sigma} + \alpha c_{k\sigma}^\dagger c_{k+Q\sigma} \right), \quad \text{where } \alpha = e^{iQ/2}.
\]

**Longitudinal dimerization.** Single electron tunneling amplitudes are modulated on the horizontal bonds and the wavevector of modulation is along the same direction (i.e. along \(x\)). The bond centered version, in which the extrema of the modulation lie on the bonds (see Fig. 1c) corresponds to: \(\Delta H_3 = V_0 \sum_{\sigma, k} \cos(k_x + \frac{Q}{2}) \left( \alpha^* c_{k+Q\sigma}^\dagger c_{k\sigma} + \alpha c_{k\sigma}^\dagger c_{k+Q\sigma} \right)\).

**Transverse dimerization.** Single electron hopping is modulated on the vertical bonds, and the wavevector of modulation is along the horizontal direction (i.e. along \(x\)). The site centered version (i.e. with extrema of the modulation realized on the vertical bonds) is shown in Fig. 1d, and corresponds to:

\[
\Delta H_4 = V_0 \sum_{\sigma k} \cos k_y \left( c_{k+Q\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{k+Q\sigma} \right).
\]
Anomalous longitudinal dimerization. The $x$-components of the $d_{x^2-y^2}$-wave pairing amplitudes are modulated in the $x$ direction. The bond centered version, shown in Fig. 1c, corresponds to: $\Delta \mathcal{H}_5 = V_0 \sum_{\sigma, \mathbf{k}} \{ \cos(k_x + \frac{Q}{2}) \left( \alpha^* c_{\mathbf{k}+Q}^\dagger c_{\mathbf{k}}^\dagger + \alpha c_{\mathbf{k}}^\dagger c_{\mathbf{k}}^\dagger - k - Q \right) \} + \text{h.c.}$.

Anomalous transverse dimerization. The $y$-components of the $d_{x^2-y^2}$-wave pairing amplitudes are modulated in the $x$ direction. The site centered version, shown in Fig. 1d, corresponds to: $\Delta \mathcal{H}_6 = V_0 \sum_{\sigma, \mathbf{k}} \{ \cos k_y \left( \alpha^* c_{\mathbf{k}+Q}^\dagger c_{\mathbf{k}}^\dagger + \alpha c_{\mathbf{k}}^\dagger c_{\mathbf{k}}^\dagger - k - Q \right) \} + \text{h.c.}$.

Note that these subdominant order parameters may appear either as a result of a phase transition in the bulk, or due to pinning by vortices, impurities or any other defects (see discussion in Section IV). Following experimental observations in [75, 74, 134], we assume that the order is unidirectional, and choose the ordering wave vector to be $Q = Q \hat{e}_x$. However, even if we were to assume checkerboard order, our analysis is carried out to linear order in perturbation theory and, by linear superposition, our results would be identical to those obtained for unidirectional order. For the STM experiments in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [72, 75], $Q = 2\pi/4$, while

---

The distinction between site and bond-centered orders is only defined for translational symmetry breaking commensurate with the lattice, i.e. when the wave vector is $Q = 2\pi/n$ with $n$ integer.
the neutron scattering experiments on YBa$_2$Cu$_3$O$_{6.35}$ [135] correspond to the smaller value: \( Q = 2\pi /8 \). We point out that the six cases listed above are, in general, not orthogonal to each other in a symmetry sense. As a result it is conceivable that more than one order parameter could be simultaneously non-zero; for example, in a microscopic model without particle-hole symmetry, a simple CDW would be expected to induce dimerization as the two order parameters are linearly coupled [98].

Upon expressing the Hamiltonians \( \Delta H \) in the basis of Bogoliubov quasiparticles, they reduce to the generic form

\[
\Delta H_i = \sum_{k\sigma} \left[ A_k^i \gamma_{k\sigma}^\dagger \gamma_{k+Q\sigma} + A_{k+Q}^i \gamma_{k\sigma}^\dagger \gamma_{k+Q\sigma} \right] + \sum_k \left[ B_k^i \gamma_{k\sigma}^\dagger \gamma_{k+Q\sigma} + B_{k+Q}^i \gamma_{k\sigma}^\dagger \gamma_{k+Q\sigma} + h.c. \right],
\]

(2.4)

where

\[
\begin{align*}
A_k^1 &= V_0 \omega_k \\
A_k^2 &= V_0 \alpha \omega_k \\
A_k^3 &= V_0 \alpha \cos(k_x + \frac{Q}{2}) \omega_k \\
A_k^4 &= V_0 \alpha \cos(k_y) \omega_k \\
A_k^5 &= -V_0 \alpha \cos(k_x + \frac{Q}{2}) \eta_k \\
A_k^6 &= -V_0 \cos(k_y) \eta_k \\
B_k^1 &= V_0 \eta_k \\
B_k^2 &= V_0 \alpha \eta_k \\
B_k^3 &= V_0 \alpha \cos(k_x + \frac{Q}{2}) \eta_k \\
B_k^4 &= V_0 \alpha \cos(k_y) \eta_k \\
B_k^5 &= V_0 \alpha \cos(k_x + \frac{Q}{2}) \omega_k \\
B_k^6 &= V_0 \cos(k_y) \omega_k
\end{align*}
\]

(2.5)

in terms of the coherence factors \( \omega_k = u_{k+Q} u_k - v_{k+Q} v_k \) and \( \eta_k = u_{k+Q} v_k + v_{k+Q} u_k \).

STM experiments measure the local density of states \( \rho(r, \epsilon) = \sum_{n\sigma} \left\{ |\langle n | c_{r\sigma}^\dagger | 0 \rangle|^2 \delta(\epsilon - \epsilon_n) + |\langle n | c_{r\sigma} | 0 \rangle|^2 \delta(\epsilon + \epsilon_n) \right\} \), where the summation over \( n \) ranges over all excited states. In particular, we are interested in the Fourier transform

\[
\rho_q(\epsilon) = \frac{1}{N} \sum_r e^{-iqr} \rho(r, \epsilon)
\]

\[
= \frac{1}{N} \sum_{n\kappa\sigma} \left[ \langle 0 | c_{k+q\sigma} | n \rangle \langle n | c_{k\sigma}^\dagger | 0 \rangle \delta(\epsilon - \epsilon_n) \right. + \left. \langle 0 | c_{k\sigma}^\dagger | n \rangle \langle n | c_{k+q\sigma} | 0 \rangle \delta(\epsilon + \epsilon_n) \right] .
\]

(2.6)

Although a full treatment of all terms in (2.4) is complicated, progress can be made if we assume that the ordering represented by \( \Delta H \) is weak, allowing us to obtain an analytic expression for the Fourier transform that is exact to linear order in \( V_0 \). This is then the sum of two contributions

\[
\rho_Q(\epsilon) = \rho_Q^A(\epsilon) + \rho_Q^B(\epsilon) + O(V_0^2),
\]

(2.7)

where \( \rho_Q^A(\epsilon) \) is obtained by ignoring the \( B_k \) term in the perturbation (2.4) and vice versa.
Chapter 2: Translational Symmetry Breaking in the Superconducting State of the Cuprates: Analysis of the Quasiparticle Density of States

A small value of \( V_0 \) leads to another important simplification: We only need to consider the pairwise mixing between states connected by \( \Delta \mathcal{H} \). For instance, in computing \( \rho^A_Q(\epsilon) \) for \( Q = 2\pi/4 \) one would have to analyze coupled equations for four quasiparticles \((k, k + Q, k + 2Q, k + 3Q = k - Q)\) connected by the perturbation. However, in the limit when \( V_0 \) is small, there is at most one pair of quasiparticles that have similar energies, and that will be hybridized appreciably by \( \Delta \mathcal{H} \). This hybridization can be analyzed by diagonalizing the corresponding two-by-two Hamiltonian, which gives the new eigenstates \(|\alpha_{\kappa\sigma}\rangle\) and \(|\beta_{\kappa\sigma}\rangle\) with energies \( \tilde{E}_{k\pm} = \frac{E_k + E_{k+Q}}{2} \pm \left[ \frac{(E_k - E_{k+Q})^2}{2} + |A_k|^2 \right]^{1/2} \). Note that these states satisfy \( \langle 0|c_{k+Q\sigma}|\alpha_{\kappa\sigma}\rangle\langle\alpha_{\kappa\sigma}|c^\dagger_{k\sigma}|0\rangle = \frac{1}{2} u_ku_k+Q \sin 2\theta_k e^{-i\chi_k} \), \( \langle 0|c_{k+Q\sigma}|\beta_{\kappa\sigma}\rangle\langle\beta_{\kappa\sigma}|c^\dagger_{k\sigma}|0\rangle = -\frac{1}{2} u_ku_k+Q \sin 2\theta_k e^{i\chi_k} \), where we have defined \( A_k = |A_k| e^{i\chi_k} \), and tan \( 2\theta_k = 2|A_k|/(E_k - E_{k+Q}) \). From these results one easily finds

\[
\rho^A_Q(\epsilon) = \frac{1}{N} \sum_k \frac{A_k^*}{\sqrt{\left( \frac{E_k - E_{k+Q}}{2} \right)^2 + |A_k|^2}} \times \left[ u_ku_{k+Q} \left( \delta(\epsilon - \tilde{E}_{k+}) - \delta(\epsilon - \tilde{E}_{k-}) \right) \right. \\
\left. + u_{k+Q}v_k \left( \delta(\epsilon + \tilde{E}_{k+}) - \delta(\epsilon + \tilde{E}_{k-}) \right) \right] \quad (2.8)
\]

When considering \( \rho^B_Q \), one would naively expect that it is always smaller than \( \rho^A_Q \), because the perturbation terms of the form \( \gamma^\dagger_{k+Q} \gamma^\dagger_{k-l} \) connect states that differ in energy by \( E_k + E_{k+Q} \), a factor that is never small. However, in some cases the coherence factors in \( A_k \) vanish at important regions of the Brillouin zone, making \( \rho^A_Q(\epsilon) \) anomalously small. In addition, as we discuss below, both \( \rho^{A,B}_Q(\epsilon) \) are large at biases corresponding to the saddle points on the degeneracy lines \( E_k = E_{k+Q} \) and van Hove singularities of the Bogoliubov quasiparticles \( \epsilon \approx \Delta_0 \). A nearly identical analysis of the one above for \( \rho^A \) yields

\[
\rho^B_Q(\epsilon) = \frac{1}{N} \sum_k \frac{B_k^*}{\sqrt{\left( \frac{E_k + E_{k+Q}}{2} \right)^2 + |B_k|^2}} \times \left[ u_kv_{k+Q} \delta(\epsilon - \tilde{E}_{k+}) + u_{k+Q}v_k \delta(\epsilon - \tilde{E}_{k-}) \right. \\
\left. - u_{k+Q}v_k \delta(\epsilon + \tilde{E}_{k+}) - u_{k+Q}v_{k+Q} \delta(\epsilon + \tilde{E}_{k-}) \right] \quad (2.9)
\]

where \( \tilde{E}_{k\pm} = \pm \frac{E_k - E_{k+Q}}{2} + \left[ \frac{(E_k + E_{k+Q})^2}{2} + |B_k|^2 \right]^{1/2} \). Equations (2.8,2.9), are two key results of this paper. In combination with Eqns (2.5), they provide an explicit expression for the energy dependence of the Fourier component of the local density of states \( \rho_Q(\epsilon) \) when the translational symmetry breaking is weak.
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From the form of \( A_k \) and \( B_k \), it is obvious that when there is no mixing between bond and site centered CDW, \( \rho_Q(\epsilon) \) can be made real at all energies by an appropriate choice of the overall phase, \( i.e. \) by a shift in the origin of coordinates when doing the Fourier transform. One obvious observation is that the results for the site-centered and bond-centered CDW are identical modulo an overall phase factor of \( e^{iQ/2} \). If one defines the Fourier transform in such a way that it is real in both cases, the origin will coincide with one of the sites of the lattice for the site-centered CDW, and it will be at the center of a bond for the bond-centered CDW. Hence careful analysis of the STM data allows one to distinguish two kinds of CDW, a task that is not possible in neutron scattering experiments with current resolution. Mixing site and bond-centered orders breaks inversion symmetry and leads to a complex-valued \( \rho_Q(\epsilon) \).

2.3 Charge order with no randomness

2.3.1 Period four CDW in \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \)

We first focus on modulations at \( Q = (2\pi/4, 0) \) that is relevant to \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) [72, 75]. Figure 2.2 shows results of the numerical evaluation of formulas (2.7), (2.8) and (2.9) for various perturbations (2.5). [As transverse and longitudinal dimerization curves are qualitatively similar, curves corresponding to the former are not displayed.] We choose the band structure and the value of \( \Delta_0 \) in (2.3) appropriate to \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \): \( t_1/t = -0.3, \mu/t = -0.99 \) (this corresponds to 14\% doping), \( \Delta_0/t = 0.14 \) and \( \Delta_0 = 40 \text{ meV} \) [127]. We set \( V_0/t = 0.02 \), although its precise value is inconsequential, as \( \rho_Q(\epsilon) \) scales linearly with \( V_0 \) when the latter is sufficiently small.

If we turn our attention to the expression for \( \rho^A \), Eqn. (2.8), we see that the energy denominator is smallest for those quasiparticles lying close to the degeneracy points \( E_k \equiv E_k+Q \), which are strongly hybridized by the \( A_k \) part of the perturbation. Figure (2.3) shows the four loci of such points, \( a \) through \( d \), that are degenerate with \( a' \) to \( d' \) respectively. The pairs \( aa' \) and \( bb' \) are obvious, since they have \( k_x = \pm\pi/4 \) and \( k_x = \pm3\pi/4 \) (for the same \( k_y \)); the other two require a more detailed analysis of the band structure. Out of the set of degeneracy points, we expect large contributions from the neighborhood of points A and B, as the dispersion of hybridized energies \( \tilde{E}_{k\pm} \) is flat at these points. These same regions of the Brillouin zone will dominate the \( \rho_B \) contribution, since the energy denominator in (2.9) will be small only if both \( k \) and \( k + Q \) lie close to the Fermi surface, which occurs only in the neighborhood of points A and B. In addition we expect, for both \( \rho^A \) and \( \rho^B \) pieces, a large contribution at \( \epsilon = \Delta_0 \), where a van Hove singularity for the Bogoliubov quasiparticles yields a logarithmic divergence in the density states.

We turn now to the numerical results displayed in Fig 2.2. Consider first the simple CDW curves. The sharp features that dominate the CDW plots can be understood in terms of the degeneracies mentioned above: the peak at energies around 0.5\( \Delta_0 \) comes
Figure 2.2: Energy dependence of the Fourier component of the local density of states $\rho_Q(\epsilon)$ at $Q = (2\pi/4, 0)$ for various cases of charge ordering. Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ type band structure is assumed. We show a direct calculation based on formulas (2.7,2.8,2.9). The curves correspond to the CDW (solid), longitudinal dimerization (dashed) and anomalous longitudinal dimerization (dotted) orders. To simplify the comparison, $\rho_Q(\epsilon)$ is multiplied by $-1$ for CDW, and by $\frac{1}{2}$ for anomalous longitudinal dimerization. In addition, subsequent curves are shifted vertically by 0.6. Results for both kinds of transverse dimerization are qualitatively similar to corresponding longitudinal results and are omitted for visual clarity.
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Figure 2.3: Fermi surface for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Dashed lines correspond to the quasiparticles that satisfy $E_{k+Q} = E_k$ and are strongly affected by $\Delta H$ when $Q = (2\pi/4, 0)$. Quasiparticles on line $a$ hybridize with quasiparticles on line $a'$ (and similarly for lines $b$ and $b'$, and curves $c$, $c'$ and $d$, $d'$). Crossings of these lines with the Fermi surface (points $A$ and $A'$, $B$ and $B'$) give the minimal energy of such quasiparticles: $0.5\Delta_0$ and $0.7\Delta_0$ respectively. Contributions from these points produce sharp peaks at energies 20 and 30 meV in Fig. 2. The Van Hove singularity for the Bogoliubov quasiparticles at energy $\Delta_0$ leads to a peak at 40 meV.

from the vicinity of the A point, the peak around $0.7\Delta_0$ comes from the vicinity of B, and the pile around $\Delta_0$ comes from the van Hove singularity near the $(0, \pi)$ and $(\pi, 0)$ points. The longitudinal dimerization results can be similarly understood by taking into account the additional minus sign in the vicinity of the point B due to the factor $\cos(k_x+\pi/4)$ in $A_k$ and $B_k$. The results for the anomalous dimerization can also be understood in this framework after taking into account the extra sign modulation in $u_kv_k$, which changes sign whenever $\Delta_k$ does. Note that, for all perturbations considered, $\rho_Q(\epsilon)$ displays approximate particle-hole symmetry for small biases, as observed in STM measurements [75]. This is not a generic property of $\rho_Q(\epsilon)$; for example, for a diamond-shaped Fermi surface $\mu = t' = 0$ the CDW signal is exactly antisymmetric. Finally, note that $\rho_Q(\epsilon)$ goes to zero at $\epsilon = 0$ in all cases; this reflects the vanishing density of low-energy quasiparticle states in an ideal $d$-wave superconductor.

While the results in Figure 2.2 describe a system with infinite quasiparticle lifetime and no disorder, in a real system disorder will smear the sharp features in $\rho_Q(\epsilon)$. To model this, these curves are re-displayed in Figure 2.4 after smearing over an energy width $w = 0.2\Delta_0$. This procedure smoothes the sharp features in the spectra, and generates finite intensity at low energies. Notice that the smeared CDW curve does not have the two large peaks surrounding zero bias, nor does it have clear zero crossings at $|\epsilon| \approx \Delta_0$, the dominant features of the STM spectra observed in
Figure 2.4: The results in Fig. 2.2 are shown after smearing over an energy range of 8 meV. To simplify the comparison, $\rho_Q(\epsilon)$ was multiplied by $-1$ for CDW and anomalous transverse dimerization, and by a factor of $-\frac{1}{2}$ for transverse dimerization.

By contrast, the signal related to longitudinal dimerization or, especially, to either kind of anomalous dimerization, share many of the qualitative properties of the data. However, neither curve by itself accounts for all the observed features in the data. This prompts us to consider a combination of several kinds of order. For example, if we assume that no pairing modulation is present, the combination of longitudinal dimerization and CDW, $(\text{long.dim.}) + 1.05(\text{CDW})$, shown as a solid curve in Figure 2.5 reproduces the STM results reasonably well, with only a small difference in the position of the peaks ($\pm 17$ meV, compared to experimentally observed $\pm 25$ meV). Alternatively we can match experimental data by considering the combination of anomalous longitudinal dimerization and CDW, $(\text{anom.long.dim}) + 0.2(\text{CDW})$, shown as a dashed curve in Figure 2.5. It slightly overestimates the peak bias to be $\pm 29$ meV, and yields a low intensity at zero bias. Any intermediate combination between these two scenarios also gives good agreement with experiments. Although CDW was used in both combinations discussed above, it can be substituted by transverse dimerization, which yields a qualitatively similar $\rho_Q(\epsilon)$ to CDW. We note that, for $\epsilon \leq 3\Delta_0$, the results come from the vicinity of the Fermi surface and are robust against variations in the band structure that do not alter qualitatively the shape of the Fermi surface (e.g. the $a$ and $b'$ lines do not move below the Fermi surface).

We note, however, that a certain care should be exercised when comparing our results to the STM spectra in [72, 75, 73, 130, 74]. An additional complication of the experiments is that for every point on the surface of the sample the height of the STM tip is adjusted to keep the tunneling current at a certain voltage fixed.
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Figure 2.5: $\rho_Q(\epsilon)$ for $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ type band structure, ordering wavevector $Q = 2\pi/4$ and a combination of charge orders: longitudinal dimerization and CDW, $1.05\text{(CDW)} + (\text{long},\text{dim.})$ (solid line); anomalous longitudinal dimerization and CDW, $(\text{anom,long,dim.}) + 0.2\text{(CDW)}$ (long-dashed line). The same smearing is assumed as in Fig.2.4. For clarity, curves have been offset vertically by 0.25.

This implies that the local density of states is not measured directly, but instead its product with some space dependent function is measured. In Section 2.5 we review how this normalization procedure can be included in analysis.

2.3.2 Period eight CDW in $\text{YBa}_2\text{Cu}_3\text{O}_{6.35}$

To model $\text{YBa}_2\text{Cu}_3\text{O}_{6.35}$ for which CDW-type peaks have been observed at $Q = 2\pi/8$ [135] we take the same band structure $t_1/t = -0.3$, but a different value of the chemical potential $\mu/t = -0.815$ (this corresponds to 6% doping). We use the same value of $\Delta_0/t = 0.14$, $\Delta_0 = 40$ meV, $V_0/t = 0.02$, and keep the energy smearing $w = 0.2\Delta_0$. The main difference with the charge order at $Q = 2\pi/4$ is that the analog of line $a$ in this case is inside the Fermi surface, so that the only contributions will come from the vicinity of point B at energies around $0.8\Delta_0$. This leads to less structure in $\rho_Q(\epsilon)$ and smaller intensity at zero energy (see Fig. 2.6).

2.4 Dispersion of the STM spectra

Recent experiments [73, 130] demonstrated that the STM spectra of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ cannot be explained by charge order at a unique wavevector. Peaks in $\rho_Q(\epsilon)$ have been observed away from $(2\pi/4, 0)$ and the wavevectors of the peaks are energy dependent.
Figure 2.6: YBa$_2$Cu$_3$O$_{6.35}$ type band structure and ordering wavevector $Q = (2\pi/8, 0)$. The inset shows $\rho_Q(\epsilon)$ for CDW (solid line), dimerization (dashed line), and anomalous dimerization (dotted line) separately. Main figure has the linear combination $(a_d + 0.2(CDW))$, which was displayed for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ in Fig. 2.5 (the other linear combination is nearly zero and thus omitted). The same smearing is assumed as in Fig. 2.4.

In this section we review and compare two possible scenarios for such dispersion of the STM spectrum: 1) randomness and pinning of charge order, 2) scattering of BCS quasiparticles by impurities and crystal defects. Both cases can be described using an extension of the formalism presented in the previous section. We consider a single particle Hamiltonian that generalizes equation (2.4)

$$\Delta \mathcal{H} = \sum_{kq\sigma} \left[ V_{kq} c_{k,\sigma}^\dagger c_{k+q,\sigma} + \text{h.c.} \right] + W_{kq} \left( c_{k,\sigma}^\dagger c_{-k-q,-\sigma} + c_{-k,-\sigma} c_{k+q,\sigma} \right) + \text{h.c.} \right].$$

(2.10)

Here $\mathbf{q}$ describes the wavevector of the potential modulation, and the $\mathbf{k}$ dependence of $V$ and $W$ gives its internal structure (e.g. simple CDW vs dimerization)$^2$. In Section II we considered charge order at a unique wavevector that corresponds to taking potentials $V$ and $W$ as $\delta(\mathbf{q} - \mathbf{Q})$. In the case of a disordered CDW we expect that these functions are no longer $\delta$-functions but are centered narrowly around some particular wavevector. By contrast, when translational symmetry breaking comes from impurities, we expect to find $V$ and $W$ that extend over a wide range of wavevectors $\mathbf{q}$. A

$^2$We only consider spin singlet interactions in (2.10), since these are the only ones contributing to $\rho_Q$ to linear order in perturbation theory.
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Figure 2.7: Dispersion in the $(0,0)$ to $(\pi,0)$ direction in a system with charge order with randomness (momentum is measured in units of $2\pi$). Charge order is assumed to have Gaussian distribution centered around wavevector $(2\pi/4,0)$ with the width $2\pi/20$. The function $V(q)$ in (2.11) is shown, up to a scale, as the thick solid curve. For visual clarity, only results corresponding to the linear combination $1.05(\text{CDW}) + (\text{ld})$ are displayed. Each curve corresponds to a different bias; starting from the bottom, the biases are 8 mV, 12 mV, 16 mV, and 20 mV. Throughout, the quasiparticle smearing is fixed at 8 meV.

The charge order observed in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [75, 74] had strong signatures of randomness and pinning in the form of lattice defects. The correlation length estimated from the distance between defects was $\approx 20a_0$. If we assume the charge order to be of the form $1.05(\text{CDW}) + (\text{long.dim.})$, we can describe it as

$$V_{kq} = V_0(q) \left(1.05 + \cos(k_x + \frac{q}{2})\right), \quad W_{kq} = 0$$

(2.11)

where $V_0(q)$ is a Gaussian distribution function centered at $(2\pi/4,0)$ with a width $2\pi/20a_0$. We display in Fig. 2.7 the signal produced by a perturbation of this kind, for bias voltages 8, 12, 16, and 20 mV, as a function of wavevectors along the $(0,0)$ to $(\pi,0)$ direction. The resulting dispersion agrees closely with that observed in [73] and [74].

In experiments of Hoffman et.al [73] and McElroy et.al [130] peaks in the LDOS were observed at very different wavevectors from $(2\pi/4,0)$ (including some in diagonal directions). This suggest that either $V_{kq}$ or $W_{kq}$ must be non-zero over a fairly wide
Figure 2.8: Dispersion in the \((0, 0)\) to \((\pi, 0)\) direction in a model with impurity induced quasiparticle scattering (momentum is measured in units of \(2\pi\)). Each curve corresponds to a different bias; starting from the bottom, the biases are 8 mV, 12 mV, 16 mV, and 20 mV. Unlike other computations in this paper, the quasiparticle smearing is fixed at 2 meV. This is done since the main features in these curves are averaged out for the usual smearing of 8 meV.

range of values of \(q\), and the most natural candidate is scattering by impurities \([73, 130, 200]\). For concreteness, we assume that the impurity induces a higher chemical potential at a single site, so the perturbation used corresponds to a simple CDW which is uniform in \(q\), \(V_{kq} = V_0\), \(W_{kq} = 0\). In Fig. 2.8 we show the signal computed along the \((0, 0)\) to \((\pi, 0)\) direction at bias voltages 8, 12, 16, and 20 mV. In all cases there is a pronounced peak that disperses with the applied bias voltage. To find the positions of these peaks we reverse the arguments given in Section II. There, we started with a potential at wavevector \(Q\) and found that only quasiparticles at certain energies were strongly affected by it. Now we need to find the modulation wavevector that affects quasiparticles at a given energy. From the band structure of \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}\) we find for the peak positions (in units of \(2\pi\)): 0.35, 0.32, 0.29, and 0.26. The curves on Fig. 2.8 show general agreement with this “quasiparticle scattering” argument \([73, 130]\), except for a consistent small shift to lower wavevector, which comes from the energy smearing procedure. This dispersion is stronger than that displayed in the data at wavevector \((2\pi/4, 0)\), but is in good agreement with the dispersion observed at other wavevectors.

In the discussion above we considered two situations: ordered CDW and non-interacting electrons with impurities. There may also be an intermediate regime of interacting electrons close to the CDW instability and with disorder \([153, 99]\).
Qualitatively, this case may be described by equation (2.10) but with the potentials $V_{kq}$ and $W_{kq}$ coming not only from the external fields but also from the density induced in the electron system. For simplicity let’s take only one of the channels discussed in Section 2.2, e.g. simple CDW (the generalization to the case of several channels is straightforward). Then

$$\Delta H = \sum_q \hat{\rho}_q U_q \hat{\rho}_q + \sum_q V_{q \text{ext}}^q \hat{\rho}^\dagger_q + \text{h.c.}$$

(2.12)

with

$$\hat{\rho}_q = \sum_{k\sigma} c^\dagger_{k\sigma} c_{k+q\sigma}$$

Response of the quasiparticles to (2.12) in the Hartree approximation is determined by the effective perturbation Hamiltonian

$$\Delta H = \sum_{kq\sigma} V_{q \text{eff}}^q c^\dagger_{k+q\sigma} c_{k\sigma} + \text{h.c.}$$

$$V_{q \text{eff}}^q = V_{q \text{ext}}^q + U_q \langle \hat{\rho}_q \rangle = \frac{V_{q \text{ext}}^q}{1 - U_q \chi_0(q, \omega = 0)}$$

(2.13)

where $\chi_0(q, \omega = 0) = \langle \hat{\rho}_q \hat{\rho}_q^\dagger \rangle$ must be computed for the non-interacting system. This corresponds to contributions to the LDOS from the class of diagrams in figure 2.9(a). When the system is close to the CDW instability, the denominator of (2.13) approaches zero around some particular wavevector $Q$. Hence, $V_{q \text{eff}}^q$ may be peaked around $Q$ even when $V_{q \text{ext}}^q$ is momentum independent. In principle we can go beyond the Hartree approximation, including diagrams such as those shown in figure 2.9(b,c). These will introduce a frequency-dependent self energy, as in the case of pinned spin density fluctuations considered in [155].

It is interesting to ask whether by analyzing experimental data one can separate contributions of disordered CDWs from those due to quasiparticle scattering off impurities. Reference [74] pointed out that the presence of a weakly dispersing signal at wavevector $(2\pi/4, 0)$ makes charge order a likely candidate at that wavevector. Here we build on this idea and suggest that a more consistent approach is to analyze $\rho_q(\epsilon)$ at many different wavevectors using a reasonable set of basis functions, e.g. simple CDW and dimerization. Such analysis will give the $q$ dependence of various components in the potentials $V_{kq}$ or $W_{kq}$. We expect that some of them will be almost uniform in momentum space and correspond to localized defects, such as impurities; whereas others will be centered around particular wavevectors and arise from the existence or at least proximity of charge order.

When the field of view of the STM measurement contains more than one impurity there are several important questions that we need to address. We must ask how
the contributions from different impurities add up and whether the system retains the property of uniformity of phase of $\rho_q(\epsilon)$ at fixed $q$ but different $\epsilon$. We consider impurities that cause an arbitrary potential $V_{kq}$ in Eqn. (2.10), i.e. they may modify the chemical potential, the electron kinetic energy, or the pairing amplitude, but first we assume that all impurities are identical. The Fourier component of the LDOS is proportional to $V_{kq}^{tot} = V_{kq} \sum r_a e^{iqr_a}$, where $r_a$ runs over impurity positions. If one impurity does not break parity symmetry, we can make $V_{kq}$ real by choosing the origin at the position of this impurity (see also discussion in Section II). This implies that $V_{kq}^{tot}$ has a phase that depends on $q$ only and is the same for all $k$, which in turn proves that, at fixed $q$, $\rho_q(\epsilon)$ has constant phase (modulo $\pi$) for all values of $\epsilon$ (see Eqns (5)-(9)). So, in the case of identical impurities we have only one phase to worry about and we can always make $\rho_q(\epsilon)$ real by an appropriate choice of origin. When impurities are different, we will have an intrinsically complex $\rho_q(\epsilon)$, with possibly energy dependent phase at different bias voltages. In either case, interference among the impurities leads to an appreciable suppression of the amplitude of $\rho_q(\epsilon)$. When there are many impurities in the area $A$ of the STM field of view, and their positions are uncorrelated, each impurity introduces a random phase to $V_{kq}^{tot}$, whose amplitude can be analyzed in terms of a random walk. Therefore, in a typical experiment we expect that with increasing the system size, $\langle |\rho_q(\epsilon)| \rangle$ will decay as $1/\sqrt{A}$, with statistical fluctuations of the same order. This argument also applies to the case of disordered CDW, where the role of impurities is played by defects in the CDW lattice.
2.5 Experimental Considerations

Our discussion in the earlier sections was restricted to models on a square lattice for which we calculated the lattice density of states in the presence of several kinds of translational symmetry breaking. In analyzing actual experimental data, additional effects need to be taken into account: the real space structure of the atomic wavefunctions, and the current normalization condition used in the STM measurements [72, 75, 73, 130, 74]. These are reviewed below.

2.5.1 Structure factors

For lattice Hamiltonians, wavevectors that differ by the reciprocal lattice vectors $\mathbf{G}$ are equivalent. For the Fourier components of the local density of states $\rho^{\text{lattice}}(\mathbf{q})$, this implies that $\rho^{\text{lattice}}(\mathbf{q} + \mathbf{G}) = \rho^{\text{lattice}}(\mathbf{q})$ for any $\mathbf{G}$. To understand why this equivalence is not observed in experiments we must take into account the real space structure of the Wannier wavefunctions of electrons in the conduction band. Here we study the effects of a single-band tight-binding model, in which Bloch states at the Fermi level can be written as a superposition of localized atomic orbitals $\psi_k(\mathbf{r}) = \sum \phi(\mathbf{r} - \mathbf{R})$. We begin by projecting the Bogoliubov-de Gennes (BdG) wavefunctions in terms of the single-band wavefunctions,

$$u_n(\mathbf{r}) = \sum_k a_n^k \psi_k(\mathbf{r}),$$
$$v_n(\mathbf{r}) = \sum_k b_n^k \psi_k^*(\mathbf{r}).$$

If we know how an operator $\Theta$ acts on the Bloch wavefunctions $\psi_k$, $\Theta \psi_k = \sum_{k'} \Theta_{kk'} \psi_{k'}$, then the above relation induces an action on $a_k$ through $\Theta a_k = \sum_{k'} a_{k'} \Theta_{kk'}$ (and similarly for $b_k$). Thus, the solutions to the BdG equation

$$\left( \begin{array}{cc} \hat{\xi} + \hat{V} & \hat{\Delta} + \hat{W} \\ \hat{\Delta}^\dagger + \hat{W}^\dagger & -\hat{\xi} - \hat{V} \end{array} \right) \left( \begin{array}{c} a_k^n \\ b_k^n \end{array} \right) = E_n \left( \begin{array}{c} a_k^n \\ b_k^n \end{array} \right)$$

will be independent of the Wannier wavefunction $\phi(\mathbf{r})$ once we determine the action of the BdG operator on the Bloch wavefunctions $\psi_k$.

For positive biases $\epsilon > 0$ (the $\epsilon < 0$ case can be analyzed analogously), the LDOS is given by

$$\rho^{\text{phys}}_\mathbf{q}(\epsilon) = \int d^2 \mathbf{r} e^{i\mathbf{qr}} \sum_n u_n^*(\mathbf{r}) u_n(\mathbf{r}) \delta(\epsilon - E_n)$$

$$= \sum_n \delta(\epsilon - E_n) \sum_{kk'} a_n^k a_n^{k'} J(k, k', \mathbf{q}).$$
where
\[
J(k, k', q) = \int d^2r e^{iqx_k} \psi^*_k(r) \psi_{k'}(r)
\]
\[
= \sum_G \delta(q - (k - k') + G) \times \sum_R e^{ik'\mathbf{R}} \int d^2r e^{iqr} \phi^*_k(r) \phi(r - \mathbf{R}).
\]

If we assume that the relevant electronic wavefunction is well localized, we can ignore terms involving the overlap across different sites \((\mathbf{R} \neq 0)\) in the last integral. Then, the only dependence of \(J\) on \(k\) and \(k'\) is through the crystal momentum conservation condition, and we find

\[
\rho_{\text{phys}}(q, \epsilon) = S_q \rho_{\text{lattice}}(q, \epsilon)
\]

with

\[
\rho_{\text{lattice}}(\epsilon) = \sum_{k,n} \delta(\epsilon - E_n) a_k^* a_{k+q}^n
\]

\[
S_q = \int d^2r |\phi(r)|^2 e^{iqr}.
\]

One immediately recognizes that in (2.14) \(\rho_{\text{lattice}}(\epsilon)\) is the Fourier component of the lattice density of states that we analyzed in the earlier sections, and \(S_q\) is the structure factor determined by the atomic wavefunctions. Peaks in the STM spectra arise from \(\rho_{\text{lattice}}(\epsilon)\), whereas \(S_q\) only provides additional wavevector dependence. Hence in our tight binding model we expect that wavevectors which differ only by reciprocal lattice vectors have peaks at the same energies, but with generally different intensities.

### 2.5.2 Current Normalization Condition

An additional subtlety of STM experiments in [72, 75, 73, 130, 74] is the space-dependent normalization used. It is natural to assume that the tunneling matrix elements do not change appreciably with energy over the energy range of interest. Thus, if \(z\) is the height of the STM tip above the sample, and \(r\) is its 2D coordinate along the plane of the sample surface, then the differential tunneling conductance \(g\) can be written as

\[
g(r, z, \epsilon) = f(r, z) \rho_{\text{phys}}(r, \epsilon),
\]

where \(\rho_{\text{phys}}(r, \epsilon)\) is the 2D density of states in the CuO plane. The experiments in [72, 75, 73, 130, 74] adjust the \(z\) coordinate at every point \(r\) along the surface, so as to
keep the current at $V_f$ fixed at a predetermined value $I_f$. The differential conductance normalized in this fashion is

$$g_{\text{meas}}(r, \epsilon) = f(r) \rho^{\text{phys}}(r, \epsilon),$$

where $f(r) = I_f / \int_0^{V_f} d\epsilon \rho^{\text{phys}}(r, \epsilon)$. Let us now discuss some properties of $g_{\text{meas}}(r, \epsilon)$.

The spatial variation in $f(r)$ is dominated by the inhomogeneous quasiparticle weight within a unit cell. To see this, write

$$\rho^{\text{phys}}(r, \epsilon) = \rho^{\text{per}}(r, \epsilon) + \rho^{\text{TSB}}(r, \epsilon),$$

where $\rho^{\text{per}}(r, \epsilon)$ is periodic with the lattice and is of order one, whereas $\rho^{\text{TSB}}(r, \epsilon)$ breaks lattice translational symmetry and is of order $V_0$ in our formalism. If we define $f^{\text{per}}(r) = I_f / \int_0^{V_f} d\epsilon \rho^{\text{per}}(r, \epsilon)$, then

$$f(r) = f^{\text{per}}(r)(1 - H(r))$$

in terms of a TSB function $H(r)$ of order $V_0$.

It is convenient to absorb $f^{\text{per}}$ into $\rho$ by introducing a new function, $\rho'(r, \epsilon) \equiv f^{\text{per}}(r)\rho^{\text{phys}}(r, \epsilon)$. Due to the symmetry properties of $f^{\text{per}}$, $\rho'$ is simply related to $\rho^{\text{lattice}}$ through a modified structure factor

$$\rho'_q(\epsilon) = S'_q \rho^{\text{lattice}}(\epsilon)$$

$$S'_q = \int d^2 r f^{\text{per}}(r)|\phi(r)|^2 e^{iqr}.$$ Expressing $g_{\text{meas}}$ in terms of $\rho'$,

$$g_q^{\text{meas}}(\epsilon) = \rho'_q(\epsilon) - \int \frac{d^2 k}{(2\pi)^2} H_{q-k} \rho'_k(\epsilon), \quad (2.15)$$

we see that $g_q^{\text{meas}}$ gets “direct” contributions from structure in the LDOS at wavevector $q$, as well as “shadow” contributions from structure in the LDOS at other wavevectors $k$, whenever $H_{q-k}$ is non-zero. Whereas (2.15) is an exact relation, it is useful to truncate it to order $V_0$ by keeping in the second term only those contributions coming from the neighborhood of the reciprocal vectors $k \approx G$,

$$g_q^{\text{meas}}(\epsilon) = \rho'_q(\epsilon) - \alpha_q \rho^{\text{lattice}}_{k=0}(\epsilon) + O(V_0^2) \quad (2.16)$$

$$\alpha_q = \sum_G H_{q-G} S'_G. \quad (2.17)$$

In this approximation the shadow contribution to $g_q^{\text{meas}}(\epsilon)$ factorizes into the space-dependent factor $\alpha_q$ and the space-averaged density of states $\rho^{\text{lattice}}_{k=0} \propto \langle g_{\text{meas}}(\epsilon) \rangle$. From (2.16) and (2.17) we can verify an important property of the tunneling spectra

$$\frac{g_{q+G}^{\text{meas}}(\epsilon)}{g_q^{\text{meas}}(\epsilon)} = \frac{S'_{q+G}}{S'_q}.$$
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when $\mathbf{G}$ is a vector of the reciprocal lattice and $\mathbf{q}$ is not. Hence, we expect $g_{\mathbf{q}}^{\text{meas}}(\epsilon)$ and $g_{\mathbf{q}+\mathbf{G}}^{\text{meas}}(\epsilon)$ to have peaks at the same energies but in general with different overall amplitudes.

An interesting question to ask is whether it is possible to analyze experimental data in a way that would allow to separate direct and shadow contributions to $g_{\mathbf{q}}^{\text{meas}}(\epsilon)$. Below we demonstrate that this is possible using an exact sum rule obeyed by $\rho_{\mathbf{q}}^{\text{lattice}}(\epsilon)$. Regardless of the model used and the nature of the symmetry breaking perturbation, the sum over all frequencies of $\rho_{\mathbf{q}}^{\text{lattice}}(\epsilon)$ should be identically zero for all $\mathbf{q}$ different from the reciprocal lattice vectors $\mathbf{G}$:

$$
\int_{-\infty}^{\infty} d\epsilon \rho_{\mathbf{q}}^{\text{lattice}}(\epsilon) = \frac{1}{N} \sum_{k\sigma} \langle 0 | \left\{ c_{k+\mathbf{q}\sigma}, c_{k\sigma}^\dagger \right\} | 0 \rangle \\
\equiv 2 \sum_{\mathbf{G}} (2\pi)^2 \delta(\mathbf{q} - \mathbf{G}).
$$

In principle, this identity can be used to remove the shadow contribution in equation (2.15). In particular, for $\mathbf{q} \neq \mathbf{G}$, combining the approximate result (2.16) and our knowledge of $\rho_{\mathbf{k}=0}^{\text{lattice}}(\epsilon)$ from experiment, we can fix $\alpha_{\mathbf{q}}$ by requiring the sum rule to be obeyed:

$$
\rho'_{\mathbf{q}}(\epsilon) = g_{\mathbf{q}}^{\text{meas}}(\epsilon) - \langle g^{\text{meas}}(\epsilon) \rangle \frac{\int_{-\infty}^{V_{\text{MAX}}} g_{\mathbf{q}}^{\text{meas}}(\epsilon) d\epsilon}{\int_{-V_{\text{MAX}}}^{V_{\text{MAX}}} \langle g^{\text{meas}}(\epsilon) \rangle d\epsilon} \\
(2.18)
$$

Here $V_{\text{MAX}}$ should be chosen sufficiently large so that the ratio of the two integrals is close to its saturated value, yet it should be small enough that we are still justified in using a single band model and a local picture of electron tunneling.

For completeness, we also list two other sum rules obeyed by tunneling spectra. By construction, at every wavevector $\mathbf{q} \neq 0$ the function $g_{\mathbf{q}}^{\text{meas}}(\epsilon)$ must satisfy the normalization condition

$$
\int_{0}^{eV_f} d\epsilon \, g_{\mathbf{q}}^{\text{meas}}(\epsilon) = 0.
$$

One can derive an independent sum rule if we restrict the class of symmetry breaking Hamiltonians to effective one-particle operators (2.10) [This includes all perturbations considered in this work.] Then the $\epsilon$-weighted average of $\rho_{\mathbf{q}}^{\text{lattice}}(\epsilon)$ will be, for $\mathbf{q} \neq \mathbf{G}$,

$$
\int_{-\infty}^{\infty} d\epsilon \epsilon \rho_{\mathbf{q}}^{\text{lattice}}(\epsilon) = \frac{1}{N} \sum_{k\sigma} \langle 0 | \left\{ [c_{k+\mathbf{q}\sigma}, H], c_{k\sigma}^\dagger \right\} | 0 \rangle \\
= \frac{2}{N} \sum_{k\sigma} V_{\mathbf{kq}}.
$$
For the basis functions discussed in Section II we find that only the $V_{kq}$ describing simple CDW gives finite contributions after summing over $k$. Hence,

$$\int_{-\infty}^{\infty} d\epsilon \epsilon \rho_{q}^{\text{lattice}}(\epsilon) = 2 V_{q}^{\text{cdw}}.$$ 

It is important to point out that this sum rule will be spoiled by shadow contributions in (2.15), and is only of use if these have been previously removed, using for example procedure in equation (2.18).

As a useful consistency check of our formalism, one can easily verify that expressions (2.7), (2.8), and (2.9) satisfy both sum rules. We emphasize, however, that although these expressions are only correct to linear order in perturbation strength, the sum rules are non-perturbative and therefore hold to all orders in perturbation theory. Furthermore, their validity is not affected by the introduction of finite quasiparticle lifetimes as, for any normalized symmetric distribution $g(\epsilon)$,

$$\int d\epsilon (\alpha + \beta \epsilon) g(\epsilon - \epsilon_0) = \alpha + \beta \epsilon_0.$$ 

By contrast, the average of $\rho_{q}(\epsilon)$ weighted by any other power of $\epsilon$ is sensitive to details of quasiparticle smearing.

Unfortunately, these sum rules are of limited immediate use, since the bulk of the integration comes from large energies, whereas current experiments only probe a relatively narrow range of biases about the chemical potential.

### 2.6 Photoemission

Before concluding, we would like to propose a way of identifying weak charge ordering in photoemission experiments that could supplement current STM studies. A common signature of a strong charge ordering in the ARPES experiments is the presence of shadow bands: the electron spectral function at momentum $k$ acquires an additional peak at the energy of the quasiparticle at momentum $k + Q$. For weak charge order the shadow bands may be difficult to observe: when the energy difference between $E_k$ and $E_{k+Q}$ is large, mixing between quasiparticles is negligible and the intensity of the shadow peaks is vanishingly small. Strong mixing only occurs when states $k$ and $k+Q$ are nearly degenerate, although in this case the two peaks are hard to distinguish since they are close in energy. Thus we expect to observe an increase of the apparent linewidth of quasiparticles when the latter satisfy the degeneracy condition $E_k = E_{k+Q}$ and are strongly affected by the charge order. For example, in the case of the Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ band structure shown on Figure 2.3 we expect an anomalous increase in the apparent quasiparticle linewidth at the points A, A', B, and B' on the Fermi surface.
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2.7 Conclusions

To summarize, we considered the effects of weak translational symmetry breaking on the $d$-wave superconducting state of the cuprates. For systems with periodic charge order we derived an explicit formula for the energy dependence of the Fourier component of the local density of states for several types of order, including simple charge density wave, electron kinetic energy and superconducting gap modulations. We argued that within a one band model the STM spectra observed in [72, 75, 74] cannot be explained by a simple charge density wave but require the existence of some form of (anomalous) dimerization, i.e. modulation in the electron hopping or in the superconducting pairing amplitude. We discussed a situation in which charge order has finite correlation length due to pinning by impurities. In this case the LDOS has Fourier components for a range of momenta around the ordering wavevector $Q$. For different wavevectors $q$, peaks in $\rho_q(\epsilon)$ will occur at different energies, although the peak dispersion is weak, in agreement with [73, 74]. We also considered systems in which translational symmetry breaking comes not from charge ordering but from impurities. We found that the Fourier components of the LDOS in this case have peaks for a wide range of wavevectors and strong dispersion of these peaks is consistent with the STM experiments of Refs. [73, 130].

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Chapter 3

Properties and Detection of Spin Nematic Order in Strongly Correlated Electron Systems

3.1 Introduction

When ordered, classical spin systems can arrange in a number of patterns, including (anti)ferromagnetic, canted, and helical structures. In addition to these, quantum mechanics allows the formation of a wealth of magnetic phases for quantum spins not available to their classical counterparts. Due to its quantum numbers, detection of such order is often difficult: For instance, Nayak has considered a generalization of spin density wave (SDW) order, in which spin triplet particle-hole pairs of non-zero angular momentum condense with a modulated density[140]. These states are characterized by spin currents rather than spin densities: thus, they do not couple at linear order to probes such as photons, neutrons, or nuclear spins. Only at second order do these phases couple to conventional probes, e.g. in two-magnon Raman scattering. Despite the challenges involved in their detection, subtle forms of magnetic ordering such as these may be necessary to explain phenomena such as the specific heat anomaly in the heavy-fermion compound URu$_2$Si$_2$[29], and the pseudogap regime in the cuprates[28].

Promising materials for the observation of exotic magnetic phases include systems with strong antiferromagnetic fluctuations such as the heavy-fermion compounds, the organic superconductors, and the cuprates. For instance, the cuprates in the absence of carrier doping are antiferromagnetic Mott insulators at low temperatures. As carriers are introduced through doping, the nature of the magnetic order evolves until, for optimally doped and overdoped samples, the system becomes a metallic paramagnet. In between these two limits, the underdoped cuprates have been argued to have spin glass[94] and stripe phases[55]. The proximity between Mott insulator
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and superconducting phases in the cuprates makes them ideal systems to study the hierarchy by which the broken symmetry of Mott insulators is restored [163, 164].

In this paper we will explore the possibility of detection of spin nematic order, a different quantum magnetic phase, in strongly correlated electron systems[67]. Nematic order has been proposed as a state originating from charge fluctuations of stripe order[207, 143]. A spin stripe is a unidirectional collinear spin density wave (SDW), and it consists of antiferromagnetically ordered domains separated by anti-phase domain walls, across which the direction of the staggered magnetization flips sign. The order parameter is

\[ S(r) = \Phi e^{i K_s \cdot r} + \Phi^* e^{-i K_s \cdot r}, \]

with \( K_s = (\pi, \pi) + \vec{\delta} \) corresponding to antiferromagnetically ordered stripes with period \( 2\pi/|\delta| \). Here, the complex vector \( \Phi = e^{i \theta} n \) takes its value within the manifold of ground-states \( S_1 \times S_2/Z_2 \); the \( Z_2 \) quotient is necessary not to overcount physical configurations, as the transformation \( e^{i \theta} \rightarrow -e^{i \theta}, n \rightarrow -n \) does not modify \( \Phi \). The real vector \( n \) gives the direction of the staggered magnetization in the middle of a domain, while the phase factor \( e^{i \theta} \) specifies the location of the domain walls. A shift in \( \theta \) by \( 2\pi \) translates the system by the periodicity of the SDW, and thus leaves the system invariant. Associated with collinear SDW order is charge order due to the modulations in the amplitude of the local spin magnetization[208], which can be described by a generalized CDW order parameter

\[ \delta \rho(r) = \varphi e^{2i K_s \cdot r} + \varphi^* e^{-2i K_s \cdot r}, \]

for some \( SU(2) \) invariant observable \( \rho \), not necessarily the electron density. In the stripe picture, this CDW usually arises from the accumulation of holes at the domain walls.

Stripes were first observed in elastic neutron scattering experiments on the spin-1 nickelate insulator \( \text{La}_2-x\text{Sr}_x\text{NiO}_4 \), and coexistence of stripes with superconductivity was first observed in underdoped \( \text{La}_{1.6-x}\text{Nd}_{0.4}\text{Sr}_x\text{CuO}_4 \)[189], where the unidirectional character was demonstrated by transport[141] and photoemission[214] measurements. In \( \text{YBa}_2\text{Cu}_3\text{O}_{6.35} \) and \( \text{La}_{1.6-x}\text{Nd}_{0.4}\text{Sr}_x\text{CuO}_4 \), it is observed that SDW order is first destroyed by spin fluctuations[135]. In this case, memory of the charge modulation can remain, even after averaging over the spin direction, resulting in a spin-invariant CDW phase, whose presence may explain recent STM measurements in \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \)[72, 75].

For other materials, however, or in other regions of the phase diagram, symmetry may be restored in a different order. In particular, Zaanen and Nussinov [207, 143] proposed that many experimental features of \( \text{La}_x\text{Sr}_{1-x}\text{CuO}_4 \) can be explained by assuming that the spin stripe order is destroyed by charge fluctuations. In this picture, dynamical oscillations in the anti-phase domain-walls of a spin stripe lead to a restoration of translational symmetry and a loss of Néel order. However, although
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Figure 3.1: Charge fluctuations of a spin stripe, provided that the domain walls (curves) maintain their integrity. A spin nematic state is a linear superposition of fluctuating domain configurations such as these. Within each domain, the staggered magnetization (arrows) is well-defined, and it flips sign across the anti-phase domain walls. Due to fluctuations, translational symmetry is restored to the system, and the magnetization has expectation value zero at every point. However, SU(2) symmetry is not restored, as there is a preferred axis in which spins align, modulo a sign.\[207, 143].

both charge and spin order seem to be destroyed in this process, $\delta \rho = 0$ and $S = 0$, full spin symmetry need not be restored: So long as neither dislocations nor topological excitations of the spin proliferate, the integrity of the domain walls allows the staggered magnetization on each oscillating domain to be well-defined. Thus, although the local magnetization does not have an expectation value, the magnetization modulo an overall sign does. This is nematic order, in which $S$ and $-S$ are identified, see Fig. 3.1. The order parameter can be chosen to be $\langle S^\alpha S^\beta - S^2 \delta^{\alpha\beta}/3 \rangle \propto \langle n^\alpha n^\beta - 1/3n^2\delta^{\alpha\beta} \rangle \neq 0$, which has a non-zero expectation value. Because translational invariance is restored in this process, the nematic order parameter is spatially uniform, instead of being modulated by some multiple of the SDW wave vector. In addition, we expect the nematic to be uniaxial, with a single preferred axis $n$ (mod $Z_2$) inherited from the nearby collinear SDW.

Direct observation of spin nematic order through conventional probes is difficult. For instance, neutrons do not couple to nematic order, which is a spin-two operator. Similarly, nematic order is translationally invariant, and does not give Bragg peaks in X-ray experiments. In principle, two-magnon Raman scattering can probe nematic order, but in practice it is difficult to separate the contribution due to the nematic from the creation of two magnons[207]. Hence, although spin nematic order can have important experimental consequences, e.g. for antiferromagnetic correlations...
in magnetic field experiments on superconducting samples [207], its direct detection remains a challenge.

The existence of other stripe liquid phases, different from the spin nematic treated in this paper, as well as proposals for their detection, are discussed in Ref. [99]. In particular, the nematic state described there originates from fluctuations of a unidirectional CDW that restore translational invariance but, by maintaining a memory of the original orientation of the CDW, break the rotational symmetry (point group) of the lattice. Hence, unlike the spin nematic, this “charge nematic” is SU(2) spin invariant, and only breaks a discrete group.

### 3.2 Spin nematic order parameter

A spin nematic is a state that breaks spin SU(2) symmetry without breaking time reversal invariance [12]. The presence of spin nematic order can be observed in the equal time spin-spin correlator

\[
\langle \hat{S}^\alpha(r_1)\hat{S}^\beta(r_2) \rangle = C(r_1, r_2)\delta^{\alpha\beta} + \epsilon^{\alpha\beta\gamma} A^\gamma(r_1, r_2) + Q^{\alpha\beta}(r_1, r_2).
\]

This expression corresponds to the SU(2) decomposition \((1) \otimes (1) \sim (0)_{\text{sym}} \oplus (1)_{\text{asym}} \oplus (2)_{\text{sym}}\). We consider the three terms appearing in eq. (3.1) in turn. The scalar function \(C\) is explicitly spin invariant. It contains important information regarding charge order, but it does not help us in defining a nematic phase. On the other hand, the pseudovector function \(A = \langle \hat{S}_1 \times \hat{S}_2 \rangle\) gives a measure of the non-collinearity of the spin vector field. However, in the case at hand where the nematic state originates from charge fluctuations of a collinear SDW phase, we expect \(A\) to vanish. This is supported by the fact that, from the point of view of the Ginzburg-Landau free energy, the pseudovector \(A\) cannot couple linearly to any function of the SDW order parameter \(\Phi\). As an aside, we note that for systems with spin exchange anisotropy of the Dzyaloshinskii-Moriya (DM) form, the DM vector will couple linearly to \(A\), as expected from the weak non-collinearity (canting) in such systems. However, the expectation value of \(A\) in this case comes from explicit breaking of the spin symmetry.

Thus, all information of interest to us is contained in the symmetric spin-2 tensor \(Q^{\alpha\beta}\). We define a symmetrized traceless spin correlator \(\hat{Q}^{\alpha\beta}\),

\[
\hat{Q}^{\alpha\beta}(r_1, r_2) = \frac{1}{2}(\hat{S}_1^\alpha \hat{S}_2^\beta + \hat{S}_1^\beta \hat{S}_2^\alpha) - \frac{\delta^{\alpha\beta}}{3} \hat{S}_1 \cdot \hat{S}_2
\]

whose expectation value yields \(Q^{\alpha\beta}\) directly,

\[
Q^{\alpha\beta}(r_1, r_2) = \langle \hat{Q}^{\alpha\beta}(r_1, r_2) \rangle.
\]
Starting from a SDW state, as domain wall fluctuations grow to destroy charge order, translational invariance is restored to the system, insuring that \( Q^{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) \) is independent of the center-of-mass coordinate, \( i.e. \ Q^{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) = Q^{\alpha\beta}(\mathbf{r} + \mathbf{R}, \mathbf{r'} + \mathbf{R}) \) for any displacement \( \mathbf{R} \). This fact alone signals the breaking of spin symmetry, since the choice of a non-trivial \( i.e. \) not proportional to \( \delta^{ab} \) tensor \( Q^{\alpha\beta} \) has been made across the system. Thus, while \( Q^{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) \) decays exponentially with distance \( |\mathbf{r}_1 - \mathbf{r}_2| \) due to the absence of long-range Néel order, the onset of nematic order is reflected in the translationally-invariant expectation value in the matrix-valued function (3.3). Since the original SDW state has a single preferred spin direction \( \hat{n} \), the ensuing nematic order will be uniaxial,

\[
Q^{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) = f(\mathbf{r}_1 - \mathbf{r}_2)Q^{\alpha\beta}_0, \\
Q^{\alpha\beta}_0 = (n^\alpha n^\beta - \delta^{\alpha\beta}/3)S.
\]

Here, we have decomposed the order parameter into three component objects: a function \( f \) describing the internal structure of the nematic; the unit vector director field \( \mathbf{n} \); and the scalar magnitude \( S \). As seen explicitly from (3.3), the function \( f \) is parity-symmetric, \( f(\mathbf{r}) = f(-\mathbf{r}) \). As will be shown below, \( f \) is dominated by the short range antiferromagnetic correlations between spins, and therefore has a large contribution at the wave vector \( (\pi, \pi) \). By definition, we choose this contribution to be positive, \( f(\pi, \pi) > 0 \). With this convention, \( S > 0 \) corresponds to a Néel vector that is locally aligned or anti-aligned with the director field \( \mathbf{n} \) (sometimes referred to as the \( N^+ \) phase in the literature of classical liquid crystals, see e.g. Ref. [39]), while \( S < 0 \) corresponds to a Néel vector that is predominantly perpendicular to \( \mathbf{n} \) (the \( N^- \) phase). We will show that, at low temperatures, \( S > 0 \) due to the local antiferromagnetic correlations whereas, for anisotropic systems at high temperatures, a phase with \( S < 0 \) is possible. Finally, we note that the unidirectional SDW state (stripe phase) breaks the discrete rotational symmetry of a tetragonal lattice. This symmetry may be restored when charge fluctuations destroy the SDW state to form the nematic. In this case \( f(\mathbf{r}) \) will be symmetric under rotations on the plane by \( \pi/2, \mathbf{r} \rightarrow R_{\pi/2}\mathbf{r} \). However, if a memory of the orientation of the stripes survives the domain wall fluctuations, \( f \) will not have such symmetry, yielding a “nematic spin-nematic”, \( i.e. \) a translationally invariant system that is anisotropic in real space and in spin space.

Sections 3.3 and 3.4 will be devoted to understanding the behavior of the three component fields of the nematic: \( f, \mathbf{n}, \) and \( S \). Then, in Section 3.5 we will explore how this detailed knowledge can be used in experimental searches for nematic order.
3.3 Nematic wave function

In order to explore the possible symmetry properties of the function $f$, we study its short wave length structure by explicit construction of a nematic operator on a small cluster. As is well known, it is impossible to describe nematic order in terms of a single spin-$1/2$ particle, as the identification of “up” and “down” results in a trivial Hilbert space for the spin degree of freedom. Another way to see this is that a spin-2 operator has a vanishing expectation value with respect to any spin-$1/2$ state, resulting in the identity $Q_{ij}^{\alpha\beta} \equiv 0$ whenever $i = j$.

This limitation can be overcome by coarse-graining a group of spins and constructing a nematic wave function out of them. In order to preserve the underlying rotational symmetry of the system, we carry this out on square $2 \times 2$ plaquettes of spins, and use energetic considerations to find the states most likely to contribute to magnetic order. We take the $t$-$J$ model as a starting point, analyzing the low energy Hilbert space in a manner similar to the projected $SO(5)$ approach of Zhang et al. [212] or the CORE approach of Altman and Auerbach [2]. In these analyses, the lattice is first split into plaquettes. On each plaquette, the Hamiltonian is diagonalized, and the $m$ lowest energy states $|\psi_{\nu}\rangle_{i}$ are kept, where $\nu \in \{1, \ldots, m\}$ and $i$ labels the plaquette. For a lattice composed of $N$ plaquettes, this allows one to define a projected subspace $\mathcal{M}$ of the Hilbert space spanned by $m^{N}$ factorizable states of the form $|\psi_{\nu_{1}}\rangle_{1} \otimes |\psi_{\nu_{2}}\rangle_{2} \cdots |\psi_{\nu_{N}}\rangle_{N}$. We assume that the ground state is well-contained in $\mathcal{M}$.

Figure 3.2 reproduces results in [2] for a $t$-$J$ model on a $2 \times 2$ plaquette. The lowest energy bosonic states are, at half filling, the $S = 0$ ground state $|\Omega\rangle$ and the $S = 1$ magnon triplet $\hat{t}_{a}^\dagger |\Omega\rangle$, and for a plaquette with two holes, an $S = 0$ state $\hat{b}^\dagger |\Omega\rangle$. In addition, there are two low-lying $S = 1/2$ fermion doublets with one hole; however, unbound holes are dynamically suppressed, as supported by DMRG calculations on larger lattices, and we shall exclude the one-hole sector in what follows. Then, to lowest order in the analysis, we only keep the low-lying bosonic states, in terms of which a general low-energy plaquette state can be written as

$$|\psi\rangle_{i} = \left(s + m^{\alpha}\hat{t}_{a,i}^\dagger + c\hat{b}_{i}^\dagger\right)|\Omega\rangle_{i}. \quad (3.5)$$

It is useful to get some intuition regarding the wave functions (3.5). Introducing the total spin and staggered spin operators on a plaquette, $\hat{S} = \hat{S}_{1} + \hat{S}_{2} + \hat{S}_{3} + \hat{S}_{4}$ and $\hat{N} = \hat{S}_{1} - \hat{S}_{2} + \hat{S}_{3} - \hat{S}_{4}$, as well as the DM-type vector, $\hat{D} = \hat{S}_{1} \times \hat{S}_{2} - \hat{S}_{2} \times \hat{S}_{3} + \hat{S}_{3} \times \hat{S}_{4} - \hat{S}_{4} \times \hat{S}_{1}$, we find

$$\hat{S}_{a} \sim i\epsilon_{\alpha\beta\gamma}\hat{t}_{a}^\dagger \hat{t}_{\beta} \hat{t}_{\gamma},$$
$$\hat{N}_{a} \sim \hat{t}_{a} + \hat{t}_{a}^\dagger,$$
$$\hat{D}_{a} \sim i(\hat{t}_{a} - \hat{t}_{a}^\dagger).$$
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Figure 3.2: Spectrum of $t$-$J$ model on a $2 \times 2$ plaquette. Adapted from [2].

up to positive multiplicative factors and up to terms lying outside of the projected low-energy space. In particular, we find the expectation values on a single plaquette

$$
\langle \hat{S}_i \rangle \sim m^* \times m,
\langle \hat{N}_i \rangle \sim \text{Re}(s^* \mathbf{m}),
\langle \hat{D}_i \rangle \sim \text{Im}(s^* \mathbf{m}),
\langle \hat{b}_i \rangle \sim s^* c,
\langle \hat{N}_i \hat{b}_i \rangle \sim m^* c.
$$

(3.6)

The last two expressions describe local singlet and triplet superconductivity, respectively.

One can build a nematic on a cluster of plaquettes by choosing a factorizable state, in which $s = 0$ and $\mathbf{m}$ is a constant real vector on every plaquette,

$$
|\psi_{\text{fact}}\rangle = \prod_i (m^\alpha \hat{a}^\dagger_{a,i} + c \hat{b}^\dagger_{b,i}) |\Omega_i\rangle
$$

(3.7)

The constraint that $\mathbf{m}$ is real insures that no long range ferromagnetic or Néel orders develop, whereas nematic order does due to the SU(2)-symmetry breaking choice of the vector $\mathbf{m}$. Note from (3.6) that $|\psi_{\text{fact}}\rangle$ is also a triplet superconducting state (except at half-filling, where $c = 0$). Order of this type is found, for instance, in the triplet superconducting state of quasi-one dimensional Bechgaard salts, where the triplet superconducting order parameter is constant along the Fermi surface due to the splitting of the Fermi surface into two disjoint Fermi sheets[149].

On the other hand, in applications to materials such as the high $T_c$ cuprates, we would like to introduce a nematic state that is a singlet superconductor, instead of triplet. For this, the use of non-factorizable states is necessary. For instance,
introducing a local angle variable $\theta_i \in [0, 2\pi)$ on each plaquette, consider the state

$$|\psi_1\rangle = \int (d\theta_1 d\theta_2 \ldots) \left[ \prod_i (s + m^\alpha \cos(Q \cdot r_i - \theta_i) \hat{t}^i_a + \hat{c}^i_b) |\Omega\rangle_i \right],$$

where $m$ is a constant real vector, and $Q$ is the wave vector of the underlying SDW. If the angle $\theta_i$ were held constant across the lattice, long range SDW order would ensue. In contrast, by integrating independently over the $\theta_i$ at different sites, we introduce charge fluctuations that average out the local magnetization to zero. Hence, the state (3.8) has restored translational and time-reversal symmetry, with only singlet superconductivity and nematic order surviving. We note that (3.8) ignores correlations between spin degrees of freedom, controlled by $\hat{t}^i_a$, and charge degrees of freedom, controlled by $\hat{b}^i$. More complex nematic wave functions that take this effect into account are given in Appendix A.1. On the other hand, in practical calculations, one may consider a slightly simpler wave function than (3.8) by replacing the $\theta_i$ by local Ising variables $\sigma_i = \pm 1$ on each plaquette. This leads to the wave function

$$|\psi_2\rangle = \sum_{\{\sigma_1, \sigma_2, \ldots\} = \pm 1} \left[ \prod_i (s + \sigma_i m^\alpha \hat{t}^i_a + \hat{c}^i_b) |\Omega\rangle_i \right].$$

As before, this state has time-reversal and translational symmetries restored, with only spin nematic and superconducting orders surviving. Finally, note that in order to produce a nematic state without any type of superconductivity (singlet or triplet), it is necessary to introduce another fluctuating Ising variable which multiplies the term $\hat{c}^i_b$ in (3.9), thus randomizing the relative phase between all three components of the wave function.

Despite the fact that we have considered many different wave functions, depending on the possible coexistence of nematic order with different types of superconductivity, the analysis above allows us to make strong predictions on the dominant short wave length dependence of $f$. This is because, of all the low energy plaquette states kept in the projected Hilbert space, only the triplet $\hat{t}^i_a |\Omega\rangle$ breaks SU(2) symmetry. Hence, only this state can contribute directly to the nematic order parameter. There are six different pairs $i \neq j$ of sites on a $2 \times 2$ plaquette, and the most general spin-2 operator $\hat{P}^{\alpha\beta}_{ij}$ on a plaquette can be written as a linear combination of the six “link” operators $\hat{Q}^{\alpha\beta}_{ij}$,

$$\hat{P}^{\alpha\beta} = \sum_{(ij) \in \square} \alpha_{ij} \hat{Q}^{\alpha\beta}_{ij}. \quad (3.10)$$

It is useful to introduce an inner product for real functions $\alpha_{ij}$ on the links of a plaquette, according to $(\alpha, \beta) = \sum_{i \neq j \in \square} \alpha_{ij} \beta_{ij}$. With this, we can write a normalized
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\[ \hat{P}_{s_1} = \left( \hat{Q}_{12} + \hat{Q}_{23} + \hat{Q}_{34} + \hat{Q}_{41} \right) / 2, \]

\[ \hat{P}_{s_2} = \frac{1}{\sqrt{2}} \left( \hat{Q}_{13} + \hat{Q}_{24} \right). \]

The solid lines denote links with weight +1, dashed lines have weight −1. Thus, for instance, \( \hat{P}_{s_1} = (\hat{e}_{12} + \hat{e}_{23} + \hat{e}_{34} + \hat{e}_{41}) / 2 \), the other basis vectors are \( \alpha_{s_2} = (\hat{e}_{13} + \hat{e}_{24}) / \sqrt{2} \). The other basis vectors are \( \alpha_{p_x} = (\hat{e}_{23} - \hat{e}_{41}) / \sqrt{2} \), \( \alpha_{d_{x^2+y^2}} = (\hat{e}_{12} - \hat{e}_{34} - \hat{e}_{41} + \hat{e}_{13}) / 2 \), and \( \alpha_{d_{xy}} = (\hat{e}_{13} - \hat{e}_{24}) / \sqrt{2} \).

It is easy to see that among the six operators (3.10), only those with \( s \)-wave symmetry get a non-vanishing expectation value with respect to the state (3.8). What’s more, the linear combination \( \hat{P}_{s_F} = (\hat{P}_{s_1} + \sqrt{2} \hat{P}_{s_2}) / \sqrt{3} \) has a vanishing expectation value, so that it is possible to write an orthonormal basis of operators in which only the basis operator,

\[ \hat{P}_{s_A} = \frac{1}{\sqrt{3}} (-\sqrt{2} \hat{P}_{s_1} + \hat{P}_{s_2}), \]

has a non-zero expectation value. This can be understood as a consequence of local antiferromagnetic correlations, since \( \hat{P}_{s_A}^{\alpha\beta} \) can be expressed in terms of the plaquette staggered magnetization \( N \) as

\[ \hat{P}_{s_A}^{\alpha\beta} = \frac{1}{2\sqrt{6}} \left( N^\alpha N^\beta - N^2 \delta^{\alpha\beta} \right). \]
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Using the relation

\[ Q_{ij} = \sum_{\eta} \alpha_{ij}^\eta \hat{P}_\eta \]  \hspace{1cm} (3.14)

which holds for \( i, j \) on the same plaquette, we see that the dominant short-range contribution to the nematic order parameter is

\[ Q_{ij}^{\alpha\beta} = \alpha_{ij}^{sA} \langle \hat{P}_{sA}^{\alpha\beta} \rangle. \]  \hspace{1cm} (3.15)

This is of the form (3.4) with

\[ f(k) = \alpha_{sA}^{sA}(k) = \frac{4}{\sqrt{6}}(\cos k_x \cos k_y - \cos k_x - \cos k_y), \]  \hspace{1cm} (3.16)

\[ Q_0^{\alpha\beta} = \langle \hat{P}_{sA}^{\alpha\beta} \rangle. \]

Note that we can relate the real vector \( \mathbf{m} \) in Eqs. (3.8) and (3.9) to the director field \( \mathbf{n} \) of the nematic, appearing in (3.4), through

\[ \langle \hat{P}_{sA}^{\alpha\beta} \rangle \propto m^\alpha n^\beta - m^2 \delta^{\alpha\beta}/3, \]  \hspace{1cm} (3.17)

from which we conclude that \( \mathbf{n} \propto \mathbf{m} \). This can be used to constrain the sign of \( S \),

\[ S = \frac{3}{2} n^\alpha n^\beta \langle \hat{P}_{sA}^{\alpha\beta} \rangle > 0. \]

Therefore, at low temperatures, where the state of the system is dominated by the low energy plaquette states, \( S \) is positive.

3.4 Mean field analysis

We now study the finite temperature phase diagram of the spin nematic. We assume that superconductivity is either present as a background phase throughout the entire region of the phase diagram that we study, or not present at all. Hence, we do not include explicitly the interaction between superconducting and nematic order parameters. As is well known (see, e.g. Ref [26]), symmetry allows the inclusion of cubic terms into the Ginzburg-Landau (GL) free energy of a nematic order parameter. Thus, the most general GL free energy for a spin-isotropic system is, up to quartic order,

\[ F_{Q,iso} = \beta \text{Tr}Q_0^2 - \gamma \text{Tr}Q_0^4 + \delta \text{Tr}Q_0^4. \]  \hspace{1cm} (3.18)

By the identity \((\text{Tr}Q_0^2)^2 = 2\text{Tr}Q_0^4\), which holds for any \( 3 \times 3 \) traceless symmetric matrix, we do not include the term \((\text{Tr}Q_0^2)^2\) in (3.18). The phase diagram is shown in
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Figure 3.4: Mean field phase diagram for a nematic without anisotropy in the spin exchange interaction. The ordered phases $N^\pm$ are uniaxial. All transitions are first order.

Fig. 3.4. At high temperatures, $\beta$ is large and positive, and the system is disordered, $Q_0 = 0$. On the other hand, as temperature is reduced and the value of $\beta$ decreases, there is spontaneous breaking of spin SU(2) symmetry as the system undergoes a first order transition into the nematic state. The nematic in this case is uniaxial as desired (see sections 3.1 and 3.2); in order to stabilize biaxial nematic order, terms of order $Q_5^0$ and $Q_6^0$ would have to be added to the free energy[26]. We note that, as discussed in sections 3.2 and 3.3, $S > 0$ in the low temperature phase. Thus, the cubic coefficient $\gamma$ must be positive.

How is the above analysis modified by the presence of spin-orbit effects? For definiteness, we concentrate on the case of the cuprate La$_x$Sr$_{1-x}$CuO$_4$ in the low temperature orthorhombic (LTO) phase. This compound displays strong evidence for fluctuating stripe order in its underdoped regime[60], and the spin exchange constants $J^{\alpha\beta}$ are known in detail from neutron scattering experiments in undoped La$_2$CuO$_{4+x}$[147, 181]. The analysis presented here can be easily generalized to other materials. In La$_x$Sr$_{1-x}$CuO$_4$, spin-orbit effects are small: The anisotropic part of the spin exchange interaction $J^{\alpha\beta}$ is less than $10^{-2}$ of the isotropic part in undoped La$_2$CuO$_{4+x}$[147, 181]. Yet, at low temperatures, this anisotropy leads to a preferred direction for the Néel order and to weak ferromagnetism [34]. Thus, although the anisotropy is a low energy effect, playing a weak role on the onset and magnitude of the nematic order parameter, it may ultimately fix the preferred spin orientation for the nematic. This aspect of the interplay between $J$ and $Q$ will be especially important when we try to separate their contributions to the anisotropy in the spin susceptibility (see Eq. (3.26) below).

The most general form of the spin-exchange interaction for spins on nearest neigh-
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bor Cu sites is

$$
\mathcal{H} = \sum_{\langle ij \rangle} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta
$$

(3.19)

$$
= \sum_{\langle ij \rangle} \left( J_{0,ij} S_i \cdot S_j + J_{s,ij}^{\alpha\beta} S_i^\alpha S_j^\beta + D_{ij} \cdot (S_i \times S_j) \right),
$$

where $J_{ij}^{\alpha\beta}$ is a traceless symmetric tensor and $D$ is the Dzyaloshinskii-Moriya (DM) vector. Neither $J_0$ nor $J_s$ depend on the bond $\langle ij \rangle$. It is convenient to work with the principal axes of the system: the vectors $a$ and $c$ lie on the CuO$_2$ planes at 45 degrees from nearest neighbor Cu-Cu bonds, and the vector $b$ is normal to the CuO$_2$ planes, see Fig. 3.5. In this basis, $J_s$ is diagonal, $J_0 + J_s = \text{diag}(J_{aa}, J_{bb}, J_{cc})$ with $J_{bb} < J_{aa} \approx J_{cc}$ [147]. For simplicity we take $J_{aa} = J_{cc}$ in what follows, corresponding to easy plane antiferromagnetic interactions along the $a$-$c$ plane. On the other hand, the DM vector $D_{ij}$ points along $\pm a$, with the sign on each bond $\langle ij \rangle$ given by the staggered pattern shown in Fig. 3.5. Thus,

$$
J_{ij} = \begin{pmatrix}
J_0 + \Delta & 0 & 0 \\
0 & J_0 - 2\Delta & \pm D \\
0 & \mp D & J_0 + \Delta
\end{pmatrix},
$$

where $\Delta = (J_{aa} - J_{bb})/3 > 0$. A useful measure of the relative importance of the anisotropies $\Delta$ and $D$ is given by the ratio $x \equiv D^2/\Delta$, which is approximately equal to one in the LTO phase of $\text{La}_2\text{CuO}_{4+x}$ [147, 181].

It is instructive to consider first the effects of spin anisotropy on an antiferromagnet. The GL free energy $F_N$ of a Néel order parameter $N$ is, to lowest order in spin-orbit coupling,

$$
F_N = -\lambda N^T J_s N + \frac{\lambda'}{J_0} (D \cdot N)^2 + \mu N^2 + \nu N^4.
$$

(3.20)

The term $D \cdot N$ is a pseudoscalar and is forbidden by parity and time-reversal symmetries. The first two terms include the effects of anisotropy, and are both quadratic in the spin-orbit coupling. The coefficient $\lambda$ is positive, as necessary to capture the tendency of spins to order along the easy plane at low temperatures. Similarly, the DM vector induces a weak canting for staggered spins that are perpendicular to it. This pushes $N$ towards the plane normal to $D$, which requires $\lambda' > 0$. Thus we see that $J_s$ chooses an easy plane for the spins, and the DM vector selects a preferred direction, $c$, within the easy plane [34], see Fig. 3.5. The ratio $\lambda'/\lambda$ is unimportant in this case.

We now turn our attention to the nematic. In addition to the usual GL free energy for a nematic order parameter, eq. (3.18), the explicit symmetry breaking due
Figure 3.5: The Dzyaloshinskii-Moriya vectors (dashed arrows) and ground state spin orientation (solid arrows) on a single CuO$_2$ plane in the LTO phase of La$_2$CuO$_{4+x}$. The black dots denote Cu sites. The DM vectors $D_{ij}$ point along $\pm a$ and are staggered between adjacent bonds. This, combined with easy plane anisotropy, yield a weakly canted AF order, where the spins on the Cu sites have a large staggered component in the $\pm c$ direction, and a small uniform component out of the plane (in the $b$ direction, not shown).
to anisotropy in the spin exchange can be taken into account, to quadratic order in the spin-orbit interaction, by adding the terms,

\[
F_Q = F_{Q,\text{iso}} + F_{Q,\text{anis}} \\
F_{Q,\text{anis}} = -\alpha \text{Tr}(J_s Q_0) + \frac{\alpha'}{J_0} D^T Q_0 D. \tag{3.21}
\]

Note that, unlike the Néel case (3.20), the order parameter \( Q \) couples linearly to the anisotropy. Thus, the symmetry is broken explicitly, and strictly speaking there is no disordered phase with \( Q_0 = 0 \). This, however, does not preclude the existence of crossovers in the order parameter, or even discontinuities at first order transitions, as we traverse the phase diagram. For weak anisotropy the order parameter will be extremely small at high temperatures, and very sharp crossovers will be observed. Another consequence of the linear coupling is that, unlike antiferromagnetic order which always lies on the easy plane of \( J^{\alpha\beta} \), uniaxial nematic order can point either in the direction of maximal coupling of \( J^{\alpha\beta} \), or in the direction of minimal coupling of \( J^{\alpha\beta} \), depending on the sign of \( S \). For the state with nematic order and \( S > 0 \), we expect the director field \( n \) to lie on the easy plane and be orthogonal to \( D \), \textit{i.e.} be parallel to the direction that the SDW state would take in the absence of charge fluctuations. This constrains the linear coefficients appearing in (3.21) to be positive, \( \alpha > 0 \) and \( \alpha' > 0 \).

In order to obtain the mean field phase diagram for a spin nematic, we compare the minima of \( F \) for the director field \( n \) pointing along the various principal axes \( \hat{e}_i \). The result is shown in Fig. 3.6. The low temperature phase \( N^+ \) is a uniaxial nematic characterized by \( S > 0 \) and \( n = \mathbf{c} \). The high temperature phase \( N^- \) is also uniaxial, but it has \( S < 0 \). The director field in \( N^- \) depends on the relative strength of the two anisotropy terms, \( w \equiv \alpha' x / \alpha \). This quantity is material dependent, and is unlikely to change significantly over the phase diagram (except, of course, across a structural phase transition), so that only one of the following scenarios should be observed within a given material: For \( w < 1 \), \( n = \mathbf{b} \), whereas for \( w > 1 \), \( n = \mathbf{a} \). The coefficient \( \beta \) increases with temperature, possibly tuning a first order phase transition between phases \( N^+ \) and \( N^- \), or otherwise moving the system through a sharp crossover within the \( N^- \) phase. In either case, the temperature dependence of the order parameter leads to strong experimental signatures discussed in Section 3.5. Figure 3.7 shows the value of \( S \) as we move across the \( N^+/N^- \) phase transition along the dashed line in Fig. 3.6.
Figure 3.6: Mean field phase diagram including anisotropy in the spin exchange $J^{\alpha\beta}$, for the case $J^{bb} < J^{aa} = J^{cc}$, $\mathbf{D} = \pm \mathbf{a}$. All transitions are first order. Phase $N^+$ is characterized by $S > 0$ and $\mathbf{n} = \mathbf{c}$, phase $N^-$ by $S < 0$. The director $\mathbf{n}$ in phase $N^-$ depends on the parameter $w \equiv \alpha'x/\alpha$: for $w < 1$, $\mathbf{n} = \mathbf{b}$, while for $w > 1$, $\mathbf{n} = \mathbf{a}$. The parameter $w$ is material-dependent and is unlikely to change across the phase diagram. Thus, only a single type of $N^-$ phase is accessible within a given material. The dashed arrow shows a possible trajectory where a first order transition is crossed as temperature is increased; alternatively, for smaller values of $\gamma$, the first order transition may be avoided and strong crossover behavior may be observed instead.

### 3.5 Detection

In the presence of a spin nematic order parameter $Q_{ij}^{\alpha\beta} \equiv Q_{ij}^{\alpha\beta}(\mathbf{r}_i, \mathbf{r}_j)$ of the form (3.4), symmetry allows the term

$$\mathcal{H}_{\text{int}} = -g \sum_{ij} Q_{ij}^{\alpha\beta} \hat{S}_i^\alpha \hat{S}_j^\beta$$  \hspace{1cm} (3.22)

to enter the Hamiltonian, which can be thought of as a local spin-spin interaction mediated by the nematic order. The coefficient $g$ is positive, as necessary for the stability of the nematic order. When the system develops long-range nematic order, electrons move in a nematic background which acts like an effective anisotropic spin exchange. This leads to anisotropy in the spin response function. In the random phase approximation (RPA), when an external magnetic field $\mathbf{B}$ is applied to the system, $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}} - \sum_i \mathbf{B}_i \cdot \hat{\mathbf{S}}_i$, the electrons see an effective field

$$B_{\text{eff}}^\alpha(\mathbf{k}) = B^\alpha(\mathbf{k}) + gQ^{\alpha\beta}(\mathbf{k}) \langle \hat{S}_j^\beta(\mathbf{k}) \rangle,$$  \hspace{1cm} (3.23)

leading to the dynamic spin response

$$\chi_{\text{RPA}}^{\alpha\beta}(\mathbf{k}, \omega) = \chi_0(\mathbf{k}, \omega) \left[ (1_{2\times2} + gQ(\mathbf{k})\chi_0(\mathbf{k}, \omega))^{-1} \right]^{\alpha\beta},$$  \hspace{1cm} (3.24)
Spin nematic order thus induces anisotropy in the spin susceptibility. We introduce a tensor $\Xi^{\alpha\beta}$, defined by

$$
\Xi^{\alpha\beta}(k, \omega) \equiv \frac{1}{2} \left[ (\chi^{-1})^{\alpha\beta} + (\chi^{-1})^{\beta\alpha} \right] - \frac{\delta^{\alpha\beta}}{3} \sum_c (\chi^{-1})^{cc}.
$$

Experimental measurements of $\chi^{\alpha\beta}$ from polarized neutron scattering experiments (for arbitrary wave vector $k$) or from Knight shift measurements (for $k = 0$) can be used to compute $\Xi^{\alpha\beta}$, which is the natural object to consider when studying nematic order. In the current approximation, we find

$$
\Xi^{\alpha\beta}_{\text{RPA}}(k, \omega) = g Q^{\alpha\beta}(k).
$$

(3.25)

Even in the absence of nematic ordering, spin-orbit coupling leads to anisotropy in the antiferromagnetic exchange $J_{ij}^{\alpha\beta}$, which enters the Hamiltonian in a term of the form (3.22) with $gQ \rightarrow -J$, see eq. (3.19). The complete expression for $\Xi^{\alpha\beta}$ is therefore

$$
\Xi^{\alpha\beta}_{\text{RPA}}(k, \omega) = g Q^{\alpha\beta}(k) - J^{\alpha\beta}(k).
$$

(3.26)

Note that only the traceless symmetric part of $J_{ij}$ contributes to $\Xi$. We face the challenge of untangling the contributions to (3.26) due to the anisotropy in $J$ from
Figure 3.8: Wave vector dependence of \( f(k) \) corresponding to the plaquette nematic operator \( \hat{P}_{sA} \). This is expected to be the dominant contribution to \( f \), and enters the anisotropy of the spin susceptibility through Eq. 3.26. The “+” and “−” regions show the sign of \( f(k) \) on the Brillouin zone.

those coming from the presence of nematic order. For this, the analysis of Section 3.3 is pivotal, in particular eq. (3.16), which gives the dominant wave vector dependence of the nematic contribution to the anisotropy in the spin response function, see Figure 3.8. This can combined with detailed knowledge of the form of \( J_s \) [147, 181], 
\[
J_s(k) = \eta(k) \Delta \text{diag}(1, 1, -2).
\]
As before, \( \Delta = (J^{aa} - J^{bb})/3 > 0 \), and we assume that anisotropy is small beyond the nearest-neighbor range to set \( \eta(k) = 2(\cos k_x + \cos k_y) \).

Thus, the contributions due to \( Q \) and \( J \) can be distinguished by the wave vector dependence of the signal, as one is proportional to \( f(k) = \frac{4}{\sqrt{6}}(\cos k_x \cos k_y - \cos k_x - \cos k_y) \) and the other to \( \eta(k) = 2(\cos k_x + \cos k_y) \). For example, experiments measuring the susceptibility at the points \( k = (\pi, 0) \) and \( (0, \pi) \) are sensitive to \( Q \), but not \( J \), see Fig. 3.8.

For completeness, we evaluate the expression (3.26) in the various phases shown in Fig. 3.6 for underdoped \( \text{La}_{x}\text{Sr}_{1-x}\text{CuO}_4 \). In the low temperature phase \( N^+ \), we expect,

\[
\Xi^{aa} = -g|S|f(k)/3 - \Delta \eta(k),
\]
\[
\Xi^{bb} = -g|S|f(k)/3 + 2\Delta \eta(k),
\]
\[
\Xi^{cc} = 2g|S|f(k)/3 - \Delta \eta(k),
\]

In the high temperature phase \( N^- \), we must consider two separate scenarios. If \( \eta > 1 \), then \( n = a \), and

\[
\Xi^{aa} = -2g|S|f(k)/3 - \Delta \eta(k),
\]
\[
\Xi^{bb} = g|S|f(k)/3 + 2\Delta \eta(k),
\]
\[ \Xi^{cc} = g|S|f(k)/3 - \Delta\eta(k), \]

whereas, if \( \eta < 1 \), then \( \mathbf{n} = \mathbf{b} \), and
\[ \Xi^{aa} = -\Xi^{bb}/2 = \Xi^{cc}, \]
\[ \Xi^{cc} = g|S|f(k)/3 - \Delta\eta(k), \]

Thus, if the system goes through a phase transition between phases \( N^+ \) and \( N^- \), the discontinuity in \( S \), shown in Fig. 3.7, together with the change in the director field \( \mathbf{n} \), would give a very clear experimental signature of nematic order in Knight shift and polarized neutron scattering experiments.

Finally, we consider the prospect of observing director density waves (DDW), the Goldstone modes corresponding to the nematic state, in neutron scattering experiments. To do this, we study the pole structure of the RPA result (3.24). Expanding (3.24) about \( k = 0 \) and \( \omega = 0 \), we find two degenerate DDW modes, with speed \( v_{DDW} \propto \sqrt{g|S|} \),
\[ \chi_{\perp\perp}(k, \omega) \propto \frac{k^2}{\omega^2 - v_{DDW}^2 k^2}, \]  
(3.27)

with \( \perp \) labelling either of the directions perpendicular to the director of the nematic. Equation (3.27) is consistent with an independent calculation of the DDW modes starting from an effective low energy quantum rotor model, see Section 3.6. We note that the DDW modes found here may be overdamped, depending on the details of the system. This would be the case, for instance, if \( v_{DDW} \) were smaller than the Fermi velocity. However, provided that the modes are underdamped, they can be detected in neutron scattering experiments. This is surprising at first, as local \( Z_2 \) invariance implies that equal-time correlators of the form \( \langle S^a_i S^b_j \rangle \) must decay exponentially at large distances \( |x_i - x_j| \). However, as (3.27) indicates, the correlator at different times need not decay exponentially. Also note that the inelastic scattering peak (3.27) has vanishing weight as \( k \to 0 \), consistent with the absence of an elastic Bragg peak. Unfortunately, this feature makes DDW modes difficult to distinguish from the low energy collective modes of a quantum paramagnet, computed in Appendix A.2.

### 3.6 Quantum rotor model

Another approach to study Goldstone modes is to introduce a quantum rotor model which captures the low energy properties of the system. This can be done by coarse-graining spins in plaquettes, as carried out in section 3.3. There we found that the low energy plaquette states at half-filling contain one singlet ground state, and one triplet state obtained by acting on the ground state by the staggered magnetization operator. This matches the low energy spectrum of a quantum rotor \( \mathbf{n} \), on the
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plaquette \(i\), which can be written in terms of the component spins of the plaquette as

\[
\hat{L}_i = \hat{S}_{i1} + \hat{S}_{i2} + \hat{S}_{i3} + \hat{S}_{i4},
\]

\[
\hat{n}_i \sim \hat{S}_{i1} - \hat{S}_{i2} + \hat{S}_{i3} - \hat{S}_{i4}.
\]

Here, the total spin \(\hat{L}\) acts as the canonical conjugate of \(\hat{n}\), satisfying the commutation relations,

\[
\begin{align*}
\left[ L_\alpha^i, L_\beta^j \right] &= i\delta_{ij} \epsilon^{\alpha\beta\gamma} L_\gamma^i, \\
\left[ L_\alpha^i, n_\beta^j \right] &= i\delta_{ij} \epsilon^{\alpha\beta\gamma} n_\gamma^i, \\
\left[ n_\alpha^i, n_\beta^j \right] &= 0.
\end{align*}
\] (3.28)

We introduce an effective Hamiltonian for these rotors, consistent with local \(Z_2\) symmetry,

\[
H_{\text{rotor}} = \frac{\nu}{2} \sum_i \hat{L}_i^2 - \tilde{g} \sum_{\langle ij \rangle} (\hat{n}_i \cdot \hat{n}_j)^2.
\] (3.29)

The dynamic spin susceptibility can be obtained, in the long wave length limit \(k \to 0\), by the linear response of \(\hat{L}\) to an external field \(\hat{B}_i = B_i e^{-i(\omega t - k \cdot r_i)}\),

\[
H_0^B = -\sum_i \hat{B}_i \cdot \hat{L}_i.
\] (3.30)

The Heisenberg equations of motion for the rotors become

\[
\begin{align*}
\frac{d\hat{L}_i}{dt} &= \tilde{g} \sum_{j \in NN(i)} (\hat{n}_i \cdot \hat{n}_j)(\hat{n}_i \times \hat{n}_j) + \hat{B}_i \times \hat{L}_i, \\
\frac{d\hat{n}_i}{dt} &= \frac{\nu}{2} (\hat{L}_i \times \hat{n}_i) - \hat{n}_i \times \hat{L}_i - \hat{B}_i \times \hat{n}_i.
\end{align*}
\] (3.31)

In the absence of an external field \(\hat{B}\), the rotor correlator is assumed to be highly local,

\[
\langle \hat{n}_i^\alpha \hat{n}_j^\beta \rangle_0 = \delta_{ij} (\delta^{\alpha\beta} n_i^2 / 3 + Q^{\alpha\beta}) \equiv \delta_{ij} G^{\alpha\beta}.
\]

The product of \(\hat{n}\) operators then differs from the mean field result by a correction,

\[
\hat{n}_i^\alpha \hat{n}_j^\beta - \delta_{ij} G^{\alpha\beta} = \delta_{ij} \rho^{\alpha\beta} + \lambda_{ij}^{\alpha\beta},
\]

which has been split into a local term \(\rho^{\alpha\beta}\), and a non-local term, \(\lambda_{ij}^{\alpha\beta} = 0\) for \(i = j\).

Linearizing the equations of motion (3.31) with respect to these corrections, we obtain

\[
\begin{align*}
-i\omega L_\alpha &= F(k) \epsilon^{\alpha\beta\gamma} G^{\beta\gamma} \rho^{\delta}, \\
-i\omega \rho^{\alpha\beta} &= (\epsilon^{\beta\gamma\delta} G^{\alpha\delta} + \epsilon^{\alpha\gamma\delta} G^{\beta\delta})(\nu L^\gamma - B^\gamma).
\end{align*}
\] (3.32)
where

\[ F(k) = 2\tilde{g} \sum_{i=1}^{d} (1 - \cos q_i). \]  \hfill (3.33)

Since we are interested in the linear response, we have excluded from Eq. (3.32) terms quadratic in \( B \). Note that, to this order in \( B \), the non-local term \( \lambda_{ij} \) drops out of the equations of motion.

For the current case of interest, a uniaxial nematic, \( G^{\alpha\beta} \) is of the form

\[ G = \frac{1}{3} \begin{pmatrix} n^2 - S & 0 & 0 \\ 0 & n^2 - S & 0 \\ 0 & 0 & n^2 + 2S \end{pmatrix}. \]

Solving (3.32) for \( L \) yields

\[ L^\perp = -\frac{SF(k^2)}{\omega^2 - \nu S^2 F(k)} B^\perp, \] \hfill (3.34)

\[ L^\hat{n} = 0, \]

where \( \perp \) is either of the directions perpendicular to \( \hat{n} \). Note that, unlike the case of antiferromagnetic order, \( \chi^{\alpha\beta} \) has no off-diagonal contributions. This is attributed to time reversal invariance. For long wave lengths \( k \to 0 \), \( F(k) \to \tilde{g}k^2 \), and poles in the susceptibility indicate the presence of two degenerate DDW modes, with velocity \( v_{\text{DDW}} = \sqrt{\nu S^2 \tilde{g}} \). This is consistent with the RPA result found above, Eq. (3.27).

Finally, we compute the dynamic spin susceptibility near \( k = (\pi, \pi) \) by replacing the term \( H_B^0 \) by a source that couples directly to the staggered magnetization,

\[ H_B^\pi = -\sum_i \mathbf{B}_i \cdot \hat{n}_i. \] \hfill (3.35)

Proceeding as above, we find the linear response

\[ n_i = -\frac{\nu G^{\alpha\beta}}{\omega^2 - z \tilde{g} n^2} B_i^\beta, \] \hfill (3.36)

where \( z = 4 \) is the coordination number of the lattice. Note that, in the current approximation, the collective modes near \( (\pi, \pi) \) are non-dispersing and gapped. The spin gap \( \omega = \sqrt{z \tilde{g} n^2} \) indicates that there is no long range Néel order in the system.

### 3.7 Lattice gauge theory

Up to now, we have ignored the possibility of fractionalization and the richer phase structure that it allows. As an example, by introducing a disclination core energy,
Figure 3.9: (a) Phase diagram for eq. (3.37) for the case \( J_n = 0 \), corresponding to a \( \mathbb{Z}_2 \) lattice gauge theory with a \( U(1) \) field. The Ising transition as \( K \) is increased corresponds to a binding of \( Q = 1/2 \) topological excitations into \( Q = 1 \) excitations. (b) Case \( J_n = 0 \), corresponding to a \( \mathbb{Z}_2 \) lattice gauge theory with an \( SO(3) \) field. The first order nematic to paramagnet transition can be split into two second order transitions, passing through a topologically ordered phase.

\[
S = -J_n \sum_{ij} n_i \sigma_{ij} n_j - J_\theta \sum_{ij} \sigma_{ij} \cos(\theta_i - \theta_j) - K \sum \prod \sigma_{ij}.
\] (3.37)

Unlike section 3.4, here we ignore the anisotropy in the tensor \( J^{\alpha\beta} \), which is weak and only affects the very low energy physics. Figures 3.9 and 3.10 display the phase diagrams for extreme values of the couplings \( J_n, J_\theta \) and \( K \). Figure 3.9 shows the phase diagrams for the cases \( J_n = 0 \) and \( J_\theta = 0 \). These correspond to \( \mathbb{Z}_2 \) lattice gauge theories with \( U(1) \) and \( SO(3) \) Higgs fields, respectively, which have been studied extensively in the literature\[107, 172, 173, 44\].

Figure 3.10 shows the situation when any of the couplings in (3.37) is infinite. In all of these cases, the auxiliary field \( \sigma_{ij} \) is completely ordered, and we can work in “minimal gauge”, where \( \sigma_{ij} = 1 \) for all bonds. This corresponds to a lack of topological
Figure 3.10: Phase diagrams when any of the couplings in eq. (3.37) is infinite. In all of these cases, topological defects in the gauge field are energetically forbidden, and we can work in minimal gauge $\sigma_{ij} = 1$. (a) Case $J_n = \infty$, insuring that at least nematic order is present. $K$ is irrelevant in this situation, as the field $\sigma_{ij}$ is frozen. As $J_\theta$ is increased, the system undergoes an XY transition from nematic to SDW order. The situation is similar to the case $J_\theta = \infty$, shown in (b), but now a Heisenberg transition is seen from CDW to SDW order. In (c), $K = \infty$, leading to a dynamical decoupling of the $\theta$ and $n$ terms in the action (3.37). For small $J_\theta$ and $J_n$, a paramagnet with only topological order survives.
defects, which are energetically forbidden. Once a value of \( n \) (or \( \theta \)) is chosen at a given lattice point, smoothness of the fields insures that the \( Z_2 \) redundancy in \( n \) (or \( \theta \)) is removed everywhere. Thus, the universality class of these transitions is the same as that of the corresponding ungauged theories. For instance, in Fig. 3.10(c), starting with the topologically ordered paramagnet at small \( J_n \) and \( J_\theta \), we can increase \( J_\theta \) until the onset of CDW order through an XY phase transition. Similarly, by increasing \( J_n \) we get the onset of nematic order through a Heisenberg transition. In these regions of phase space, the simultaneous presence of both CDW and nematic orders imply SDW order. To see this, suppose that \( \langle n \rangle_m \) and \( \langle e^{i\theta} \rangle_m \) are simultaneously non-zero, where the subscript \( m \) indicates that we are working in minimal gauge. Then \( \langle e^{i\theta n} \rangle_m \) is non-zero, but this quantity is in fact independent of the gauge used.

Let us now consider the phase diagram when \( K = 0 \). In this case the auxiliary gauge field fluctuates strongly, and it is useful to sum (3.37) over \( \sigma_{ij} \) configurations to get

\[
S_{\text{eff}} = -\frac{J_n^2}{2} \sum_{\langle ij \rangle} (n_i - n_j)^2 - \frac{J_\theta^2}{2} \sum_{\langle ij \rangle} \cos^2(\theta_i - \theta_j) - J' \sum_{\langle ij \rangle} n_i \cdot n_j \cos(\theta_i - \theta_j) + \ldots
\] (3.38)

In this particular model, \( J' = J_n J_\theta \). An analysis of two dimensional algebraic order in a model of this sort (with XY spins) has been carried out in Ref. [102]. There, the only phases present are paramagnet, CDW, nematic, and SDW, and there is a direct transition between paramagnetic and SDW phases. Thus, for the action (3.37), although we only look at the boundary of the phase diagram, in all the limits considered, the simultaneous appearance of nematic and CDW order implies SDW order.

However, it is possible to have a state with nematic and CDW orders without simultaneously stabilizing SDW order. To see this, notice that \( J' \) in (3.38) can be tuned by adding an extra gauge invariant term to the original action (3.37)

\[
\Delta S = -J_e \sum_{\langle ij \rangle} n_i \cdot n_j \cos(\theta_i - \theta_j).
\] (3.39)

In particular, when \( J' = 0 \), Eq. (3.38) leads to two independent transitions for \( n \) and \( \theta \), yielding paramagnetic, CDW, nematic, and nematic+CDW phases. The latter phase breaks SU(2) spin symmetry and translational symmetry, but leaves time reversal invariant. How can such a state arise from fluctuations of a spin stripe? In the stripe picture, an anti-phase domain wall serves a dual role, both as a region where charge accumulates and as a boundary between domains of opposite staggered magnetization. The effect of (3.39) is to disentangle these two roles to obtain two separate objects, a charge line component and a magnetic anti-phase line component.
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Figure 3.11: Five faces of the phase diagram of the action (3.37): $J_\theta = 0$, $J_\theta = \infty$, $J_n = 0$, $J_n = \infty$, and $K = \infty$. We do not compute the phase diagram along the sixth face, $K = 0$, explicitly. However, there are indications from XY spins in 2d that the only phases present there are paramagnet, CDW, SDW, and nematic[102]. However, introduction of a new term (3.39) can spit the SDW into a CDW+nematic phase. Note that, for large values of $K$, a topologically ordered phase becomes available.
Then, fluctuations of the anti-phase line component can restore time reversal symmetry without restoring translational invariance. Note that, as the extra coupling $J_e$ is decreased, an Ising phase transition between nematic+CDW and SDW phases begins to occur in the corner of the phase diagram $J_\theta, J_n \to \infty$ until, for small enough $J_e$, the nematic+CDW phase disappears entirely in favor of the SDW phase.

### 3.8 Summary

In this paper we have considered the prospect of direct detection of a quantum spin nematic in strongly correlated electron systems, such as heavy-fermion compounds, the cuprates, and the organic superconductors. The spin nematic order parameter is a spin-2 operator, and it does not couple, to linear order, to many of the conventional probes, such as neutrons, photons, or nuclear spins. However, we show that electrons moving in a nematic background have an anisotropic spin susceptibility, which can be detected in polarized neutron scattering and Knight shift experiments. In addition, we discuss the possibility of observing the Goldstone modes associated with nematic ordering in inelastic neutron scattering experiments.

In Section 3.2, we defined the nematic order parameter in terms of the equal-time spin-correlation function, and argued for uniaxial nematic order in systems with collinear spin correlations. In Section 3.3, we introduced wave functions to describe nematic order in a number of situations, including a stand-alone nematic, and nematic order coexisting either with spin-singlet or spin-triplet superconductivity. In order to do this, we followed a coarse-graining and low energy projection procedure, as done in Refs. [212] and [2]. We used these wave functions to constrain the short distance and low energy structure of the nematic order parameter. In Section 3.4, we considered the finite temperature phase diagram of the nematic through a mean-field analysis of the GL free energy. Here, we included the effects of the spin-orbit interaction which, even when weak, ultimately fix the director of the nematic. We illustrated this principle using spin-exchange constants measured in undoped La$_2$CuO$_{4+x}$. In Section 3.5, we computed the anisotropic spin response of electrons in the nematic phase, and discussed prospects for its observation. There, we also computed the spectrum of Goldstone modes of a quantum spin nematic. In Section 3.6, these results were supported by the analysis of an effective quantum rotor model. Finally, in Section 3.7, we considered the possible presence of topologically-ordered phases, as well as an exotic CDW+nematic phase, in a system of fractionalized electrons.

### 3.9 Acknowledgements

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Chapter 4

SO(4) Theory of Antiferromagnetism and Superconductivity in Bechgaard Salts

A common feature of many strongly correlated electron systems is proximity of a superconducting state to some kind of magnetically ordered insulating state. Examples include organic materials[82, 114], heavy fermion superconductors[129, 97], and high T\textsubscript{c} cuprates[124]. Several theoretical analyses suggest that a strong repulsion between the two orders plays an important role in determining the phase diagram and low energy properties of these materials[165]. The idea of competing orders was developed into the SO(5) theory of high T\textsubscript{c} superconductivity of S.C. Zhang[211]. SO(5) symmetry has also been applied to study competition of ferromagnetism and p-wave superconductivity in Sr\textsubscript{2}RuO\textsubscript{4}[139], and antiferromagnetism and d-wave superconductivity in κ-BEDT-TTF salts[138].

In this paper we consider the interplay of antiferromagnetism (AF) and triplet superconductivity (TSC) in quasi one-dimensional (Q1D) electron systems. Our study is motivated by Q1D Bechgaard salts (TMTSF)	extsubscript{2}X. The most well studied material from this family, (TMTSF)	extsubscript{2}PF\textsubscript{6}, is an antiferromagnetic insulator at ambient pressure and a superconductor at high pressures[83, 5, 198, 100]. The symmetry of the superconducting order parameter in (TMTSF)	extsubscript{2}PF\textsubscript{6} is not yet fully established, but there is strong evidence that electron pairing is spin triplet: the superconducting T\textsubscript{c} is strongly suppressed by disorder[31]; critical magnetic field H\textsubscript{c2} in the interchain direction exceeds the paramagnetic limit[112]; the electron spin susceptibility, obtained from Knight shift measurements, does not decrease below T\textsubscript{c}[111]. In another material from this family, (TMTSF)	extsubscript{2}ClO\textsubscript{4}, superconductivity is stable at ambient pressure and also shows signatures of triplet pairing[179, 69, 84, 144]. Insulator to superconductor transition as a function of pressure has also been found in(TMTSF)	extsubscript{2}AsF\textsubscript{6}[23].
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The phase diagram of interacting electrons in one dimension was obtained in Ref. [64] using bosonization and renormalization group (RG) analyses. At incommensurate filling, this system has a phase boundary between spin density wave (SDW) and TSC phases when $K_\rho = 1$ and $g_1 > 0$ ($K_\rho$ is the Luttinger parameter in the charge sector, $g_1$ the backward scattering amplitude). The starting point of our discussion is the observation that, in the absence of umklapp, 1D Luttinger liquids have an “isospin” SO(4)$_{\text{iso}}$ symmetry[54] at the boundary between SDW and TSC phases. To define this symmetry, we introduce the charge of left and right moving electrons, $Q_\pm$, and two new operators, $\Theta_\pm$, ($r = \pm$)

\[
Q_r = \frac{1}{2} \sum_{ks} \left( a_{r,ks}^\dagger a_{r,ks} - \frac{1}{2} \right)
\]

\[
\Theta_r^\dagger = r \sum_k a_{r,k\uparrow}^\dagger a_{r,-k\downarrow}.
\]

Here $a_{\pm,ks}^\dagger$ creates right/left moving electrons of momentum $\pm k_f + k$ and spin $s$. Combining these according to $J_r^x = (\Theta_r^\dagger + \Theta_r)/2$, $J_r^y = (\Theta_r^\dagger - \Theta_r)/2i$, and $J_r^z = Q_r$, we see that the generators satisfy two independent chiral SO(3) algebras, $[J_r^a, J_{r'}^b] = i\delta^{rr'}\epsilon^{abc}J_r^c$. The product of left and right algebras yields the total isospin group SO(4)$_{\text{iso}} \approx$SO(3)$_R \times$SO(3)$_L$. The Luttinger Hamiltonian at incommensurate filling, $\mathcal{H}$, generically commutes with the charge operators $Q_\pm$. Using a bosonized form of $\mathcal{H}$, it can be shown that at $K_\rho = 1$, the $\Theta_\pm$ operators also commute with $\mathcal{H}$[54, 148]. Thus, at $K_\rho = 1$, SO(4)$_{\text{iso}}$ forms an exact symmetry of $\mathcal{H}$. In addition, for spin-symmetric interactions, which describe Bechgaard salts to a very good approximation[148, 186], the system has SO(3)$_{\text{spin}}$ symmetry, $[S_\alpha, S_\beta] = i\epsilon^{\alpha\beta\gamma}S_\gamma$, generated by the total spin

\[
S_\alpha = \frac{1}{2} \sum_{r,ks s'} a_{r,ks}^\dagger \sigma_{ss'}^\alpha a_{r,ks'}.
\]

Hence, for $K_\rho = 1$, i.e. the line separating SDW and TSC phases, the system has full SO(3)$_{\text{spin}} \times$SO(4)$_{\text{iso}}$ symmetry. We emphasize that for Luttinger liquids at incommensurate filling, this symmetry always appears at the SDW/TSC phase boundary and does not require fine-tuning of the parameters.

This symmetry can be used to unify SDW and TSC order parameters. SDW order away from half filling is described by a complex vector order parameter,

\[
\Phi_\alpha = \sum_{ks s'} a_{+ks}^\dagger \sigma_{ss'}^\alpha a_{-ks'}.
\]

Q1D band structure restricts the orbital component of triplet superconducting order to be $\Psi(\vec{p}) \propto p_x$, with $x$ the coordinate along the chains. Thus, the TSC order
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The parameter is also a complex vector,

$$\Psi_\alpha^\dagger = \frac{1}{i} \sum_{kss'} a_{++,ks}^\dagger \sigma_{ss'}^\alpha a_{--,ks'}^\dagger$$

The four vector order parameters $\text{Re}\Phi$, $\text{Im}\Phi$, $\text{Re}\Psi$, and $\text{Im}\Psi$ can be combined into a $4 \times 3$ matrix,

$$P_{\bar{a}\alpha} = \begin{pmatrix} (\text{Re}\Psi)_x & (\text{Im}\Psi)_x & (\text{Re}\Phi)_x & (\text{Im}\Phi)_x \\ (\text{Re}\Psi)_y & (\text{Im}\Psi)_y & (\text{Re}\Phi)_y & (\text{Im}\Phi)_y \\ (\text{Re}\Psi)_z & (\text{Im}\Psi)_z & (\text{Re}\Phi)_z & (\text{Im}\Phi)_z \end{pmatrix}$$

Each column (row) of $\hat{P}$ transforms independently as a vector under the action of $SO(3)_{\text{spin}}$ ($SO(4)_{\text{iso}}$).

The $\Theta_r$ operators are reminiscent of Yang’s $\eta$ operator, which generates an $SO(4)$ symmetry for the Hubbard model[205]. Unlike $\eta$, whose center of mass momentum is always the commensurate wave vector $\pi$, the $\Theta_r$ have their momenta at the wave vectors $\pm 2k_f$. This is crucial for defining the symmetry at arbitrary electron density; in contrast, Yang’s $SO(4)$ applies only at half-filling.

Real materials are only Q1D and coupling between chains gives rise to finite temperature phase transitions. However, as long as 3D coupling is weaker than the intrachain tunnelling and interactions, the nature of the ordered state is determined by the most divergent susceptibility within individual chains. Hence, for Q1D materials near the SDW/TSC boundary we expect to find $K_\rho$ close to one, and to find approximate $SO(3)_{\text{spin}} \times SO(4)_{\text{iso}}$ symmetry. Then, the phase diagram in three spatial dimensions is obtained from a Ginzburg-Landau (GL) free energy whose form is strongly constrained by symmetry,

$$F = \frac{1}{2} (\nabla P_{\alpha\alpha})^2 + \bar{r} P_{\alpha\alpha}^2 + \delta r \left( P_{1\alpha}^2 + P_{2\alpha}^2 - P_{3\alpha}^2 - P_{4\alpha}^2 \right) + \tilde{u}_1 P_{\alpha\alpha}^2 P_{\beta\beta} + \tilde{u}_2 P_{\alpha\alpha} P_{\beta\beta} P_{\alpha\beta} P_{\beta\alpha}$$

This is the most general expression with $SO(3)_{\text{spin}} \times SO(4)_{\text{iso}}$ symmetric quartic coefficients. We follow the common assumption that changing the external control parameters of the system, e.g. temperature and pressure, only affects the quadratic coefficients. These are thus allowed to break the symmetry and tune the phase transition. For $\delta r \neq 0$, the symmetry is broken down to $SO(3)_{\text{spin}} \times SO(2)_c \times SO(2)_t$, where $SO(2)_c$ is generated by the total charge $Q = Q_+ + Q_-$, and $SO(2)_t$ comes from the lattice translational symmetry[213].

At half-filling, umklapp scattering must be taken into consideration. This is the case for Bechgaard salts, where structural dimerization splits the conduction band into a full lower band, and a half-filled upper band. Umklapp turns two right movers into left movers, and vice versa,

$$\mathcal{H}_3 = \frac{g_3}{2L} \sum_{k,k+q} a_{++,k+q}^\dagger a_{++,k}^\dagger a_{--,q} a_{--,k+q} + h.c.$$
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The term (4.6) pins the phase of the SDW, reducing it to the real Néel vector \( \vec{N} = \text{Re}\bar{\Phi} \) (for \( g_3 > 0 \)). In the presence of umklapp there is still a direct AF/TSC transition at \( K_p = 1[82] \). On the other hand, \( Q_+ \) and \( Q_- \) are no longer conserved separately, and SO(4)\(_{\text{iso}}\) symmetry of the free energy is broken. However, to linear order in \( g_3 \), SO(4)\(_{\text{iso}}\) is not broken all the way down to SO(2)\(_c\). The contribution of \( H_3 \) to the free energy is \( \Delta F = \frac{g_3}{4} \left( (\text{Re}\Phi)^2 - (\text{Im}\Phi)^2 \right) \), which preserves a residual symmetry SO(3)\(_{\text{iso}}\), given by the diagonal subgroup of SO(4)\(_{\text{iso}}\) \( \approx \text{SO}(3)_{\text{R}} \times \text{SO}(3)_{\text{L}}[148] \). The generators of SO(3)\(_{\text{iso}}\) are \( I_a = J_a^+ + J_a^- \). Together with SO(3)\(_{\text{spin}}\) invariance, the total symmetry defined by these operators is SO(4)\(_{\text{spin}}\) \( \times \) SO(3)\(_{\text{iso}}\).

The justification for considering small \( g_3 \) is as follows. The bare value of \( g_3 \) is proportional to dimerization, which is only of order of 1% in (TMTSF)\(_2\)PF\(_6[183]\). Furthermore, the GL free energy depends on the renormalized value \( g_3,_{\text{eff}} \) at the crossover scale between 1D and 3D physics, which is even smaller than the bare value of \( g_3 \). Umklapp is irrelevant inside the TSC phase, as well as on the AF/TSC phase boundary. Even in the AF phase, where umklapp is a relevant perturbation, \( g_3 \) flows near zero before diverging, and this divergence may be cut off by the onset of 3D coupling. Therefore, everywhere close to the AF/TSC phase boundary, we can assume that \( g_3,_{\text{eff}} \) is small.

SO(4) symmetry unifies AF and TSC orders, which are now combined into a 3 \( \times \) 3 tensor order parameter,

\[
Q_{aa} = \begin{pmatrix}
(\text{Re}\tilde{\Psi})_x & (\text{Im}\tilde{\Psi})_x & N_x \\
(\text{Re}\tilde{\Psi})_y & (\text{Im}\tilde{\Psi})_y & N_y \\
(\text{Re}\tilde{\Psi})_z & (\text{Im}\tilde{\Psi})_z & N_z
\end{pmatrix}
\]

(4.7)

The columns (rows) of \( \tilde{Q} \) transform as a vector under the spin (isospin) SO(3) algebra, \([S_a, Q_{b\beta}] = i\epsilon_{abc} Q_{c\beta} (I_a, Q_{b\beta}) = i\epsilon_{abc} Q_{c\beta}\). In analogy with (4.5), the GL free energy near the AF/TSC phase boundary is

\[
F = \frac{1}{2} (\nabla Q_{aa})^2 + \bar{r} Q_{aa}^2 + \delta r (Q_{z,\alpha}^2 - Q_{x,\alpha}^2 - Q_{y,\alpha}^2) \\
+ \tilde{u}_1 Q_{aa}^2 Q_{b\beta}^2 + \tilde{u}_2 Q_{aa} Q_{a\beta} Q_{b\alpha} Q_{b\beta}
\]

(4.8)

When \( \delta r = 0 \) the model has full SO(4) symmetry. Away from this line it only has spin and charge SO(3)\(_{\text{spin}}\) \( \times \) SO(2)\(_c\) symmetry. A derivation of the GL free energy for weakly interacting Q1D electrons yields the model in (4.8) with \( \tilde{u}_1 = 21\zeta(3)/16\pi^2 v_f T^2 \) and \( \tilde{u}_2 = -7\zeta(3)/8\pi^2 v_f T^2[148] \).

The properties of model (4.8) depend strongly on the sign of \( \tilde{u}_2 \), which determines whether the triplet superconductor is unitary (\( \text{Re}\tilde{\psi} \propto \text{Im}\tilde{\psi} \)) or non-unitary (\( \text{Re}\tilde{\psi} \times \text{Im}\tilde{\psi} \neq 0 \)). We expect the unitary case, \( \tilde{u}_2 < 0 \), to be of experimental relevance to (TMTSF)\(_2\)PF\(_6\), and in the remainder of this paper we primarily concentrate on it. The mean field diagram is then composed of an AF phase separated from a TSC.
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Figure 4.1: Mean field phase diagram of eq. (4.8) in the unitary case $\tilde{u}_2 < 0$. There is a first order transition (thick line) between AF and TSC phases. Inset: Corresponding diagram for non-unitary case $\tilde{u}_2 > 0$. M denotes a mixed AF/TSC phase.

phase by a first order phase transition, and a disordered (Normal) phase separated from the two other phases by second order lines (see Fig. 4.1). For completeness, we include in the inset the mean field phase diagram for the non-unitary case.

To understand the role of thermal fluctuations in model (4.8) and in slightly perturbed models where the quartic coefficients do not lie exactly on the SO(4) symmetric manifold, we use $4 - \epsilon$ RG analysis. We find that the RG equations have only two fixed points: a trivial Gaussian fixed point, $\bar{r} = \delta r = \tilde{u}_1 = 0$, and an SO(9) Heisenberg point, $\bar{r} \neq 0$, $\delta r = 0$, $\tilde{u}_1 \neq 0$, $\tilde{u}_2 = 0$. In Fig. 4.2 we show RG flows in the SO(4) symmetric plane, where we find runaway flows whenever $\tilde{u}_2 \neq 0$. The analysis can be generalized to order parameters $\vec{N}$ and $\vec{\Psi}$ that are $N$-component vectors, in which case the SO(4)$\approx$SO(3)$_{spin}$×SO(3)$_{iso}$ symmetry becomes SO($N$)$_{spin}$×SO(3)$_{iso}$. We find that even in the large $N$ limit, all flows with $\tilde{u}_2 < 0$ are runaway flows, indicating the absence of fixed points with unitary TSC.

The absence of a fixed point in the RG flow often implies that fluctuations induce a first order phase transition, thus precluding a multicritical point in the phase diagram. In order to inspect this possibility, we study model (4.8) directly in 3D in the large $N$ limit[148]. The idea of the large $N$ expansion is to sum self-consistently all bubble diagrams. We find (inset of Fig. 4.3) a first order transition between AF and TSC phases along the SO(4) symmetric line $\delta r = 0$, in agreement with mean field theory. A new feature of the large $N$ limit is the first order transition between the Normal and AF phases in the vicinity of the critical point. If we assume that the experimentally controlled pressure changes an extensive variable conjugate to $\delta r$, such as the volume
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Figure 4.2: Renormalization group flow of the SO(4) symmetric theory eq. (4.8) in $d = 4 - \epsilon$. There are no stable fixed points. Instead, there are two types of runaway flow, corresponding to unitary ($\tilde{u}_2 < 0$) and non-unitary ($\tilde{u}_2 > 0$) TSC.

of the system, the first order transition broadens into a coexistence region of TSC and AF. This is consistent with the experimental phase diagram of (TMTSF)$_2$PF$_6$ (Fig. 4.3). An unusual feature of the theoretical phase diagram (inset, Fig. 4.3) is the first order transition between Normal and TSC phases. This is similar to the fluctuation-driven first order transition between Normal and superfluid phases proposed for $^3$He by Bailin et al. [8]. In bulk $^3$He, the coherence length is very long and the transition is mean-field like. The fluctuation region is so small that tiny discontinuities at the transition caused by fluctuations would be impossible to observe. In Q1D systems, such as Bechgaard salts, the fluctuation region is expected to be large[170] and the discontinuous nature of the Normal to TSC transition may be experimentally accessible. This transition has been investigated through specific heat measurements in (TMTSF)$_2$ClO$_4$[61]. The results were interpreted as a mean-field BCS transition, although the amplitude of the specific heat jump was unusually large. Since $T_c$ in these materials is very sensitive to impurities, the extra amplitude in the specific heat jump might be attributed to broadening due to disorder of a $\delta$-function peak in specific heat. Experimental observation of the coexistence region of Normal and TSC phases, or of hysteresis effects in resistivity measurements may also be very difficult. Nearly equal strains in the TSC and the Normal phases and the nearly temperature independent superconducting transition temperature can make such a coexistence region very small. On the other hand, it is possible that spin anisotropy present in real materials, but not included in our theoretical analysis, stops the runaway RG flows leading to the first order transition. Another possibility
Figure 4.3: Schematic temperature-pressure phase diagram of (TMTSF)$_2$PF$_6$ [198, 100]. AF/N and AF/TSC correspond to coexistence regimes of the appropriate phases. **Inset:** Phase diagram for competing AF and unitary TSC states for model (4.8) in the large $N$ limit. $\delta r$ tunes the system across the two phases. Thick lines represent first order transitions.

is that one loop $4 - \epsilon$ RG calculations and the large $N$ expansion do not capture the correct behavior of model (4.8) for $\epsilon = 1$ and $N = 3$. For the Normal to unitary TSC transition, De Prato *et al.* argued that a stable fixed point describing the second order phase transition appears in the six-loop expansion of the GL free energy[156]. We hope that future experiments will investigate the nature of the Normal to TSC transition in Bechgaard salts in more detail.

The most dramatic consequence of enhanced symmetry at the phase transition is the prediction of new low energy collective excitations. In the vicinity of the AF/TSC phase transition, SO(4) symmetry leads to a new collective mode, corresponding to the $\Theta$ operator that rotates AF and TSC orders into each other[148]. As pressure is varied toward the phase transition, breaking of the SO(4) symmetry is reduced, leading to a decrease in the energy of the $\Theta$ excitation. Mode softening is not expected generically at a first order phase transition and identifies the $\Theta$-resonance as a generator of the SO(4) quantum symmetry. Weak symmetry breaking due to interchain coupling and higher order umklapp terms may lead to a small gap and to finite broadening of $\Theta$, even at the AF/TSC phase boundary. Deep in the normal phase the $\Theta$ excitation cannot be probed by conventional methods, such as electromagnetic waves or neutron scattering, as these only couple to particle-hole channels (e.g. spin or density) and $\Theta$ is a collective mode in the particle-particle channel. The situation changes when the system becomes superconducting. In the presence of a conden-
sate of Cooper pairs, charge is not a good quantum number and particle-particle and particle-hole channels mix. The $\Theta$ excitation should thus appear as a resonance in inelastic neutron scattering experiments\cite{148}, and its intensity should be proportional to the square of the superconducting amplitude $|\Psi|^2$. For Q1D Bechgaard salts, we expect strong pairing fluctuations even above $T_c$. Hence, precursors of the $\Theta$ resonance may be visible in the normal state, with strong enhancement of the resonant scattering intensity appearing when long range TSC order develops.

It is useful to put the SO(4) model of AF/TSC competition in Bechgaard salts in the general perspective of electron systems with competing orders. In the case of the SO(5) theory of AF and $d$-wave SC in 2d systems\cite{211,138}, it is difficult to construct realistic microscopic models with such symmetry (see e.g. Refs. \cite{180,71}). By contrast, SO(4) symmetry in Bechgaard salts arises naturally from a conventional Luttinger description. We also point out that tuning across the AF/TSC phase boundary in $(\text{TMTSF})_2\text{PF}_6$ can be done in the same sample by varying pressure, whereas tuning the AF/SC transition in the cuprates requires using different samples. Thus, we consider $(\text{TMTSF})_2\text{PF}_6$ a good candidate for experimental observation of emergence of higher symmetry in a strongly correlated electron system.

In the discussion above, we assumed Luttinger liquid behavior in individual chains to motivate the approximate SO(4) symmetry at the AF/TSC phase boundary. It has been suggested that for the superconducting phase of Bechgaard salts, inter-chain hopping is strong enough to turn the system into a strongly anisotropic Fermi liquid\cite{195,19}. The decreased nesting condition in this case strongly affects antiferromagnetism. For the classical symmetry of the GL free energy, this effect can be absorbed into the normalization of the field $\vec{N}$, so that the GL parameters only display a small deviation from SO(4) symmetry at the mean-field level. Thus, we do not expect a qualitative change in the phase diagram presented in Fig. 4.3 (see Ref. \cite{148} for a detailed discussion). To verify the approximate quantum SO(4) symmetry for the strongly anisotropic Fermi liquid, one can study the spectrum of collective excitations using an RPA-type analysis and verify the existence of the $\Theta$ excitation\cite{43}. These results will be presented elsewhere.

In summary, we introduced an SO(4) framework for the competition between AF and TSC in Q1D electron systems. The microscopic origin of the SO(4) symmetry at the transition between AF and TSC orders was identified in the Luttinger liquid model. Our results have direct implications for Q1D organic superconductors from the $(\text{TMTSF})_2\text{X}$ family. For example, first order transitions between AF and TSC phases, and between AF and Normal phases, explain the AF/TSC and the AF/Normal coexistence regions found in the phase diagram of $(\text{TMTSF})_2\text{PF}_6$ \cite{198}. We also argue that the Normal/TSC transition in these materials could be weakly first order. We predict a sharp resonance in neutron scattering, whose characteristics identify it unambiguously as a generator of SO(4) symmetry.
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Chapter 5

Competition between Triplet Superconductivity and Antiferromagnetism in Quasi One-Dimensional Electron Systems

5.1 Introduction

Quasi one-dimensional compounds can display a rich variety of phases, including spin-Peierls, charge density wave, spin density wave, and superconducting orders[78, 82, 35, 14, 120]. Due to the large anisotropy in their crystal structure, these materials are often modelled as a collection of weakly coupled Luttinger liquids. The wealth of phases seen in these compounds is then attributed to the intrinsic instability of one dimensional electron systems towards the formation of quasi long range order[11]. As temperature is lowered, correlations along individual chains grow, until the coupling between chains stabilize true long range order. In the current paper, we follow this approach to study the interplay between triplet superconductivity (TSC) and antiferromagnetism (AF) in quasi one-dimensional electron systems. The starting point of our discussion is an observation that, for weak umklapp scattering, one-dimensional Luttinger liquids at half-filling have SO(4) symmetry at the boundary between AF and TSC phases. Near this boundary, the two order parameters can be unified using SO(4) symmetry, leading to strong constrains on the topology of the phase diagram and on the spectrum of low energy collective excitations.

Our analysis is motivated by quasi one-dimensional Bechgaard salts (TMTSF)$_2$X, and their sulphurated counterparts (TMTTF)$_2$X. The most well studied material from this family (TMTSF)$_2$PF$_6$ is an antiferromagnetic insulator at ambient pressure and becomes a superconductor at high pressure[83, 5, 178, 198, 100]. The symmetry of the superconducting order parameter in (TMTSF)$_2$PF$_6$ is not yet fully established[49],
but there is strong evidence that electron pairing is spin triplet: the superconducting \( T_c \) is strongly suppressed by disorder \([31, 32, 185, 36, 1]\); critical magnetic field \( H_{c2} \) in the interchain direction exceeds the paramagnetic limit \([112, 65]\); the electron spin susceptibility, obtained from the Knight shift measurements, does not decrease below \( T_c \) \([111]\). In another material from this family, \((\text{TMTSF})_2\text{ClO}_4\), superconductivity is stable at ambient pressure and also shows signatures of triplet pairing\([179, 69, 84, 144]\). Insulator to superconductor transition as a function of pressure has also been found for \((\text{TMTSF})_2\text{AsF}_6[23]\) and \((\text{TMTTF})_2\text{PF}_6[80]\).

There are two aspects of the SO(4) symmetry between antiferromagnetism and triplet superconductivity that we address in this paper.

**Classical SO(4) Symmetry.** We consider the possible emergence of the classical (static) symmetry at a finite temperature critical point. We introduce a Ginzburg-Landau (GL) free energy to describe the interaction between the AF and TSC orders, and we study the effects of thermal fluctuations through a large \( N \) expansion and renormalization group (RG) analyses in \( d = 4 - \epsilon \) and \( d = 2 + \epsilon \) dimensions. For a unitary TSC, which we argue to describe Bechgaard salts, we find a first order transition between AF and TSC phases, a first order transition between AF and normal phases ending in a tricritical point, and a weakly first order transition between TSC and normal phases. For a non-unitary TSC we find a mixed phase in which AF and TSC orders are present simultaneously. We argue that the system is close to having an SO(4) symmetric tetracritical point, but there is a narrow line of direct first order transitions between the normal and the mixed phase. (For a detailed discussion of the distinction between unitary and non-unitary TSC, see Sec. 5.3.1.)

**Quantum SO(4) Symmetry.** We introduce a quantum SO(4) rotor model which encapsulates key features of the competition between AF and TSC orders. We use this model to study collective excitations in the system in various phases. We argue that the \( \Theta \)-excitation, which gives one of the generators of the SO(4) algebra, should give rise to a sharp resonance in spin polarized neutron scattering in the TSC phase. We further predict that in the case of a unitary TSC the energy of the \( \Theta \)-resonance should decrease to nearly zero at the phase boundary with the AF phase. Such mode softening is not expected generally near a first order transition and would be a unique signature of the enhanced symmetry at the transition point.

Bechgaard salts belong to a class of strongly correlated electron systems displaying proximity of a superconducting state to some kind of magnetically ordered insulating state. Other examples include the high \( T_c \) cuprates\([124]\), heavy fermion superconductors\([129, 97]\), and in most cases the superconducting (SC) order parameter is spin singlet (\( s \) or \( d \) wave) and the insulating state has antiferromagnetic or spin density wave order. Symmetry principles have been introduced to study the competition of order parameters in some of these systems. In S.C. Zhang’s SO(5) theory of high \( T_c \) superconductivity\([211]\), antiferromagnetism and \( d \)-wave superconductivity
are treated as components of a five dimensional order parameter. In addition to the generators of the usual charge SO(2) and spin SO(3) symmetries, new $\pi$-operators are introduced, which rotate superconductivity and antiferromagnetism into each other. A combination of analytical approximations and numerical results can be used to argue an approximate SO(5) theory of a class of two dimensional lattice models, such as the Hubbard and the $t$-$J$ model [131, 53]. The SO(5) symmetry has also been used to discuss quasi two-dimensional organic $\kappa$-BEDT-TTF salts[138]. The unification approach based on higher symmetries has been generalized to several other types of competing states. SO(5) and SO(8) symmetries have been used to classify possible many-body ground states in electronic ladders [166, 116]. SO(6) symmetry has been introduced to discuss competing striped phases and superconductivity in the cuprates[126] SO(4) symmetry has been used to combine $s$-wave superconductivity and charge density wave orders in the negative $U$ Hubbard model[204, 210], as well as $d$-wave superconductivity and $d$-density wave phases [113, 140]. It was also suggested that the SO(5) algebra can be used to combine ferromagnetism and triplet superconductivity in quasi two-dimensional Sr$_2$RuO$_4$ [139], although the existence of microscopic models with such symmetry has not been demonstrated.

There are several reasons why Bechgaard salts, and (TMTSF)$_2$PF$_6$ in particular, are promising candidates for experimental observation of the emergence of high symmetry from the competition of two orders. The insulator to superconductor transition in these materials is tuned by pressure, so the entire phase diagram can be explored in a single sample. This compares favorably to the cuprate superconductors, where the AF/SC transition appears as a function of doping and different samples are required to investigate various regimes. Another important advantage of Bechgaard salts is that they may be well described by a microscopic Luttinger liquid Hamiltonian, for which we can demonstrate the existence of SO(4) symmetry using standard bosonization analysis. This is in contrast to the high Tc cuprates, in which approximations need to be made in order to even define generators of the SO(5) symmetry [211, 71, 158]. A related issue is the question of quasiparticles in the AF insulating state and in the $d$-wave superconducting phase. In the former case the quasiparticle spectrum is fully gapped while in the latter case there are nodal quasiparticles. It is not presently known how this difference affects a quantum SO(5) symmetry for collective bosonic degrees of freedom. An advantage of the SO(4) symmetry in (TMTSF)$_2$PF$_6$ is that quasiparticles are fully gapped in both the superconducting and the insulating phases.

Recent neutron scattering experiments demonstrated the existence of strong AF fluctuations in a triplet superconductor Sr$_2$RuO$_4$[122, 21, 59]. This material is not quasi one-dimensional, but it has nested pieces of the Fermi surface (see e.g. Ref. [122]). Thus, we expect that this material may also show some qualitative features of the competition between AF and TSC discussed in this paper.

We note that our approach is phenomenological in nature, since we do not attempt to obtain Luttinger parameters starting from microscopic considerations. Instead, we observe that Bechgaard salts remain strongly anisotropic even close to the AF/TSC
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Phase boundary. Hence, we argue that the Luttinger parameter should be such that individual 1d chains should be in the vicinity of such phase transition. By starting with the Luttinger Hamiltonian, we derive the SO(4) symmetry as its immediate consequence. We note, however, that the Luttinger liquid physics is not a necessary requirement for observing SO(4) symmetry near the AF/TSC phase boundary. Several groups have argued that near the TSC phase of Bechgaard salts, the interchain tunneling is sufficient to suppress Luttinger liquid behavior in favor of a strongly anisotropic Fermi liquid[19, 51]. We will argue below that an approximate classical SO(4) symmetry will be present near the AF/TSC boundary even if the ordered phases arise from a Fermi liquid state, although we still rely on the assumption that interchain hopping of electrons is much smaller than intrachain hopping (this condition is satisfied for Bechgaard salts, see Sec. 5.8). Similarly, we expect that the Θ resonance will be present even in a strongly anisotropic Fermi liquid, whose observation will verify the approximate quantum SO(4) symmetry. In this paper, for concreteness, we will concentrate on the case where the ordered phases emerge from Luttinger liquid behavior on individual chains.

This paper is organized as follows. In section 5.2 we discuss the Luttinger liquid model for interacting electrons in one dimension. For incommensurate band filling, we show that along the transition line between the TSC and the SDW phases, this model has SO(3)×SO(4) symmetry. At half-filling we argue that, for weak umklapp, this symmetry is reduced to SO(4) symmetry. For quasi one-dimensional systems such as Bechgaard salts we argue that this SO(4) symmetry provides a unified description of AF and TSC orders. In section 5.3 we discuss a general GL free energy for the interplay between magnetism and triplet superconductivity at finite temperatures, and present mean field diagrams for these orders. In section 5.4 we analyze thermal fluctuations using 4 − ε RG analysis and demonstrate the absence of stable fixed points, which could control multicritical points in the phase diagram. In section 5.5 we analyze the case of unitary TSC competing with AF by extending the spin SO(3) group to an SO(N) algebra and using large N analysis. In section 5.6 we investigate the interplay of non unitary TSC and AF using large N approach and RG analysis for N > 3 in 4 − ε and 2 + ε dimensions. We also discuss a physically relevant case of N = 3. In Section 5.7 we introduce an effective SO(4) quantum rotor model that condenses the essential features of the competition between the two phases. We use this model to study collective excitations in various phases. In section 5.8 we discuss SO(4) symmetry in highly anisotropic Fermi liquids. In section 5.9 we review experimental implications of the SO(4) symmetry for Bechgaard salts. Finally, in section 5.10 we summarize our results.
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Figure 5.1: Phase diagram for a one dimensional system of interacting spin-1/2 fermions [64]. Here \( K_\rho^2 = (2\pi v_f + 2g_4 + g_1 - 2g_2)/(2\pi v_f + 2g_4 - g_1 + 2g_2) \). SDW and CDW correspond to spin and charge density wave states, SS and TS to singlet and triplet superconducting phases.

5.2 Microscopic origin of the symmetry

5.2.1 \( \text{SO}(3) \times \text{SO}(4) \) symmetry at incommensurate filling

Consider a one dimensional electron gas with the Hamiltonian

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_4
\]

\[
\mathcal{H}_0 = \sum_{rks} (\epsilon_{r,ks} - \mu) a_{r,ks}^\dagger a_{r,ks}
\]

\[
\mathcal{H}_1 = \frac{g_1}{L} \sum a_{+,ks}^\dagger a_{-p,ks}^\dagger a_{+,p+q,ks} a_{-,k-q,ks}
\]

\[
\mathcal{H}_2 = \frac{g_2}{L} \sum a_{+,k+qs}^\dagger a_{-,p+q,ks}^\dagger a_{-,p+q,ks} + \frac{g_4}{L} \sum a_{-,k+qs}^\dagger a_{-,p+q,ks}^\dagger a_{+,p+q,ks} + \frac{g_4}{L} \sum a_{-,k+qs}^\dagger a_{-,p-qs} a_{+,k+qs}^\dagger a_{-,p-qs}
\]

(5.1)

Here \( a_{\pm,ks}^\dagger \) create right/left moving electrons with momenta \( \pm k_f + k \) and spin \( s \), and we assume linearized dispersion of electrons \( \epsilon_{r,ks} - \mu = rv_f k \). In the Hamiltonian (5.1) the interaction term \( g_1 \) describes backward scattering and terms \( g_2 \) and \( g_4 \) describe forward scattering. For now, we assume that the system has incommensurate filling, so that umklapp processes are not allowed. The phase diagram for this system obtained from the renormalization group analysis has been discussed extensively before (see e.g. Refs. [174] and [64]) and is shown in Fig. 5.1. For the current discussion, we concentrate on the region of the phase diagram near the transition line between the TSC and the SDW phases at \( K_\rho = 1 \), i.e.

\[
g_1 = 2g_2
\]

(5.2)
We demonstrate that on this line the system has an SO(3)×SO(4) symmetry that unifies order parameters of the two phases.

The total spin operators are defined as

\[ S_\alpha = \frac{1}{2} \sum_{r,k,s,s'} a^\dagger_{r,ks} \sigma_\alpha^{ss'} a_{r,k's'} \]  \hspace{1cm} (5.3)

where \( \sigma_\alpha^{ss'} \) are the usual Pauli matrices. These operators form a spin SO(3) algebra

\[ [S_\alpha, S_\beta] = i \epsilon^{\alpha\beta\gamma} S_\gamma \]  \hspace{1cm} (5.4)

We can also combine the charge operators for right and left movers \((r = \pm)\),

\[ Q_r = \frac{1}{2} \sum_{ks} \left( a^\dagger_{r,ks} a_{r,k's'} - \frac{1}{2} \right) \]  \hspace{1cm} (5.5)

and the operators

\[ \Theta^\dagger_r = r \sum_k a^\dagger_{r,k\uparrow} a^\dagger_{r,-k\downarrow} \]  \hspace{1cm} (5.6)

to form two separate isospin SO(3) algebras

\[ J^r_x = \frac{1}{2}(\Theta^\dagger_r + \Theta_r) \]
\[ J^r_y = \frac{1}{2i}(\Theta^\dagger_r - \Theta_r) \]
\[ J^r_z = Q_r \]
\[ [J^r_a, J^r_b] = i \delta_{r,r'} \epsilon^{abc} J^r_c \]  \hspace{1cm} (5.7)

The total isospin group is therefore SO(4)\textsubscript{isospin} = SO(3)\textsubscript{R}×SO(3)\textsubscript{L}. Note that, since spin and isospin operators commute, \([S_\alpha, J^r_b] = 0\), they jointly define the closed algebra of the SO(3)\textsubscript{spin}×SO(4)\textsubscript{isospin} group.

The total spin, \(S_\alpha\), and the total charge, \(Q_+ + Q_-\), always commute with the Hamiltonian (5.1). In addition, due to the absence of umklapp at incommensurate filling, \(Q_+\) and \(Q_-\) are conserved separately. As shown in Appendix B.1 using bosonization, when the condition (5.2) is satisfied, the \(\Theta_r\) operators also commute with the Hamiltonian. Hence, the system has full SO(3)×SO(4) symmetry at the phase boundary between TSC and SDW phases. We emphasize that the SO(3)×SO(4) symmetry of Luttinger liquids at the SDW/TSC boundary is generic and does not require fine tuning of the parameters. SO(4)\textsubscript{isospin} invariance has been discussed in quasi one-dimensional systems with highly anisotropic spin interactions[161, 25]. The \(\Theta_r\) operators in (5.6) are reminiscent of the \(\eta\) operators introduced by C.N. Yang to study...
the Hubbard model[204, 210], but we will show in Sec. 5.3.2 that the two sets of operators define different symmetry groups and apply to different systems.

Spin density wave order away from half-filling is described by a complex vector order parameter,

$$\Phi_\alpha = \sum_{kss'} a_{+,ks}^\dagger \sigma_{s's}^\alpha a_{-,ks'}.$$  

(5.8)

For quasi one-dimensional systems, the band structure restricts the orbital component of the triplet superconducting order to be $$\tilde{\Psi}(\vec{p}) \propto p_x$$, where $$x$$ is the direction parallel to the chains. Thus, the TSC order parameter is also described by a complex vector,

$$\Psi_\alpha^\dagger = \frac{1}{i} \sum_{kss'} a_{+,ks}^\dagger (\sigma^\alpha \sigma_2)_{s's} a_{-,ks'}^\dagger.$$  

(5.9)

The factor of $$-i$$ is introduced for convenience, $$-i\sigma_2 \equiv \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$. The four vector order parameters $$\text{Re} \tilde{\Psi}, \text{Im} \tilde{\Psi}, \text{Re} \tilde{\Phi}, \text{Im} \tilde{\Phi}$$ can be combined into a $$4 \times 3$$ matrix,

$$\hat{P} = \begin{pmatrix} (\text{Re} \tilde{\Psi})_x & (\text{Im} \tilde{\Psi})_x & (\text{Re} \tilde{\Phi})_x & (\text{Im} \tilde{\Phi})_x \\ (\text{Re} \tilde{\Psi})_y & (\text{Im} \tilde{\Psi})_y & (\text{Re} \tilde{\Phi})_y & (\text{Im} \tilde{\Phi})_y \\ (\text{Re} \tilde{\Psi})_z & (\text{Im} \tilde{\Psi})_z & (\text{Re} \tilde{\Phi})_z & (\text{Im} \tilde{\Phi})_z \end{pmatrix}$$  

(5.10)

Each column of $$\hat{P}$$ transforms independently as a vector under the action of the spin group,

$$[S_\alpha, P_\beta] = i\epsilon^{\alpha\beta\gamma} P_\gamma$$  

(5.11)

The action of the isospin group on $$\hat{P}$$ is easiest to understand in terms of the operators $$I_a = J^+_a + J^-_a$$ and $$\Lambda_a = J^+_a - J^-_a$$. For a fixed row of $$\hat{P}$$, the action of the isospin generators in the basis $$(\text{Re} \Psi_\alpha, \text{Im} \Psi_\alpha, \text{Re} \Phi_\alpha, \text{Im} \Phi_\alpha)$$ is represented by

$$I_x = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$  

$$\Lambda_x = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$  

$$I_y = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$  

$$\Lambda_y = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}$$  

$$I_z = \begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$  

$$\Lambda_z = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}$$  

(5.12)
Once the fourth component is identified as the “time-like” direction, this is the (Euclidean) Lorentz group, with the \( I_a \) acting as rotations and the \( \Lambda_a \) acting as boosts. Hence, the rows of order parameter \( \bar{P}_{\alpha a} \) transform in the vector representation of the \( \text{SO}(4) \) isospin group.

### 5.2.2 SO(4) symmetry at half filling

In Bechgaard salts (TMTSF)$_2$X, three out of every four conduction states are occupied. At quarter filling, umklapp processes involving interactions of four electrons are allowed. Such interactions are weak, and furthermore are irrelevant in the RG sense for \( K_\rho > 1/4 \) (we remind the readers that we are interested in the regime near the SDW/TSC boundary, where \( K_\rho \approx 1 \))[62]. On the other hand, due to structural dimerization in Bechgaard salts[183], a gap splits the conduction band into a completely filled lower band and a half-filled upper band. Hence, Bechgaard salts are half-filled systems. At half filling, the Hamiltonian (5.1) must be modified to include two-electron umklapp scattering processes,

\[
\mathcal{H}_3 = \frac{g_3}{2L} \sum_{a} a_{+,k+qs}^\dagger a_{+,p-qt}^\dagger a_{-,p} a_{-,ks} + \frac{g_3}{2L} \sum_{a} a_{-,k-qs}^\dagger a_{-,p+qt}^\dagger a_{+,p} a_{+,ks} \tag{5.13}
\]

Analysis of the phase diagram of Luttinger liquids at half-filling reveals that there is still a direct transition between AF and TSC orders at \( K_\rho = 1 \), although this condition now corresponds to \( g_1 - 2g_2 = |g_3| \). The umklapp term allows scattering of two right moving electrons into two left moving ones, and vice versa. Thus, it does not commute with the operator \( \Lambda_z = Q_+ - Q_- \), which leads to breaking of the \( \text{SO}(3) \times \text{SO}(4) \) symmetry. To understand the nature of this symmetry breaking, it is useful to rewrite (5.13) in the form,

\[
\mathcal{H}_3 = \frac{g_3}{2L} \sum_{q} \left( \text{Re} \hat{\Phi}(q) \cdot \text{Re} \hat{\Phi}(-q) - \text{Im} \hat{\Phi}(q) \cdot \text{Im} \hat{\Phi}(-q) \right), \tag{5.14}
\]

where \( \hat{\Phi}(\vec{q}) \) is the SDW order parameter at center of mass momentum \( 2k_f + \vec{q} \),

\[
\hat{\Phi}(\vec{q}) = \sum_{kss'} a_{+,kq}^\dagger \sigma_{ss'} a_{-,k-q}s'. \tag{5.15}
\]

Equation (5.14) shows explicitly that umklapp tends to pin the phase of the SDW order parameter at either 0 or \( \pi \), depending on the sign of \( g_3 \). This is in agreement with the observation that period two antiferromagnetic order can be described by a single real Néel vector.

We will show in Section 5.3.2 that, whereas the Ginzburg-Landau free energy is no longer \( \text{SO}(3)_{\text{spin}} \times \text{SO}(4)_{\text{isospin}} \) symmetric at half-filling, to linear order in \( g_3 \) it maintains an \( \text{SO}(4) = \text{SO}(3)_{\text{spin}} \times \text{SO}(3)_{\text{isospin}} \) symmetry. The unbroken part of the
isospin group, $\text{SO}(3)_{\text{isospin}}$, is the diagonal subgroup of $\text{SO}(3)_{R} \times \text{SO}(3)_{L}$, which is generated by the three $I_\alpha$ operators, $I_x = \frac{1}{2}(\Theta^\dagger + \Theta)$, $I_y = \frac{1}{2i}(\Theta^\dagger - \Theta)$, $I_z = Q$, where

$$Q = \frac{1}{2} \sum_{ks} \left( a^\dagger_{+,ks} a_{+,ks} + a^\dagger_{-,ks} a_{-,ks} - 1 \right)$$

$$\Theta^\dagger = \sum_k \left( a^\dagger_{+,k} a^\dagger_{+,k} - a^\dagger_{-,k} a^\dagger_{-,k} \right).$$  (5.16)

Without loss of generality we consider the case $g_3 < 0$, where the order parameter for antiferromagnetism is given by the real part of $\vec{\Phi}$,

$$N_\alpha = \frac{1}{2} \sum_{kss'} \left( a^\dagger_{+,ks} \sigma^\alpha_{ss'} a_{-,ks'} + a^\dagger_{-,ks'} \sigma^\alpha_{ss'} a_{+,ks} \right)$$  (5.17)

It is easy to verify that $\{ \vec{N}, \text{Re} \vec{\Psi}, \text{Im} \vec{\Psi} \}$ transform as vectors under both spin and isospin $\text{SO}(3)$ symmetries. We define

$$\hat{Q} = \begin{pmatrix} (\text{Re} \vec{\Psi})_x & (\text{Im} \vec{\Psi})_x & N_x \\ (\text{Re} \vec{\Psi})_y & (\text{Im} \vec{\Psi})_y & N_y \\ (\text{Re} \vec{\Psi})_z & (\text{Im} \vec{\Psi})_z & N_z \end{pmatrix}$$  (5.18)

$\hat{Q}$ transforms as a vector under both $\text{SO}(3)$ algebras

$$[I_\alpha, Q_\beta] = i \epsilon^{abc} Q_c \delta^\beta_\gamma$$

$$[S_\alpha, Q_\beta] = i \epsilon^{\alpha\beta\gamma} Q_\gamma$$  (5.19)

so it describes an order parameter that transforms as a (1,1) representation of the $\text{SO}(4)$ algebra. Since we are mostly interested in applying our results to Bechgaard salts, we focus mostly on this $\text{SO}(4)$ symmetry in Ref. [149], as well as on the remainder of this paper.

Unlike the $\text{SO}(3) \times \text{SO}(4)$ symmetry discussed in the incommensurate case, the $\text{SO}(4)$ symmetry at half-filling is not a rigorous symmetry of the system. The generators of this group do not commute with the Hamiltonian of the system exactly. However, the main emphasis of our work is to understand the finite temperature phase diagram of (TMTSF)$_2$PF$_6$. This is obtained from the classical GL free energy, which at the AF/TSC phase boundary has $\text{SO}(4)$ symmetry if we retain umklapp processes to linear order in $g_3$ (see discussion in Section 5.3.2). In addition, with regards to quantum properties, $\text{SO}(4)$ symmetry is a good starting point to study the collective modes of the system when $g_3$ is small. The latter assumption is well justified for (TMTSF)$_2$PF$_6$, since the observed dimerization in this material is less than 1%[183]. For small $g_3$, modes found assuming $\text{SO}(4)$ symmetry will have a finite overlap with the actual excitations of the system. In particular, the quantum numbers of the $\Theta$
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mode discussed in Section 5.7, including charge two and center of mass momentum \(2k_f\), are not affected by umklapp. These properties determine which experimental probes couple to \(\Theta\). We must keep in mind, however, that the explicit breaking of \(\text{SO}(4)\) due to higher order corrections in \(g_3\), and also due to interchain coupling, may give a small energy gap and finite broadening to \(\Theta\), even at the AF/TSC phase boundary. We also point out that, from the point of view of \(\Theta\) excitations, the difference between \(\text{SO}(3)\times\text{SO}(4)\) and \(\text{SO}(4)\) symmetries corresponds to the question whether \(+2k_f\) and \(-2k_f\) excitations are the same (\(\text{SO}(4)\) symmetry at half filling) or different (\(\text{SO}(3)\times\text{SO}(4)\) symmetry away from half filling).

Thus far in the analysis we have ignored spin-orbit effects. Microwave absorption experiments in \((\text{TMTSF})_2\text{AsF}_6\) measured [186] the anisotropy in the exchange couplings to be \(10^{-6}\). This ultimately determines the preferred axes for the Néel vector \(\vec{N}\) (along the b-axis of the crystal [136]) and the spin component of the TSC order \(\vec{\Psi}\) (along either the a- or c-axis [112]). However, we do not expect such tiny anisotropy to play a significant role in determining the competition between AF and TSC phases. We also point out that NMR experiments in \((\text{TMTSF})_2\text{PF}_6\) find a divergence of \(T_{1}^{-1}\) at the Néel temperature that is well-described by the \(O(3)\) isotropic Heisenberg model [20]. Thus, even for critical fluctuations of the AF order parameter, spin anisotropy coming from spin-orbit coupling is unobservably small.

Before concluding this section we point out that the isospin algebra defined by equations (5.5), (5.6), and (5.7) can be also used to relate charge density wave order and singlet superconductivity in quasi one-dimensional electron systems[54]. This is relevant for the lower half of Fig. 5.1.

5.3 Ginzburg-Landau Free Energy

The main goal of this section is to investigate consequences of the \(\text{SO}(4)\) symmetry for the true finite temperature phase transitions, when we need to consider three dimensional fluctuations of the order parameter. One may be concerned that by introducing interchain couplings, we will immediately destroy the \(\text{SO}(4)\) symmetry. As we will show in section 5.8, even in the case where the interchain coupling \(t_b\) is large enough to make the system into a highly anisotropic Fermi liquid, approximate \(\text{SO}(4)\) symmetry prevails in the Ginzburg-Landau (GL) free energy (see e.g. Eq. (5.29). This feature of the AF/TSC GL free energy implies that our analysis of the phase diagram, based on classical \(\text{SO}(4)\) symmetry, is valid even when the normal state is described by a highly anisotropic Fermi liquid rather than a collection of weakly coupled Luttinger liquids. A review of the normal state properties of organic superconductors at low magnetic fields is given in Ref. [19], and low temperature transport properties have been reported recently in Ref. [51].

We illustrate the effects of interchain coupling in Fig. 5.2. As the temperature is reduced on either side of \(K_{\rho} = 1\), the correlation length along a chain in the ap-
propriate correlation function grows due to intrachain interactions. At some finite temperature, before this length diverges, coupling between the chains becomes relevant and a true three dimensional transition can take place. At the crossover between one and three dimensions, the description of the system in terms of a Luttinger liquid is supplanted by a GL free energy describing the interactions of the order parameters in three spatial dimensions. In this picture, for small enough $t_b$ the presence of a phase boundary between AF and TSC implies that the intrachain Hamiltonian is close to the SO(4) symmetric point $K_\rho = 1$.

An important assumption of our analysis is that pressure varies the value of $K_\rho$ and tunes the transition across the AF/TSC phase boundary. We note that measurements of $K_\rho$ based on optical conductivity measurements have been carried out at ambient pressure, i.e. deep inside the SDW phase in (TMTSF)$_2$PF$_6$. For instance, in Refs. [40] and [171], the value $K_\rho = 0.23$ is obtained. Ref. [171] point out that this value of $K_\rho$ assumes that the dominant umklapp contribution is due to commensurability at quarter filling. They acknowledge that if umklapp is dominated by commensurability at half-filling, these measurements then imply $K_\rho = 0.925$. They also point out that a half-filled model has the drawback of predicting a gap energy that is too small. However, it is equally difficult to justify the assumption that quarter filling makes the commensurability dominant: for $K_\rho = 0.23$, the rate of divergence in the RG of commensurability at one quarter is exponentially smaller than the corresponding rate for commensurability at half-filling. Thus, we feel that the question of the value of $K_\rho$ is not yet settled.

### 5.3.1 Incommensurate filling

At incommensurate filling, a translation by one lattice constant multiplies the SDW order parameter by a complex phase factor,

$$\bar{\Phi} \rightarrow e^{2ik_{\mathbf{r}} \cdot \mathbf{a}} \bar{\Phi} = e^{2\pi i \nu} \bar{\Phi},$$

where $\nu$ is the filling fraction of the conduction band. For a completely incommensurate case, when $\nu$ is an irrational number, the GL free energy must be SO(2) symmetric with respect to the phase of $\Phi$\textsuperscript{213}. In the absence of pinning terms, the operator $\Lambda_z = Q_+ - Q_-$ generates continuous rotations between the real and imaginary parts of $\bar{\Phi}$, eq. (5.12).

\textsuperscript{1}This is in contrast with rational fillings, such as $\nu = 1/4$, for which translational symmetry allows terms of the form

$$\text{Re} \left( e^{i\theta} (\bar{\Phi})^{4n} \right)$$

for any positive integer $n$ and for an arbitrary fixed phase $\theta$. These terms tend to pin the phase of the SDW order, and they reduce the SO(2) symmetry of translations to the discrete group $Z_4$. Note that SO(4)$_\text{isospin}$ symmetry does not allow pinning terms such as these. This is because the operator $\Lambda_z = Q_+ - Q_-$ generates continuous rotations between the real and imaginary parts of $\bar{\Phi}$, eq. (5.12).
Figure 5.2: Proposed phase diagram for weak inter-chain coupling $t_b$. When inter-chain coupling is present, $t_b \neq 0$, long range order at finite temperatures becomes possible. In the unitary case, the second order quantum critical point of a Luttinger liquid becomes a first order transition between AF and unitary TSC. As $t_b$ grows, the AF phase shrinks due to reduced nesting of the Fermi surface. Throughout we assume positive backscattering $g_1 > 0$.

The most general GL free energy with SO(3)$_{\text{spin}}$×SO(2)$_{\text{charge}}$×SO(2)$_{\text{translation}}$ is

$$F = \frac{1}{2} |\nabla \Psi|^2 + \frac{1}{2} |\nabla \Phi|^2 + \frac{r_1}{2} |\Psi|^2 + \frac{r_2}{2} |\Phi|^2 + u_1 (|\Psi|^2)^2 + u_2 (|\Phi|^2)^2$$

$$+ u_3 |\Psi|^2 |\Phi|^2 + u_4 |\Psi|^2 |\Phi|^2 + 2v_1 |\Psi|^2 |\Phi|^2 + 2v_2 |\Psi|^2 |\Phi|^2 + 2v_3 |\Psi|^2 |\Phi|^2$$

Near the phase boundary between SDW and TSC phases, for quasi one dimensional systems the form of the free energy is strongly constrained by the SO(3)$_{\text{spin}}$×SO(4)$_{\text{isospin}}$ symmetry. We expect the properties of the system to be well described by the free energy,

$$F = \frac{1}{2} \sum_{\alpha} \nabla P_{\alpha} \cdot \nabla P_{\alpha} + \frac{\bar{r}}{2} \sum_{\alpha} P_{\alpha} P_{\alpha} + \frac{\delta r}{2} \sum_{\alpha} (P_{1\alpha}^2 + P_{2\alpha}^2 - P_{3\alpha}^2 - P_{4\alpha}^2)$$

$$+ \bar{u}_1 \sum_{\alpha\beta} P_{\alpha\beta} P_{\beta\alpha} + \bar{u}_2 \sum_{\alpha\beta} P_{\alpha\beta} P_{\beta\alpha} P_{\alpha\beta} P_{\beta\alpha}.$$

This is the most general free energy with SO(3)$_{\text{spin}}$×SO(4)$_{\text{isospin}}$ symmetric quartic coefficients, where we have used the order parameter defined in equation (5.10) to display this invariance explicitly. We follow the common assumption that changing the external control parameters of the system only affects the quadratic coefficients.
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Figure 5.3: Mean-field phase diagram of (5.22) and (5.29) for $\tilde{u}_2 < 0$. At half filling, SDW order reduces to AF order.

Thus, these are allowed to break the symmetry and tune the phase transition. For $\delta r \neq 0$, the symmetry is broken down to $\text{SO}(3)_{\text{spin}} \times \text{SO}(2)_{\text{charge}} \times \text{SO}(2)_{\text{translation}}$.

There is an explicit duality between antiferromagnetism and triplet superconductivity under reversal of the sign of $\delta r$ in (5.22). The mean field phase diagram of (5.22) depends crucially on the sign of $\tilde{u}_2$. For negative $\tilde{u}_2$, there is a tendency for all vector order parameters to point along a common axis. The order parameters in this case can be described by a single real vector times a complex phase, $\vec{\Psi} = e^{i\varphi} \vec{n}$ and $\vec{\Phi} = e^{i\theta} \vec{n}$. This is referred to in the $^3\text{He}$ literature as unitary triplet superconductivity[115], and in magnetism as collinear spin density order[213]. On the other hand, for positive $\tilde{u}_2$, all vector order parameters tend to be mutually orthogonal. The real and imaginary parts of the order parameters can no longer be set to be parallel, $\text{Re}\vec{\Psi} \times \text{Im}\vec{\Psi} \neq 0$ and $\text{Re}\vec{\Phi} \times \text{Im}\vec{\Phi} \neq 0$. This is the non-unitary/non-collinear case. The mean-field phase diagrams for (5.22) for $\tilde{u}_2$ negative and positive are shown in Figs. 5.3 and 5.4.

In principle, the parameters of the GL free energy (5.21) can be obtained from a microscopic Hamiltonian. In Appendix B.2 we consider a quasi one dimensional electron systems with weak interactions and obtain a free energy as in (5.22) with

$$
\tilde{u}_1 = \frac{21\zeta(3)}{16\pi^2 v_f T^2}
$$

$$
\tilde{u}_2 = -\frac{7\zeta(3)}{8\pi^2 v_f T^2}
$$

(5.23)

The quadratic coefficients depend on coupling constants in the TSC and SDW channels, and on temperature. They are typically parameterized in terms of the pressure-
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Figure 5.4: Mean-field phase diagram of (5.22) and (5.29) for $\tilde{u}_2 > 0$. At half filling, SDW order reduces to AF order.

dependent mean-field transition temperature

$$
\begin{align*}
  r_1(T, P) &= \alpha_{TSC}(T - T_C(P)) \\
  r_2(T, P) &= \alpha_{SDW}(T - T_N(P))
\end{align*}
$$

The analysis of Appendix B.2 shows that weakly interacting Fermi liquids favor unitary TSC and collinear SDW order, $\tilde{u}_2 < 0$.

5.3.2 Half-filling

As is well known, the physics of period two antiferromagnetic order is captured by a single real Néel vector. It is interesting to study how this comes about from the point of view of the microscopic Luttinger Hamiltonian. As pointed out in Section 5.2, the Hamiltonian at half-filling includes a new contribution due to umklapp scattering, Eq. (5.14). This gives a correction to the GL free energy, which to linear order in $g_3$ can be written as

$$
\Delta F = h \left( (Re \bar{\Phi})^2 - (Im \bar{\Phi})^2 \right)
$$

where $h = \frac{g_3}{2L}$. The new term pins the SDW, and breaks the $SO(4)_{isospin} = SO(3)_R \times SO(3)_L$ symmetry down to its diagonal subgroup $SO(3)_{isospin}$. In agreement with the Feynman-Hellman theorem, the quartic coefficients derived in Appendix B.2 are not modified to linear order in $g_3$. Therefore, in the linear order in $g_3$, the free energy has $SO(4) = SO(3)_{spin} \times SO(3)_{isospin}$ symmetry. In principle, the higher order contributions
of the umklapp $g_3$ term can break the original SO(4)_{iso} spin symmetry all the way down to SO(2)_{charge}, generated by the total charge $Q$.

The bare value of $g_3$ in (TMTSF)$_2$PF$_6$ is small, since it is proportional to dimerization, which in this compound is very weak[183]. Assuming that Coulomb interactions are of the order of the bandwidth, this leads to a bare value of $g_3$ of about 0.01. Furthermore, it is not the bare value of $g_3$ that enters the GL free energy, but its effective (renormalized) value at the 1d to 3d crossover scale. At high temperatures one-dimensional physics is observed. As temperature is reduced, everywhere on the TSC side of the phase diagram, as well as on the AF/TSC phase boundary, $g_3$ flows to zero. This allows us to approach the critical region from the TSC side, along which the GL free energy is SO(3)_{iso} symmetric. Even on the AF side of the phase diagram, where $g_3$ is relevant, the flow of $g_3$ passes near zero before diverging. Therefore, near the AF/TSC phase boundary, the flow spends a lot of time near zero, and the eventual upturn of $g_3$ may not be reached for realistic systems, in which the 3d coupling may cut off the 1d RG flow at low temperatures. Hence, it is reasonable to take small $g_3$ everywhere near the AF/TSC phase boundary, and to consider a model with SO(3)_{iso} symmetry.

In what follows, we will assume that the umklapp term favors the real part of the SDW, which becomes the Néel order parameter $\vec{N}$,

$$\vec{N} = \text{Re} \vec{\Phi}. \quad (5.26)$$

From now on we assume that $\text{Im} \vec{\Phi}$ is sufficiently well gapped, so that it does not need to be included in the analysis of the competition between AF and TSC. This is justified since the pinning term (5.25) is relevant in the 3d theory, and thus any fixed point of the theory will be characterized by strong pinning.

It is useful to consider the relation between our SO(4) symmetry and the SO(4) symmetry introduced by C.N. Yang for the Hubbard model[205]. The symmetry generators of Yang’s SO(4) is the $\eta$ operator,

$$\eta^\dagger = \sum_k c^\dagger_{k+\pi \uparrow} c^\dagger_{-k \downarrow}. \quad (5.27)$$

$k$ summation goes over the entire Brillouin zone. This operator should be compared to our $\Theta$ operators defined in eq. (5.6) for incommensurate filling, and eq. (5.16) for half-filling. Away from half filling, the difference between the two operators is obvious. $\Theta$ has momentum equal to the nesting wave vector $2k_f$, in contrast to $\eta$, which always has center of mass momentum $\pi$. This allows us to have SO(4) symmetry for any electron density, in contrast to Yang’s SO(4), which only applies at half-filling. At half-filling, however, $2k_f = \pi$, and the only difference is the relative sign between the left and right moving contributions. This difference is substantial. The Néel order parameter transforms as a singlet under the action of $\eta$,

$$[\eta, \vec{N}] = 0. \quad (5.28)$$
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This should be contrasted with $\Theta$, which rotates $\vec{N}$ into the TSC order parameter $\vec{\Psi}$, see eq. (5.19). The two SO(4) symmetries thus differ in the order parameters which they unify, and in the microscopic models for which they apply. Yang’s SO(4) applies to the negative $U$ Hubbard model, for which singlet SC and CDW are degenerate lowest energy states at half-filling. Our SO(4) unifies AF and TSC orders, which are not degenerate for the Hubbard model. As we discussed earlier, we expect these to be nearly degenerate phases for half-filled systems with small umklapp (e.g. quarter filled systems with small dimerization, such as (TMTSF)$_2$PF$_6$ and with $K_\rho$ close to one).

In analogy with the incommensurate case, at half-filling we expect that quasi one-dimensional systems near the AF/TSC phase boundary have a Ginzburg-Landau free energy with SO(4)-symmetric quartic coefficients. The symmetry can be made explicit in terms of the matrix order parameter $\hat{Q}$:

\[
F = \frac{1}{2} \sum_{a} \nabla Q_{aa} \nabla Q_{aa} + \frac{r}{2} \sum_{a} Q_{aa} Q_{aa} + \delta r \sum_{a} (Q_{3a}^2 - Q_{1a}^2 - Q_{2a}^2) + \bar{u}_1 \sum_{a \alpha \beta} Q_{aa} Q_{a \beta} Q_{a \beta} + \bar{u}_2 \sum_{a \alpha \beta} Q_{aa} Q_{a \beta} Q_{b \beta}
\]

\[
= \frac{1}{2} |\nabla \vec{\Psi}|^2 + \frac{1}{2} (\nabla \vec{N})^2 + \frac{r_1}{2} |\vec{\Psi}|^2 + \frac{r_2}{2} \vec{N}^2 + (\bar{u}_1 + \bar{u}_2)(|\vec{\Psi}|^2 - |\vec{N}|^2)^2
\]

(5.29)

Changing temperature and some other parameter of the system (e.g. pressure in (TMTSF)$_2$PF$_6$) allows to control $r_1$ and $r_2$. The SO(4) symmetry is recovered on the line $r_1 = r_2$.

Equation (5.29) is a special case of the most general free energy with the SO(3) $\times$ SO(2) symmetry of spin and charge rotations\(^2\),

\[
\tilde{F} = \frac{1}{2} |\nabla \vec{\Psi}|^2 + \frac{1}{2} (\nabla \vec{N})^2 + \frac{r_1}{2} |\vec{\Psi}|^2 + \frac{r_2}{2} \vec{N}^2 + u_1(|\vec{\Psi}|^2)^2 + u_2(|\vec{\Psi}|^2)^2 + u_3|\vec{\Psi}|^2 |\vec{N}|^2 + 2u_2|\vec{\Psi} \cdot \vec{N}|^2
\]

(5.30)

Translational symmetry rules out $\vec{N} \cdot \vec{\Psi}^* \times \vec{\Psi}$ because this term has a non-zero wave vector. Similarly, $|\vec{N} \times \vec{\Psi}|^2$ can be reduced to terms already present in (5.30). When the conditions

\[
r_1 = r_2, \\
u_2 - u_3 = u_1
\]

\(^2\)Triplet pairing in Bechgaard salts does not have orbital degree of freedom. Quasi one-dimensional electron band structure requires $\vec{\Psi}(\vec{p}) \propto p_x$, where $x$ is the direction parallel to the chains. This provides considerable simplification in writing effective models, such as the Ginzburg-Landau free energy (5.30).
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\[ u_2 - 2u_3 = v_1 \]
\[ v_2 = 2u_3 \quad (5.31) \]

are satisfied, we recover SO(4) symmetry. In addition, if we supplement the conditions (5.31) by

\[ v_2 = 0 \quad (5.32) \]

there is an even higher SO(9) symmetry, which allows rotations between any components of vectors \( \vec{N} \), \( Re\tilde{\Psi} \), and \( Im\tilde{\Psi} \)

\[ \bar{F} = \frac{1}{2} |\nabla \tilde{\Psi}|^2 + \frac{1}{2} (\nabla \vec{N})^2 + \frac{r}{2} (|\tilde{\Psi}|^2 + \vec{N}^2) + \bar{u}(|\tilde{\Psi}|^2 + \vec{N}^2)^2 \quad (5.33) \]

At half-filling, there is no distinction between collinear and non-collinear magnetism. However, the sign of \( \tilde{u}_2 \) still determines the nature of the triplet superconductivity, as well as the topology of the mean-field phase diagrams. These are similar to those displayed for incommensurate filling, Figs. 5.3 and 5.4, the only difference being that SDW order is reduced to AF order. The mean-field phase diagrams for (5.29) for \( \tilde{u}_2 \) negative and positive are shown in Fig. 5.3. The analysis of Appendix B.2 can be easily modified to half-filling, and yields an SO(4) symmetric free energy of the form (5.29) with coefficients still given by (5.23). Thus, weakly interacting Fermi liquids favor the case \( \tilde{u}_2 < 0 \). Strong interactions, however, can modify the quartic coefficients (5.29), including a possible change of sign of \( \tilde{u}_2 \). In the subsequent discussion we consider both possibilities. It is useful to note that all experimentally known cases of triplet pairing between fermions, such as \( ^3He \) [115, 4], and \( Sr_2RuO_4 \), correspond to the unitary case. Hence, negative \( \tilde{u}_2 \) appears more likely.

5.4 Thermal fluctuations

We now consider the free energy (5.30) and address how fluctuations affect the mean-field phase diagram shown in Figs. 5.3 and 5.4. For instance, when the quartic coefficients do not lie exactly on the SO(4) symmetric manifold, we will study whether such symmetry appears as we go to longer length scales and integrate out short wave length fluctuations. The possibility of enhanced static symmetry at the critical point has been discussed previously for several solid state systems. For easy axis AF in a magnetic field, SO(3) symmetry was suggested to appear at the spin flop critical point [56, 101]. For systems with competing singlet superconducting and antiferromagnetic orders Zhang suggested a static SO(5) symmetry as the bicritical point[211, 42]. This SO(5) symmetry has also been used to study the quasi-two dimensional \( \kappa \)-BEDT-TTF salts[138]. Yang and Zhang introduced an SO(4) symmetry for the Hubbard model at half-filling which unifies singlet superconductivity with charge density wave order [204, 210].
To understand the role of fluctuations in models (5.30) and (5.29) we use $4 - \epsilon$ renormalization group (RG) analysis. For subsequent discussion it is useful to extend the spin SO(3) symmetry of the equation (5.30) to a more general SO(N) symmetry. This is achieved by considering vectors $\vec{N}$ and $\vec{\Psi}$ as $N$-component vectors. The RG equations can be derived using the standard approach \[26\]

\[
\begin{align*}
\frac{dr_1}{dl} &= 2r_1 + \frac{8K_d}{1 + r_1} \{(N + 1)u_1 + 3u_3\} + \frac{4K_d}{1 + r_2} \{Nv_1 + 2v_2\} \\
\frac{dr_2}{dl} &= 2r_2 + \frac{8K_d}{1 + r_1} \{Nv_1 + 2v_2\} + \frac{4K_d}{1 + r_2} (N + 2)u_2 \\
\frac{du_1}{dl} &= \epsilon u_1 - K_d (8N + 32)u_1^2 + 32u_1u_3 + 32u_3^2 + 4Nv_1^2 + 8v_1v_2 + 2v_2^2 \\
\frac{du_2}{dl} &= \epsilon u_2 - K_d \{4(N + 8)u_2^2 + 8Nv_1^2 + 16v_1v_2 + 8v_2^2\} \\
\frac{du_3}{dl} &= \epsilon u_3 - K_d \{8Nu_3^2 + 48u_1u_3 + 2v_2^2\} \\
\frac{dv_1}{dl} &= \epsilon v_1 - K_d \{(8N + 8)u_1v_1 + (4N + 8)u_2v_2 + 16u_3v_1 + 16u_1v_2 + 8v_1v_2 + 4v_2u_2 + 4v_2^2\} \\
\frac{dv_2}{dl} &= \epsilon v_2 - K_d \{8u_1v_2 + 8u_2v_2 + 16u_3v_2 + 32v_1v_2 + (4N + 8)v_2^2\} \\
\end{align*}
\] (5.34)

Here $dl = d\Lambda/\Lambda$, where $\Lambda$ is a momentum cut-off, and $K_d = \ldots$ is a surface of a unit sphere in $d = 4 - \epsilon$ dimension.

For the physically relevant $N = 3$ equations (5.34) have only two fixed points. One is a trivial Gaussian fixed point

\[ r_{\{1,2\}} = u_{\{1,2,3\}} = v_{\{1,2\}} = 0 \] (5.35)

and the other is an SO(9) Heisenberg point

\[
\begin{align*}
r_{\{1,2\}} &= -\frac{(3N + 2)\epsilon}{6N + 16} \\
u_1 &= u_2 = v_1 = \frac{\epsilon}{(6N + 16)K_d} \\
u_3 &= v_2 = 0 \\
\end{align*}
\] (5.36)

The Gaussian fixed point is completely unstable. The SO(9) Heisenberg point has five unstable directions (for general $N$, the Heisenberg point has $SO(3N)$ symmetry, but it remains unstable in five directions for all $N > 1$). The critical point should have only two unstable directions: $r_{\{1,2\}}$ should flow away from the critical point, but all the interaction coefficient should flow toward the fixed point. So, neither the Gaussian nor the SO(9) Heisenberg fixed points are good candidates for the critical point. In Fig. 5.5 we show RG flows in the SO(4) symmetric plane. We find two types of run-away flows. When we start with $\tilde{u}_2$ positive, it continues increasing. For $\tilde{u}_2$
negative, the RG flow make it even more negative. In both cases $\tilde{u}_1$ flows to negative values.

In many cases absence of a fixed point in the RG flows implies that we do not have a multicritical point in the phase diagram, but instead fluctuations induce a first order phase transition. Below we discuss consequences of the run-away flows in equations (5.34). We point out that two types of the run-away flows in the SO(4) symmetric manifold shown in Fig. 5.5 correspond to unitary ($\tilde{u}_2 < 0$) and non-unitary ($\tilde{u}_2 > 0$) TSC. These two cases are considered separately.

### 5.5 Finite temperature analysis: Unitary case

We consider model (5.29) with $N$-component vectors and with negative $\tilde{u}_2$. In the $4 - \epsilon$ expansion there are run-away flows even for large $N$. Thus, we do not find a fixed point that could give a critical point. To understand the phase diagram in this case we employ large $N$ calculations in $d = 3$. In the large $N$ expansion, all bubble diagrams are summed self-consistently\[215, 85\]. The large $N$ approach for unitary triplet superconductors without coupling to magnetic order has been discussed previously in [8] in the context of $^3$He.

Let us start by analyzing the superconducting phase. In the mean-field approximation the order parameter factorizes as $\tilde{\Psi} = e^{i\theta} \tilde{u}$. Hence, we take the average value of the order parameter in the ordered phase to be $\tilde{\Psi}_0 = (0, ..., 0, \sigma)$ and
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separate the longitudinal and transverse components of the fluctuating part \( \delta \tilde{\Psi} = (\tilde{A}_T + i \tilde{B}_T, A_L + i B_L) \). For the Néel order parameter we also separate \( \tilde{N} = (\tilde{N}_T, \tilde{N}_L) \). Effective masses for \( \tilde{A}_T, \tilde{B}_T, \) and \( \tilde{N}_T \) are given by

\[
\begin{align*}
  r_A &= r_1 + 4(\tilde{u}_1 + \tilde{u}_2)\sigma^2 + 4(\tilde{u}_1 + \tilde{u}_2)N \int_0^\Lambda \frac{d^3k}{(2\pi)^3} \frac{1}{k^2 + r_A} \\
  &+ 4\tilde{u}_1N \int_0^\Lambda \frac{d^3k}{(2\pi)^3} \left( \frac{1}{k^2 + r_B} + \frac{1}{k^2 + r_N} \right) \\
  r_B &= r_1 + 4\tilde{u}_1\sigma^2 + 4(\tilde{u}_1 + \tilde{u}_2)N \int_0^\Lambda \frac{d^3k}{(2\pi)^3} \frac{1}{k^2 + r_B} \\
  &+ 4\tilde{u}_1N \int_0^\Lambda \frac{d^3k}{(2\pi)^3} \left( \frac{1}{k^2 + r_A} + \frac{1}{k^2 + r_N} \right) \\
  r_N &= r_2 + 4\tilde{u}_1\sigma^2 + 4(\tilde{u}_1 + \tilde{u}_2)N \int_0^\Lambda \frac{d^3k}{(2\pi)^3} \frac{1}{k^2 + r_N} \\
  &+ 4\tilde{u}_1N \int_0^\Lambda \frac{d^3k}{(2\pi)^3} \left( \frac{1}{k^2 + r_A} + \frac{1}{k^2 + r_B} \right)
\end{align*}
\]

(5.37)

where \( \Lambda \) is the ultraviolet (short distance) cut-off of the free energy in equation (5.29). In writing equations (5.37) we used that in the large \( N \) limit, \( \tilde{u}_{1,2} \sim 1/N, \sigma \sim \sqrt{N} \), and we neglected terms of the order of \( 1/N \), including contributions from longitudinal fluctuations. A requirement of the cancellation of tadpole diagrams for \( A_L \) gives the condition \( r_A = 0 \), as one would expect from the Goldstone theorem. It is convenient to define parameter \( r_c \) from the condition

\[
0 = r_c + (12\tilde{u}_1 + 4\tilde{u}_2)N \int_0^\Lambda \frac{d^3k}{(2\pi)^3} \frac{1}{k^2}
\]

(5.38)

If we measure \( r \)'s with respect to \( r_c \)

\[
\begin{align*}
  t_\psi &= r_1 - r_c \\
  t_N &= r_2 - r_c
\end{align*}
\]

(5.39)

we can absorb all the cut-off dependence of equations (5.37) into definitions of \( t_\psi \) and \( t_N \)

\[
\begin{align*}
  0 &= t_\psi + 4(\tilde{u}_1 + \tilde{u}_2)\sigma^2 + 4\tilde{u}_1N \int \frac{d^3k}{(2\pi)^3} \left( \frac{1}{k^2} - \frac{1}{k^2 + r_B} \right) \\
  r_B &= t_\psi + 4\tilde{u}_1\sigma^2 + 4(\tilde{u}_1 + \tilde{u}_2)N \int \left( \frac{1}{k^2} - \frac{1}{k^2 + r_B} \right) \\
  &+ 4\tilde{u}_1N \int \frac{d^3k}{(2\pi)^3} \left( \frac{1}{k^2} - \frac{1}{k^2 + r_N} \right)
\end{align*}
\]
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Figure 5.6: Phase diagram of (5.29) with $\tilde{u}_2 < 0$ in three dimensions in the large $N$ limit including fluctuations. Parameters are $\tilde{u}_1 = 1/N \tilde{u}_2 = -1/2N$.

\[
\begin{align*}
r_N &= t_N + 4\tilde{u}_1\sigma^2 + 4\tilde{u}_1N \int \frac{d^3k}{(2\pi)^3} \left( \frac{1}{k^2} - \frac{1}{k^2 + r_B} \right) \\
&\quad + 4(\tilde{u}_1 + \tilde{u}_2)N \int \left( \frac{1}{k^2} - \frac{1}{k^2 + r_N} \right)
\end{align*}
\]

(5.40)

Integrals are now convergent for large $k$, so upper limits of integration can be extended to infinity. Solutions to equations (5.40) correspond to extremal points of free energy as a function of $\sigma$. When both $t_\psi$ and $t_N$ are large, there are no solutions to equations (5.40). This is a disordered phase. Once we decrease $t_\psi$ sufficiently, a single solution appears at $t_\psi,M$ and splits into two for $t_\psi < t_\psi,M$. This describes the appearance of the TSC phase as a locally stable state. The point $t_\psi,M$, where two solutions merge into one and disappear, correspond to the boundary of the local stability region of the TSC phase. As $t_\psi$ is lowered further, at a temperature $t_\psi,L$ one of the solutions approaches $\sigma = 0$ and then disappears. This is a spinodal point below which a disordered phase is unstable to developing TSC order parameter. The actual first order phase transition occurs somewhere between $t_\psi,M$ and $t_\psi,L$.

Fig. 5.6 shows a phase diagram constructed from the arguments presented above, for both TSC and AF phases. We note that the mixed phase with simultaneous TSC and AF orders is only possible on the $t_\psi = t_N$ line. Thus, the first order phase transition between two types of ordered phases remains even when we include fluctuations. The most interesting feature of this phase diagram is that the transition between the disordered and the antiferromagnetic phases becomes first order in the vicinity of the critical point.
5.6 Finite temperature analysis: non-unitary case

Mean-field calculations for the free energy (5.29) with $\tilde{u}_2 > 0$ demonstrated that the TSC phase is non-unitary and there is a mixed phase with both TSC and AF order (see Section 5.3 and figure 5.4). Within mean field theory, the mixed phase terminates at a tetracritical point with $SO(4) = SO(3) \times SO(3)$ symmetry. The goal of this section is to examine how the tetracritical point is affected by thermal fluctuations.

To this end we extend the $SO(3)$ spin symmetry to $SO(N)$ and approach the problem with three different methods: A large $N$ analysis, a renormalization group calculation in $d = 4 - \epsilon$ and in one in $d = 2 + \epsilon$. The physical picture that emerges from all of these approaches is that a $SO(3) \times SO(N)$ critical point exists for sufficiently large $N$, but probably does not survive down to the physical $N = 3$. We argue that in this case the tetracritical point is stretched to a line of direct first order transition from the normal state to the mixed phase.

5.6.1 Large $N$ phase diagram in three dimensions

We consider the model (5.29) in three dimensions for large $N$ and with $\tilde{u}_2 > 0$. We note that the quartic terms give a free energy that is bounded from below for $\tilde{u}_1 + \tilde{u}_2/3 > 0$. Thus, in this section we will always assume that this condition is satisfied. In appendix B.3 we also discuss that when $\tilde{u}_1 + \tilde{u}_2/3$ becomes small, of the order of $1/N^2$ (in the large $N$ limit both $\tilde{u}$s are of the order of $1/N$), the phase diagram may change qualitatively.

In the mixed phase the TSC and AF both have non-zero expectation values and are orthogonal to each other. Hence, in the ordered phase we can choose

$$\langle \tilde{\Psi} \rangle = (0, \ldots, 0, \sigma_\psi, i\sigma_\psi, 0)$$
$$\langle \tilde{N} \rangle = (0, \ldots, 0, 0, 0, \sigma_N) \quad (5.41)$$

Following the discussion in Section 5.5 we introduce longitudinal and transverse fluctuations for all order parameters. It is easy to verify that the requirement of cancellation of tadpole diagrams for longitudinal components implies zero effective masses for the transverse components. Shifting $r_1$ and $r_2$ as in equation (5.39) we obtain self-consistency conditions for expectation values of the order parameters

$$t_\psi + (12\tilde{u}_1 + 4\tilde{u}_2)\sigma_N^2 + 4\tilde{u}_1\sigma_N^2 = 0$$
$$t_\psi + (4\tilde{u}_1 + 4\tilde{u}_2)\sigma_N^2 + 8\tilde{u}_1\sigma_N^2 = 0 \quad (5.42)$$

These equations can be easily solved and we obtain a phase diagram shown in figure 5.7. We observe that in this case the only effect of fluctuations is to shift the tetracritical point from $r_1 = r_2 = 0$ to $r_1 = r_2 = r_c$. 
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5.6.2 Renormalization Group analysis in $d = 4 - \epsilon$. $SO(3) \times SO(N)$ fixed point

As shown in Fig. 5.5 for $N = 3$, all fixed points with symmetry $SO(4) \sim SO(3) \times SO(3)$ are unstable within a $4 - \epsilon$ expansion. In contrast, as $N$ is increased a fixed point with $SO(3) \times SO(N)$ symmetry appears that is fully stable with respect to changes in the quartic interaction parameters, including those perturbations that destroy $SO(3) \times SO(N)$ symmetry. Such fixed point exists for $N \geq 33$ and has

$$v_1 = -\frac{3\epsilon}{2K_d} h(N)$$

$$v_2 = \frac{\epsilon}{4K_d} \frac{1 - 72h(N)}{N + 7}$$

$$r_1 = r_2 = -2K_d \{(3N + 2)v_1 + (N + 6)v_2\}$$

(5.43)

where $u_1$, $u_2$ and $u_3$ are related to $v_1$ and $v_2$ by the constraints (5.31), and the function $h(N) = \left( N^2 + 8N - 65 + (N + 7)\sqrt{N^2 - 34N + 49} \right)^{-1} \sim 1/2N^2 + O(1/N^3)$ is real only for $N > 32$.

The two quadratic parameters $r_1$ and $r_2$ are relevant, tuning the transition on a two dimensional phase diagram. The RG flow equations (5.34), linearized about the fixed point (5.43), yield two principal directions, $(\delta r_1, \delta r_2) \propto (1, 1)$ associated with the thermal exponent $\lambda_t$, and $(\delta r_1, \delta r_2) \propto (-1, 2)$ associated with the anisotropy...
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exponent $\lambda_g$. From these we find the critical exponents,

$$\frac{1}{\nu} = \lambda_t = 2 - \epsilon \left( 1 - \frac{10}{N} + \frac{28}{N^2} \right) + O\left( \frac{\epsilon}{N^3} \right),$$

$$\phi = \lambda_g \nu = 1 - \epsilon \left( \frac{3}{2N} + \frac{51}{2N^2} \right) + O\left( \frac{\epsilon}{N^3} \right).$$

(5.44)

Note that the crossover exponent $\phi$ for the anisotropy is always less than one. This implies [26] that the phase boundaries meet as straight lines at the critical point, and we find the same topology of the phase diagram as shown in Fig. 5.7.

5.6.3 Renormalization Group analysis in $d = 2+\epsilon$. SO(3)×SO(N) fixed point

The runaway flows in the equations (5.34) mean that the system goes to strong coupling. In this limit the magnitudes of the vectors $Re\vec{\psi}$, $Im\vec{\psi}$, and $\vec{N}$ have already developed locally but the directions can still fluctuate on long length scales. For $N = 3$ one of the runaway directions of equations (5.34) corresponds to $u_3$, $v_2 > 0$ and $u_1, v_1 < 0$. The corresponding strong coupling limit can be described by a triad of vectors that are all mutually orthogonal.

$$F = -\sum_{(xy)} \left\{ K_1 \vec{e}_1(x) \cdot \vec{e}_1(y) + K_2 (\vec{e}_2(x) \cdot \vec{e}_2(y) + \vec{e}_3(x) \cdot \vec{e}_3(y)) \right\}$$

(5.45)

Here $\vec{e}_1$, $\vec{e}_2$, and $\vec{e}_3$ correspond to $\vec{N}$, $Re\vec{\Psi}$, and $Im\vec{\Psi}$ respectively. The free energy (5.45) has an explicit SO(2) charge symmetry of rotations between $\vec{e}_2$ and $\vec{e}_3$. The continuum version of this model is given by

$$F = \int d^d x \left\{ \frac{1}{2g_1} (\nabla \vec{e}_1)^2 + \frac{1}{2g_2} (\nabla \vec{e}_2)^2 + (\nabla \vec{e}_3)^2 \right\}$$

(5.46)

Here $g_i \propto K_i^{-1}$ and the constraints $\vec{e}_i \cdot \vec{e}_j = \delta_{ij}$ are implied.

Let us now discuss the phase diagram of (5.45) and (5.46). For $K_{1,2} \to 0$ we have a fully disordered phase. For $K_{1,2} \to \infty$ we have a fully ordered phase that is a mixture of TSC and AF. When $K_2 = \infty$ the vectors $\vec{e}_1$ and $\vec{e}_2$ are ordered and there is an Ising type transition between TSC and TSC+AF phases. For $K_1 = \infty$ vector $\vec{N}$ is ordered and there is an O(2) transition between the AF and TSC+AF states. For $K_2 = 0$ there is a Heisenberg transition between the disordered and the AF phases. For $K_3 = 0$ there is a transition between the fully disordered and the TSC phases. What happens in the interior of the phase diagram, however, is not clear.

When we apply the $d - 2 = \epsilon$ RG analysis to the model (5.46) [58, 7, 90, 38, 93] we obtain the flow equations

$$\frac{dg_1}{dl} = -\epsilon g_1 + \frac{g_1^2 (g_2^2 + g_1 g_2 - g_1^2)}{2\pi (g_1 + g_2)^2}$$

$$\frac{dg_2}{dl} = -\epsilon g_2 + \frac{g_2^2 (g_1^2 + g_1 g_2 - g_2^2)}{2\pi (g_1 + g_2)^2}$$

$$\frac{dg_3}{dl} = -\epsilon g_3 + \frac{g_3^2 (g_1^2 + g_2^2 - g_3^2)}{2\pi (g_1 + g_2)^2}$$
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Figure 5.8: Renormalization group flow of non-linear model eq. (5.46), corresponding to equations (5.47).

\[
\frac{dg_2}{dl} = -\epsilon g_2 + \frac{g_1^2 g_2^2}{2\pi (g_1 + g_2)^2} \quad (5.47)
\]

The flow diagram is shown in fig. 5.8. We can see that it lacks the Ising and O(2) phase transitions. This is not surprising, since the \(d - 2 = \epsilon\) analysis works well only for the spin-wave excitations of order parameters with \(N \geq 3\).

To shed some light on the phase diagram of (5.45) and (5.46) we consider the large \(N\) generalization of this model. We assume that all vectors \(\vec{e}_i\) have \(N\) components

\[
F = \int d^d x \left\{ \frac{1}{2g_1} (\nabla \vec{e}_1)^2 + \frac{1}{2g_2} ((\nabla \vec{e}_2)^2 + (\nabla \vec{e}_3)^2) + \frac{1}{g_3} ((\vec{e}_1 \cdot \nabla \vec{e}_2)^2 + (\vec{e}_1 \cdot \nabla \vec{e}_3)^2) + \frac{1}{g_4} (\vec{e}_2 \cdot \nabla \vec{e}_3)^2 \right\} \quad (5.48)
\]

The last two terms in equation (5.48) are generated in the RG flow, even if they are absent in the microscopic model (such terms are linearly independent of the first two only for \(N > 3\)). The symmetry breaking pattern of the non-linear model (5.48) is

\[
O(N) \times O(2)/O(N-3) \times O(2)_{\text{diag}}. \quad (5.49)
\]

In order to express the RG equations in a simple form we introduce the variables \(\eta_i\),

\[
\eta_1 = \frac{1}{g_1}, \\
\eta_2 = \frac{1}{g_2},
\]
These variables arise naturally in a matrix formulation of the non-linear model Eq. (5.48), see Appendix B.4, where the RG calculation is outlined. To one loop order we find the RG flow

\[
\begin{align*}
\frac{d\eta_1}{dl} &= \epsilon \eta_1 - \frac{1}{2\pi} \left(N - 2 + \frac{\eta_1^2 - \eta_2^2 - \eta_3^2}{2\eta_1 \eta_3}\right) \\
\frac{d\eta_2}{dl} &= \epsilon \eta_2 - \frac{1}{2\pi} \left(N - 2 + \frac{\eta_2^2 - \eta_3^2 - \eta_4^2}{2\eta_2 \eta_3} - \frac{\eta_4}{2\eta_2}\right) \\
\frac{d\eta_3}{dl} &= \epsilon \eta_3 - \frac{1}{2\pi} \left(N - 2 + \frac{N - 3 \eta_3^2 - \eta_1^2 - \eta_2^2}{2\eta_1 \eta_2} - \frac{\eta_2}{2\eta_3}\right) \\
\frac{d\eta_4}{dl} &= \epsilon \eta_4 - \frac{1}{2\pi} \left(\frac{N - 3 \eta_4^2}{2\eta_2} + \frac{\eta_2^2}{2\eta_3}\right)
\end{align*}
\] (5.51)

The conditions \( g_1 = g_2 \) and \( g_3 = g_4 \) define a two dimensional subspace over which the free energy (5.48) has the enhanced symmetry \( SO(3) \times SO(N) \). For arbitrary \( N \), the RG equations (5.51) have an \( SO(3) \times SO(N) \) fixed point

\[
\begin{align*}
\eta_1 &= \eta_2 = (N - 2 - x)/\epsilon, \\
\eta_3 &= \eta_4 = x \eta_1,
\end{align*}
\] (5.52)

where \( x = (N - 2 + \sqrt{N^2 - 5N + 5})/(N - 1) \). Independent of \( N \), this point has one stable direction and one unstable direction within the symmetric plane. The flow in directions perpendicular to the symmetric plane depends on the value of \( N \). The case \( N = 4 \) is special and is discussed in Appendix B.4. For all other \( N \geq 5 \), the RG flow away from the \( SO(3) \times SO(N) \) plane has one stable and one unstable direction. Two relevant parameters are therefore necessary to tune the transition, just as we found in the \( d = 4 - \epsilon \) analysis for large \( N \), eq. (5.43). Computing the critical exponents \( \nu \) and \( \phi \), just as we did in the case \( d = 4 - \epsilon \), eq. (5.44), we find,

\[
\begin{align*}
1/\nu &= \epsilon, \\
\phi &= 1 - \frac{63}{16N^2} - O\left(\frac{1}{N^3}\right).
\end{align*}
\] (5.53)

Just as before, we find that for all finite \( N \), \( \phi \) is less than one, leading to a phase diagram that is topologically equivalent to that found in large \( N \) expansion and in \( 4 - \epsilon \) RG analysis (see Fig. 5.7). What’s more, to leading order in \( 1/N \), expansions about the upper and lower critical dimension, eqs. (5.44) and (5.53), lead to the same
critical exponents,

\[ \frac{1}{\nu} = d - 2 + O\left(\frac{1}{N}\right) \]
\[ \phi = 1 - O\left(\frac{1}{N}\right) \]

This supports the fact that for large \( N \) the \( SO(3) \times SO(N) \) fixed point changes adiabatically with dimension.

5.6.4 Phase Diagram for \( N = 3 \) in three dimensions

We employed three approaches to study classical fluctuations in systems with competing AF and non-unitary TSC: large \( N \) expansion, \( d = 4 - \epsilon \) and \( d = 2 + \epsilon \) RG analyses. When \( N \) is large all three consistently predict a tetracritical point with enhanced \( SO(3) \times SO(N) \) symmetry. In the physically relevant case \( N = 3 \) and \( d = 3 \) the situation is less clear. For example, expansion from the upper critical dimension \( (d = 4 - \epsilon) \) shows that such fixed point appears only for \( N \geq 33 \). Expansion from the lower critical dimension \( (d = 2 + \epsilon) \) gives an \( SO(3) \times SO(N) \) fixed point in the RG flow for any \( N \geq 3 \), but these fixed points become tetracritical points on the phase diagram only for \( N \geq 5 \). It is possible that in three dimensions even for \( N = 3 \) there is a tetracritical \( SO(3) \times SO(3) \) point. The reason why perturbative expansions in dimension fail to see it, is that they work well for small \( \epsilon \) and extrapolations to \( d = 3 \) should be treated with caution\[93\]. Such scenario, however, would contradict the results of classical Monte Carlo simulations in Ref. \[47\], in which the model (5.45) has been analyzed for \( K_1 = K_2 \). In that paper the bimodal distribution in the energy histogram has been interpreted as a signature of the first order transition.

The phase diagram that we propose for the model (5.45) and for systems with competing AF and non-unitary TSC in general is shown in Fig. 5.9. Thermal fluctuations turn a tetracritical point into a line of direct first order transitions between a disordered and a mixed TSC/AF phase. We expect, however, that the width of such first order line is small and the transition is very weakly first order. We conjecture that when approaching the transition between the normal and the AF/TSC mixed phase, susceptibilities for the AF and TSC order parameters start increasing as if dominated by the \( SO(3) \times SO(3) \) tetracritical point. Only very close to the transition line the divergencies are cut-off due to the transition being first order.

Finally, we note that eq. (5.45) with \( K_1 = 0 \) is among a class of closely related models that have been studied extensively in the context of frustrated magnetism\[41, 91, 103, 92, 123, 16, 118, 146, 119, 117, 79\]. Numerical studies of these models in \( d = 3 \) dimensions yield non-universal critical properties at the boundary of normal and TSC phases\[91, 103, 92, 123, 16, 118, 146, 119, 117\], and even evidence of a first order transition\[79\]. The non-perturbative theoretical analysis of Ref. \[184\] supports the latter scenario, claiming that the critical point observed in non-linear
Figure 5.9: Phase diagram for systems with competing AF and non-unitary TSC orders described by the model (5.45) in three dimensions. The tetracritical point in the mean-field phase diagram of the GL free energy in equation (5.29) (see Fig. 5.4) is replaced by a line of direct first order transitions between a disordered and a mixed TSC/AF phase.

Sigma models in $d = 2 + \epsilon$ disappears at $d_c = 2.87$ in one such model, being replaced by a weakly first order transition above $d_c$. The exact nature of the transition seems to be very strongly model-dependent near $d = 3$, and we leave open the possibility that the transition between non-unitary TSC and normal phases is weakly first order.

5.7 Quantum SO(4) symmetry

The microscopic system that motivated our discussion is an assembly of Luttinger liquids weakly coupled in three dimensions. It is useful to condense this system to a simpler effective quantum model that concentrates on the low energy collective degrees of freedom, such as AF and TSC order parameters and rotations between them (such a description only applies in the vicinity of the AF/TSC phase boundary shown in Fig.1). Effective quantum models have been discussed previously for spin systems (see Ref [162] for a review), and systems with singlet superconductivity competing either with charge density wave order [204, 205, 210, 46] or with antiferromagnetism [211, 212, 125, 2, 163].

A simple form for such an effective model is an SO(4) quantum rotor model

$$\mathcal{H}_r = \frac{1}{2\chi_1} \sum_i \mathbf{S}_i^2 + \frac{1}{2\chi_2} \sum_i \mathbf{I}_i^2 - J \sum_{\langle ij \rangle} Q_{ia} Q_{ja}$$
The model is obtained by coarse-graining the original lattice so that, for a half-filled system, each site of the rotor model includes two (or a larger even number, as necessary to include an integer number of spin-triplet Cooper pairs) adjacent sites along the intrachain direction of the original lattice. By combining the electronic operators that make up each rotor model site, one can build three local spin and three local isospin operators $\vec{S}_i$ and $\vec{I}_i$, and an SO(4) tensor order parameter $Q_{i,a\alpha}$. Following a procedure similar to Ref. [2], one can show that the low energy properties of the system are given by the rotor commutation relations,

$$\begin{align*}
[S_{i,\alpha}, S_{j,\beta}] &= i\delta_{ij}\epsilon_{\alpha\beta\gamma} S_{i,\gamma} \\
[I_{i,a}, I_{j,b}] &= i\delta_{ij}\epsilon_{abc} I_{i,c} \\
[S_{i,\alpha}, Q_{j,a\beta}] &= i\delta_{ij}\epsilon_{\alpha\beta\gamma} Q_{j,a\gamma} \\
[I_{i,a}, Q_{j,b\alpha}] &= i\delta_{ij}\epsilon_{abc} Q_{j,c\alpha} \\
[Q_{i,a\alpha}, Q_{j,b\beta}] &= 0
\end{align*}$$

These relations are analogous to equations (5.4), (5.7), and (5.19). In equation (5.55) the unit length constraint of the rigid rotor models is replaced by the interaction terms $\tilde{u}_1$ and $\tilde{u}_2$. For $\delta r$ negative the system favors the AF state and for $\delta r$ positive the TSC state is preferred. When $\delta r = 0$ all generators of SO(4) ($\vec{I} = \sum_i \vec{I}_i$ and $\vec{S} = \sum_i \vec{S}_i$) commute with the Hamiltonian (5.55) and the system is exactly SO(4) symmetric.

We can use equation (5.55) to discuss excitation spectra in various phases of the system. We choose to orient the AF order parameter ($Q_{zz}$) in the $z$ direction so that $\langle Q_{zz} \rangle = N$. Similarly we take $\langle Q_{xx} \rangle = \psi$ to describe unitary TSC, and $\langle Q_{xx} \rangle = \langle Q_{yy} \rangle = \psi$. For non-unitary TSC. With these choices we can linearize the equations of motion for the fluctuations to obtain:

$$\begin{align*}
\frac{dQ_{j,b\beta}}{dt} &= -\frac{1}{\chi_1} \sum_{\alpha} S_{j,a\alpha} \epsilon_{\alpha\beta\gamma} b \langle Q_{bb} \rangle - \frac{1}{\chi_2} \sum_{\alpha} I_{j,a\alpha} \epsilon_{\alpha\beta\gamma} \langle Q_{\beta\beta} \rangle \\
\frac{dS_{j,a\alpha}}{dt} &= J \sum_{\beta'\beta''} \epsilon_{\alpha\beta'\beta''} \langle Q_{\beta'\beta''} \rangle \sum_{\delta} (Q_{j,\beta'\beta''+\delta} - Q_{j,\beta'\beta''-\delta}) \\
\frac{dI_{j,a\alpha}}{dt} &= J \sum_{\beta'\beta''} \epsilon_{\alpha\beta'\beta''} \langle Q_{\beta'\beta''} \rangle \sum_{\delta} (Q_{j,\beta'\beta''} - Q_{j,\beta'\beta''+\delta}) \\
&\quad + 4\delta r (\epsilon_{az\beta'} \langle Q_{a\beta',z} \rangle Q_{j,z\beta'} + \epsilon_{az\beta'} Q_{j,z\beta'} \langle Q_{a\beta',z} \rangle).
\end{align*}$$

The above equations define a linear eigenvalue problem for the frequencies of the
collective modes and for the second quantized operators

$$b^\dagger(k) = \sum_{\gamma \neq \gamma} A^1_{\gamma\gamma} Q_{\gamma\gamma}(k) + \sum_a A^2_a S_a(k) + \sum_a A^3_a I_a(k), \quad (5.60)$$

which obey $b^\dagger(k) = i[H, b^\dagger(k)] = i\omega_k b^\dagger(k)$. The Fourier transforms of lattice operators are defined by $\hat{O}(k) = N^{-1/2} \sum_j \hat{O}_j e^{ik \cdot \delta x_j}$. In the effective model, neutrons couple to the spin order parameter $Q_{za}$, so that the low energy scattering intensity of polarized neutrons is given by:

$$\chi''_a(k + 2k_f, \omega) = \sum_n |\langle n|Q_{za}(k)|0\rangle|^2 \delta(\omega - \omega_n) \quad (5.61)$$

The momentum is shifted by $2k_f$ because a uniform $Q_{za}$ in (5.55) corresponds to a SDW order of momentum $2k_f$ in the microscopic model. The weight associated with a particular collective mode created by $b^\dagger(k)$ is

$$|\langle 0|b(k)Q_{za}(k)|0\rangle|^2 \delta(\omega - \omega_k) = |\langle 0|b(k), Q_{za}(k)|0\rangle|^2 \delta(\omega - \omega_k) \quad (5.62)$$

However, in the following, we focus on neutron scattering near $2k_f$.

The nature of collective excitations in the various phases is summarized in Figs. 5.10, 5.12 and Table 5.1. We now provide a detailed analysis of the collective modes and the associated neutron scattering intensity in each phase. A complementary calculation of the neutron scattering intensity of the $\Theta$-excitations in the unitary TSC, based on the microscopic model, is given in Ref. [149].

### 5.7.1 Antiferromagnet

In the AF phase $\langle Q_{zz} \rangle = N$ and all other order parameters vanish. Then Eqs. (5.57-5.59) decouple to four independent collective modes. The equations of motion for the pairs $\{Q_{zx}, S_y\}$ and $\{Q_{zy}, S_x\}$ yield the usual AF spin waves with linear dispersion reflecting broken SO(3) spin symmetry:

$$\omega_{AF,S}(k + 2k_f) = N \sqrt{J z \chi_1 (1 - \gamma_k)} \approx \sqrt{\frac{J}{2\chi_1}} |k|. \quad (5.64)$$

Here $J_k = J z / (2\chi_1)$, $z$ is the lattice coordination ($z = 6$ for a cubic lattice in three dimensions), $\gamma_k = z^{-1} \sum_\delta e^{ik \delta}$, and $\delta$ are bond vectors. Although $k$ and $k + 2k_f$
are related by reciprocal lattice vectors in the rotor model (5.55), they are not in the microscopic Hamiltonian, and the addition of \(2k_f\) to the argument of (5.64) serves as a mnemonic for the fact that the spin mode is centered primarily around \(2k_f\).

Similarly the equations of motion for \(\{Q_{xz}, I_y\}\) and \(\{Q_{yz}, I_x\}\) describe two massive isospin waves:

\[
\omega_{AF,I}(k + 2k_f) = N \sqrt{\frac{4|\delta r|}{\chi_2} + \frac{J}{2\chi_2} k^2}
\]

These excitations correspond to rotations between the AF and the TSC states and indicate proximity of the two ground states. When \(\delta r\) goes to zero, the mass of the isospin waves vanishes reflecting an enhanced SO(4) symmetry. The isospin modes in the AF phase do not couple to neutrons.

### 5.7.2 Unitary triplet superconductor

In the unitary TSC (\(\delta r > 0, \tilde{u}_2 < 0\)) we choose \(\langle Q_{xz}\rangle = \psi\), while all other order parameters vanish. Eqs. (5.57) and (5.58) for the pairs \(\{Q_{xy}, S_z\}\) and \(\{Q_{xz}, S_y\}\) yield two spin wave modes reflecting the broken spin symmetry:

\[
\omega_{uTSC,S}(k) = \psi \sqrt{\frac{J}{2\chi_1}} |k|.
\]

The creation operators for the two spin waves involve the generators \(S_y\) and \(S_z\) respectively. Substitution into (5.62) immediately shows that the neutron scattering weight of these modes at \(2k_f\) vanishes.

Eqs. (5.57) and (5.59) for the pair \(\{Q_{yx}, I_z\}\) yields a gapless phase fluctuation mode reflecting the broken charge U(1) symmetry in the TSC phase:

\[
\omega_{uTSC,\varphi}(k) = \psi \sqrt{\frac{J}{2\chi_2}} |k|.
\]

With the inclusion of Coulomb interactions, this mode becomes massive through the Higgs phenomenon, with a mass of the order of the plasma frequency. The creation operator of this isospin mode involves the generator \(I_z\). Substitution into (5.62) shows that it does not couple to \(2k_f\) neutrons.

Finally, the equations of motion for the pair \(\{Q_{zx}, I_y\}\) give the massive \(\Theta\)-mode:

\[
\omega_{uTSC,\Theta}(k + 2k_f) = \psi \sqrt{\frac{J}{2\chi_2} k^2 + \frac{4\delta r}{\chi_2}}
\]

The operator that creates this mode from the ground state is given by

\[
b^\dagger_\Theta(k) = \frac{1}{\sqrt{1 + \chi_2(Jk^2/2 + 4\delta r)}} \left( \sqrt{\chi_2(Jk^2/2 + 4\delta r)} Q_{zx}(k) + iI_y(k) \right)
\]
When substituted into Eq. (5.62) it gives a neutron scattering intensity at $k + 2k_f$:
\[
|\langle 0 | [b_{\Theta}(k), Q_{z\alpha}(k)] | 0 \rangle|^2 \delta(\omega - \omega_{nTSC,\Theta}) = \delta_{\alpha\gamma} \frac{\psi^2}{1 + \chi_2(\frac{Jk^2}{2} + 4\delta r)} \delta(\omega - \omega_{nTSC,\Theta}(k+2k_f)) \tag{5.70}
\]

As we approach the point $\delta r = 0$ with SO(4) symmetry, the gap of the $\Theta$-mode vanishes as $\sqrt{\delta r}$. Hence, the spectrum of the Hamiltonian (5.55) with $\hat{u}_2 < 0$ is such that on both sides of the AF/TSC transition we observe mode softening. Mode softening at the first order transition is a property of the higher symmetry quantum critical points [46, 211, 212]. Exactly at the SO(4) symmetric point $\delta r = 0$ the system has gapless spin and isospin wave doublets.

### 5.7.3 Non unitary triplet superconductor

For the case $\hat{u}_2 > 0$ the TSC phase is non-unitary. We choose $\langle Q_{xx} \rangle = \langle Q_{yy} \rangle = \psi$. There is also a mixed phase where a non-vanishing AF order parameter $\langle Q_{zz} \rangle = N$ appears in addition to the non unitary TSC order, considered below. In the pure non-unitary TSC we find two spin wave modes $\{Q_{xz}, S_y\}$ and $\{Q_{yz}, S_x\}$ with linear dispersion:
\[
\omega_{nTSC,S}(k) = \psi \sqrt{\frac{J}{2\chi_1}} |k| \tag{5.71}
\]

As in the unitary case, these spin waves do not couple to neutrons around $2k_f$.

The non unitary TSC also supports two degenerate massive $\Theta$-modes $\{Q_{zx}, I_y\}$ and $\{Q_{zy}, I_x\}$ with dispersion
\[
\omega_{nTSC,\Theta}(k + 2k_f) = \psi \sqrt{\frac{J}{2\chi_2}} \frac{1}{k^2 + 4\delta r} \tag{5.72}
\]

These correspond to rotations of the real and the imaginary parts of the TSC order parameter toward the AF. These excitations are created by the operators:
\[
\begin{align*}
b_{\Theta_x}(k) &= \frac{1}{\sqrt{1 + \chi_2(\frac{Jk^2}{2} + 4\delta r)}} \left( \sqrt{\chi_2(\frac{Jk^2}{2} + 4\delta r)} Q_{zy}(k) - i I_x(k) \right) \\
b_{\Theta_y}(k) &= \frac{1}{\sqrt{1 + \chi_2(\frac{Jk^2}{2} + 4\delta r)}} \left( \sqrt{\chi_2(\frac{Jk^2}{2} + 4\delta r)} Q_{zx}(k) + i I_y(k) \right) \tag{5.73}
\end{align*}
\]

Substituting the $b_{\Theta_n}$ operators in (5.62) we find the neutron scattering weight near $2k_f$:
\[
|\langle 0 | [b_{\Theta_x}(k), Q_{z\alpha}(k)] | 0 \rangle|^2 \delta(\omega - \omega_{nTSC,\Theta}) = \delta_{\alpha\gamma} \frac{\psi^2}{1 + \chi_2(\frac{Jk^2}{2} + 4\delta r)} \times \delta(\omega - \omega_{nTSC,\Theta}(k+2k_f))
\]
Figure 5.10: Collective excitations in various phases. (a) In the AF phase, the excitation spectrum consists of two massless spin waves and two massive isospin waves. Due to translational symmetry breaking, $2k_f$ is a reciprocal lattice vector, and these modes also have non-zero weight at the dashed curves near $k = 0$. The spectrum in the TSC phase contains massless phase and spin modes, as well as massive $\Theta$ modes. For unitary TSC, there is only one such mode. The non-unitary TSC (as well as the mixed phase) contains a second, degenerate $\Theta$ mode, represented by the dotted curve. (b) The SO(4) symmetric point ($\delta r = 0$). In a unitary TSC this point corresponds to the transition between AF and TSC. It is characterized by four gapless (Goldstone) modes (2 isospin and 2 spin). In the non-unitary case the SO(4) symmetric point is inside the mixed AF/TSC phase. It supports only 3 (degenerate) Goldstone modes. This is because the order parameter has a residual SO(3) symmetry as described in the text.
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\[ |0\rangle [b_{\Theta y}(k), Q_z \Theta(k)] |0\rangle^2 \delta(\omega - \omega_{nTSC,\Theta}) = \delta_{xy} \frac{\psi^2}{1 + \chi_2(Jk^2/2 + 4\delta \rho)} \times \delta(\omega - \omega_{nTSC,\Theta}(k + 2k_f)) \] (5.74)

The phase fluctuation mode in the non-unitary TSC phase differs from its counterpart in the unitary case. The Eqs. (5.57-5.59) for \{Q_{xy}, Q_{yx}, S_z, I_z\} cannot be decoupled, giving a mode that involves both spin and isospin generators. Due to the residual symmetry generated by \(S_z + I_z\), the mode with \(Q_{xy} - Q_{yx}\), drops out of the spectrum. The remaining excitation follows the dispersion

\[ \omega_{nTSC,\Theta}(k) = \psi \sqrt{J \left( \frac{1}{\chi_1} + \frac{1}{\chi_2} \right)} k. \] (5.75)

As in the unitary case, Coulomb interactions make this a massive mode, with a mass of the order of the plasma energy. The creation operator of this mode involves the generators \(I_z, S_z\). Substitution into (5.62) gives vanishing neutron scattering intensity at \(2k_f\).

5.7.4 Mixed phase

In the AF/non-unitary TSC mixed phase, the order parameters form an orthogonal triad \(\tilde{\psi}_1 = \psi_x, \tilde{\psi}_2 = \psi_y, \tilde{N} = N \hat{z}\), i.e. \(\langle Q_{xx} \rangle = \langle Q_{yy} \rangle = \psi, \langle Q_{zz} \rangle = N\). It is easy to verify that the phase fluctuation mode remains unchanged, its dispersion given by Eq. (5.75). However, other modes are complicated due to the fact that Eqs. (5.57-5.59) couple the coordinates \{Q_{xx}, Q_{zx}, S_y, I_y\} and similarly \{Q_{yz}, Q_{zy}, S_x, I_x\}. Solution of the eigenvalue equations yields two collective modes for each of the above coordinate sets. One is a massive “\(\Theta\)” mode and the other a gapless spin wave-like mode:

\[ \omega_{S,\Theta} = \sqrt{\left( \frac{2\delta \rho \phi}{\chi_2} + \frac{J_k \rho}{2\chi_t} \right)^2 + \left( \frac{2\delta \rho \phi}{\chi_2} + \frac{J_k \rho}{2\chi_t} \right)^2 - \frac{J_k}{\chi_1 \chi_2} (J_k \phi^2 + 4\delta \rho \phi \rho)} \] (5.76)

Where \(\chi_t^{-1} \equiv \chi_1^{-1} + \chi_2^{-1}\), \(J_k \equiv J_z/2(1 - \gamma_k)\), \(\phi \equiv \psi^2 - N^2\), and \(\rho \equiv \psi^2 + N^2\). To calculate the spectrum in the mixed phase as a function of the tuning parameter \(\delta \rho\), we find the values of the order parameters at a given \(\delta \rho\) from the mean field theory of (5.55). Specifically we use the result \(\psi^2 - N^2 = \delta r/\tilde{u}_2\). Fig. 5.11(a) gives an example of the dispersions obtained for a particular value of \(\delta r\) within the mixed phase. The asymptotic form of the excitation energies at small wave vectors is given by:

\[ \omega_S \sim \sqrt{\frac{J_k \rho}{2\chi_1} k} \]
\[ \omega_{\Theta} \sim \frac{J_k \rho}{2\chi_2} k^2 + \frac{4\delta \rho^2}{\tilde{u}_2 \chi_2}. \] (5.77)
Figure 5.11: Spin waves and Θ-modes in the mixed phase. (a) Dispersions ($\delta r > 0$) of the mode clearly show mixing between the Θ-mode and the spin wave. Each of the shown modes is doubly degenerate. (b) Neutron scattering intensity of the modes at wave-vector $k = 2k_f + 0.1\pi$ as a function of the tuning parameter $\delta r$. Note that the weight of the spin wave modes goes to zero at the SO(4) symmetric point $\delta r = 0$. Θ-modes are strongly enhanced near $\delta r = 0$. 
Figure 5.12: Gap of the $\Theta$ modes softens toward $\delta r = 0$ reflecting the enhanced SO(4) symmetry at that point. (a) The gap decreases as $\sqrt{|\delta r|}$ in the case $\tilde{u}_2 < 0$ (unitary TSC). (b) In the case $\tilde{u}_2 > 0$ there is a change from $\sqrt{|\delta r|}$ behavior in the pure phases to linear decrease at smaller $|\delta r|$, inside the mixed non-unitary TSC and AF phase.

Fig. 5.11, demonstrates that the exact dispersion (5.76) deviates from these asymptotic forms already at relatively small wave vectors. This is due to the strong mixing between spin and isospin modes. Due to this mixing, both spin waves and $\Theta$-modes carry some weight in the neutron scattering intensity (see Fig. 5.11(b)). The scattering intensity associated with the spin wave mode vanishes in the vicinity of $\delta r = 0$. On the other hand the intensity of the $\Theta$ modes becomes dramatically enhanced. Another unique feature of the phase with mixed non-unitary TSC and AF order is a linear with $|\delta r|$ softening of the $\Theta$-excitation gap. Compare this to the $\sqrt{\delta r}$ softening in the unitary TSC (See also Fig. 5.12).

The SO(4) symmetric point $\delta r = 0$ needs special consideration. Here $N^2 = \psi^2$ and the order parameter is invariant under the SO(3) group generated by $I + S$. This implies that there are only three Goldstone modes at this point. Indeed, a direct calculation at the SO(4) symmetric point gives three degenerate modes with dispersion:

$$\omega_{nSO(4)}(k) = \psi \sqrt{\frac{J}{2} \left( \frac{1}{\chi_1} + \frac{1}{\chi_2} \right) |k|} \quad (5.78)$$

Note that the number of Goldstone modes at the SO(4) point is different in a unitary and non-unitary TSC. In the unitary case the spin and isospin SO(3) symmetries are broken separately with a residual $U(1) \times U(1)$ symmetry of the order parameter. local gauge freedom associated with each. This leads to four Goldstone modes. In the non unitary case, on the other hand, there is residual SO(3) symmetry of the order parameter, corresponding to $I + S$ rotations as discussed above. Consequently, this system has only three Goldstone modes.

The gapless spin waves and phase modes that we found away from the SO(4) symmetry are generic to systems that break spin SO(3) and charge U(1) symmetries.
However, Θ excitations, which can be thought of as massive isospin waves, are not. Their presence shows the proximity of AF and TSC phases and their softening at the point δr = 0 should provide a unique signature of the SO(4) symmetry of the system.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Order parameter</th>
<th>Residual symmetry, generators</th>
<th>Goldstone (massless) modes</th>
<th>Pseudo-Gold. (massive) modes</th>
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</thead>
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<tr>
<td>AF</td>
<td>⟨Qzz⟩</td>
<td>U(1)×U(1) Sz, Iz</td>
<td>2 Sx, Sy</td>
<td>2 Ix, Iy</td>
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<tr>
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<td>⟨Qxx⟩</td>
<td>U(1) Sx</td>
<td>3 Sy, Sz, Iz</td>
<td>1 Iy</td>
</tr>
<tr>
<td>nuTSC</td>
<td>⟨Qxx⟩ = ⟨Qyy⟩</td>
<td>U(1) Sx + Iz</td>
<td>3 Sy, Sz, Sx − Iz</td>
<td>2 Ix, Iy</td>
</tr>
<tr>
<td>nuTSC + AF</td>
<td>⟨Qxx⟩ = ⟨Qyy⟩, ⟨Qzz⟩</td>
<td>U(1) Sx + Iz</td>
<td>3 Sy, Sz, Sx − Iz</td>
<td>2 Ix, Iy</td>
</tr>
<tr>
<td>u SO(4)</td>
<td>⟨Qxx⟩</td>
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<td>4 Sy, Sx, Iy, Iz</td>
<td>0</td>
</tr>
<tr>
<td>nu SO(4)</td>
<td>⟨Qxx⟩ = ⟨Qyy⟩ = ⟨Qzz⟩</td>
<td>SO(3) I + S</td>
<td>3 I − S</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 5.1: Symmetry breaking and collective modes. Here uTSC and nuTSC stand for unitary and non-unitary TSC respectively, nTSC+AF corresponds to a mixed phase of non-unitary TSC and antiferromagnetism away from the SO(4) symmetric point.

5.8 SO(4) symmetry in a strongly anisotropic Fermi liquid

Thus far in the analysis we have treated the case of weakly coupled Luttinger liquids, where we showed that SO(4) symmetry describes the phase diagram and collective modes of a system near the AF/TSC phase transition. However, there is a tendency away from Luttinger behavior as pressure is increased towards the superconducting state, as supported by the observation of field-induced SDW phases at high magnetic fields[104, 9, 22, 66, 52, 203], by optical measurements[195], and by low temperature transport experiments[51]. A review of the normal state of Bechgaard salts at low magnetic fields is given in Ref. [19]. In this section, we will consider the effects of interchain hopping in the extreme case where it is large enough to destroy all remnants of Luttinger liquid physics, and make the system into a highly anisotropic
Fermi liquid instead. We will see that even in this limit, despite the loss of nesting, an approximate SO(4) symmetry remains.

We begin by looking at the classical SO(4) symmetry of the GL free energy. In order to investigate this symmetry, it is sufficient to consider the quartic GL terms. This follows from the fact that our analysis of the phase diagram includes explicitly anisotropy in the quadratic terms, see eq. (5.29), which is tuned to zero by pressure at the AF/TSC transition. As shown in Appendix B.2, a microscopic derivation of the GL parameters starting from a weakly interacting Fermi liquid leads to the following form for the quartic GL terms,

$$F_4 = A \left( 2(|\Psi|^2)^2 - |\Psi|^4 \right) + B (N^2)^2 + 2(C + D)|\Psi|^2 N^2 - 4D|\Psi| \cdot N|^2, \quad (5.79)$$

where, for a perfectly nested Fermi surface, $A = B = C/2 = D = \frac{7\zeta(3)}{16\pi^2 v_f T^2}$ satisfy the SO(4) symmetry conditions (5.31)

$$A = D, \quad B = D, \quad C/2 = D,$$

and the sign of the coefficients corresponds to the unitary TSC case. In the presence of interchain coupling $t_b$, the single electron spectrum becomes

$$\xi_k = -2t_a \cos k_a - 2t_b \cos k_b - \mu. \quad (5.80)$$

Although Bechgaard salts are triclinic, and expression (5.80) applies to rectangular lattices only, it gives a good approximation to the low energy quasiparticle states of the system. Here, we take $t_a = 250$ meV, $t_b = 20$ meV, as estimated from plasma frequency measurements[81] and band structure calculations[68]. In addition, we take $\mu = \sqrt{2}t_a$, corresponding to a quarter-filled band and a nesting vector $Q = (2k_f, \pi) \approx (\pi/2, \pi)$. We note that, in the Fermi liquid description, dimerization only affects very high energy quasiparticles, and we exclude it from (5.80).

At first glance, interchain hopping seems to have a devastating effect on the SO(4) symmetry. The nesting vector $Q$ no longer connects the right and left moving Fermi surfaces exactly. Hence, while the coefficient $A$ is insensitive to $t_b$, the low temperature divergence in the coefficients $B$, $C$, and $D$ is preempted by the loss of nesting. Instead, these coefficients saturate at a temperature of the order of $t_b^2/t_a \approx 20$ K, changing the ratio $A/B$ from unity at high temperatures to about 10 at $T_c = 1.2$ K. However, nesting strongly affects antiferromagnetism only, and not superconductivity. Hence, it’s effects on the GL parameters grow in proportion to the number of times that each GL parameter multiplies $\vec{N}$ in (5.79). Thus, most of the effect can be absorbed into the normalization of the field $\vec{N}$. While the fields $\vec{N}$ and $\vec{\Psi}$ cannot be normalized independently in the full GL free energy, as this would change the ratio of gradient
Figure 5.13: Quartic Ginzburg-Landau coefficients (5.79) for a strongly anisotropic Fermi liquid, for the choice of parameters $t_a = 250 \text{ meV}$, $t_b = 20 \text{ meV}$. The solid curve shows $\sqrt{AB}$, the dashed curve $D$, and the dash-dotted curve $(C + D)/3$. Although the three curves do not coincide, as would be required by SO(4) symmetry, they trace similar trajectories all the way down to the critical temperature $T_c = 1.2 \text{ K}$ (vertical dotted line). At temperatures higher than shown, the three curves converge as nesting is restored.

terms $\frac{1}{2}(|\nabla \Psi|^2 + (\nabla \vec{N})^2)$, such scaling is allowed when considering the mean-field properties of the system. The conditions for SO(4) symmetry at mean-field level are then

\[
\sqrt{AB} = D, \\
(C + D) = 3D.
\] (5.81)

Thus, at the mean-field level, SO(4) symmetry is only broken weakly. This is illustrated in Fig. 5.13, where the left and right hand sides of the conditions (5.81) are evaluated explicitly. Despite the strong variation in the values of the different GL coefficients, the curves shown in Fig. 5.13 trace similar trajectories, indicating the approximate SO(4) symmetry. At $T_c = 1.2 \text{ K}$, we find $A = 7.0 \times 10^4$, $B = 7.3 \times 10^3$, $C = 3.1 \times 10^4$, and $D = 2.1 \times 10^4$, leading to $\sqrt{AB}/D = 1.06$ and $(C + D)/(3D) = 0.82$ ($\vec{N}$ was rescaled by a factor of 1.76). Thus, the conditions (5.81) deviate from exact SO(4) symmetry by less than 20% at $T_c = 1.2 K$.

While classical SO(4) symmetry is no longer exact, the phase diagram derived in previous sections does not change in important ways. At the mean-field level, the 20% variation from the SO(4) conditions (5.81) can open a very narrow mixed phase...
between the TSC and AF phases. Hence, as pressure is varied from the AF phase to the TSC phase, there will no longer be a discontinuity in the order parameters or in the density. Instead, these quantities will show a smooth but very rapid variation as pressure transverses the mixed phase. Therefore, due to the narrowness of the mixed phase, the system will be very sensitive to disorder. For realistic systems, which have impurities and crystal defects, the mixed phase will segregate into inhomogeneous regions of AF and TSC, just as found in the coexistence phase in the strictly first order case. However, unlike the case of a first order transition, the inhomogeneous behavior will be apparent even when the phase diagram is tuned by experimental variables that are intrinsic. We note that the narrowness of the mixed phase, and the corresponding sensitivity to disorder, is a direct consequence of the proximity of the system to SO(4) symmetry.

We now consider the fluctuation-induced first order transition between the AF and normal phases near the SO(4) symmetric point. We note that in order to alter the topology of the phase diagram, the bare GL parameters must differ enough from the SO(4) symmetric values to divert the RG flow near a new critical point. While symmetry can play an important role in an RG flow, it is difficult to conceive of a situation where reduction of symmetry would lead to softening of the first order transitions into second order. Thus, we expect the first order transition between AF and normal phases discussed earlier to still be present. Finally, we note that the case we consider in this section is extreme, in that we look study the system as a weakly interacting, strongly anisotropic Fermi liquid. This probably gives a strong overestimate of the magnitude of the breaking of classical SO(4) symmetry in real systems, which are likely to lie between the Fermi liquid limit and the weakly coupled Luttinger liquid limit, where SO(4) is a good symmetry.

Before concluding this section, we briefly discuss the effects of interchain coupling on the quantum SO(4) symmetry. One can look for this symmetry by verifying the existence of the \( \Theta \) resonance in a strongly anisotropic Fermi liquid formalism. Inside the TSC phase, this can be done using RPA type calculations, which include the AF particle-hole and \( \Theta \) resonance particle-particle channels (see e.g. Ref. [43]). Results of these calculations will be reported elsewhere. The main effect of interchain hopping is to fix the transverse components of the nesting vector to \( Q = (2k_f, \pi, \pi) \). Thus, the \( \Theta \) resonance for quasi-one dimensional systems is a collective mode, whose quantum numbers are spin zero, charge two, and wave vector \( Q \). The presence of interchain coupling also introduces broadening of the \( \Theta \) mode, and prevents it from softening all the way down to zero energy at the AF/TSC phase transition. Instead, we expect the minimum energy of the excitation to be of the order of \( t_b^2/t_a = 16 \text{ meV} \).
5.9 Experimental signatures of SO(4) symmetry

The interplay of AF and SC in the organic material (TMTSF)$_2$PF$_6$ has been a subject of active investigation [83, 5, 178]. There is strong experimental evidence supporting that superconducting order is spin triplet, as discussed in Section 5.1. In addition, (TMTSF)$_2$PF$_6$ has a quasi one-dimensional structure, as the anisotropy of electron tunneling along the chains (a), in the planes (b), and perpendicular to the planes (c) is of the order of $t_a : t_b : t_c = 250 : 25 : 1$. Hence, (TMTSF)$_2$PF$_6$ is a good candidate for comparison with the theoretical model discussed in this paper. Following the discussion in Section 5.3 and Appendix B.2 we expect the triplet order parameter in this material to be unitary. The phase diagram for this case was obtained in Section 5.5. In Ref. [149] we compare this to the experimental phase diagram of (TMTSF)$_2$PF$_6$[198, 100]. One consequence of having enhanced symmetry at a phase transition is the suppression of the critical temperature due to fluctuations of one order parameter into the other. This may contribute to the drastic drop in $T_{AF}$ as pressure is increased near the AF/TSC phase boundary in Bechgaard salts[198].

The first order transition between AF and TSC phases near the critical point, Fig. 5.6, leads to a regime of frustrated phase separation, with domains of one phase inside the other. The volume fractions of each phase are governed by the Maxwell construction, while the size of individual domains is determined by the competition between short-range and long-range parts of the Coulomb interaction[24]. If the domains are distributed randomly, the total resistance of the system may be found using an effective medium approximation. This implies, for example, that the system is superconducting when the TSC phase is beyond the percolating threshold. On the other hand, it is possible that the TSC domains are not distributed uniformly in the system, and are more favorable on the surface of the sample. In this case, the TSC regions can “short-circuit” the system even before they reach the percolation condition for the bulk. Transport properties consistent with this scenario of an inhomogeneous system have been reported in Ref. [198].

An interesting direction for exploring competition between AF and TSC phases is to use magnetic field experiments in the superconducting state near the AF/TSC phase boundary. Magnetic field produces orbital currents that strongly suppress electron pairing and leads to a formation of an Abrikosov vortex lattice. Suppression of the AF order by Zeeman effect is much smaller. Thus, we expect magnetic fluctuations to become strongly enhanced in the mixed state[211, 6, 45, 213, 88]. Since the critical field along the c-axis is $H_{c2}^c = 100mT[112]$, an applied magnetic field along the c-axis on the order of a few mT can have a strong effect, see Fig. 5.14. This is in contrast with effects such as field induced SDW’s and reentrant superconductivity, which require fields of at least 5 T for their observation[78, 104, 9, 22, 66, 52, 203]. For pressures close to the AF/TSC phase boundary and for slightly larger magnetic fields there may also be a quantum phase transition in which long range AF order develops inside the vortex phase. We note that strong sensitivity of $1/T_1$ to magnetic fields in
Figure 5.14: The effect of a magnetic field on the superconducting state. For points (A) far from the AF/TSC boundary, the magnetic field destroys superconductivity leading to a normal state. For points (B) close to the boundary, a magnetic phase is stabilized instead. The double line denotes a first order transition, which expands into a AF/TSC coexistence region in the experimental phase diagram. Here we focus on the unitary case, but similar effects can be seen for the non-unitary case near the AF/TSC mixed phase. Fields of the order of 100 mT are sufficient for a significant enhancement in antiferromagnetism to be observed. This is in contrast with field-induced SDW phases, which require fields in excess of 5 T.

the superconducting state of (TMTSF)$_2$PF$_6$ have been reported in Ref. [111]. Here, increasing the magnetic field along the b-axis from 12.8 mT to 232 mT results in a large increase of $1/T_1$, consistent with the enhancement of antiferromagnetism that we propose. Earlier specific heat measurements in Ref. [61] already showed that when the superconducting order in (TMTSF)$_2$ClO$_4$ is suppressed by a magnetic field, the system goes into a semimetallic state with a suppressed quasiparticle density of states. This is consistent with developing AF order, thus opening a gap in the quasi particle spectrum. It may be interesting to study further the enhancement of magnetic order in the mixed state with neutron scattering [89, 105, 106, 96], NMR [37, 133, 86], and µSR[132] experiments.

In Ref. [149] (see also section 5.7 of this paper) we discuss that direct observation of the $\Theta$ mode in the superconducting phase should be possible through neutron scattering. The most important feature of the $\Theta$-resonance, which identifies it as a generator of the SO(4) symmetry, is the pressure dependence of the resonance energy inside the TSC phase. When the pressure is reduced and the system is brought toward the phase boundary with the AF phase, we predict the energy of the $\Theta$-resonance to be dramatically decreased. Mode softening is not expected generically at first order phase transitions and provides a unique signature of the SO(4) quantum symmetry.
Figure 5.15: Tunneling experiment for detecting the Θ excitation in (TMTSF)$_2$ClO$_4$ material. A singlet superconducting material with a higher transition temperature than (TMTSF)$_2$ClO$_4$ provides a reservoir of Cooper pairs that can couple resonantly to Θ pairs. Momentum mismatch between the Cooper pairs in SC and Θ pairs in (TMTSF)$_2$ClO$_4$ is compensated by scattering of electrons in a layer of the SP material (TMTTF)$_2$PF$_6$.

We note that due to interchain hopping, the center of mass momentum of the Θ excitation in quasi-one dimensional systems is $(2k_f, \pi, \pi)$.

Another approach to detect the Θ excitation involves tunneling experiments with the SSC/(TMTSF)$_2$ClO$_4$ junction shown in Fig. 5.15 (analogous experiments in the context of π excitations in the high Tc cuprates are discussed in Ref. [13]). A singlet superconductor provides a reservoir of Cooper pairs that can couple to Θ pairs in (TMTSF)$_2$ClO$_4$. One needs to overcome, however, the momentum mismatch between the two types of pairs. A possible approach is to use an intermediate layer of the quasi 1d material (TMTTF)$_2$PF$_6$. This salt is quarter filled and displays spin-Peierls (SP) order. The modulations of the SP order thus have a periodicity of four TMTTF sites, matching the $(2k_f, \pi, \pi)$ wave vector of (TMTSF)$_2$ClO$_4$. The small mismatch between the two wave vectors, due to differences in the lattice constant in these compounds, can be compensated by a parallel magnetic field [167]. We expect peaks in the current-voltage characteristics of the junction when the voltage bias compensates the energy difference between Cooper and Θ pairs

$$2eV = \omega_{\Theta}$$

Peaks in $IV$ should be present even above the superconducting transition temperature of (TMTSF)$_2$ClO$_4$ and only require the other material to be superconducting. The choice of (TMTSF)$_2$ClO$_4$ is made as this material is likely to be close to the AF/TSC transition at ambient pressure [18]. This eliminates the need for pressure cells, which would make the experiments much more difficult.
5.10 Summary

The primary purpose of this paper has been to discuss the competition of antiferromagnetism and triplet superconductivity in quasi one-dimensional systems, such as Bechgaard salts (TMTSF)$_2$X. The point of departure of our work is the existence of enhanced symmetry, that unifies the two order parameters, in one dimensional systems of interacting electrons. Analysis of the Luttinger liquid model presented in Section 5.2 showed that the usual charge and spin $U(1) \times SO(3)$ symmetry is enhanced to a higher $SO(3) \times SO(4)$ symmetry on the transition line between the two phases for incommensurate band filling. For half-filled systems and weak umklapp scattering, the enhanced symmetry group becomes $SO(4)$. Weak coupling between chains, that enables true long range order, is expected to perturb the $SO(4)$ symmetry only slightly.

In sections 5.3, 5.4, 5.5, and 5.6 we studied the finite temperature phase diagram for systems with $SO(4)$ symmetry. For the unitary case, a mean field analysis shows that $SO(4)$ symmetry requires a direct first order transition between TSC and AF phases. In addition, fluctuations of the order parameters turn a portion of the boundary between AF and normal phases into a first order transition and also lead to a weakly first order transition between TSC and normal phases. For the non-unitary case, $SO(4)$ symmetry requires two second order transitions between TSC and AF phases. We find that the system is close to having an $SO(4)$ symmetric tetracritical point, but thermal fluctuations stretch this point into a short line of direct first order transitions from the normal state to the mixed state. Our results have direct implications for quasi one-dimensional organic superconductors from the (TMTSF)$_2$X family, which are likely to be unitary triplet superconductors. For example, first order transitions between the AF and the TSC phases, and between the Normal and the AF phases explain the AF/TSC and the AF/Normal coexistence regions found in the phase diagram of (TMTSF)$_2$PF$_6$.

In section 5.7 we analyze collective excitations in various phases and demonstrate that $SO(4)$ leads to the existence of a new collective mode, the $\Theta$ excitation, which describes rotations between the AF and the TSC phases. In section 5.9 we study possible experimental tests of the $SO(4)$ symmetry. We propose that the $\Theta$ excitation should be observed as a sharp resonance in spin polarized inelastic neutron scattering experiments in the superconducting phase. We predict that the energy of the peak decreases toward the first order phase transition to AF order. Such softening of modes is not expected in general near a first order transition and would be a unique signature of the enhanced symmetry at the transition point.
5.11 Acknowledgements

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Appendix A

Appendices to Chapter 3

A.1 Correlations of spin and charge

While equation (3.8) gives the simplest wave function that describes a state with both superconducting and nematic orders, it does not incorporate correlations between charge and spin degrees of freedom. In the stripe picture, domain walls are not only regions where holes accumulate, they are also regions across which the staggered magnetization changes sign. One can modify (3.8) to include this effect, by relating $\sigma_i$ to the number of domain walls crossed:

$$|\psi_3\rangle = \sum_{\{\sigma_1, \sigma_2, \ldots\} = \pm 1} \prod_k \delta \left( \sigma_k - \sigma_1 (-1) \sum_{j=1}^k \delta_{jk} \right) g \left[ \hat{b}_j \hat{b}_j \right] \times \left[ \prod_i \left( s + \sigma_i m^a \hat{t}_a, i + c \hat{b}_i \right) \right]|\Omega\rangle_i.$$  \hspace{1cm} (A.1)

In this case, the sum over sites inside the delta function runs over a path on the plane joining site 1 to site $k$. This forces a change of sign in $\sigma_k$ every time a new domain wall intervenes between those two sites. The path sum is only independent of path whenever the domain walls run continuously through the sample instead of ending up abruptly, and when an odd number of them do not intersect, as would happen, for instance, in a “T-junction”. The functional $g$ is chosen to destroy all configurations that violate these constraints, thus enforcing the integrity of the fluctuating domain walls. The simplest choice for $g$ is a projection operator that gives equal weight to all allowed configurations. In this case, the wave function (A.1) can be rewritten as

$$|\psi_4\rangle = \sum_{D} \prod_{i \in D} \left( s + \sigma_{D,i} m^a \hat{t}_a, i \right) |\Omega\rangle_i \prod_{j \in D} c \hat{b}_j |\Omega\rangle_j,$$  \hspace{1cm} (A.2)

where $D$ denotes an allowed domain-wall configuration, and $\sigma_{D,i}$ is the sign of the staggered magnetization on site $i$ in configuration $D$. Equations (A.1) and (A.2) are alternate descriptions of the nematic state of Zaanen and Nussinov [207, 143].
A.2 Collective modes of a quantum paramagnet

We would like to see if the director density waves (DDW) of a nematic state can be easily distinguished from the collective modes of a quantum paramagnet. These latter modes can be derived, in the RPA approximation, by substituting $-gQ_{ij}^{\alpha\beta} \rightarrow J_0 \delta^{\alpha\beta} \eta_{ij}$ in equations (3.22) and (3.24). Here, $\eta_{ij}$ is equal to 1 if $i$ and $j$ are nearest neighbors, and zero otherwise; and $J_0 > 0$ is the antiferromagnetic spin exchange. We find an isotropic spin response,

$$\chi^{\alpha\beta}_{\text{RPA}}(k, \omega) = \frac{\chi^0(k, \omega)}{1 - J_0 \eta(k) \chi^0(k, \omega)} \delta^{\alpha\beta}, \tag{A.3}$$

where $\eta(k) = 2(\cos k_x + \cos k_y)$. In the limit $k \rightarrow 0$, $\omega \rightarrow 0$, the free spin susceptibility tends to $\chi_0 \rightarrow k^2/\omega^2$, leading to the long wavelength result,

$$\chi^{\alpha\beta}_{\text{RPA}} \sim \frac{k^2}{\omega^2 - 4J_0 k^2} \delta^{\alpha\beta}.$$ 

Thus, there are three degenerate gapless paramagnon poles (with vanishing weight at $k = 0$). On the other hand, the poles of Eq. (A.3) near $k = (\pi, \pi)$ have a spin gap $\Delta$ due to the lack of long-range Néel order,

$$\omega_{k \sim (\pi, \pi)} = \sqrt{4J_0^2 (k - (\pi, \pi))^2 + \Delta^2}.$$
Appendix B

Appendices to Chapter 5

B.1 Derivation of SO(3) × SO(4) symmetry in Luttinger liquids

In this Appendix we demonstrate that along the line $g_1 = 2g_2$, the Luttinger liquid Hamiltonian (5.1) has an exact SO(3)$_{\text{spin}}$ × SO(4)$_{\text{isospin}}$ symmetry. For this, we use bosonization to write the $\Theta^\dagger_r$ operators (5.6) as

$$\Theta^\dagger_r = r \int dx \eta^\dagger \eta r e^{-r A(x)},$$

(B.1)

where $A(x) = i \sqrt{2} (\phi_\rho(x) + \theta_\rho(x))$ and $\theta_\rho = \pi \int x' \Pi_\rho(x')$. Note that $\Theta^\dagger_r$ are independent of the spin fields $\phi_\sigma$ and $\theta_\sigma$. Hence, the spin sector of the bosonized Hamiltonian commutes trivially with $\Theta^\dagger_r$, and we need only keep track of the charge sector,

$$\mathcal{H}_\rho = \int dx \left( \frac{\pi u_\rho K_\rho}{2} \Pi_\rho^2 + \frac{u_\rho}{2\pi K_\rho} (\partial_x \phi_\rho)^2 \right).$$

(B.2)

Whenever $g_1 = 2g_2$, corresponding to $K_\rho = 1$, the commutator $[\mathcal{H}_\rho, A]$ takes on a simple form,

$$[\mathcal{H}_\rho, A(x)] = \sqrt{2} u_\rho (\partial_x \phi_\rho(x) + \pi \Pi_\rho(x))$$

$$= -iu_\rho \partial_x A(x),$$

(B.3)

so that commuting $\mathcal{H}_\rho$ with an arbitrary function of $A(x)$ is equivalent to taking the derivative with respect to $x$. For example,

$$[\mathcal{H}_\rho, e^A] = \sum_n \frac{1}{n!} [\mathcal{H}_\rho, A^n]$$
\[
\mathcal{H} = [\mathcal{H}_\rho, A] + \frac{1}{2} (A [\mathcal{H}_\rho, A] + [\mathcal{H}_\rho, A] A(x)) + \ldots
\]
\[
= -iu_\rho \left( \partial_x A + \frac{1}{2} (A \partial_x A + \partial_x AA) \right) + \ldots
\]
\[
= -iu_\rho \partial_x e^A. \quad \text{(B.4)}
\]

Hence,
\[
\left[ \mathcal{H}_\rho, \int dx \ e^{A(x)} \right] = -iu_\rho \int dx \ \partial_x e^{A(x)}
\]
\[
= -iu_\rho \left[ e^{A(L)} - e^{A(0)} \right], \quad \text{(B.5)}
\]

which vanishes if periodic boundary conditions are imposed on \( \phi(x) \) and \( \theta(x) \). Thus, for \( K_\rho = 1 \),
\[
\left[ \mathcal{H}, \Theta^\dagger_\pm \right] = 0, \quad \text{(B.6)}
\]

and the Luttinger liquid has full \( \text{SO}(3)_{\text{spin}} \times \text{SO}(4)_{\text{isospin}} \) symmetry, generated by \( \Theta_\pm \), the total spin operators \( S_\alpha \), and the charge of left and right movers,
\[
Q_\pm = \sum_{k_s} (a^\dagger_{\pm,k_s} a_{\pm,k_s} - \frac{1}{2}) \quad \text{(B.7)}
\]

The enlarged symmetry relies on the independent conservation of total number of right- and left-movers. This is not a good conservation law, for instance, in the presence of impurity scattering, dimerization, or umklapp. For general \( K_\rho \), we find
\[
\left[ \mathcal{H}, \Theta^\dagger_\pm \right] = \frac{K_\rho^2}{2} \int dx \left( \sqrt{2} u_\rho (\partial_x \phi_\rho(x) - \pi \Pi_\rho(x)) \right) \frac{\eta^\dagger_\pm \eta_\dagger_\pm}{2\pi} e^{\mp A(x)}. \quad \text{(B.8)}
\]

We would like to thank Daw-Wei Wang for helpful discussions on results presented in this section.

\section*{B.2 Ginzburg-Landau free energy for weak interactions}

To extract parameters of the GL free energy we consider a mean-field Hamiltonian
\[
\mathcal{H} = \sum_{k_s} (\epsilon_k - \mu) a^\dagger_{k_s} a_{k_s} + \bar{\Psi} \cdot \sum_k w_k a^\dagger_{k_s} a^\dagger_{-k_s} (\bar{\sigma} \sigma_2)_{ss'} + \bar{\Psi}^* \cdot \sum_k \bar{w}_k a_{-k_s} a_{k_s} (\sigma_2 \bar{\sigma})_{ss'}
\]
\[
+ \bar{\Phi} \cdot \sum_k a^\dagger_{-k_f s'} a_{k_f s} (\bar{\sigma}_s a^\dagger_{-k_f s'} a_{k_f s} + \bar{\sigma}'_s a^\dagger_{-k_f s'} a_{k_f s}) \quad \text{(B.9)}
\]
where $w_k = |k|/k$ gives the sign of $k$. Integrating out the fermions yields an effective action for the order parameter fields. We obtain the fourth order terms:

$$ F_4 = A \left( 2(|\vec{\psi}|^2)^2 - |\vec{\psi}|^2 \right) + B \left( 2(|\vec{\Phi}|^2)^2 - |\vec{\Phi}|^2 \right) $$

$$ + 2C |\vec{\psi}|^2 |\vec{\Phi}|^2 + 2D \left( |\vec{\psi}|^2 |\vec{\Phi}|^2 - |\vec{\Phi}^* \cdot \vec{\Phi}|^2 \right) \quad (B.10) $$

where

$$ A = \frac{1}{2\beta} \sum_{\omega_n} \int \frac{dk}{2\pi} G^2(-k, -\omega_n) G^2(k, \omega_n) $$

$$ B = \frac{1}{\beta} \sum_{\omega_n} \int \frac{dk}{2\pi} G^2(k, \omega_n) G(k + 2k_f, \omega_n) \{ G(k + 2k_f, \omega_n) + 2G(k - 2k_f, \omega_n) \} $$

$$ C = \frac{-1}{\beta} \sum_{\omega_n} \int \frac{dk}{2\pi} G^2(k, \omega_n) G(-k, -\omega_n) \{ G(k + 2k_f, \omega_n) + G(k - 2k_f, \omega_n) \} $$

$$ D = \frac{1}{\beta} \sum_{\omega_n} \int \frac{dk}{2\pi} G(k, \omega_n) G(-k, -\omega_n) G(k + 2k_f, \omega_n) G(-k - 2k_f, -\omega_n) w_{-k} w_{k + 2k_f} $$

For instance, the diagram giving the coefficient $A$ is shown in Fig. B.1. For the Luttinger liquid type model with linearized spectrum around $k = \pm k_f$ we obtain

$$ A = B = C/2 = D. \quad (B.11) $$

The relationship among coefficients (B.11) implies that the effective GL free energy (B.10) is SO(3)$_{\text{spin}} \times$SO(4)$_{\text{isospin}}$ symmetric, as expected from the discussion in Section 5.2. $F$ can thus be parameterized in the form (5.22), with $\tilde{u}_1 = 3A$ and $\tilde{u}_2 = -2A$. In the clean limit,

$$ A = \frac{7\zeta(3)}{16\pi^3 v_f T^2} $$
Figure B.2: Corrections to coefficient of $|\Phi_z|^2|\Psi_z|^2$ term in GL free energy, to linear order in umklapp scattering (dashed line). The two diagrams add up to zero. Inspection of all such diagrams shows that the quartic coefficients of the GL free energy are not modified to linear order.

where $\zeta(3) = 1.202\ldots$, and $v_f$ is the Fermi velocity.

Note that, as was pointed out in section 5.3.2, to linear order in $g_3$, umklapp does not affect the quartic coefficients of the free energy. For instance, the diagrams in Fig. B.2 could contribute to the coefficient of the term $|\Phi_z|^2|\Psi_z|^2$. However, although they do not vanish individually, the two add up to zero. This is consistent with the Feynman-Hellman theorem which requires that the only corrections to the free energy to linear order in $g_3$ be given by the expectation value of the perturbation (5.14).

**B.3 Non-unitary triplet superconductivity and antiferromagnetism: Expansion from the lower critical dimension.**

Here we outline some of the methods used in the RG calculation of the non-linear model (5.48) in $d = 2 + \epsilon$ dimensions. The RG flow equations of a general non-linear
model can be computed using the formalism of Friedan[58]. The fields in such models must satisfy constraints which force them to lie on some target space manifold $\mathcal{M}$. For instance, the usual non-linear $\sigma$ model deals with a single $N$-component vector with a constrained fixed length, and $\mathcal{M}$ in this case is the $N-1$ dimensional sphere describing the locus of possible values of such vector. A local set of coordinates $\phi_i$ can be introduced on a patch of $\mathcal{M}$, in terms of which the free energy becomes

$$F = \int dx \, g_{ij}(\phi(x)) \partial_\mu \phi^i(x) \partial_\mu \phi^j(x).$$

Unlike the original fields used to define the model, the fields $\phi_i(x)$ are unconstrained; all information regarding the original constraints is contained in the metric $g_{ij}$. The metric also contains the coupling constants of the system. In Friedan’s formalism, the RG flow is thought of as a gradual deformation of the manifold as the short length degrees of freedom are integrated out. The RG equations can be written in a covariant way; to one loop order,

$$\frac{\partial g_{ij}}{\partial \ell} = \epsilon g_{ij} - R_{ij},$$

where $\epsilon = d - 2$ and $R_{ij}$ is the Ricci tensor, determined uniquely by the metric.

In practice, whenever the manifold is a homogeneous space $G/H$, as in our case, it is simplest to work directly in the tangent space of the manifold, see [7] for a detailed discussion. In terms of the metric on the tangent space, $\eta_{ab}$, the RG equations become

$$\frac{\partial \eta_{ab}}{\partial \ell} = \epsilon \eta_{ab} - R_{ab},$$

where the Ricci tensor in the tangent space is given by

$$R_{ab} = \sum_{Ic} f_{ac} \, f_{Ib} + \sum_{cd} \eta_{cc} - (\eta_{cc} - \eta_{dd})^2 \frac{1}{4 \eta_{cc} \eta_{dd}} f_{ac} \, f_{bc} \, f_{cd}$$

in terms of the structure factor constants of the group $G$

$$[T_a, T_b] = f_{ab} \, T_c + f_{ab} \, T_I$$

$$[T_I, T_b] = f_{Ib} \, T_c.$$

Generators labelled by upper case indices are elements of Lie $H$, while lower case indices denote generators in Lie $G$-Lie $H$. In applying expression (B.15), we assume that the generators have been chosen so that the structure factor constants (B.16) are antisymmetric with respect to exchange of any two indices; such a choice is always possible. Equation (B.15) is written in a non-covariant way to make the dependence on the coupling constants $\eta_{ab}$ explicit, and it shows the advantage of working in tangent space: the Ricci tensor is given directly in terms of the Lie algebra of $G$. 
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We briefly digress to discuss the Lie algebra of the group \( SO(N) \), which has \( N(N-1)/2 \) generators corresponding to infinitesimal rotations in the planes \( \langle m, m' \rangle \). The indices \( m \neq m' \) run through the \( N \) independent axes. For instance, \( SO(3) \) has three generators, \( T_x = \langle \hat{y}, \hat{z} \rangle \), \( T_y = \langle \hat{z}, \hat{x} \rangle \), and \( T_z = \langle \hat{x}, \hat{y} \rangle \). Keeping in mind that \( \langle m, m' \rangle = \langle -m', m \rangle \) (“a clockwise rotation in the \( x - y \) plane is a counterclockwise rotation in the \( y - x \) plane”), we introduce a graphical representation: if we draw \( N \) points on a sheet of paper, an arbitrary generator \( \langle m, m' \rangle \) can be represented by an arrow from point \( m \) to point \( m' \). The structure factor constants of the Lie algebra

\[ [\langle m, m' \rangle, \langle n, n' \rangle] = \delta_{mn'} \langle m, n' \rangle - \delta_{m'n} \langle m, n \rangle - \delta_{mn} \langle m', n \rangle + \delta_{mn'} \langle m', n \rangle \]

can be written as a “generalized \( \epsilon \) tensor”,

\[ [\langle m, m' \rangle, \langle n, n' \rangle] = \epsilon_{\langle m, m' \rangle \langle n, n' \rangle} \langle p, p' \rangle \theta(p, p'), \]

(B.17)

which has a simple interpretation in terms of the arrows described above: \( \epsilon \) vanishes unless \( \langle m, m' \rangle, \langle n, n' \rangle, \) and \( \langle p, p' \rangle \) are the edges of a closed triangle. If they do form a closed triangle, count the number of times that the directions of the arrows must be flipped to turn it into an oriented triangle, i.e. one satisfying \( m' = n, n' = p \), and \( p' = m \). For an even number of flips, \( \epsilon = 1 \); otherwise \( \epsilon = -1 \). With this in mind, inspection of (B.15) shows that, for groups \( G \) based on \( SO(N) \), where \( f_{ab} c \sim \epsilon_{ab} c \), the calculation of the Ricci tensor reduces almost entirely to the counting of triangles.

Armed with these tools, consider the non-linear model (5.48),

\[ F = \int d^4 x \left\{ \frac{1}{2g_1} (\nabla \vec{e}_1)^2 + \frac{1}{2g_2} ((\nabla \vec{e}_2)^2 + (\nabla \vec{e}_3)^2) + \frac{1}{g_3} ((\vec{e}_1 \cdot \nabla \vec{e}_2)^2 + (\vec{e}_1 \cdot \nabla \vec{e}_3)^2) + \frac{1}{g_4} (\vec{e}_2 \cdot \nabla \vec{e}_3)^2 \right\}. \]

(B.18)

Model (B.18) has the symmetry \( SO(N) \) of rotations of the \( N \)-component vectors, and the symmetry \( SO(2) \) of internal rotations between \( \vec{e}_2 \) and \( \vec{e}_3 \). Hence, the symmetry group of (B.18) is \( G = SO(N) \times SO(2) \). The order parameter is a triad of mutually orthogonal vectors, \( \Phi = (\vec{e}_1 \ \vec{e}_2 \ \vec{e}_3) \), and the ordered phase has residual symmetry \( H = SO(N-3) \times SO(2)_{\text{diag}} \). The generators of \( H \) leave the triad \( \Phi \) invariant, whereas the generators in Lie \( G \)-Lie \( H \) rotate the triad and are in one-to-one correspondence with the spin waves of the system.

We identify four types of spin waves, corresponding to the following classes of generators: \( T_{a_1} \), which leave \( \vec{e}_1 \langle 2,3 \rangle \) untouched but rotate \( \vec{e}_1 \) into one of the remaining \( N - 3 \) directions; \( T_{a_2} \), which leave \( \vec{e}_1 \) untouched, but rotate either \( \vec{e}_2 \) or \( \vec{e}_3 \) into one of the remaining \( N - 3 \) directions; \( T_{a_3} \), of rotations in either the \( \vec{e}_1, \vec{e}_2 \) plane or the \( \vec{e}_1, \vec{e}_3 \) plane; and \( T_{a_4} \), composed of the single generator of rotations in the \( \vec{e}_2, \vec{e}_3 \) plane. Each class furnishes an independent irreducible representation under the action of the
group $H$, leading to four different spin wave velocities, and to four different coupling constants, $\eta_1 \ldots \eta_4$,

$$
\eta_{bc} = \sum_{a_1} \eta_1 \delta_{ba_1} \delta_{ca_1} + \sum_{a_2} \eta_2 \delta_{ba_2} \delta_{ca_2} + \sum_{a_3} \eta_3 \delta_{ba_3} \delta_{ca_3} + \eta_4 \delta_{ba_4} \delta_{ca_4}.
$$

The RG flow equations (B.14) become

$$
\frac{d\eta_1}{dl} = \epsilon \eta_1 - \frac{1}{2\pi} \left( N - 2 + \frac{\eta_1^2 - \eta_2^2 - \eta_3^2}{\eta_2 \eta_3} \right)
$$

$$
\frac{d\eta_2}{dl} = \epsilon \eta_2 - \frac{1}{2\pi} \left( N - 2 + \frac{\eta_2^2 - \eta_3^2 - \eta_4^2}{2\eta_1 \eta_3} - \frac{\eta_4}{2\eta_3} \right)
$$

$$
\frac{d\eta_3}{dl} = \epsilon \eta_3 - \frac{1}{2\pi} \left( N - 2 + \frac{N - 3}{\eta_1 \eta_2} - \frac{\eta_2^2}{2\eta_3} \right)
$$

$$
\frac{d\eta_4}{dl} = \epsilon \eta_4 - \frac{1}{2\pi} \left( \frac{N - 3}{\eta_2} \eta_4^2 + \frac{\eta_2^2}{2\eta_3^2} \right), \tag{B.19}
$$

The fixed $SO(N) \times SO(3)$ symmetric point of (B.19) is described in the body of the text for $N \geq 5$. For $N = 4$, the fixed point is stable with respect to arbitrary perturbations away from the $SO(N) \times SO(3)$ symmetric plane [incidentally, in this case the fixed point has a larger symmetry than expected, $SO(4) \times SO(4)$]. On the other hand, within the plane, it has one stable and one unstable direction. This suggests the RG flows and the phase diagram that are shown schematically in Fig. B.3. Note that we have a whole line of direct transitions between the disordered and the TSC+AF phases. This whole line is controlled by the point O that has a high $SO(4) \times SO(4)$ symmetry. This is quite remarkable: a higher symmetry appears not at a single point but at the whole transition line.

### B.4 Non-unitary triplet superconductivity and antiferromagnetism: Large $N$ analysis

In Section 5.6.1 we pointed out that a free energy in (5.29) in the large $N$ limit should be considered with care, when $\tilde{u}_1 + \tilde{u}_2/3$ is close to zero. Here we assume that
\( \tilde{u}_2 > 0 \), so, this requires negative \( \tilde{u}_1 \). The complications arise when the system goes outside the basin of attraction of the tetracritical fixed point, and the RG flows carry \( \tilde{u}_1 \) to large negative values. As we discuss below, this leads to a first order transition which is similar to what was suggested in Ref. [8] for the normal to \( \text{A}_1 \) transition in liquid \( ^3\text{He} \). We take

\[
\tilde{u}_1 + \frac{\tilde{u}_2}{3} = \frac{\delta}{4N},
\]

where \( \delta \) is positive and is of order \( \frac{1}{N} \). We now extend the calculations presented in Section 5.6.1 to the next order in \( \frac{1}{N} \). For all order parameters we separate expectation values and fluctuations

\[
\vec{\Psi} = (\vec{a}_T + i\vec{b}_T, \sigma_\psi + a_L + ib_L, a_1 + ib_1), \quad \vec{N} = (\vec{N}_T, N_0, N_1, \sigma_N + N_L),
\]

We can expand equation (5.29) to order \( \frac{1}{N} \) and obtain tadpole equations for \( a_L \) and \( N_L \). In addition to the counterterms and loops due to fluctuations of the transverse components, we need to include fluctuations of the longitudinal components. Note, that loops of longitudinal components may be terminated by bubble chains coming from \( \tilde{u}_2(\tilde{a}_T\tilde{b}_T)a_0 \) vertices. We also need to include diagrams that arise from \( \tilde{u}_2(\tilde{a}_T\tilde{b}_T)b_La_L \) vertices. Special attention should be paid to diagonalization of propagators, since the free energy has terms which introduce mixing between fluctuating components in (B.21).

If we want to absorb the cut-off dependence into renormalization of quadratic coefficient (compare to equation (5.38)), we need to define the latter relative to

\[
r_{c^{'}} = r_c - \langle 40\tilde{u}_1 + 24\tilde{u}_2 \rangle \int_0^\Lambda \frac{d^3k}{(2\pi)^3} \frac{1}{k^2} + \langle 4\tilde{u}_1 + 8\tilde{u}_2 \rangle \frac{j}{2\pi^2} \log \Lambda,
\]

where

\[
j = \frac{\tilde{u}_2N}{4}.
\]

Integrals in tadpole equations can not be calculated exactly. Hence, we expand them in two cases: \( j^2 \gg 32\tilde{u}_2\sigma^2 \) and \( j^2 \ll 32\tilde{u}_2\sigma^2 \) (\( \sigma^2 \) corresponds to \( \sigma_N^2 \) or \( \sigma_\psi^2 \) or \( (\sigma_N^2 + \sigma_\psi^2)/2 \) depending on terms in the integrals). Also, while solving final system of equations, expansions under conditions \( \sigma_\psi^2 \gg \sigma_N^2, \sigma_\psi^2 \ll \sigma_N^2, \sigma_N^2 \approx \sigma_\psi^2 \) were made. To be concrete, we took the values \( \tilde{u}_1 = -1/(4N) + \delta/(4N) \) and \( \tilde{u}_2 = 3/(4N) \).

Transition from disordered phase to superconductive and antiferromagnetic phases outside the vicinity of \( r_{c^{'}} \) remains of the second order, though transition border shifts such that

\[
t_{N,\psi} = \frac{15}{16\pi^2N} \log \frac{16}{3}.
\]

In the vicinity of full \( \text{SO}(3) \times \text{SO}(N) \) symmetry line \( t_N = t_\psi \) we expanded equations under conditions

\[
|\sigma_N^2 - \sigma_\psi^2| \sim \sigma^2/N,
\]

where

\[
\tilde{u}_2 > 0, \quad \tilde{u}_1 < 0, \quad \tilde{u}_1 + \frac{\tilde{u}_2}{3} = \frac{\delta}{4N},
\]

and

\[
\tilde{u}_1 > 0, \quad \tilde{u}_2 = 0, \quad \tilde{u}_1 + \frac{\tilde{u}_2}{3} = \frac{\delta}{4N}.
\]
Figure B.4: Phase diagram for large N under conditions (B.20). Solid line is a I order phase transition, dashed – II.

resulting in first order phase transition, limited by boundaries

\[ t_{N,L} + 2t_{\Psi,L} = 0 \]  \hspace{1cm} (B.26)

and

\[ t_{N,M} + 2t_{\Psi,M} = \frac{C_0^2}{4N^2\delta}, \]  \hspace{1cm} (B.27)

where \( C_0 = (1 + 3\sqrt{3}/2)/\pi \).

Condition (B.25) for solution obtained, appears to be valid not only for small deviations from the line of symmetry, but for entire line of transition. Thus solution (B.26,B.27) is self-consistent in the entire region, resulting in phase diagram shown on Fig. B.4. In comparison with solution of the first order expansion, boundary of mixed phase becomes a first order phase transition, and there is no angle between \( N\Psi \leftrightarrow N \) and \( N\Psi \leftrightarrow \Psi \) boundaries (which is \( \propto \delta \) in first order expansion). Boundary of the basin of attraction of stable fixed point is determined by the validity of expansion for different conditions for \( j^2 \). In our case it is \( N\delta \sim 1 \).

On the other hand, expansion under condition \( \sigma_N^2 \gg \sigma_\Psi^2 \) for \( N\Psi \leftrightarrow N \) transition, and \( \sigma_N^2 \ll \sigma_\Psi^2 \) for \( N\Psi \leftrightarrow \Psi \) also results in self-consistent solution with phase transition boundary of a different geometry. On the boundary minor component drops to zero, while major almost does not change. In our opinion, this solution does not have a physical sense.
Bibliography


