Transport Properties in the Vicinity of Mott Insulators

by

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Abstract

Understanding the states in the vicinity of the Mott insulator is crucial to understanding both the physics of the transition between a Mott insulating phase and a metallic phase and the physics of the cuprate high-temperature superconductors. In this thesis, we start from the standard Mott insulating regime of the two dimensional Hubbard model. We then study the physics of nearby states where transport has been restored.

First we consider doping of the Hubbard model in the strong coupling limit, i.e. the $t-J$ model. Using the variational Monte Carlo technique, we study Gutzwiller projected states. In particular, studying the projected BCS quasiparticles, we calculate the renormalization of the quasiparticle current and the spectral weight. Both are investigated as a function of momentum and doping. Finally, we discuss the relation between this model and the cuprate superconductors.

In the second half of this thesis, we return to the half-filled Hubbard model but now at intermediate values of $U/t$. In this regime, we study the spin liquid phase, a state that possibly lives between the Mott insulator and the normal metal. Motivated by the recently created organic compound $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, we study a particular spin liquid where there is a spinon Fermi surface coupled to a $U(1)$ gauge field. While still a charge insulator, this model has many metallic-like properties. We first develop a quantum Boltzmann equation for this model from which we calculate the spin resistivity and the more experimentally accessible thermal conductivity. We then proceed to consider spinon pairing and calculate the gauge field contribution to the spin susceptibility. We find that the theoretical result is consistent with experiments giving further evidence that at low temperatures this compound is described by this particular $U(1)$ spin liquid.

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Chapter 1

Introduction

1.1 Background

One of the simplest models for studying systems with strong electron correlation is the single-band Hubbard model. The Hubbard model describes a system of particles hoping on a lattice with an energy cost \( U \) when two particles occupy the same site. Here we consider the Hubbard model for spin 1/2 electrons, where \( U \) is an effective on-site repulsion due to the Coloumb interaction. Despite its simplicity, the physics of the Hubbard model is only well understood in one dimension. The two and three dimensional cases remain open problems even after decades of research. In this thesis, we focus on the two dimensional Hubbard model which is thought to contain a variety of interesting phases at the heart of many current problem in strongly correlated systems. In particular, we focus on the relation between the Hubbard model and both the superconducting phase seen in the cuprates and the proposed spin-liquid phase.

The Hubbard Hamiltonian is given by

\[
\mathcal{H}_{\text{Hub}} = -\sum_{i,j,\sigma} t_{ij} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \( c_{i,\sigma}^\dagger \) is the electron creation operator at lattice site \( i \) with spin \( \sigma = (\uparrow, \downarrow) \) and \( n_{i\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma} \) is the corresponding number operator. The \( t_{ij} \) term is a standard tight
binding model for electron hopping between lattice sites $i$ and $j$. While in general the hopping integral $t_{ij}$ can be non-zero over arbitrarily long range and can also be complex, for simplicity we consider only isotropic nearest neighbor hopping. Thus $t_{ij} = t$ if $i$ and $j$ are nearest neighbors, and $t_{ij} = 0$ otherwise.

In this thesis, we explore the Hubbard Hamiltonian as a function of the relative energy scales $U/t$ and as a function of doping. We begin by considering the half-filled Hubbard model where there are exactly as many electrons in the system as lattice sites. In the two limits of small and large $U/t$, the expected solutions are then relatively straightforward. For small $U/t$, the energy scale for on-site repulsion is much smaller than the bandwidth $W = 2zt$, where $z$ is the number of nearest neighbors for a given site on the lattice under consideration. Thus we expect that in this limit the system is in a metallic phase and that a Fermi liquid description is accurate. Note that while this argument holds in general, for the specific case of the two-dimensional square lattice, the Fermi surface exhibits perfect nesting and is thus unstable to an antiferromagnetic instability for arbitrary $U$. The system therefore remains an insulator even for small $U/t$.

For large $U/t$, the energy scale for on-site repulsion outweighs the kinetic energy and the system is in a regime where the strong interaction between electrons dominates the physics of the problem. In the extreme limit of $U/t \to \infty$, no double occupancy is allowed due to the infinite energy cost of two electrons occupying the same lattice site. In the strong coupling limit at half-filling, there is exactly one electron per site and thus the electrons are frozen in place. This leads to an insulating phase known as a Mott insulator. In general, a Mott insulator is a system which one would expect to be a conductor based on standard band theory, but becomes insulating due to the strong Coulomb interaction between electrons. If we assume that $t$ is fixed, then we can define a critical $U_c$, such that for $U > U_c$ the system is in a Mott insulating phase.
1.2 Hole doping and $t$–$J$ model

We now turn to study the strong-coupling limit of the Hubbard model more precisely. As mentioned above, doubly occupied sites are strictly forbidden in this limit. In fact they can only enter through virtual processes when there is a finite hole density. One can treat this limit perturbatively in $t/U$ through a unitary transformation which eliminates the terms in the Hamiltonian that couple states with different numbers of doubly occupied sites. [1] Working to lowest order in $t/U$ and dropping the three site terms, we arrive at the standard Hamiltonian considered in the strong-coupling limit, the $t$–$J$ model

$$\mathcal{H}_{tJ} = -t \sum_{\langle i,j \rangle,\sigma} \left( c_{i,\sigma}^+ c_{j,\sigma} + \text{h.c.} \right) + J \sum_{\langle i,j \rangle} (S_i \cdot S_j - n_i n_j / 4), \quad (1.2)$$

where $n_i = \sum_{\sigma} n_{i\sigma}$ is the total particle number and $J = 4t^2 / U$ relates the exchange coupling to the Hubbard model on-site repulsion. Note that in the $t$–$J$ model the electron creation and annihilation operators are subject to the additional constraint that no double occupancy is allowed. In Chapter 2, we discuss further the unitary transformation relating the $t$–$J$ and Hubbard models and explore the consequences of retaining higher order terms in the expansion.

Although we have simplified the problem by greatly reducing the Hilbert space that must be considered, this Hamiltonian is still extremely non-trivial and inaccessible to perturbative methods. Ignoring an overall energy shift, we see that at half-filling the $t$–$J$ model reduces to the spin 1/2 Heisenberg model. Thus for non-frustrated lattices, we expect that at half-filling the system has antiferromagnetic order and the low-energy excitations are spin waves. In fact for all two dimensional lattices the Heisenberg model gives rise to an antiferromagnetically ordered ground state wave function. Thus in general, in the strong coupling limit, the Hubbard model enters a magnetically ordered Mott insulating phase since the electrons themselves are unable to move due to the no double occupancy constraint.

Another motivation for studying the strong coupling limit is that the $t$–$J$ model
on the square lattice is often taken as a good starting point for exploring the essential physics of the cuprate high-temperature superconductors. Experimentally the cuprates show a rich phase diagram as a function of doping and temperature. In particular at zero temperature, as the hole concentration increases the system moves from an antiferromagnetically ordered phase to a d-wave superconducting phase and finally into a metallic phase. At finite temperatures, the cuprates also exhibit other phases which are currently not as well-understood such as the strange metal and pseudo-gap phases.

We thus turn to study the $t-J$ model as a function of hole doping. In general when the hole density is large, we expect that the $t-J$ model returns to the metallic phase, barring the presence of an antiferromagnetic instability due to nesting of the Fermi surface. The interesting case is the regime with small but finite hole doping where the cuprates are found to enter a superconducting phase. Recently it has been established that this superconducting phase can be reasonably well-described by considering Gutzwiller-projected wave functions, in particular the projected d-wave BCS ground state.[2] We use this model as a starting point for exploring the properties of the low-energy excitations in this state.

The Gutzwiller projection $P_D$ takes a wave function $|\psi_0\rangle$ and restricts it to the subspace where doubly occupied states are forbidden,

$$|\psi\rangle = P_D |\psi_0\rangle = \prod_i [1 - n_i, n_i,] |\psi_0\rangle.$$ (1.3)

The projected states are thus consistent with the no double occupancy constraint inherent in the $t-J$ model. While the original mean-field states $|\psi_0\rangle$ are amenable to analytic study, in general the Gutzwiller projection leads to strong correlations in the wave function and makes analytic calculations intractable. We are thus left to approximate and numerical solutions, which we now discuss.

For a particular Gutzwiller projected state $|\psi\rangle$, we are interested in calculating the expectation of some operator $A$. This can be done approximately by relating the expectation value in the projected state to the expectation value in the unprojected
state through some factor $g_A$,

$$\langle \psi | A | \psi \rangle = g_A \langle \psi_0 | A | \psi_0 \rangle.$$  \hspace{1cm} (1.4)

The calculation of the expectation value in the unprojected state is straightforward and a variety of approximation methods have been developed to estimate $g_A$.\cite{3, 4}

We do not use these techniques however, and instead proceed to calculate the expectation value numerically. While at first this seems to be impossible on any reasonably sized lattice due to the exponential growth of the number of states with lattice size, it turns out that the computation can be done quickly and to high precision using Monte Carlo methods. The key is to write the expectation value $\langle A \rangle$ as

$$\langle A \rangle = \sum_\alpha f(\alpha)\rho(\alpha)$$ \hspace{1cm} (1.5)

where

$$f(\alpha) = \sum_\beta \langle \alpha | A | \beta \rangle \frac{\langle \beta | \psi \rangle}{\langle \alpha | \psi \rangle},$$ \hspace{1cm} (1.6)

$$\rho(\alpha) = \frac{|\langle \alpha | \psi \rangle|^2}{\langle \psi | \psi \rangle}.$$ \hspace{1cm} (1.7)

Here $\alpha$ and $\beta$ denote particular spin configurations constrained to the subspace with no doubly occupied sites. Writing the expectation value in this way, we can calculate $\langle A \rangle$ by considering a random walk through configuration space using the weight $\rho(\alpha)$. Since we are interested in calculating the expectation value of operators that contain a small number of creation and annihilation operators, the expression $\langle \alpha | A | \beta \rangle$ is only nonzero for a few configurations $\beta$ for any given $\alpha$. We consider unprojected wave functions $\psi$ where $\langle \alpha | \psi \rangle$ can be evaluated as the determinant of a matrix. Thus the whole calculation can be done relatively quickly on a desktop computer. For further details on this method see Ref. [5].

Using this Monte carlo method, one can consider the Gutzwiller-projected d-wave
BCS wave function as a variational state with variational parameters $\mu$ and $\Delta$. We then find the optimal values of these parameters which minimize the $t-J$ Hamiltonian and calculate the expectation value of physical operators in this optimal state. In this thesis, we extend this idea to look at the possible structure of low-lying excitations, by studying the Gutzwiller-projected d-wave BCS quasiparticle. We are interested in the renormalization of the current carried by the quasiparticle and in the spectral weight of this excitation. Moreover, we relate these quasiparticle results to the superfluid density as a function to temperature, allowing us to make some comparison between the calculations from the variational Monte carlo method (VMC) and experimental results.

1.3 Spin Liquids

We now return to the half-filled Hubbard model which, as mentioned above, reduces to the Heisenberg model in the strong coupling limit. Regardless of the frustration inherent in the lattice, the Heisenberg model always has a magnetically ordered ground state. Thus for large $U$, deep in the Mott insulating phase, we expect that the system enters an antiferromagnetic Mott insulating state where the low-energy transport is described by spin waves.

Moving away from the strong coupling limit and considering $U$ near $U_c$ so that the system is just on the Mott insulating side of the metal-insulator transition, the higher order terms derived in the expansion of the strong coupling limit can no longer be ignored. This results in the spin Hamiltonian containing long range spin-spin interactions as well as loop interactions.[5, 6] These terms provide another important source for frustration in system. It has been proposed that by considering such a frustrated Hamiltonian on a frustrated lattice, that it may be possible to stabilize an insulating ground state where there is no spin order, a state known as a spin-liquid. Describing the system in terms of spins, since in the insulating phase the charge degrees of freedom are gapped, this state would be a ground state of a spin Hamiltonian that does not break any of the symmetries of the Hamiltonian or the
lattice. One of the earliest and most famous examples of such a state is the uniform RVB state proposed by Anderson as the possible ground state for the Heisenberg model on the triangular lattice.[7] Since then however it has been established that this is not the ground state for this system and in fact the triangular lattice Heisenberg model has a 120 degree antiferromagnetically ordered ground state. In fact, so far only specially engineered Hamiltonians have been shown to have a spin-liquid ground states. However there has been much recent theoretical work studying frustrated spin systems with more realistic Hamiltonians that may exhibit spin-liquid ground states.[8, 9, 10]

One of the main differences between the spin-liquid and the magnetically ordered Mott insulator, is the nature of the low-energy excitations. While in both cases the charge degrees of freedom are gapped, in the spin-liquid the excitations do not necessarily have to be Bosonic since they do not arise as Goldstone modes. In general the spin excitations in a spin-liquid can be either gapped or gapless and either Fermionic or Bosonic. These distinctions are related to many interesting questions involving the presence of topological order which we do not discuss in this work.

While the theoretical existence of a spin-liquid ground state for a realistic microscopic Hamiltonian remains an open question, there has been recent progress in the search for experimental realizations of spin-liquid phases in two dimensions. Two of the most promising candidates are the organic compound $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ (Ref. [11]) and the compound ZnCu$_3$(OH)$_6$Cl$_2$ (Ref. [12]). Both systems involve highly frustrated lattices. The organic compound can be described by a quasi-two dimensional triangular lattice, while the ZnCu$_3$(OH)$_6$Cl$_2$ forms a Kagome lattice. In this thesis, we focus on the spin-liquid proposed to describe the organic compound. While it is an interesting question to take the triangular lattice and consider either the Hubbard Hamiltonian at $U$ near $U_c$ or a spin Hamiltonian with additional terms that enhance frustration in order to see if a spin liquid ground state can be stabilized, we do not address this issue here. Instead we focus on the proposed spin-liquid and calculate the experimentally accessible quantities and compare to the results from $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$. 

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The particular spin-liquid proposed to describe \( \kappa \)-\((BEDT-TTF)_{2}\text{-Cu}_{2}(CN)_{3} \) at low temperatures can be derived from the Hubbard Hamiltonian through the slave-particle formalism, see Ref. [13] (slave-boson) and Ref. [14] (slave-rotor). In both cases one begins by breaking the electron up into a spin 1/2, charge neutral spinon plus a second bosonic piece. This however enlarges the Hilbert space for the problem. To solve this issue one considers the partition function for the system. By adding a Lagrange multiplier to the Lagrangian, we can enforce a constraint that returns us to the original Hilbert space. We then consider fluctuations around this mean-field state. One finds that at this saddle point the system is described in terms of Fermionic spin 1/2 spinons coupled to a \( U(1) \) gauge field. In the insulating phase the charge degrees of freedom are gapped; however, the spinons are still able to form a Fermi surface and thus we expect this organic compound to exhibit many metallic like properties that only depend on the presence of a Fermi surface.

1.4 Outline

In this thesis, we are interested in studying transport properties of systems in the vicinity of the Mott insulating phase. If the Mott insulator is magnetically ordered then transport is the result of magnetic excitations in the system that can be described with standard spin wave theory. In the case of finite doping, the system can enter a superconducting phase that we study using the VMC technique previously mentioned. Finally, we consider a frustrated system near the metal-insulator transition where a possible spin liquid phase is present. In realistic systems, one would ideally consider the effects of hole-doping and decreasing \( U/t \) simultaneously, here however, for the sake of simplicity we study each of these two cases independently.

This thesis is organized as follows. In Chapter 2, we study the strong coupling limit of the Hubbard model away from half-filling, the doped \( t-J \) model on the two dimensional square lattice, which can be taken as a starting point for exploring the physics of high-temperature superconductors. With the use of Gutzwiller-projected variational states, we study the renormalization of the current carried by the quasiparticles
in high-temperature superconductors and of the quasiparticle spectral weight. The renormalization coefficients are computed by the variational Monte Carlo technique, under the assumption that quasiparticle excitations may be described by Gutzwiller-projected BCS quasiparticles. We find that the current renormalization coefficient decreases with decreasing doping and tends to zero at zero doping. The quasiparticle spectral weight $Z_+$ for adding an electron shows an interesting structure in $k$ space, which corresponds to a depression of the occupation number $n_k$ just outside the Fermi surface. The perturbative corrections to those quantities in the Hubbard model are also discussed.

In Chapters 3 and 4, we return to the Hubbard model but now study the half-filled case at smaller values of $U/t$ that are still in the Mott insulating regime but that are close to the metal-insulator transition. We also move from the square lattice to the triangular lattice where the effects of frustration are much stronger. Applying the slave-particle formalism to the Hubbard model on a triangular lattice, one can arrive at a spin liquid state that contains a spinon Fermi surface coupled to a $U(1)$ gauge field. Our choice to study this particular spin liquid is motivated by the recent proposal that the organic compound $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ may be well described at low temperatures by this spin liquid state.[14, 6]

In Chapter 3, we use the non-equilibrium Green's function formalism, to derive the Quantum Boltzmann Equation (QBE) for this state. In this system, however, one cannot \textit{a priori} assume the existence of Landau quasiparticles. We show that even without this assumption we can still derive a linearized equation for a generalized distribution function. We show that the divergence of the effective mass and of the finite temperature self-energy do not enter these transport coefficients and they remain well-defined. Moreover, using a variational method, we calculate the temperature dependence of the spin resistivity and thermal conductivity of this system due to the spinons. In the final section of chapter 3, in analogy to phonon-drag, we study the gauge boson contribution to the thermal conductivity.

In Chapter 4, we consider the susceptibility of this spin liquid at low temperatures. In particular, we examine the proposal that below some small temperature ($\sim 10K$)
the spinons pair. We calculate the effect on the susceptibility due to the development of a gap in the gauge field. We find that the proposed spinon pairing is consistent with the observed susceptibility measurements in $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$.

Note that most of the work in this thesis is presented in materials published elsewhere. Chapter 2 is adapted from work that was published as Ref. [15]. Chapter 3 details work from a paper that is currently in preparation for publication, Ref. [16]. Finally, Chapter 4 details work that has been submitted for publication and appears online as Ref. [17].
Chapter 2

Variational Monte Carlo Study of the Current Carried by a Quasiparticle

2.1 Introduction

In recent years, it has been acknowledged that ground-state properties of high-temperature superconductors may be reasonably well described with the help of Gutzwiller-projected wave functions [2]. However the main challenge of any candidate theory of high-temperature superconductivity is the description of finite-temperature properties such as the superconducting transition and the pseudogap phenomenon in underdoped cuprates. One of the first issues related to the finite-temperature physics of high-temperature superconductors is the structure of low-lying excitations. Within the framework of Gutzwiller-projected wave functions, the first steps in studying the excitations have been recently made: the quasiparticle spectrum and the quasiparticle spectral weight have been calculated [18, 19]. In this chapter, we complement the previous studies with the analysis of the current carried by the quasiparticles. The magnitude of the quasiparticle current has a direct physical implication in reducing the superfluid density at finite temperature, which eventually determines the super-
conducting transition temperature in the underdoped regime [20, 21]. Furthermore, the deviation of the quasiparticle current from the prediction of the BCS theory may provide a helpful insight in the physics of high-temperature superconductivity.

The reduction of the superfluid density \( n_s(T)/m \) by thermal quasiparticles at the nodes of a \( d \)-wave superconductor has been computed by Lee and Wen [20, 21] as

\[
\frac{\hbar^2 n_s(T)}{m} = \frac{\hbar^2 n_s(0)}{m} - \frac{2}{\pi} \alpha^2 \frac{v_F}{v_{\Delta}} k_B T,
\]

where \( v_F \) and \( v_{\Delta} \) are the velocity of the nodal quasiparticles perpendicular and parallel to the underlying Fermi surface, and \( \alpha \) is the phenomenological Landau parameter [22] which renormalizes the current carried by the quasiparticle

\[
j(k) = -e\alpha v_F.
\]

Experimentally, \( n_s(T)/m \) can be related to the London penetration depth \( \lambda \), and the ratio \( v_F/v_{\Delta} \) may be extracted independently from a thermal-conductivity measurement [23]. This makes \( \alpha \) an experimentally accessible quantity for a variety of doping values [24, 25].

In the first part of this chapter, we focus on computing the current renormalization \( \alpha \) for different doping values. We find that it decreases with decreasing doping, and that it is roughly constant along the Fermi surface at all dopings. The contribution of particles and holes to the total quasiparticle current allows us to picture the “effective Fermi surface” where the electron contribution crosses over to the hole contribution. We observe that this “effective Fermi surface” deviates considerably from the original Fermi surface of the unprojected BCS state. This reveals the particle-hole asymmetry produced by the Gutzwiller projection.

In the second part of this chapter, we discuss another renormalization parameter: the quasiparticle spectral weight \( Z_+ \) for adding an electron. The momentum dependence of \( Z_+ \) shows a pocket structure at the diagonal of the Brillouin zone just outside the Fermi surface. We further discuss the relations and bounds on \( Z_+ \) in the \( t-J \) model, as well as corrections arising from the rotation to the Hubbard model.
For our analysis, we take the minimal two dimensional model for strongly interacting electrons on a lattice, the Hubbard model. Following the usual procedure (see, e.g., Refs. [18, 26]), we first study the wave function for its strong-coupling limit, the $t-J$ model and then include the first-order correction in $t/U$ due to the doubly-occupied sites. The Hamiltonian for the $t-J$ model for our system is defined on the two-dimensional square lattice by

$$\mathcal{H}_{tJ} = -t \sum_{\langle i,j \rangle, \sigma} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.} \right) + J \sum_{\langle i,j \rangle} \left( S_i \cdot S_j - n_i n_j / 4 \right),$$  

with $t/J = 3$. $J = 4t^2/U$ gives the relation between the exchange coupling $J$ and the Hubbard Hamiltonian on-site repulsion term $U$. We have defined $S_i = \frac{1}{2} c_{i,\alpha}^\dagger \sigma_{\alpha,\beta} c_{i,\beta}$, and $n_i = \sum_\alpha c_{i,\alpha}^\dagger c_{i,\alpha}$. Since we are in the strong-coupling limit, the Hamiltonian (2.3) is also supplemented with the constraint that no double occupancy is allowed, unlike the original Hubbard model Hamiltonian (1.1).

We use the variational Monte Carlo technique to calculate expectation values of operators given our trial wave functions. [5, 27] For the $t-J$ model, we consider two related trial wave functions: the ground state wave function $|\Psi_{GS}\rangle$ and the wave function for the excited state $|\Psi_{EX}\rangle$. For the ground state, we use the Gutzwiller-projected $d$-wave singlet,

$$|\Psi_{GS}\rangle = P_D P_N |\Psi_{BCS}\rangle$$

where $P_D = \prod_i [1 - n_i n_i]$ is the Gutzwiller projection operator onto the subspace with no doubly occupied states, and $P_N$ is the projection operator onto the subspace with $N$ particles. $|\Psi_{BCS}\rangle = \prod_k \left[ 1 + a_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger \right] |0\rangle$, where $c_{k,\sigma}^\dagger$ is the Fourier transform of real-space electron creation operator $c_{i,\sigma}^\dagger$. Following the standard BCS definitions for a $d$-wave singlet state,

$$a_k = \frac{v_k}{u_k} = \frac{\Delta_k}{\xi_k + \sqrt{\xi_k^2 + \Delta_k^2}},$$

$$\Delta_k = \Delta_{\text{var}}(\cos k_x - \cos k_y),$$

$$\xi_k = \epsilon_k - \mu_{\text{var}},$$
with $c_k = -2(\cos k_x + \cos k_y)$. Not only has this $d$-wave Gutzwiller-projected wave function been shown to give good variational energies for the $t-J$ model relative to other possible phases, but also it has correctly reproduced many properties of the superconducting state.\cite{28, 18}

For the trial wave function of the low-lying excited states, we take the natural ansatz of the Gutzwiller-projected Bogoliubov quasiparticle \cite{29, 19}

$$|\Psi_{\text{EX}}(k, \sigma)\rangle = P_D P_N \gamma_k^\dagger |\Psi_{\text{BCS}}\rangle. \quad (2.8)$$

Since the overall normalization of the wave function is of no importance, we may also rewrite the trial excited state as

$$|\Psi_{\text{EX}}(k, \sigma)\rangle = P_D P_N c_k^\dagger |\Psi_{\text{BCS}}\rangle. \quad (2.9)$$

Throughout the rest of this chapter, we suppress the $k$ and $\sigma$ variables on $|\Psi_{\text{EX}}\rangle$ for notational convenience. The expectation values of any operator $\mathcal{O}$ in the variational ground and excited states is often denoted as $\langle \mathcal{O} \rangle_{\text{GS}}$ and $\langle \mathcal{O} \rangle_{\text{EX}}$ respectively.

In our simulations, we use the optimal values of $\Delta_{\text{var}}$ and $\mu_{\text{var}}$ calculated for the ground state trial wave function \cite{30}, both for the ground state and for the excited state. These values minimize the expectation value $\langle \mathcal{H}_{tJ} \rangle_{\text{GS}}$ of the physical $t-J$ Hamiltonian at a fixed concentration of holes.

We assume boundary conditions that are anti-periodic in the $x$ direction and periodic in the $y$ direction so that we avoid the singularity in $a_k$ along the nodal diagonal, $(0, 0)$ to $(\pi, \pi)$. A drawback of this choice of boundary conditions is that we are unable to calculate quantities exactly on the nodal diagonal, and instead calculate expectation values for nearby $k$ points. This becomes an important source of error when we compute expectation values at the nodal point. We try to lower this error by looking at larger systems in order to get better resolution; however, we are limited by our computing resources.

This trial excited state and various related ones have been studied previously by other groups \cite{31, 32, 33, 19}. The energy dispersion of the low-energy quasiparticles
has been found to be of the BCS type $E(k) = (\xi^2 + \Delta_k^2)^{1/2}$, but with renormalized values of the gap and bandwidth. The nodal point obviously coincides with the nodal point of the unprojected wave function $\Psi_{BCS}$ and slowly shifts inwards from $(\pi/2, \pi/2)$ along the diagonal of the Brillouin zone as the hole doping increases.

### 2.2 Current Carried by the Quasiparticles

In this section, we investigate the current carried by quasiparticles as a function of their momenta and doping. The current carried by the excited state $|\Psi_{EX}(k, \sigma)\rangle$ is defined as

$$j_{k,\sigma} = \langle \sum_{\langle ij \rangle, \alpha} it(c_{\alpha,i}^\dagger c_{\alpha,j} - c_{\alpha,j}^\dagger c_{\alpha,i}) \rangle_{EX},$$

where $\langle ij \rangle$ represents a sum over all links. Note that the orientation and direction of the link determines its contribution to the vector $j$. We can interpret the excited state trial wave function as the ground state for a system of $N$ particles to which we add one unpaired electron so that our state has a net spin and charge. The Gutzwiller projection enforces strong correlation between the added electron and the $N$-electron ground state, so that we expect an effective quasiparticle with renormalized parameters.

In the standard BCS theory (without the Gutzwiller projection), the current carried by the quasiparticles is $j_k = e\nu_k$ where $\nu_k = dE_k/dk$ is the velocity from the underlying normal state and not the velocity from the quasiparticle dispersion $dE/dk$. This is the result of the fact that in BCS theory the excitations are a superposition of particle and hole states and that these states carry opposite charge but also move in opposite directions. The underlying metallic state can have some Fermi liquid correction to the current carried by the particles and holes. This correction is then carried through to the quasiparticle current in the superconducting state, $j_k = \alpha e\nu_k$. In the case of the Gutzwiller projected trial excited state that we are studying, we see that current does still approximately follow the shape of the dispersion of the underlying metal and that the quasiparticle current renormalization $\alpha$ can be calculated from.
Figure 2-1: The top middle and bottom figures are respectively plots of the current $j$, $j_{\parallel}$, and $j_{\perp}$ as a function of the wave vector $k$ for a 12x12 system with 13 holes, $x = 0.09$. The vectors are drawn starting at the k-point at which the current is calculated, their length is proportional to the current magnitude.
Figure 2-2: The magnitude of the current $|j|$ measured in units of $t$ along the nodal diagonal, $(0,0)$ to $(\pi, \pi)$. These runs were done on the $10 \times 10$ system with the dopings of $x = 0.01, 0.05, 0.09$ and $0.17$ (increasing magnitude).

the ratio of $j/v_k$.

### 2.2.1 Current as a function of $k$

First we examine $j$, the current carried by the quasiparticle, as a function of $k$ for various dopings. At most dopings, we find a distribution with a structure similar to what one would expect from the tight binding model. In the top plot of Fig. 2-1, a typical example of the current carried by the quasiparticle as a function of wave vector is plotted. We compare the direction of the current as a function of momentum to both the quasiparticle dispersion, $dE(k)/dk$, and to the underlying dispersion of the normal state $v_k$. We find that the shape of the current indeed approximately follows the dispersion of the normal state and not the dispersion of the quasiparticles. This is the same as in the BCS theory so the Gutzwiller projection does not change this aspect of the physics.

For intermediate doping values, the magnitude of the current reaches its maximum value near the center of the Brillouin zone, and therefore near the nodal point. However, for strongly underdoped simulations, $x < 0.05$, we find that the maximum moves inward along the nodal direction, becoming closer to $(\pi/4, \pi/4)$ as the doping approaches zero. (See Fig. 2-2)

We also look at how much of the total current is being carried by the up spins and
down spins individually. By restricting the $\sum_\alpha$ in equation 2.10 so that we consider $\alpha = \uparrow$ and $\alpha = \downarrow$ separately, we can investigate this property of our trial excited state. Since we are now distinguishing between these two spins, it is important to note that we define our trial wave function as adding an up-spin to the system. Given this, we find that the current of our state is almost entirely carried by either the up spins or the down spins depending on whether or not we are inside or outside of the effective Fermi surface as can be seen in the lower two plots of Fig. 2-1. Inside of the Fermi surface, all of the current is carried by the down spins and outside of the Fermi surface all of the current is carried by the up spins. This is the qualitatively the same as in the unprojected case where the up and down spin currents have factors of $u_k^2$ and $v_k^2$ respectively.

To make a more detailed comparison to the BCS theory, we define the “particle contribution” to the current as

$$n_j = \frac{j_\uparrow(k) \cdot j_{\text{tot}}(k)}{|j_{\text{tot}}(k)|^2}, \quad (2.11)$$

where $j_{\text{tot}} = j_\uparrow + j_\downarrow$ is the total current carried by the quasiparticle. In the BCS theory, $n_j(k) = |v_k|^2$, it takes the values between zero and one, and the isoline $n_j(k) = 0.5$ coincides with the Fermi surface. In Fig. 2-3 we show the contour plots of $n_j(k)$ for different values of doping, together with the Fermi surface for the corresponding unprojected BCS wave functions. We see that the “effective Fermi surface” defined by $n_j(k)$ does not follow the original Fermi surface of the BCS state, but bends outwards in the $(0, \pi)$ regions. Thus it effectively acquires an inward curvature similar to the effect of the negative $t'$ hopping term.

### 2.2.2 Current as a function of doping

We noted earlier that the magnitude of the current has a maximum near the nodal point and that this maximum decreases as a function of doping. In Fig. 2-4, we plot the magnitude of the nodal current $j_{\text{nodal}} = j(k = (\pi/2, \pi/2))$ versus doping for both $10 \times 10$ and $20 \times 20$ systems. Because of our choice of boundary conditions,
we do not calculate the current at the true nodal point. For a 10×10 system, the “nodal point” is actually evaluated at \( k = (0.5\pi, 0.4\pi) \) and for a 20×20 system at \( k = (0.45\pi, 0.5\pi) \). In Fig. 2-4, we see that there is agreement to within the error between the data calculated for two lattices of different size, and we expect that the actual nodal current would also be within these errors.

In the 20×20 system, we can study the doping as low as 0.005 (2 holes), and our results indicate that the current apparently decreases down to zero with decreasing
Figure 2-4: Magnitude of the nodal current, $|j_{nodal}|$ measured in units of $t$, plotted as a function of doping. The solid lines are the data from a 10x10 lattice and the dashed lines from a 20x20 one. The lower curves are for the trial wave function for the $t$-$J$ model and the upper curves are for the trial wave function for the Hubbard model (to the lowest order in $t/U = 1/12$).

doping.

2.2.3 Rotation to the Hubbard model

So far we have studied the properties of fully projected wave functions. We would now like to extend our simulations from the $t$-$J$ model back to the Hubbard model. This can be done in the standard way by employing a unitary transformation $e^{is}$ that decouples the Hilbert space of the Hubbard Hamiltonian so that there are no matrix elements connecting those subspaces with different numbers of doubly occupied sites. Following MacDonald et al.[1], we determine this transformation as a power series in $(t/U)$, so that the subspaces are decoupled order by order. To the first order, the rotation generator is given by

$$iS = \frac{1}{U} (T_1 - T_{-1}) , \quad (2.12)$$

where $T_1$ and $T_{-1}$ are defined to be the parts of the kinetic energy operator that increase and decrease, respectively, the number of doubly occupied sites by one.

With the use of this rotation, we can replace computing the expectation value of any operator $O$ in the ground state of a Hubbard model by computing the expectation
value of the rotated operator \( e^{iS}Oe^{-iS} \) in the ground state of the \( t-J \) model. We use the same variational wave function for the \( t-J \) model as described above and compute the lowest-order correction (linear in \( t/U \)) to the \( t-J \) expectation value. This procedure has been applied, for example, in the work of Paramekanti et al. [26] for calculating the expectation value of the occupation-number operator.

We compute the rotation correction to the value of the nodal current and find that it does not qualitatively change its doping dependence. The corrected value of the current is plotted as the upper curves in Fig. 2-4 (for \( t/U = 1/12 \)).

### 2.2.4 Quasiparticle current renormalization \( \alpha \)

Beyond just studying the current itself, we are particularly interested in the quasiparticle current renormalization factor \( \alpha \). As we noted earlier the current and the slope of the dispersion are collinear within the error of our simulations, so we can define \( \alpha = j/v_k \).

We look at the quasiparticle current renormalization parameter \( \alpha \) as a function of doping. We are interested in \( \alpha \) for the lowest lying excitations, i.e., for those at the nodal point. Although we have calculated the Fermi velocity at the nodal point, more precise data for this velocity as a function of doping are available from the work by Yunoki et al. Ref. [19]. We use those Fermi velocity data in conjunction with our nodal current results to calculate \( \alpha \) at the nodal point.

In Fig. 2-5, we plot the nodal value of \( \alpha \) as a function of doping. We find that \( \alpha \) goes to zero at zero doping.

It is interesting to compare our results with the predictions of slave-boson theory. In this theory, the low lying excitations are \( x \) bosons which carry charge with an effective hopping matrix element proportional to \( t \) and fermions which carry spin with an effective hopping proportional to \( J \). These excitations are coupled to gauge fluctuations. When the gauge fluctuations are treated at the Gaussian level, we obtain the Ioffe–Larkin composition rule which states that the inverse of the superfluid density
Figure 2-5: The renormalization of the quasiparticle current $\alpha = |j_{\text{nodal}}|/v_F$ as a function of doping. The open circles are for runs on a $10 \times 10$ lattice and the solid ones are for runs on a $20 \times 20$ one. The solid line is the fit to the $20 \times 20$ data by Eq. (2.16) at $x^* = 0.09$.

$\rho_s = n_s/m$ is given by adding the inverses of the fermion and boson contributions:

$$\rho_s^{-1} = (\rho_s^F)^{-1} + (\rho_s^B)^{-1}$$

(2.13)

where $\rho_s^B \approx \pi t$ and $\rho_s^F \approx J(1 - aT)$ with $a \approx \Delta^{-1}$. [34] Note that the linear temperature dependence comes from thermal excitations of the nodal fermions. Expanding Eq. 2.13 at small $T$, we obtain

$$\rho_s(T) \approx \rho_s(0) - \frac{[\rho_s(0)]^2}{\rho_s^F(0)} aT.$$  

(2.14)

On the other hand, the quasiparticle dispersion is given by that of the fermions and we can identify $v_F/v_\Delta$ in Eq. 2.1 as being proportional to $aJ \sim a\rho_s^F(0)$. Comparison of Eq. 2.14 with Eq. 2.1 results in the simple expression

$$\alpha \sim \frac{\rho_s(0)}{\rho_s^F(0)},$$

(2.15)

in particular $\alpha \propto x(t/J)$ for $xt < J$. [35] We did not keep track of the numerical coefficients. If we assume that at full doping ($x = 1$) $\alpha$ should approach one (the
BCS value), Eq. (2.15) suggests the form

$$\alpha(x) = \frac{x}{x + x^*}(1 + x^*),$$  \hfill (2.16)

which for \(x^* = 0.09\) produces a qualitatively good fit of our results for \(\alpha\) (see Fig. 2-5). Note that the order-of-magnitude estimates above gives \(x^* \sim J/t\), and our best-fit value of \(x^*\) is several times smaller.

The shape and the magnitude of the current renormalization parameter \(\alpha\) as a function of doping is currently a topic of much experimental work. While there still remain large uncertainties in the experimental data, two useful comparisons can be made to our work. In Ref. [23], the measurements of thermal conductivity and of the penetration depth were used to determine the ratio \(v_F/v_\Delta\) and the superfluid density. Combining those data resulted in the the values of \(\alpha = 0.66\) and \(\alpha = 0.68\) for optimally doped samples of BSCCO and YBCO, respectively. Those numbers are in close agreement with our results around \(x = 0.15\) doping.

Our results also qualitatively agree with the decrease of \(\alpha\) as the doping decreases in underdoped YBCO, as reported in Refs. [24, 25]. However, earlier data on YBCO films indicated that the linear \(T\) slope of \(n_s/m\) is relatively insensitive to doping over a broad range of critical temperatures. [36, 37] Since \(v_F/v_\Delta\) decreases with decreasing \(x\) [38], this trend is in disagreement with Fig. 2-5 and Eq. (2.16). It will be desirable to have single crystal data for \(n_s(T)/m\) over a broad range of \(x\) to settle this point.

On the theoretical side, the recent study of a \(U(1)\) slave-boson theory with spinon-holon binding [39] predicted a sub-linear dependence of \(\alpha\) on the doping. The sub-linear form of \(\alpha(x)\) disagrees with our proposal (2.16), but is also consistent with our numerical results shown in Fig. 2-5.

We further look at \(\alpha\) along the Fermi surface for a given doping. We are interested in how the shape and size of this curve changes as a function of doping. While we expect the integral of the whole curve to decrease with \(x\), there are several possibilities for how this could occur. Two such scenarios are that the curve decreases in magnitude everywhere along the Fermi surface uniformly as doping decreases or that
\( \alpha \) is small almost everywhere along the Fermi surface but that there is a region of large \( \alpha \) around the nodal point whose width increases with \( x \). Our numerical results indicate the former of those scenarios. In the upper graph of Fig. 2-6, we plot the \( t-J \) model current magnitude along the Fermi surface. Due to the low finite resolution of our system, we just calculate the current at those points nearest to the line connecting \((\pi,0)\) and \((0,\pi)\). To calculate \( \alpha \), we use the value of \( v_F \) found by Yunoki \textit{et al.} [19] along the nodal direction for a given doping and accordingly renormalize the tight binding dispersion to calculate \( v_k \) along these points. We plot \( \alpha \) obtained in this way in the lower plot of Fig. 2-6. We see that \( \alpha \) is approximately flat along the Fermi surface.
2.3 Quasiparticle weight and Occupation Number

In this section we examine the quasiparticle weight $Z$ and the occupation number $n$ as a function of momentum and doping. The quasiparticle weight is defined as in Fermi liquid theory and gives a measure of how close our trial wave function quasiparticle is to being a free electron (or a free hole).

We begin with the definitions,

$$Z_+(k, \sigma) = \frac{|\langle \Psi_{\text{EX}} | c_{k,\sigma}^\dagger | \Psi_{\text{GS}} \rangle|^2}{\langle \Psi_{\text{EX}} | \Psi_{\text{EX}} \rangle}$$

(2.17)

$$Z_-(k, \sigma) = \frac{|\langle \Psi_{\text{EX}} | c_{k,\sigma} | \Psi_{\text{GS}} \rangle|^2}{\langle \Psi_{\text{EX}} | \Psi_{\text{EX}} \rangle}$$

(2.18)

where $|\Psi_{\text{EX}}\rangle$ also carries momentum $k$, and the electron operators are normalized as $\{c_{k,\sigma}, c_{k,\sigma}^\dagger\} = 1$. In the BCS theory (without Gutzwiller projection), $Z_+ = u_k^2$ and $Z_- = v_k^2$. Along the nodal diagonal (where the gap vanishes), $u_k^2 = 1$ outside the Fermi surface and 0 inside and $v_k^2$ is the opposite. If one defines $Z = Z_+ + Z_-$, then in the BCS model $Z = 1$ everywhere.

In the projected wave functions, these simple expressions do not apply. However, some of the properties of the spectral weights $Z_+$ and $Z_-$ may be still proven. Using the identity

$$P_D c_k^\dagger P_D = P_D c_k^\dagger$$

(2.19)

and the $d$-wave symmetry of the gap, we can prove that along the nodal diagonal,

$$Z_+ = 0 \quad \text{on} \quad (0,0) - (k_F, k_F),$$

(2.20)

$$Z_- = 0 \quad \text{on} \quad (k_F, k_F) - (\pi, \pi),$$

(2.21)

where $(k_F, k_F)$ is the nodal point. Furthermore, $Z_+$ may be rewritten as the ground-state expectation value

$$Z_+(k, \sigma) = \langle c_{k,\sigma} P_D c_{k,\sigma}^\dagger \rangle_{\text{GS}}.$$
Figure 2-7: Contour plots of $Z_+(\mathbf{k})$ in the $t$–$J$ model for dopings 0.03 (upper plot) and 0.21 (lower plot), 10 and 68 holes in a $18 \times 18$ system, respectively. The thick dashed lines denote the Fermi surface of the unprojected wave function, the big solid dot marks the position of the node. Crosses indicate data points used in plotting (available values of the $\mathbf{k}$ vector). In the upper plot, the contour lines correspond to $Z_+ = 0.01, 0.02, \ldots, 0.09$ (left to right – the maximal value of $Z_+$ is 0.09). In the lower plot, the contour lines are $Z_+ = 0.05, 0.10, \ldots, 0.35$ (with the maximal value $Z_+ = 0.38$).
Figure 2-8: **Upper plot:** contour plot of $Z_+(k)$ (or, equivalently, of $n(k)$) in the $t$–$J$ model at the doping 0.12 (24 holes in the 14×14 system). The isolines correspond to $Z_+ = 0.03, 0.06, \ldots, 0.27$ [$n(k) = 0.53, 0.50, \ldots, 0.29$ respectively, left to right]. The maximal value of $Z_+$ (near the node) is 0.27. **Middle plot:** $Z_H^+$ in the same system rotated to the Hubbard model (to the first order in $t/U = 1/12$), Eq. (2.28). The isolines correspond to $Z_H^+ = 0.05, 0.10, \ldots, 0.35$. The maximal value of $Z_H^+$ (near the node) is 0.37. **Bottom plot:** $n_k^H$ in the same system rotated to the Hubbard model (to the first order in $t/U = 1/12$), Eq. (2.29). The isolines are $n_k^H = 0.8, 0.7, \ldots, 0.2$ (left to right). The Fermi surface, the nodal point and the positions of data points are denoted in the same way as in Fig. 2-7.
We note that

\[ \langle c_i \sigma^+ c_j \sigma \rangle_{GS} = \langle c_i \sigma P c_j^\dagger \sigma \rangle_{GS} \quad i \neq j \]  
\[ = \langle c_i \sigma P c_j^\dagger \sigma \rangle_{GS} + n_{\sigma} \quad i = j. \]  

(2.23)

(2.24)

Thus \( Z_+(k, \sigma) \) is further related to the occupation number

\[ n_{k,\sigma} = \langle c_{k,\sigma}^\dagger c_{k,\sigma} \rangle \]  

(2.25)

as

\[ Z_+(k, \sigma) = \frac{1 + x}{2} - n_{k,\sigma}. \]  

(2.26)

This relation has also been given by Yunoki in Ref. [40]. In particular, from this relation follows the upper bound on the spectral weight \( Z_+ \):

\[ Z_+ \leq \frac{1 + x}{2} \]  

(2.27)

and, as a consequence, the same upper bound applies to the nodal spectral weight \( Z_{\text{nodal}} = Z_+(k_F + \epsilon, k_F + \epsilon) \) studied by Paramekanti et al. in Refs. [18, 26].

The quasiparticle weight \( Z_- \) requires a more complicated Monte Carlo calculation, since it cannot be rewritten as a simple ground-state average like (2.22). We therefore restrict ourselves to discussing only the quasiparticle weight \( Z_+ \).

The above relations for \( Z_+ \) have been derived for the fully projected wave function. If we perform a rotation to the Hubbard model, the relations (2.22) and (2.26) no longer hold, and the upper bound (2.27) cannot be proven. Specifically, for the Hubbard model we keep the same definitions of the quasiparticle weights and the occupation number (2.17), (2.18), (2.25), but with the ground and excited states rotated from the fully-projected state to the Hubbard-model state by the unitary rotation \( e^{-iS} \), as explained in the previous section. Then the lowest-order Hubbard-
model corrections to $Z_+$ and to $n_k$ may be easily computed as

\begin{equation}
Z_+^H = Z_+ + 2 \text{Re} \left\langle c_{k,\sigma} P_D [iS, c_{k,\sigma}^\dagger] \right\rangle \tag{2.28}
\end{equation}

and

\begin{equation}
n_k^H = n_k - 2 \text{Re} \left\langle c_{k,\sigma} [iS, c_{k,\sigma}^\dagger] \right\rangle. \tag{2.29}
\end{equation}

Even though the two expressions look nearly identical, the correction to $n_k$ does not contain an intermediate projector $P_D$ and, because of that, has a very different structure than that to $Z_+$. The relation between $Z_+$ and $n_k$ (2.26) no longer holds for the Hubbard model, as we shall see below.

Figs. 2-7 and 2-8 show $Z_+(k)$ for $x = 0.03, 0.12, \text{ and } 0.21$. As noted in Eq. (2.20), $Z_+$ is zero along the diagonal between (0, 0) and $(k_F, k_F)$ and jumps to a finite value $Z_{\text{nodal}}$ at the nodal point. The projected wave function inherits the essential singularity of $Z_+$ at the nodal point from the underlying BCS wave function. The value of $Z_{\text{nodal}}$ has been studied as a function of doping by Paramekanti et al. in Refs. [18, 26]. The doping dependence of $Z_{\text{nodal}}$ (Fig. 2 of Ref. [18] and Fig. 6 of Ref. [26]) is qualitatively similar to that we find for $\alpha$ (Fig. 2-5): both $Z_{\text{nodal}}$ and $\alpha$ decrease to zero with decreasing doping, with a strong upward curvature. However we are not aware of any a priori relation between $\alpha$ and $Z_{\text{nodal}}$.

Using (2.26), the plots of $Z_+(k)$ may also be interpreted as those of $n_k$ (see, e.g., the upper plot in Fig. 2-8). Note the region of depression in $n_k$ just outside the Fermi surface, which resembles a hole “pocket.” The existence of this pocket may already be inferred from the non-monotonous behavior of $n_k$ along the zone diagonal found in Refs. [18, 26] but the full $k$ dependence shown in Figs. 2-7 and 2-8 gives a more complete picture. Remarkably, a similar “pocket” structure has been found in the $U(1)$ slave-boson model with spinon-holon-binding by Ng [39]. The pocket is more pronounced at lower dopings and appears consistent with the bending of the “effective Fermi surface” defined in Section 2.2 from $n_j$, Eq. 2.11. However, to define a meaningful Fermi surface from the quasiparticle spectral weight, one needs an access also to the spectral weight $Z_-$ which goes beyond the scope of the present work.
Figure 2-9: Plot of $Z_+$ and $Z_+^H$, the solid and dashed lines respectively, along the nodal diagonal for an $18 \times 18$ system with 40 holes, $x = 0.12$. The data are calculated on the discrete grid points closest to the diagonal.

If we include the $t/U$ correction from the rotation to the Hubbard model, the pocket structure in $n_H^k$ disappears, see our Fig. 2-8 (lower plot) and Refs. [18, 26]. On the other hand, including the $t/U$ correction to $Z_+(k)$ preserves the pocket structure, see Fig. 2-8 (middle plot). This shows that in the Hubbard model the relation (2.26) between $Z_+^H(k)$ and $n_K^H$ no longer holds.

In Refs. [18, 26], it was reported that the rotation to the Hubbard model does not change the magnitude of the the jump in $n_k$ at the Fermi surface. Our results on $n_k$ and $n_K^H$ confirm this statement, however the spectral weight defined as $Z_+$ increases when rotated to the Hubbard model. In Fig. 2-9, we show $Z_+$ and $Z_+^H$ along the nodal diagonal for an $x = 0.12$ system.

### 2.4 Conclusion

In this chapter, we have studied hole doping of the strong coupling limit of the the Hubbard model. In particular, we have analyzed the properties of the excited states in the $t$–$J$ model and, to lowest order, the Hubbard model using the framework of Gutzwiller-projected variational wave functions. The quantities of main interest are the renormalization of the current and spectral weight of the quasiparticles. Both those renormalizations decrease with decreasing doping and exhibit strongly non-BCS behavior. We also find that the total current is renormalized approximately
uniformly along the Fermi surface.

The renormalization of the quasiparticle current allows us to define the effective Fermi surface as a crossover region between the electron- and hole-supported current. We observe that such a Fermi surface bends outwards in the $(0, \pi)$ regions. Such a curvature has been observed in ARPES measurements (see, e.g., Ref. [41] for a recent data on LSCO) and is normally ascribed to a negative-$t'$ hopping term. Our observation of an effective renormalization of the Fermi surface by projection suggests another possibility: that the observed hole-like shape of the Fermi surface may appear as a result of strong correlations in a $t-J$ (or Hubbard) Hamiltonian with only nearest-neighbor hopping.

We can further see a signature of the Fermi-surface renormalization in the quasiparticle spectral weight $Z_+(\mathbf{k})$. This spectral weight is peaked near the nodal point and exhibits a pocket-like structure with this feature becoming more pronounced at lower doping values. We now assume that $Z = Z_+ + Z_-$, where $Z_+$ and $Z_-$ are related to $Z$ as in the BCS case, i.e. $Z_+ = Z u_k^2$ and $Z_- = Z v_k^2$. If we now further assume that the total $Z$ is a relatively smooth function of $\mathbf{k}$, then the shape of the pocket is due to the structure of $u$. Since $u_k^2 = \frac{1}{2}(1 + \frac{\partial u}{\partial k})$, we see that the shape of $u$ is dependent on the underlying dispersion. The shape of the pocket in $Z_+$ thus implies a dispersion that has an outward curving Fermi surface. This is consistent with the results from the renormalized outward curving Fermi surface. This is consistent with the shape of the pocket in $Z_+$.

Having looked at the shape of the pocket in $Z_+$, we now examine its origin. At half-filling the projected staggered-flux (SF) state [30] is identical to the projected d-wave BCS state. Therefore, we expect that away from half-filling but still at low dopings that $n(\mathbf{k})$ in the two states are similar. In the SF state, we know that there are Fermi pockets around $(\pi/2, \pi/2)$, thus we expect some semblance of these pockets in $n(\mathbf{k})$ for the projected d-wave state. Using the relation in the $t-J$ model between $n$ and $Z_+$, we see that this is consistent with the the pocket structure that we found and points to a possible source. We also note that, since the peak falls off smoothly with increasing $|k|$, it agrees with the proposal of Wen and Lee that the Fermi arc is
part of a pocket where the backside arc is unobservable because it has a much lower spectral weight. [21]

Finally, comparing the results for the $t$–$J$ model and for the Hubbard model (to the lowest order in the $t/U$ correction), we find that the rotation to the Hubbard model does not qualitatively affect the renormalizations of the quasiparticle spectral weight and of the current.

In this chapter, we have studied the $t$–$J$ model on the square lattice as a function of doping. We have looked at the d-wave superconducting phase that exists at finite hole concentrations and investigated its low-energy excitations and transport properties. In the following chapters, we return to the half-filled Hubbard model and consider instead smaller values of $U/t$ and lattices with a higher degree of frustration. This leads us to consider the properties of the paramagnetic insulating spin liquid phase. Motivated by a particular experimental system, we now turn to study the transport properties of a system of Fermionic spinons coupled to a $U(1)$ gauge field.
Chapter 3

Transport Properties of a spinon
Fermi surface coupled to a U(1)
gauge field

3.1 Introduction

The organic compounds $\kappa$-(BEDT-TTF)$_2$-$X$ are an interesting class of materials. These large organic molecules form a quasi two-dimensional system that can be effectively modeled by the spin 1/2 Hubbard model on an anisotropic triangular lattice. Like the cuprates, these systems are found to exhibit insulating, superconducting, and metallic phases. Unlike the cuprates the system here always remains at half-filling and the relevant external parameter is the pressure. As the pressure increases, $t$ increases and the system moves towards the metallic phase. Through the choice of the anion $X$, one can modify the anisotropy of the hopping and also the ambient value of $U/t$. Initially, all of the anions tried led to zero temperature states that were either superconductors or antiferromagnetic insulators. However, consideration of the anion $X = \text{Cu}_2(\text{CN})_3$ was found to have many interesting features.

These recent experiments have shown promise that the particular compound $\kappa$-(BEDT-TTF)$_2$-$\text{Cu}_2(\text{CN})_3$ maybe the first experimentally realized spin liquid in di-
mension greater than one. Unlike for other anions, this material can be described as an effectively isotropic spin 1/2 system on a triangular lattice and thus exhibits the strongest frustration. It is found experimentally to be insulating and shows no evidence of long range magnetic order down to mK temperatures. Fitting the susceptibility using the high temperature series expansion of the spin 1/2 Heisenberg model on a triangular lattice, the exchange coupling $J$ is roughly $250K$. The static spin susceptibility also remains finite down to the lowest temperatures measured. Because of the lack of magnetic order even at temperatures many orders of magnitude lower than the exchange coupling $J$ and the experimental evidence for abundant low energy spin excitations, there has been a proposal that this system may be well described by a spin-liquid where a spinon Fermi surface is coupled to a $U(1)$ gauge field. We start with a Lagrangian describing such a two dimensional system and proceed to develop a version of the quantum Boltzmann equation (QBE). Despite potential pitfalls that we discuss below, we show that the QBE is well-defined and apply it to systems with steady-state thermal and spin currents. We show that the transport coefficients are finite and in particular calculate the temperature dependence of the spin resistivity and the more experimentally accessible thermal conductivity.

We begin by considering the $t-J$ model on the triangular lattice. We construct a mean-field state by applying the slave-boson formalism and enforcing the local constraint of no double occupancy exactly. It is known that considering fluctuations around this mean-field state leads to a $U(1)$ gauge theory. More recently, the slave-rotor representation has been applied to the Hubbard model on a triangular lattice and it was shown that again one can arrive at a $U(1)$ gauge theory. Because of the large number of low energy excitations due to presence of the spinon Fermi surface, we assume that a deconfined state occurs and thus we consider a non-compact $U(1)$ gauge theory. In other words, we assume that instanton effects are negligible. Thus our starting point is the Lagrangian for a 2-D spinon Fermi surface system coupled to a non-compact $U(1)$ gauge field given by

$$\mathcal{L} = \psi_\sigma^* \left( \partial_0 - i a_0 - \mu \right) \psi_\sigma + \frac{1}{2m} \psi_\sigma^* \left( -i \nabla - a \right)^2 \psi_\sigma,$$  \hspace{1cm} (3.1)
where the gauge field kinetic energy term has been dropped because its strength is inversely proportional to the charge gap which is large since we are assuming we are in the insulating phase. $\psi_\sigma$ is the spinon field and the gauge field is $a = (a_0, a)$. $\mu$ is the chemical potential. We work in Coulomb gauge $\nabla \cdot a = 0$.

We can then proceed to integrate out the spinons in order to generate dynamics for the gauge field. This cannot be done exactly; however, we can work in the Gaussian approximation also known as the random-phase approximation (RPA). We then consider spinons coupled to the effective action for the gauge field coming from the spinon bubbles. The use of the RPA can be formally arranged in the standard way through the $1/N$ expansion by introducing $N$ species of fermions.[43]

The longitudinal part of the gauge propagator is related to the density-density response and thus does not show any singular behavior for low energies and momentum. The transverse part however does give rise to long range interactions. After integration, we find that the effective action for the gauge field is $S(a) = \sum_q \Pi(q) a_q^\dagger a_q$, where

$$\Pi(q) = \frac{\gamma \nu_F q_0}{\sqrt{\nu_F^2 q^2 + q_0^2 + q_0}} + \chi_D q^2,$$  \hspace{1cm} (3.2)

where $\chi_D = \frac{1}{4\pi m}$ and $\gamma = \frac{k_F}{\pi}$. Details of this calculation are presented in the appendix. Thus the effective gauge field propagator is given by $D(q) = \Pi(q)^{-1}$. Rotating back to real time, $q_0 = i\nu$, and working in the limit that $\nu \ll \nu_F q$, the gauge propagator becomes

$$D(q, \nu) = \frac{1}{-i\gamma q + \chi_D q^2},$$  \hspace{1cm} (3.3)

where $q$ is now the magnitude of $q$.[34, 13]

For the remainder of the chapter we consider the effective theory given by taking the Lagrangian of Eq. 3.1 and adding gauge field dynamics through the RPA propagator of Eq. 3.3. This particular gauge theory has been studied previously in the context of the half-filled Landau level (Ref. [44]) and high-temperature superconductors (Refs. [13] and [45].) In particular, the spinon self-energy correction due to the RPA gauge propagator has been examined. Again one finds that the most singular correction comes from considering the transverse gauge field fluctuations. To one-
loop order, the self-energy $\Sigma(k, \omega)$ is found to be $\text{Re}\Sigma \sim \text{Im}\Sigma \sim \omega^{2/3}$. We note that this implies a vanishing quasiparticle spectral weight, i.e. the Landau criterion for quasiparticles is violated and thus the Fermi liquid picture is invalid for this system. Moreover, the effective mass is found to diverge at the Fermi surface as $\xi_k^{-1/3}$ where $\xi_k = \epsilon_k - \mu = k^2/2m - \mu$.\[44\]

Despite the fact that quasiparticles are ill-defined in this system, we examine the standard expressions for the spin resistivity and thermal conductivity. The spin resistivity is given by $\rho_S = \frac{m}{n\tau}$ where $1/\tau$ is the momentum relaxation rate. From the self-energy correction to the fermion propagator, we calculate the momentum relaxation rate $1/\tau \sim T^{-4/3}$.\[13\] Beyond the assumption of the validity of the quasiparticle picture, in order to arrive at $\rho_S$, we also need to consider the effective rather than bare mass for the spinons; however, as mentioned above the effective mass is divergent. In section IV, we find that $\rho_S \sim T^{4/3}$, a result which is consistent with the calculation when the quasiparticles are assumed to be well-defined and the renormalization of the mass is ignored.

The standard simple result for the thermal conductivity gives $\kappa \sim Cv^2\tau_E$ where $C$ is the specific heat, $v$ is the particle velocity and $1/\tau_E$ is the energy relaxation rate. Again from the self-energy correction to the spinon propagator, we calculate the energy relaxation rate $1/\tau_E \sim T^{2/3}$.\[13\] For a system of fermions $C = \gamma T$ and the velocity would be temperature independent. Thus $\kappa/T \sim T^{-2/3}$. However this result is again not justified in view of the divergent effective mass and lack of well-defined quasiparticles. Considering the mass renormalization leads to a specific heat $C \sim T^{2/3}$ and thus $\kappa/T \sim T^{-1}$; moreover, the velocity goes to zero as the effective mass diverges. Thus it is unclear how to proceed. In section 3.5, we see that the power law $T$ dependence of the thermal conductivity given by the naive arguments ignoring the effects of the effective mass turns out to be correct.

Because of these issues, we are forced to consider the interactions between the spinons and gauge bosons more carefully and thus turn to a quantum Boltzmann description of the system. As mentioned above, we cannot derive a QBE using the Landau quasiparticle picture because Fermi-liquid theory is invalid for this system.
We find however that we can proceed by following the work of Prange and Kadanoff who studied the electron-phonon system at temperatures high compared to the Debye temperature. [46] At high temperatures, the electrons rapidly emit phonons so that their precise energy is not well defined. Thus they deal with an analogous situation where the quasiparticle picture breaks down. Closely following their work, we find that if the self-energy at small frequencies is independent of $\xi_k$, we can define a generalized distribution function and derive a closed equation describing the dynamics of this generalized distribution function. This equation is analogous to the standard Fermi-liquid QBE. We note that the derivation of the QBE for this system is very closely related to the work done by Kim et al. in Ref. [47] studying the $\nu = 1/2$ fraction quantum Hall state, except that we derive the QBE in a different coordinate system and linearize in a different way, which allows us to use variational methods to calculate the transport properties. Note that a similar derivation of the QBE for generalized distribution functions is also considered in the work by Mahan.[48]

3.2 Deriving the QBE

To derive the QBE for this system, we work in the standard non-equilibrium Green’s function formulation. We begin with two matrices of Green’s functions $\tilde{G}$ and $\tilde{\Sigma}$ that satisfy Dyson’s equation

$$\tilde{G} = \tilde{G}_0 \tilde{\Sigma} \tilde{G},$$ (3.4)

where

$$\tilde{G} = \begin{bmatrix} G_t & -G^< \\ G^> & -G_t^< \end{bmatrix}$$ (3.5)

with $\tilde{\Sigma}$ defined similarly. Note that following Ref. [50], in Eq. 3.4 the product of two functions actually implies an integration over a shared space-time variable. Also here
we use the standard definitions, following Refs. \[49\] and \[50\],

\[
G^>(x_1, x_2) = -i \left\langle \psi(x_1) \psi^\dagger(x_2) \right\rangle \tag{3.6}
\]
\[
G^<(x_1, x_2) = i \left\langle \psi^\dagger(x_2) \psi(x_1) \right\rangle \tag{3.7}
\]
\[
G_t(x_1, x_2) = \Theta(t_1 - t_2) G^>(x_1, x_2) + \Theta(t_2 - t_1) G^<(x_1, x_2) \tag{3.8}
\]
\[
G_t(x_1, x_2) = \Theta(t_2 - t_1) G^>(x_1, x_2) + \Theta(t_1 - t_2) G^<(x_1, x_2), \tag{3.9}
\]

with associated self energies \(\Sigma^>, \Sigma^<, \Sigma_t\) and \(\Sigma_i\). Here \(x = (r, t)\). \(G_0\) denotes the non-interacting Green’s functions. These Green’s functions are related to the standard retarded \((G^R)\) and advanced \((G^A)\) Green’s functions through

\[
G^R = G_t - G^< = G^> - G_t \tag{3.10}
\]
\[
G^A = G_t - G^> = G^< - G_t. \tag{3.11}
\]

We perform a change of variables so that all the Green’s functions are expressed in terms of relative and center of mass like coordinates. Throughout this chapter, we work with the Fourier transform of the relative coordinates so that we can write \(G^<(k, \omega, r, t)\).

For a general system of fermions in thermal equilibrium, we can write that

\[
G^<(k, \omega) = i f_0(\omega) A(k, \omega) \tag{3.12}
\]
\[
G^>(k, \omega) = -i(1 - f_0(\omega)) A(k, \omega) \tag{3.13}
\]

where \(f_0(\omega)\) is the Fermi distribution function at some temperature \(T\). \(A(k, \omega) = -i(G^R(k, \omega) - G^A(k, \omega))\) is the spectral function given by

\[
A(k, \omega) = \frac{-2 \text{Im} \Sigma^R(k, \omega)}{[\omega - \xi_k - \text{Re} \Sigma^R(k, \omega)]^2 + (\text{Im} \Sigma^R(k, \omega))^2}. \tag{3.14}
\]

In Fermi liquid theory, the quasiparticles are well defined because \(\text{Im} \Sigma^R \sim \omega^2 \ll \omega\)
for small $\omega$. This means that the equilibrium spectral function is sharply peaked as a function of $\omega$, so that ignoring the incoherent background, it can be written as

$$A(k, \omega) = 2\pi \delta (\omega - \xi_k - \text{Re}\Sigma^R(k, \omega)). \quad (3.15)$$

In this chapter we are considering linear response, so we assume that the system is slowly varying in space and time and that therefore there is a notion of a local equilibrium temperature $T$ for every $(r, t)$. Assuming that the system remains close enough to equilibrium that the sharp $\omega$ peaking of the spectral weight remains valid, the standard Landau quasiparticle QBE for the fermion distribution function $f(k, r, t)$ then follows.

As mentioned in the Introduction, in this model which is described by Eqs. 3.1 and 3.3, both the real and the imaginary parts of the self-energy of the spinons scale as $\omega^{2/3}$ for small $\omega$. This violation of the Landau criterion for the existence of well-defined quasiparticles invalidates the normal derivation of the QBE since the spectral weight is no longer sharply peaked in $\omega$ and thus cannot be written in the form of Eq. 3.15.

We find that we can still proceed to derive a QBE for this system due to the form of the self-energy. First we change variables from $k$ to $\xi \equiv \xi_k$ and $\hat{k}$. Then we note that since the self-energy is independent of the magnitude of $k$, we can write $\Sigma^R(k, \omega) = \Sigma^R(\hat{k}, \omega)$, and that then for small enough $\omega$, $A(k, \omega)$ is a peaked function of $\xi$ around $\xi = 0$. This property of the invariance of the self-energy with the magnitude of $k$, i.e. that it is only a function of $\omega$ and $\hat{k}$, is exactly the same property that Prange and Kadanoff used in Ref. [46] to derive a generalized QBE for the electron-phonon system that is valid at temperatures high relative to the Debye temperature.

Following the work of Ref. [46], we assume that the system remains close enough to local equilibrium that the self-energy is independent of $\xi$ at all times. Combining this assumption with the fact that the $\int \frac{d\xi}{2\pi} A = 1$, it follows that $G^<$ and $G^>$ are sharply peaked functions of $\xi$. Integrating over the region of peaking in $\xi$, we can
then define the generalized distribution function $f(\hat{k}, \omega, r, t)$ as

$$
\int \frac{d\xi}{2\pi} \left[ -i G^<(\xi, \hat{k}, \omega, r, t) \right] = f(\hat{k}, \omega, r, t),
$$

(3.16)

where $f(\hat{k}, \omega, r, t)$ is the density of spinons with momentum in the $\hat{k}$ direction, energy $\omega$ at a given position $r$ and time $t$. Similarly we have

$$
\int \frac{d\xi}{2\pi} \left[ i G^>(\xi, \hat{k}, \omega, r, t) \right] = 1 - f(\hat{k}, \omega, r, t).
$$

(3.17)

Having established the definition of the generalized distribution function in a system without well-defined Landau quasiparticles, we now proceed to derive the QBE that governs this distribution. We begin with the matrix form of Dyson’s equation (Eq. 3.4.) In particular, we need to derive the equation of motion for $G^<$. After a standard short derivation, see for instance Refs. [50] and [47], and working in the gradient expansion, we arrive at the expression,

$$
\left[ \omega - \frac{k^2}{2m} - \text{Re} \Sigma^R, G^< \right] - [\Sigma^<, \text{Re} G^R] = \Sigma^> G^< - G^> \Sigma^<,
$$

(3.18)

which describes the evolution of $G^<$. Here $[A, B]$ is a generalized Poisson bracket defined as

$$
[A, B] = \frac{\partial A}{\partial \omega} \frac{\partial B}{\partial t} - \frac{\partial A}{\partial t} \frac{\partial B}{\partial \omega} + \nabla_r A \cdot \nabla_k B - \nabla_k A \cdot \nabla_r B.
$$

(3.19)

Note that in Eq. 3.18, we have suppressed the variables $(k, \omega, r, t)$ for the self-energies and Green’s functions.

From standard perturbation theory working to one-loop order, the self-energies
\( \Sigma^< \) and \( \Sigma^> \) are given by

\[
\Sigma^< = \sum_q \int_0^\infty \frac{d\nu}{\pi} \left| \frac{k \times \hat{q}}{m} \right|^2 \text{Im} D(q, \nu) \times \\
[(n_0(\nu) + 1)G^<(k + q, \omega + \nu) + n_0(\nu)G^<(k + q, \omega - \nu)]
\]

\[
\Sigma^> = \sum_q \int_0^\infty \frac{d\nu}{\pi} \left| \frac{k \times \hat{q}}{m} \right|^2 \text{Im} D(q, \nu) \times \\
[n_0(\nu)G^>(k + q, \omega + \nu) + (n_0(\nu) + 1)G^>(k + q, \omega - \nu)],
\]

where for notation convenience, we have dropped the variables \((r, t)\). Note that we have assumed that the gauge bosons are always in local thermal equilibrium and that \(n_0(\nu) = 1/(e^{\beta\nu} - 1)\), the standard boson equilibrium distribution function at temperature \(T\). We therefore are studying the contributions to the transport coefficients arising from spinons. In Section 3.6 we study the validity of this assumption for the particular case of the thermal conductivity.

To derive the QBE for the generalized distribution function defined in Eq. 3.16, we need to write Eq. 3.18 in terms of \(f(k, \omega, r, t)\). We integrate both sides of Eq. 3.18 over the magnitude \(\xi\) and rely on the assumption of the peaking as a function of \(\xi\). From the Kramer’s Kroenig relation,

\[
\text{Re} G^R(k, \omega) = -\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Im} G^R(\xi, k', \omega')}{\omega - \omega'}.
\]

Since \(-2 \text{Im} G^R = A\), the condition that \(\int \frac{d\xi}{2\pi} A = 1\) implies that

\[
\int \frac{d\xi}{2\pi} \text{Re} G^R = \mathcal{P} \int \frac{d\omega'}{2\pi} \frac{1}{\omega - \omega'} = 0.
\]

Therefore with the assumption that \(\Sigma^<\) is independent of \(\xi\), we can drop the second term on the LHS in Eq. 3.18 and we are left with

\[
\int d\xi \left[ \omega - \frac{k^2}{2m} - \text{Re} \Sigma^R, G^< \right] = \int d\xi (\Sigma^> G^< - G^> \Sigma^<).
\]

We expand the remaining generalized Poisson bracket on the LHS and the QBE
becomes,

\[
\int d\xi \left[ \left( 1 - \frac{\partial \text{Re}\Sigma^R}{\partial \omega} \right) \frac{\partial G^\prec}{\partial t} + \frac{\partial \text{Re}\Sigma^R}{\partial t} \frac{\partial G^\prec}{\partial \omega} - \nabla_r \text{Re}\Sigma^R \cdot \nabla_k G^\prec + \nabla_k \left( \epsilon_k + \text{Re}\Sigma^R \right) \cdot \nabla_r G^\prec \right] = I_{\text{coll}},
\]

where the collision integral, \( I_{\text{coll}} \), is defined below. Using our assumptions that the self-energies depend only on \( \omega \) even when the system is not in equilibrium and that \( G^\prec \) remains a well-peaked function of \( \xi \), we can perform the integration over \( \xi \) and find that

\[
\left( 1 - \frac{\partial \text{Re}\Sigma^R}{\partial \omega} \right) \frac{\partial f}{\partial t} + \frac{\partial \text{Re}\Sigma^R}{\partial t} \frac{\partial f}{\partial \omega} - \nabla_r \text{Re}\Sigma^R \cdot \nabla_{kF} f + \nabla_{kF} \left( \epsilon_k + \text{Re}\Sigma^R \right) \cdot \nabla_r f = I_{\text{coll}}.
\]

where \( I_{\text{coll}} \) and \( \Sigma \) now contain the generalized distribution function \( f(\hat{k}, \omega, r, t) \) instead of the associated Green's functions. We have introduced the notation \( \nabla_{kF} g(k, \omega) \) which is defined as \( \nabla_k g(k, \omega) \) evaluated at \( k = kF \hat{k} \). Note that the term \( \nabla_{kF} \text{Re}\Sigma^R \cdot \nabla_r f \) is not zero in general because the self-energy can still depend on \( \hat{k} \), however, for this particular model the self-energy only depends on \( \omega \) so this term can be dropped.

Eq. 3.26 is the full QBE for the generalized distribution function \( f(\hat{k}, \omega, r, t) \). We see that despite the lack of a well-defined quasiparticle, this QBE looks very similar to the standard QBE derived for Landau Fermi liquid theory. Instead of the normal energy variable \( \epsilon_k \), the QBE now contains \( \omega \) which is independent of \( \hat{k} \). Moreover the QBE now involves renormalized time and energy derivatives of the distribution function.[46]

We are interested in calculating the transport coefficients in the linear response regime. In fact, we have already assumed that the deviations from equilibrium are small, so that the generalized distribution functions are well-defined even out of equilibrium. We therefore proceed to linearize the QBE of Eq. 3.26. By linearizing the QBE in a particular way, we are able to use a variational method to estimate the transport coefficients. Focusing on the RHS of Eq. 3.26, i.e. the collision integral,
we introduce \( k' \) and \( \omega' \) as the energy and momentum of the intermediate spinon in the 1-loop self-energy diagram and find that the collision term, after the integration over \( \xi \) from Eq. 3.24, becomes

\[
I_{\text{coll}} = N(0) \int d\omega' d\hat{k}' d\nu d\hat{q} \text{Im} D(\mathbf{q}, \nu) \left| \frac{\mathbf{k}' \times \hat{q}}{m} \right|^2 \delta(k_F \hat{k}' - k_F \hat{k} - \mathbf{q}) \times
\]

\[
\left\{ \delta(\omega' - \omega - \nu) \left[ n_0(\nu)(1 - f(\hat{k}', \omega'))f(\hat{k}, \omega) - (n_0(\nu) + 1)(1 - f(\hat{k}, \omega))f(\hat{k}', \omega') \right] +
\delta(\omega' - \omega + \nu) \left[ (n_0(\nu) + 1)(1 - f(\hat{k}', \omega'))f(\hat{k}, \omega) - n_0(\nu)f(\hat{k}', \omega')(1 - f(\hat{k}, \omega)) \right] \right\},
\]

(3.27)

where \( N(0) = m/\pi \) is the density of states at the Fermi level for the up and down spins combined. Here we have rearranged the terms from \( \Sigma^> \) and \( \Sigma^< \) into the two processes corresponding to absorbing and emitting a gauge boson of energy \( \nu \). Note that from Eq. 3.3,

\[
\text{Im} D(\mathbf{q}, \nu) = \frac{\gamma \nu q}{\gamma^2 \nu^2 + \chi_D^2 q^4},
\]

(3.28)

where \( q = |\mathbf{q}| \).

We define \( f(\hat{k}, \omega) = f_0(\omega) + \delta f(\hat{k}, \omega) \), where \( f_0(\omega) \) is some local equilibrium distribution,

\[
f_0(\omega, r, t) = \frac{1}{e^{\beta(r,t)(\omega - \mu(r,t))} + 1}.
\]

(3.29)

We re-iterate that all of the distribution functions both in and out of equilibrium are also functions of \( r \) and \( t \). In particular the local equilibrium distribution \( f_0(\omega) \) can depend on space and time through the local temperature, \( \beta(r,t) \). This local equilibrium solution has the property that it sets the collision terms on the RHS of the QBE to be zero.[49] Thus from detailed balance, we derive the relations

\[
n_0(1 - f'_0)f_0 = (n_0 + 1)(1 - f_0)f'_0
\]

(3.30)
and

\[(n_0 + 1)(1 - f'_0)f_0 = n_0f'_0(1 - f_0),\]  

(3.31)

for the $\delta(\omega' - \omega - \nu)$ and $\delta(\omega' - \omega + \nu)$ processes respectively. Note that for notational convenience we have introduced the definitions $n_0 \equiv n_0(\nu)$, $f_0 \equiv f_0(\omega)$ and $f'_0 \equiv f_0(\omega')$. We expect that for a fermion system the deviation from equilibrium $\delta f(\mathbf{k}, \omega)$ is sharply peaked around the Fermi surface, $w = \mu$. Therefore, we introduce a new function $\phi(\mathbf{k}, \omega)$ defined by

\[f = f_0 - \phi \frac{\partial f_0}{\partial \omega}\]  

(3.32)

\[= f_0 + \phi\beta f_0(1 - f_0).\]  

(3.33)

Thus the function $\phi$ is much smoother than the original $\delta f$. Writing the generalized distribution function in this way is also critical in deriving the variational method that we use to calculate the transport properties.

Since we know that the local equilibrium distributions set the collision terms to be zero, we can expand out the distribution functions and using Eqs. 3.30 and 3.31 find that

\[I_{\text{coll}} = \int d\omega' d\mathbf{k}' d\nu d\mathbf{q} \text{ Im} D(\mathbf{q}, \nu) \times \left| \frac{\mathbf{k}' \times \mathbf{q}}{m} \right|^2 \delta(k_F \mathbf{k}' - k_F \mathbf{k} - \mathbf{q}) \times \]

\[\{ \delta(\omega' - \omega - \nu)\beta(\phi - \phi')n_0f_0(1 - f'_0) + \delta(\omega' - \omega + \nu)\beta(\phi - \phi')n_0(1 - f_0)f'_0 \},\]  

(3.34)

where $\phi \equiv \phi(\mathbf{k}, \omega)$ and $\phi' \equiv \phi(\mathbf{k}', \omega')$.

### 3.3 Finite Temperature

Before proceeding to calculating the transport coefficients using the linearized QBE, we must consider carefully what happens at finite temperatures in this system. This problem was addressed by Kim et al. in Ref. [47]. We explain their argument here so
that we can see how it effects our derivation of the QBE and later our derivation of
the transport coefficients. While in principle the derivations in section 3.2 are valid
for both zero and finite temperatures, in this system we need to take special care at
finite temperatures because at any finite temperature T, the self-energy, ImΣ^R(k, ω),
is divergent even in equilibrium.[13] This is an infrared divergence and since it arises
when the small q and ω limits have been treated exactly in cannot be alleviated
through some sort of cutoff. One can show in fact that this divergence is an artifact
of gauge invariance in the system.

The divergence of the self-energy implies that the spectral weight A(k, ω) and the
Green's functions are technically not well defined at finite temperature, which seems
to invalidate the basis of our derivation of the QBE. This problem can be addressed
however by carefully considering the source of this divergence. In particular, we see
that the source of the divergence is the gauge field fluctuations where the energy
carried by the gauge field ν is such that ν < T. We proceed then by breaking up
the gauge field fluctuations into two pieces. Following Kim, we define a_+(q, ν) to be
the fluctuations for ν > T and a_-(q, ν) to be the fluctuations for ν < T. We then
treat the a_- field as a vector potential which corresponds to a static applied random
magnetic field b_- = V × a_. We only consider the dynamics of the a_+ field. It is then
understood that all equations need to be averaged over all possible configurations of
this random magnetic field b_-.

Kim et al. showed that after breaking up the gauge field one can regain the
original QBE if the momentum k is shifted to k_- = k - a_- and the self-energy is
understood to only include fluctuations of the a_+ field. Since the self-energy now
contains only fluctuations with ν > T, it is no longer divergent. One then recovers
the original QBE of Eq. 3.25 with an additional term on the LHS

\[ \frac{k_-}{m} \cdot b_- \times \nabla_{k_-} G^< \]  

(3.35)
corresponding to an applied random field b_- . The original divergence of the full self-
energy can be understood as a consequence of the non-gauge invariance of the original
Green’s function. We note that the extra term added to the QBE by breaking up the
gauge fluctuations depends only on the gauge invariant quantity \( b_- \) and not on the
potential \( a_- \).

We now proceed to consider the effect of this applied random field on transport
calculations using the linearized QBE that we have derived. In principle, we calculate
the transport properties separately for each possible configuration of the random field
and then averages over them all. Because of this averaging, the field \( b_- \) cannot give
rise to a linear response unlike an applied “electric field” or thermal gradient. It
can however affect the transport coefficients of these quantities by contributing an
additional source of scattering. We can estimate the effect of this scattering by
calculating a scattering rate due to \( a_- \) fluctuations. Kim et al. show that these
fluctuations give rise to a scattering rate \( \tau^{-1} \sim T^{4/3} \). We can then use this estimate
to calculate how this scattering affects the low temperature forms of the transport
coefficients.

### 3.4 Spin Resistivity

The first transport property that we calculate is the spin resistivity. While less
experimentally accessible than the thermal conductivity, it is technically simpler and
thus serves to illustrate our method. We assume that there is some uniform applied
force field \( F \) that couples linearly to the spinons. One possible way of realizing such
a field is by applying a spatially varying magnetic field. Assuming that \( B \) is uniform
along one direction and has a constant slope along the other direction, the spinons
see a uniformly applied force field, \( F = \nabla B \). This field pushes up spins and down
spins in opposite directions and thus leads to a net spin current, \( J_s \).

This effective applied force field \( F \) couples to the spinons just as an electric field
couples to an electron with unit charge. Thus we can borrow the result from a system
of electrons in an applied electric field to determine the form of the driving term in
the QBE. Following the work of Mahan in Ref. [48], we find that in the presence
of a scalar potential, the energy of the particle depends on its location, where as in
steady state we expect the system to be spatially uniform. Mahan shows that this problem can be eliminated through a change of variables which has the secondary effect of changing the derivative $\nabla_r$ to $\nabla_r + \mathbf{F} \frac{\partial}{\partial \omega}$. This change of variables generates the driving term in the LHS of the QBE.

We again linearize the QBE using the earlier definitions of $f_0(\omega, r, t)$ and $\phi(\mathbf{k}, \omega, r, t)$. Since the applied force field $\mathbf{F}$ is independent of position and time, we expect that the steady state solutions for both $f_0(\omega)$ and $\phi(\mathbf{k}, \omega)$ are independent of $r$ and $t$. Thus returning to Eq. 3.26, we see that the first two terms are zero. Using the spatial invariance of the distribution functions and the fact that the equilibrium distribution function is independent of $\mathbf{k}$, we are left with

$$-\mathbf{F} \cdot \mathbf{k} v_F \frac{\partial f_0}{\partial \omega} = I_{\text{coll}}.$$  

(3.36)

This is the QBE that we consider for calculating the spin resistivity. Note that all of the terms containing the self-energy on the LHS have disappeared from the QBE. Thus the divergent effective mass does not even enter this calculation and should have no effect on the spin resistivity. We also note that Eq. 3.36 is almost identical to the linearized Boltzmann equation in an applied electric field with the change that $\mathbf{k}$ is now $(\mathbf{k}, \omega)$. Thus we proceed by following Ref. [51] to derive a variational method for calculating the transport coefficients.

We begin with defining the LHS of the linearized QBE, here Eq. 3.36, to be $X(\mathbf{k}, \omega)$. We then rewrite the collision term by defining a function $P(\mathbf{k}, \omega, \mathbf{k}', \omega')$ that is the analogue of the equilibrium transition rate between the states $(\mathbf{k}, \omega)$ and $(\mathbf{k}', \omega')$. Therefore the linearized QBE of Eq. 3.36 can be written as

$$X(\mathbf{k}, \omega) = N(0) \int d\mathbf{k}' d\omega' (\phi - \phi') P(\mathbf{k}, \omega, \mathbf{k}', \omega').$$  

(3.37)

In order to proceed to derive the variational method we first define an inner product of functions of $(\mathbf{k}, \omega)$ given by

$$\langle g, h \rangle = N(0) \int d\mathbf{k} d\omega \ g(\mathbf{k}, \omega) h(\mathbf{k}, \omega).$$  

(3.38)
We also define the operator $\mathcal{P}$ which takes the function $\phi$ and returns the function given by

$$\mathcal{P}\phi \equiv N(0) \int d\hat{k}'d\omega' (\phi - \phi') P(\hat{k}, \omega, \hat{k}', \omega').$$

(3.39)

We note that the equilibrium transitional rate $P$ is symmetric in the exchange of $(\hat{k}, \omega)$ with $(\hat{k}', \omega')$. It is easy to see that the operator $\mathcal{P}$ is linear and $\langle \phi, \mathcal{P}\phi \rangle \geq 0$. From these properties, we can derive that the solution $\phi$ of any linearized QBE that can be written in the form of Eq. 3.37 is such that it minimizes the quantity, [51]

$$\Delta = \frac{\langle \phi, P\phi \rangle}{\langle \phi, X \rangle^2}.$$  

(3.40)

We now return to consider the specific case of the QBE given by Eq. 3.36. Since the up and down spins contribute identically to the spin current $J_s$ and we are interested in $\rho_S$ only up to a numerical prefactor, we can consider the current due to the motion of only one type of spin which we denote by $J$. For a current density $J$ the energy density dissipation rate is $\rho_s J^2$. This can in turn be related to the rate of entropy density production, so that we are left with

$$T\dot{S} = \rho_s J^2,$$

(3.41)

Looking at the definition of the spin current in terms of the generalized distribution function, we find that

$$J = N(0) \int d\hat{k}d\omega v_F \phi(\hat{k}, \omega).$$

(3.42)

It is important to note that none of the renormalizations from the self-energy enter this expression. These renormalization factors instead appear on the time derivative of the particle density.[46] This fact is critical for relating the variational principle to the transport coefficients and also helps explain why the diverging effective mass does make the transport coefficient ill-defined.

Because of the $\hat{k}$ independence of $f_0(\omega)$,

$$J = -N(0) \int d\hat{k}d\omega v_F \phi(\hat{k}, \omega) \frac{\partial f_0(\omega)}{\partial \omega}.$$  

(3.43)
Thus if \( X \) is evaluated for unit applied force field, \(|F| = 1\), we are left with

\[
|J|^2 = \langle \phi, X \rangle^2.
\] (3.44)

Following Ref. [51], we now consider how the entropy is related to the distribution function \( f \). In general the Boltzmann equation balances the rate of change of the distribution function due to diffusion, external fields and scattering. We can view the QBE of Eq. 3.26 in the same light. From statistical mechanics we know that the entropy of a system of fermions in equilibrium is given by

\[
S = -k_B N(0) \int [f \ln f + (1 - f) \ln(1 - f)] \, dk \, d\omega.
\] (3.45)

We assume that this formula holds for small deviations around equilibrium. Differentiating with respect to time and linearizing, the rate of entropy production is given by

\[
\dot{S} = \frac{-N(0)}{T} \int \phi \dot{f} \, dk \, d\omega.
\] (3.46)

Thus from the collision term, we see that the rate of entropy production due to scattering is given by

\[
T \dot{S} = \langle \phi, \mathcal{P} \phi \rangle.
\] (3.47)

In steady state the macroscopic rate of entropy production, \( i.e. \) the Joule heating, is equal to the entropy production due to scattering. Thus we can solve Eq. 3.41 for \( \rho_s \) and using Eqs. 3.44 and 3.47, we find

\[
\rho_s = \frac{\langle \phi, \mathcal{P} \phi \rangle}{\langle \phi, X \rangle^2}.
\] (3.48)

Comparing Eq. 3.48 to the earlier definition of \( \Delta \), we see that the solution \( \phi \) that solves the linearized QBE of Eq. 3.36 minimizes \( \rho_s \). We thus proceed using the standard variational method. By making a reasonable ansatz for the deviation from local equilibrium \( \phi \), we can calculate an estimate for the spin resistivity \( \rho_s \).

Although the collision term includes the two distinct processes of absorbing and
emitting a gauge boson, we note that we need only calculate \( \rho_s \) for one of the two processes since they contribute identically to the spin resistivity. We consider the trial function

\[
\phi(\mathbf{k}, \omega) = \eta (\mathbf{k} \cdot \mathbf{F})
\]

where \( \mathbf{F} \) is a unit vector in the direction of the applied field \( \mathbf{F} \) and \( \eta \), which has units of \( k_F/m \), is small. This particular deviation from equilibrium \( \phi \) can be interpreted as a shift of the Fermi surface in the \( \mathbf{F} \) direction which is a reasonable guess since the shifted Fermi surface is the ansatz used to derive the standard \( T^5 \) dependence of the low temperature resistivity in a metal.

Both the numerator and the denominator of Eq. 3.48 contain factors of \( \eta^2 \) so they cancel and we drop this factor from the rest of our calculation. Plugging in the particular form of the trial function \( \phi \) from Eq. 3.49 into Eq. 3.43, it is straightforward to calculate the denominator which is independent of \( T \) and given by

\[
\langle \phi, X \rangle^2 = (mv_F)^2.
\]

Looking back at the definition of the operator \( \mathcal{P} \) given in Eq. 3.39 and using its symmetry properties, the numerator of Eq. 3.48 up to a numerical prefactor is given by

\[
\langle \phi, \mathcal{P} \phi \rangle = \beta \int d\omega d\omega' d\nu dq d\mathbf{k} d\mathbf{k}' |\mathbf{k}' \times \mathbf{q}|^2 \text{Im} D(q, \nu)(\phi - \phi')^2 f_0(\omega) \times
\]

\[
(1 - f_0(\omega'))n_0(\nu)\delta(\omega' - \omega - \nu)\delta(\mathbf{k}' - \mathbf{k} - \frac{\mathbf{q}}{k_F}).
\]

We first perform the integration over \( \omega \) and \( \omega' \), using the result that

\[
\int d\omega d\omega' \delta(\omega' - \omega - \nu)f_0(\omega)(1 - f_0(\omega')) = \frac{z}{\beta(1 - e^{-z})},
\]

where \( z = \beta \nu \). We define \( \theta \) and \( \theta' \) as the angles between \( \mathbf{k} \) and \( \mathbf{u} \), and \( \mathbf{k}' \) and \( \mathbf{u} \) respectively. We then define \( \alpha = \theta' - \theta \). The integration over \( \mathbf{q} \) just enforces the
condition from the momentum delta function, so that we are left with

\[ \langle \phi, P \phi \rangle = \beta \int d\nu d\theta d\theta' \frac{m^2 v_F^2}{2} \frac{\sin^2(\alpha)}{1 - \cos(\alpha)} \text{Im}D(q(\alpha), \nu) \times \]

\[ (\cos \theta - \cos \theta')^2 \frac{z}{\beta(1 - e^{-z})(e^z - 1)}, \quad (3.53) \]

where we have defined the function \( q(\alpha) \) which gives the magnitude of \( q \) for a particular angle \( \alpha \). We shift the integration over \( \theta \) and \( \theta' \) to \( \alpha = \theta' - \theta \) and \( \alpha' = \theta' + \theta \). Integrating over \( \alpha' \) gives

\[ \langle \phi, P \phi \rangle = \beta \int d\nu d\alpha \frac{m^2 v_F^2}{1 - \cos(\alpha)} \text{Im}D(q(\alpha), \nu) \times \]

\[ \sin^2(\frac{\alpha}{2})(2\pi - \alpha + \sin \alpha) \frac{z}{\beta(1 - e^{-z})(e^z - 1)}. \quad (3.54) \]

We now assume that since \( \text{Im} D(q, \nu) \) is peaked for small \( q \ll k_F \) that we can take \( \alpha \) to be small. Re-introducing \( q \) through a change of variables of \( \alpha \), we find

\[ \langle \phi, P \phi \rangle = \beta \int d\nu dq \frac{q^2}{k_F} \text{Im}D(q, \nu) \frac{z}{\beta(1 - e^{-z})(e^z - 1)}. \quad (3.55) \]

Inserting the RPA propagator from Eq. 3.28, we arrive at

\[ \langle \phi, P \phi \rangle = \left( \frac{\gamma^{1/3}}{\chi_D^{4/3} k_F^{3/3}} \right) \left( \int_1^\infty dz \frac{z^{4/3}}{1 - e^{-z}} \right) \frac{z^{4/3}}{(1 - e^{-z})(e^z - 1)} \times \]

\[ \left( \int_0^{y(q=2k_F)} \frac{d y \cdot y^{1/3}}{1 + y^2} \right). \quad (3.56) \]

The lower limit of the integration over \( z \) is an artifact of our treatment of the divergence of the self-energy at finite temperatures as noted in section 3.3. The self-energies in the QBE are taken to only include gauge fluctuations with \( \nu > k_B T \). We consider the effect of the low energy gauge fluctuations below.

Looking at the integrand of the \( z \) integral in Eq. 3.56, we see that it is sharply peaked for small \( z \). Since \( y \sim 1/z \) we can thus take the limit of the integration over \( y \) to be \( \infty \). The integrals over \( y \) and \( z \) are thus numerical prefactors of order unity that
we ignore. Combining Eqs. 3.48, 3.50 and 3.56, and reinserting the correct factors of \( \hbar \), we find that the spin resistivity is, up to a constant of order one,

\[
\rho_s = \hbar \left( \frac{k_B T}{E_F} \right)^{4/3}.
\] (3.57)

The final result for the spin resistivity takes exactly the form predicted by naive arguments assuming the existence of quasiparticles and ignoring the effects of the mass renormalization. Thus the only effect of the gauge bosons is through the relaxation rate. However, we have now derived this result without assuming the existence of quasiparticles and we have shown that a possible divergence due to the effective mass does not enter the expression for the spin resistivity.

Finally, we briefly discuss the effect of the low energy gauge fluctuations that cause the divergence of the self-energy at finite temperatures. As described in section 3.3, these fluctuations enter the QBE as an applied static random magnetic field \( \mathbf{b}_\perp \). Averaging over all possible configurations of this field does not lead to a linear response. Its only effect is through the transport scattering rate \( \tau_\perp \sim T^{-4/3} \). Taking the result from the QBE derivation, we assume that we can use the naive form for the spin resistivity ignoring the mass renormalization. Thus we expect that the low energy fluctuations in the self-energy loop do not change the overall scaling of \( \rho_s \) and only enter through the numerical prefactor.

### 3.5 Thermal Conductivity

We now proceed to calculate the more experimentally relevant transport coefficient, the thermal conductivity. We consider the situation where a uniform thermal gradient is applied to the system giving rise to a heat current density \( \mathbf{U} \) which is related to the thermal gradient through \( \mathbf{U} = \kappa \nabla_T T \) where \( \kappa \) is the thermal conductivity. The heat current density \( \mathbf{U} \) is defined in terms of the energy current density \( \mathbf{J}_E \) and the
particle current density $J_p$, where

$$U = J_E - \mu J_p. \quad (3.58)$$

Note that the particle current is not equivalent to the spin current $J_s$. Despite the fact that the quasiparticle is not well defined, these currents can be related to the generalized spinon distribution function $f(k, \omega)$ through

$$J_E = N(0) \sum_{\sigma} \int \omega v_F \hat{k} \tilde{f}_\sigma(\omega, \hat{k}) d\hat{k} d\omega \quad (3.59)$$

$$J_p = N(0) \sum_{\sigma} \int v_F \hat{k} f_\sigma(\omega, \hat{k}) d\hat{k} d\omega. \quad (3.60)$$

As in the case of the spin current, we again see that the renormalizations due to the self-energy do not enter the expressions for the currents and instead appear on the associated time derivatives of density or energy.[46]

Thus the heat current density $U$ is given by

$$U = N(0) \sum_{\sigma} \int v_F \hat{k}(\omega - \mu) f_\sigma(\omega, \hat{k}) d\hat{k} d\omega. \quad (3.61)$$

In the case of an applied thermal gradient, spin up and spin down react identically so we can drop the spin index for the remainder of the calculation.

For a system in steady state in an applied thermal gradient, its clear that the local equilibrium $f_0(\omega)$ defined in Eq. 3.29 depends on position $r$ through a local temperature $\beta(r)^{-1}$. The distribution function however remains time independent. Thus the QBE for the system under these conditions is

$$-\nabla_r \text{Re}\Sigma^R \cdot \nabla_{k_F} f + \nabla_{k_F} \epsilon_k \cdot \nabla_r f = I_{\text{coll}}. \quad (3.62)$$

We again linearize, assuming that $f$ is expanded into $f_0$ and $\phi$ as defined in Eq. 3.33 and that $\nabla T/T$ is small. Because $f_0(\omega)$ is assumed to be $\hat{k}$ independent, the
linearized QBE becomes

\[ \nabla_k \epsilon_k \cdot \nabla_r f_0 = I_{\text{coll}}. \] (3.63)

The earlier derivation of the variational principle remains true for Eq. 3.63 as well. Thus the quantity \( \Delta \), defined in Eq. 3.40 is still minimized by the solution \( \phi \) of the linearized QBE. Note that \( \Delta \) is dependent on the particular QBE that we are considering. To proceed, we relate \( \Delta \) for the linearized QBE of Eq. 3.63 to the thermal conductivity and then, in an identical way to the spin conductivity calculation, guess a reasonable \( \phi \) and calculate the associated thermal conductivity \( \kappa \).

We again start with an expression for the rate of entropy density production. For a given thermal current density, we have an entropy flux given by \( U/T \). This leads to a rate of entropy density production

\[ \dot{S} = \nabla \left( \frac{1}{T} \right) \cdot U = \frac{U^2}{\kappa T^2}, \] (3.64)

since \( U \) is constant throughout the sample. Note that we are assuming that there is no particle current due to the applied thermal gradient and thus no entropy production associated with a dissipation due to the presence of such a current. This assumption is valid for this system as long as there is no source of spinons. To see this we return to the Lagrangian of Eq. 3.1. Integrating out the gauge field \( a \) leads to the constraint that the spinon particle current density is conserved. Thus, the thermal resistivity \( W = \kappa^{-1} \) is given by

\[ W = \frac{T^2 \dot{S}}{U^2}. \] (3.65)

The derivation of \( \dot{S} \) in terms of \( \phi \) and \( \mathcal{P} \phi \) from Eq. 3.47 is still valid here. Thus we only need to consider \( \langle \phi, X \rangle \) and see if it is related to the heat current density \( U \). We again define the LHS of the linearized QBE, now Eq. 3.63, to be \( X \). Thus,

\[ \langle \phi, X \rangle = N(0) \int d\mathbf{k} d\omega \phi_p \mathbf{k} \nabla_r f_0 \] (3.66)

\[ = -N(0) \int d\mathbf{k} d\omega \phi_p \beta (\omega - \mu) \frac{\partial f_0}{\partial \omega} \nabla_r T \cdot \mathbf{k}. \] (3.67)
Inserting the expression for \( f \) from Eq. 3.32 into the expression for the heat current density \( U \) from Eq. 3.61, gives an identical expression up to a factor of \( \beta \). We find that

\[
\langle \phi, X \rangle = -\beta \nabla_x T \cdot U,
\]

and \( U^2 \) is thus equal to the denominator of \( \Delta \) up to some temperature independent constant. Therefore the \( \phi \) that solves the linearized QBE of Eq. 3.63 minimizes the thermal resistivity \( W \). Given an arbitrary \( \phi \), \( W \) can be calculated, up to some numerical prefactor, with

\[
W = \frac{T \langle \phi, P\phi \rangle}{\langle \phi, X \rangle^2}.
\]  

We need a trial function \( \phi \) that leads to a net flow of heat but no spinon particle current. A trial function that almost realizes this condition is

\[
\phi = \eta (\omega - \mu) \hat{k} \cdot \hat{u},
\]  

where \( \hat{u} \) is a unit vector in the direction of the heat current and \( \eta \) is small. This trial function can be interpreted as taking the original local temperature \( \beta(r) \) and giving it a \( \hat{k} \) dependence, \( \beta(\hat{k}) = \beta + \eta \hat{k} \cdot \hat{u} \). Physically at some point \( r \), the spinons with momentum pointing in the direction that the temperature decreases are hotter than average and on the opposite side of the Fermi surface the spinons are colder than average.

With the trial function \( \phi \) we now proceed to calculate the thermal resistivity \( W \). First it is again clear that \( W \) has no \( r \) dependence. Inserting the definition of the trial function \( \phi \) from Eq. 3.70, we find that \( |U| \sim n_\nu F(k_B T)^2 \). In order to calculate \( \langle \phi, P\phi \rangle \), we must recalculate \( (\phi - \phi')^2 \) for the new trial function. Using the relations imposed by the energy and momentum delta functions, we find

\[
(\phi - \phi')^2 = \nu^2 (\hat{k} \cdot \hat{u})^2 + (\omega' - \mu)^2 (q/k_F \cdot \hat{u})^2 + 2\nu(\omega - \mu)(\hat{k} \cdot \hat{u})(q/k_F \cdot \hat{u}).
\]

Each of these terms can now be integrated individually in an analogous way to the calculation of the numerator of the spin resistivity. It is again necessary to use
the fact that \( \text{Im}D(q, \nu) \) is peaked for small \( q \) in order to arrive at an analytic result. In evaluating these integrals, we need to calculate integrals of the form

\[
I(n) = \int d\omega d\omega' \delta(\omega' - \omega - \nu) f_0(\omega)(1 - f_0(\omega'))(\omega - \mu)^n,
\]

for \( n = 0, 1, 2 \). The integrals can be evaluated and we find

\[
I(0) = \frac{z}{\beta(1 - e^{-z})}, \quad I(1) = \frac{-z^2}{2\beta^2(1 - e^{-z})}, \quad I(2) = \frac{\pi^2 z + z^3}{3\beta^3(1 - e^{-z})}.\]

Using these results, we can now calculate the integrals, \( \langle \phi, \mathcal{P}\phi \rangle \) for each of the three terms in Eq. 3.71. Dropping numerical prefactors, the first term in Eq. 3.71, i.e. the \( \nu^2 \) term, contributes \( \nu_F^2 (mk_F)^{2/3} (k_B T)^{8/3} \) while the remaining two terms both contribute \( m^{4/3}k_F^{-2/3}(k_B T)^{10/3} \). Combining this result with our earlier result for \( \langle \phi, X \rangle^2 \) and plugging them into the definition of \( W \) from Eq. 3.69, we find that, restoring the correct factors of \( \hbar \),

\[
W = \frac{\hbar}{k_B \epsilon_F} \left[ \left( \frac{\epsilon_F}{k_B T} \right)^{1/3} + \left( \frac{k_B T}{\epsilon_F} \right)^{1/3} \right].
\]

Thus to leading order the low temperature thermal conductivity \( \kappa \) per layer is

\[
\frac{\kappa}{T} = \frac{k_B^2}{\hbar} \left( \frac{\epsilon_F}{k_B T} \right)^{2/3}.
\]

Thus we see that the QBE result for the thermal conductivity agrees with the result we found by making the unjustified assumption that quasiparticles were well-defined and that we can ignore the effects of mass renormalization. Note that these are the same assumptions that gave the correct result for the spinon resistivity.

With these assumptions we can show that \( \kappa/T \sim \tau_E \). We now use this result to consider the effects of the low energy \( a_- \) fluctuations. The applied static random
field b_ again only enters the thermal conductivity through a relaxation rate since it cannot lead to a linear response. We therefore are interested in the contribution to the energy relaxation rate due to b_ fluctuations. This contribution goes as $T^{-2/3}$. Thus if we assume that the QBE result that $\kappa/T \sim \tau_E$ is valid, the low energy gauge fluctuations only change the numerical prefactor of $\kappa$ and not its temperature dependence.

The form of the thermal conductivity from Eq. 3.77 is valid for clean systems only. In reality the divergent behavior of $\kappa/T$ at low $T$ is cutoff by the impurity scattering rate $1/\tau_0$. Again assuming that the QBE result is valid we thus find that the overall result for the thermal conductivity per layer in the presence of impurities is

$$\frac{\kappa}{T} \sim \left( \frac{\hbar}{k_B^2} \left( \frac{k_B T}{\epsilon_F} \right)^{2/3} + mA \frac{1}{k_B \tau_0} \right)^{-1},$$

(3.78)

where $A$ is the area of the layer.

### 3.6 Thermal Conductivity of Gauge Bosons

In all of the calculations up to this point we have assumed that the gauge bosons are always in local thermal equilibrium. Thus when we wrote down the QBE for the spinons, we assumed there was no deviation from the standard form for $n_0(\nu)$. In this section we examine the validity of this approximation and in particular look at the corrections to the thermal conductivity that arise when this assumption is relaxed.

As mentioned in the introduction, in the simplest derivation of the thermal conductivity, one finds that $\kappa$ is proportional to the heat capacity of the particles. It is known that for the model of Eqs. 3.1 and 3.3 the abundance of soft gauge field fluctuations produce a $T^{2/3}$ contribution to the specific heat.[6] As we showed in the previous section the effective mass drops out of the expression for the thermal conductivity due to the spinons. Ignoring the mass renormalization, the specific heat from the spinons is linear in $T$. Therefore, it is possible that at low temperatures, the largest contribution to the thermal conductivity comes from the gauge bosons. We
now consider the effect of allowing them to deviate from thermal equilibrium. This effect is the equivalent of phonon-drag in the electron-phonon system.

In order to describe the gauge bosons when they are not in thermal equilibrium, we derive the equation of motion for the gauge boson propagator that is analogous to Eq. 3.18. We then define a boson distribution function and derive an associated QBE. Thus we are left with two coupled differential equations that describe the system.

Exactly as in section 3.2, we begin by defining a number of different gauge boson propagators, in analogy to the spinon propagators in Eqs. 3.6 through 3.11 except with \( \psi \) replaced by \( a \). We denote these propagators with \( D \) rather than \( G \). Note that this is consistent with the definition from Eq. 3.3 which we now associate with \( D^R \). We also define an associated self-energy \( \Pi(q, \nu) \) which arises from the spinon bubble. In order to avoid double counting we consider the integration that lead to the gauge propagator in a renormalization group sense. In other words, we consider integrating out the high energy spinons to generate the gauge propagator and then consider coupling of the gauge propagator back to the low energy Fermionic modes.

Following the steps of section 3.2, we consider the expression

\[
D^>(q, \nu) - D^<(q, \nu) = -2 \text{Im} D^R = \frac{-2 \nu q}{\gamma^2 \nu^2 + \chi_D q^6}. \tag{3.79}
\]

It is clear that this expression is peaked at \( \nu = \nu_q = (\chi_D/\gamma)q^3 \). We can integrate \( \nu \) over the region of peaking and define the gauge boson distribution function as

\[
n(q, r, t) = \int \frac{d\nu}{2\pi} D^<(q, \nu, r, t). \tag{3.80}
\]

Note that unlike in the derivation of the generalized spinon distribution function, here we integrate over energy just as one does in the standard Fermi liquid case.

We now extended the assumption of the peaking of \( D \) to situations near thermal equilibrium as well. We see that despite the over-damped mode, the system looks as if it has quasiparticles at \( \nu = \nu_q \). This leaves us with the QBE for the gauge boson
distribution function, analogous to Eq. 3.26, described by

\[
\frac{\partial n}{\partial t} + \nabla_q \nu_q \cdot \nabla_r n = \Pi < (n + 1) - \Pi > n. \tag{3.81}
\]

We can now consider the two coupled QBEs of Eqs. 3.26 and 3.81 to calculate the thermal conductivity. Before proceeding, we linearize the gauge boson QBE. In analogy to Eq. 3.33, we define the deviation from equilibrium to be

\[
n(q) = n_0(\nu) - \zeta(q) \frac{\partial n_0(\nu)}{\partial \nu}
\]

\[
= n_0(\nu) + \beta \zeta(q) n_0(\nu) (1 + n_0(\nu)). \tag{3.83}
\]

Note that in the above expressions \(\nu\) is technically \(\nu(q)\) since we have defined the gauge boson distribution function as \(n(q, r, t)\).

In principle, we would need to solve the coupled set of QBEs given by Eqs. 3.26 and 3.81. However, in the case of thermal conductivity there is an important simplification. We can calculate the thermal conductivity due to the spinons and gauge bosons independently, assuming in each case that the other type of excitations remain in thermal equilibrium. This is valid because in this assumption, the terms that are ignored can be shown to be smaller by a factor of \(k_B T/\epsilon_F\) which is small for the temperatures under consideration in this system.[51]

Thus to proceed we only need to calculate the additional contribution to the thermal conductivity from the gauge bosons scattering off of spinons that can be assumed to be in thermal equilibrium. With this assumption one can evaluate \(\Pi <\) and \(\Pi >\). Remembering that the gauge propagator \(D(q, \nu)\) of Eq. 3.3 was derived from the spinon bubble, we find that after linearizing, \(I_{\text{coll}}\) for the boson QBE is given by

\[
I_{\text{coll}} = \int d\omega' d\omega d\hat{k} d\omega' d\hat{k} \text{Im} D(q, \omega - \omega) \beta \zeta(q) n_0(1 - f_0) f'_0 \delta(k_F \hat{k}' - k_F \hat{k} - q). \tag{3.84}
\]

We now make the ansatz \(\zeta(q) = \eta q \cdot \hat{u}\). Exactly as before one can derive an
expression for the thermal conductivity in terms of a variational method where

\[
\frac{1}{\kappa_g} = \frac{T^2 \dot{S}}{U^2}. \tag{3.85}
\]

Just as in section 3.5, the numerator can be related to the collision integral using Eq. 3.47, with \( \phi(\hat{k}, \omega) \) replaced by \( \zeta(q) \) and \( P \) now defined based on the gauge boson QBE. In order to use the variational method, we also must consider the left-hand side of the linearized form of the gauge boson QBE in Eq. 3.81 and relate it to \( U \).

\[
\langle \zeta, X \rangle = \int dq \zeta(q)v_q \cdot \nabla \tau n_0(\nu_q) \tag{3.86}
\]

\[
= \int dq \zeta(q) (v_q \cdot \nabla T) \frac{\nu}{T} n(q) \tag{3.87}
\]

\[
= \frac{\nabla T}{T} \cdot U \tag{3.88}
\]

since for the gauge bosons

\[
U = \int dq n(q) \nu_q v_q. \tag{3.89}
\]

Therefore we can use the variational method to calculate the gauge boson contribution to the thermal conductivity.

Returning to the denominator of Eq. 3.85, we see that

\[
\langle \zeta(q), X \rangle^2 \sim T^2 \left| \int dq \zeta(q)v_q \frac{\partial n_0}{\partial T} \right|^2. \tag{3.90}
\]

Plugging in our variational ansatz for \( \zeta(q) \), one can show that

\[
\langle \zeta(q), X \rangle^2 \sim T^2 C^2 \tag{3.91}
\]

where, as mentioned above the specific heat due to the gauge bosons \( C \sim T^{2/3} \).
We now plug in the integral form of $\langle \zeta, \mathcal{P}\zeta \rangle$ into Eq. 3.85 giving

$$
\frac{1}{\kappa_g} \sim \frac{1}{TC^2} \int d\omega d\omega' dq d\mathbf{k} d\mathbf{k}' \text{Im} D(q, \omega' - \omega) \beta \zeta^2(q) \times 
$$

$$
n_0(1 - f_0) f_0' \delta(k_F\mathbf{k}' - k_F\mathbf{k} - \mathbf{q}).
$$

(3.92)

For the particular ansatz $\zeta$ that we are considering, this integral is nearly identical to the calculation of the spin resistivity. After some work and borrowing the results from earlier calculations in this chapter, we find

$$
\frac{1}{\kappa_g} \sim \frac{1}{TC^2} T^{4/3} \sim \frac{1}{T}.
$$

(3.93)

Therefore the total thermal conductivity is

$$
\kappa \sim c_s T^{1/3} + c_g T.
$$

(3.94)

At low temperatures the thermal conductivity is thus dominated by the contribution from the spinons and one can ignore the equivalent of the phonon-drag.

### 3.7 Conclusion

Motivated by the organic compound $\kappa$-(BEDT-TTF)$_2$-Cu$_2$(CN)$_3$ which is a quasi two-dimensional effectively isotropic spin 1/2 Heisenberg model on the triangular lattice, we studied a particular $U(1)$ spin liquid defined by Eqs. 3.1 and 3.3, that has been recently proposed to describe this system at low temperatures. From this model, a variety of properties that can be compared to experiment such as the specific heat and static spin susceptibility have been calculated. In this chapter we have continued along these lines by calculating the transport properties of this spin liquid.

In addition to the physical relevance of this calculation, it is also interesting from a theoretical point of view because of problems that arise in deriving these coefficients. In particular, there are three main issues that we had to circumvent. First, the renormalized spinons are not well-defined Landau quasiparticles because the one-loop
correction to the spinon self-energy scales as $\omega^{2/3}$. Second, the effective mass diverges at the Fermi surface. And finally, as an artifact of gauge-invariance, the self-energy is divergent at finite temperature. These issues clearly invalidate the results one finds from naive arguments using renormalized parameters.

Despite these problems, we were able to proceed by deriving a QBE for this system. Starting from Dyson’s equation, we showed that even though there is no well-defined concept of a quasiparticle, we can construct a generalized distribution function based on the peaking of the spectral weight as a function of $\xi_k$, instead of the standard $\omega$ peaking. Using this peaking, we derived the QBE for this system in terms of the generalized distribution function.

We then proceeded to linearize the spinon QBE and to calculate the transport properties. Applying the variational method for solving the Boltzmann equation to the QBE, we solved for the transport coefficients. In particular, we showed that the transport coefficients are well-defined despite the diverging effective mass. Moreover, we calculated the temperature dependence of the spin resistivity and thermal conductivity. Assuming the gauge bosons remain in thermal equilibrium, we found that at low temperatures, the spin resistivity goes as $T^{4/3}$ and the thermal conductivity goes as $T^{1/3}$. In both cases, the result is identical to the one derived from naive arguments, where all the renormalizations due to the one loop corrections are ignored and the only effect of spinon-boson interaction is through a scattering rate $1/\tau$.

In the final section of this chapter, we relaxed the assumption that the gauge bosons are in thermal equilibrium. We showed that one can follow a similar method to the derivation of the spinon QBE and derive a QBE for the gauge bosons. In principle, we would then need to solve a coupled set of differential equations; however, for the specific case of the thermal conductivity we can decouple the equations if we ignore terms of order $k_B T/\epsilon_F$. Under this assumption we showed that the gauge bosons contribution to the thermal conductivity is sub-dominant to the spinon contribution.

Finally, we comment on the specific measurement of these transport coefficients in $\kappa$-(BEDT-TTF)$_2$-Cu$_2$(CN)$_3$. As mentioned in the beginning of section 3.3, the spin resistivity is difficult to measure because of the problem of creating a source and
drain of spinons. The thermal conductivity however is experimentally accessible. As discussed in the next chapter, recent experimental and theoretical work on the specific heat and spin susceptibility has lead to the suggestion that the spinons undergo a non-BCS pairing transition at low temperatures (around 6K). Clearly the results from these QBE calculations are invalid in the pairing regime where the spinons are no longer the correct particle to consider. However, as derived from the high temperature spin susceptibility, the exchange coupling is estimated to be $J \sim 250K$, which is two orders of magnitude greater than the pairing temperature. Thus there is a wide region of temperatures where one could see evidence of the spin liquid state through the temperature dependence of the thermal conductivity.
Chapter 4

Susceptibility of a spinon Fermi surface coupled to a U(1) gauge field

In this chapter, we again focus on the organic compound $\kappa$-(BEDT-TTF)$_2$-Cu$_2$(CN)$_3$, and the proposal that it can be well described by a spinon Fermi surface coupled to a $U(1)$ gauge field. In particular, we look at the static spin susceptibility at low temperatures and compare the experimental results to those predicted by this model. As mentioned before, the susceptibility can be well fit at high temperatures by the high-temperature series expansion of the spin 1/2 Heisenberg model on a triangular lattice with exchange coupling $J \sim 250K$. In addition, the susceptibility is found to drop sharply at low temperatures around 10 K before saturating to a finite value as the temperature goes to zero.[11] We show that this data is consistent with the proposed spin-liquid state when the possibility of spinon pairing is taken into consideration.

Recent measurements of the specific heat have suggested the existence of a peak in the electronic specific heat at around 6 K, once the phonon contribution has been subtracted away.[52] Led by this discovery, it was proposed that the $U(1)$ spin liquid state may have some kind of pairing instability.[53] Since the specific heat was also found to be unaffected by a magnetic field of up to 8T, conventional singlet pairing is unlikely. The pairing could, however, be ordinary BCS triplet pairing or a new kind
of pairing. Recently Lee et al.[53] proposed that this system may exhibit “Amperean” pairing. Unlike normal BCS pairing across the Fermi surface, this pairing is between two spinons on the same side of the Fermi surface. In particular, in the Amperean paired state, one pairs the spin with momentum $Q + p$ with the spin with momentum $Q - p$ where $|Q| = k_F$ and $|p|$ is small. The Amperean pairing can occur between two particles carrying almost parallel momenta due to the attractive interaction mediated by the magnetic fluctuations of the emergent gauge field. As a result the pairs carry net momentum $2k_F$ unlike the zero momentum pairs in the BCS state. In particular, the authors showed that it is possible for there to be an instability to this kind of pairing for the spinon Fermi surface coupled to a $U(1)$ gauge field. They also derived a number of experimental consequences of this model and show how they could explain many of the features seen in the experiments on $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$. Here we calculate the effect of pairing on the zero-field spin susceptibility of such a system and compare the result to what is seen experimentally in this organic compound.

Starting from a spinon Fermi surface, it is clear that at $T = 0$ the spinons give rise to a Pauli paramagnetic term due to the non-zero density of states. Standard BCS singlet pairing, however, leads to the reduction of this paramagnetism as a gap opens. At first sight, this seems to provide a natural explanation of the sharp drop in susceptibility below 10 K. However we have already excluded BCS singlet pairing because it is inconsistent with the observed insensitivity of the specific heat to magnetic field. Both triplet BCS pairing and alternate types of pairing such as LOFF and Amperean are consistent with the specific heat measurement. However it turns out that for such pairing states, the spinon contribution to the Pauli paramagnetism is unaffected by the onset of pairing, which seems inconsistent with the observed drop of susceptibility at low temperatures. In this chapter, we show that the drop of susceptibility can be explained if the effect of gauge fluctuations is taken into account. Before we include the effect of gauge fluctuations, below we ignore the gauge fluctuations and explain why the onset of pairing does not affect the contribution of spinons to the spin susceptibility in the Amperean, LOFF and triplet BCS pairing states.
We begin with a spinon system with a well defined Fermi surface. Applying a magnetic field creates two different Fermi seas for the up and down spinons, as shown in Fig. 4-1. First we consider the case of Amperean pairing, where pairing occurs on the same side of the Fermi surface. It is possible for both of these spinons to lie near the Fermi surface even after the magnetic field has been applied (Fig. 4-1). This is achieved by pairing the spin up spinon with momentum \( \mathbf{Q} + \Delta \mathbf{Q} + \mathbf{p} \) with the spin down spinon with momentum \( \mathbf{Q} - \Delta \mathbf{Q} - \mathbf{p} \), where \( |\mathbf{p}| \ll k_F \) and \( \Delta \mathbf{Q} = (\mu_B H/v_F) \hat{Q} \). Moreover, the phase space available for \( \mathbf{p} \) is unchanged with the applied field \( H \), as long as the curvature difference between spin up and down Fermi surfaces when \( H \neq 0 \) can be ignored. Thus in this approximation, there is no Zeeman limiting field for this pairing. Furthermore, the susceptibility is not reduced by pairing because although the opening of the pairing gap does smear out the momentum distribution \( n_k \), it leaves the occupied area of up and down spins unchanged. Thus the magnetization remains unchanged despite the opening of the pairing gap, and the underlying spinon paramagnetism is not destroyed.

We also note that this same argument holds for both the LOFF state \([54, 55]\) and the BCS triplet state. In the LOFF state the pairing is between a spin up on the spin up Fermi surface and a spin down on the opposite side of the spin down Fermi surface. This state as well only smears the momentum distribution leaving the occupied area unchanged and again the underlying paramagnetism survives. In the particular case of BCS triplet pairing where only the equal spin pairings \( \Delta_{\uparrow\uparrow} \) and \( \Delta_{\downarrow\downarrow} \) are nonzero, it is again clear that the pairing is unaffected by magnetic field and thus the magnetization remains fixed despite the opening of a pairing gap. In general triplet pairing there is also a non-zero pairing between the up and down spins. However, due to weak spin-orbit coupling the spin quantization axis favors a particular direction. When the applied field exceeds some small pinning field, the quantization axis rotates in such a way that the equal spin pairing description is appropriate and the thus the susceptibility remains unchanged despite the pairing gap.

For completeness, we now show how this argument fails for the BCS singlet state. After splitting the spin up and spin down with a magnetic field, the paired spins do
Figure 4-1: In the Amperean pairing state, the spinons at a and b are paired. We see that by choosing $\Delta \mathbf{Q} + \mathbf{p}$ correctly, both a and b lie near their respective Fermi surfaces. If one insists on pairing $(\mathbf{k}, \uparrow)$ with $(-\mathbf{k}, \downarrow)$, the gap does not develop at the Fermi surface. This is no longer the BCS singlet state, but in fact the breeched pairing state, which is not energetically favorable for small $H$.[56]

Thus we conclude that the naive application of triplet or Amperean pairing does not explain the sharp drop in the spin susceptibility below 10 K. In order to explain the data, we consider the effect of gauge fluctuations in the Amperean pairing state. We show that in this model of a spinon Fermi surface coupled to a $U(1)$ gauge field, the gauge field fluctuations give rise to a substantial paramagnetic contribution to the susceptibility. The onset of Amperean pairing driven by the gauge fluctuations introduces a gap in the gauge field by the Anderson-Higgs mechanism and suppress the gauge field contribution to the susceptibility. This suppression would account for the measured drop in susceptibility that occurs around 10 K. We note that this mechanism is independent of the form of pairing, whether it is triplet or Amperean.

We begin with the Lagrangian for a 2-D spinon Fermi surface system coupled to a $U(1)$ gauge field,

$$\mathcal{L} = \psi_\sigma^* (\partial_0 - ia_0 - \mu) \psi_\sigma + \frac{1}{2m} \psi_\sigma^* (-i \nabla - a)^2 \psi_\sigma. \quad (4.1)$$

We have dropped the gauge field kinetic energy term because its strength is inversely proportional to the charge gap and we are working in the insulating phase. $\psi_\sigma$ is the spinon field and the gauge field is $a = (a_0, a)$. $\mu$ is the chemical potential. We work
in Coulomb gauge $\nabla \cdot a = 0$.

We begin by calculating the random-phase approximation (RPA) for this model. By artificially introducing $N$ species of fermions, the RPA can be viewed formally as the lowest order terms in a $1/N$ expansion. [34, 13, 43] We need to calculate the bare spinon polarization bubble shown in Fig. A-1 which generates the gauge propagator. Working with this bare spinon bubble, i.e. not dressed by further fields inside the spinon loop, is equivalent to working to lowest order in the $1/N$ expansion. The scalar i.e. longitudinal part of the gauge propagator is related to the density-density response and does not show singular behavior for small $q$ and $\omega$. In other words the scalar part is screened out by spinon density fluctuations and we can focus on just the transverse part of the gauge field. Because the gauge field is now purely transverse, the spinon-gauge field vertex carries a vector index.

The gauge propagator is generated by a sum of spinon loops carrying a given spin. We define the bare spinon polarization bubble to be

$$\Pi(q) = \sum_{\sigma} \Pi_{\sigma}(q),$$

where

$$\Pi_{\sigma}(q) = \frac{1}{\beta} \sum_{k_0} \int \frac{d\mathbf{k}}{(2\pi)^2} G_{\sigma} \left( k + \frac{q}{2} \right) G_{\sigma} \left( k - \frac{q}{2} \right) \left| \frac{\mathbf{k} \times \mathbf{q}}{m} \right|^2,$$

with $q = (q_0, \mathbf{q})$ and $k$ similary defined. Again, we show the details of this calculation in the appendix, but in the end we find that

$$\Pi_{\sigma}(q) = \frac{1}{2} \left( \frac{\gamma \sqrt{v_F^2 |q_0|}}{\sqrt{(v_F^2 q)^2 + q_0^2 + |q_0|}} + \chi_d q^2 \right),$$

where $\chi_d = \frac{1}{12 \pi m}$ and $\gamma = \frac{k_F^2}{\pi}$. $k_F$ and $v_F$ are the Fermi momentum and velocity respectively for a spinon with spin $\sigma$ in an applied magnetic field. We find that we need to keep the curvature of the Fermi surface so we use that $k_F^\sigma = \sqrt{k_F^2 \pm 2m\mu_B H}$, where $\sigma = (+, -)$ for the up and down spins respectively.

In order to calculate the susceptibility, we compute the free energy of the La-
grangian from Eq. 4.1. We first note that because of the vector nature of the gauge propagator, there are no tadpole diagrams. The diagram we consider then is the standard RPA which is a closed string of bubbles. This is equivalent to calculating the free energy by integrating out the spinon fields and obtaining an effective action for the gauge field. The effective action is $S(a) = \sum_q \Pi(q) a_q^* a_q$ with $\Pi(q)$ from Eq. 4.2. Thus the partition function is

$$Z = e^{-\beta F} = \int \mathcal{D}a \, e^{-S(a)}, \quad \text{(4.5)}$$

where $F$ is the thermodynamic potential. Performing the functional integral, we find

$$F = \frac{1}{\beta} \sum_{q_0} \int \frac{dq}{(2\pi)^2} \ln \Pi(q). \quad \text{(4.6)}$$

We need to calculate the susceptibility $\chi = -\frac{\partial^2 F}{\partial H^2}|_{H=0}$. The spinon bubble in Eq. 4.2 only depends on $H$ through the parameters $v_F^2$ and $k_F^2$ of $\Pi(q)$. Inserting Eq. 4.4 into Eq. 4.2, we then Taylor expand to get

$$\Pi(q) = \Pi_0(q) + A(q)H^2 + O(H^3) \quad \text{(4.7)}$$

where

$$\Pi_0(q) = \frac{|q_0| k_F^2}{\pi m \left(q_0 + \sqrt{q_0^2 + \frac{q^2 k_F^2}{m^2}}\right)} + \chi d q^2 \quad \text{(4.8)}$$

and

$$A(q) = -\frac{q^3 m^3 q_0 \sqrt{q_0^2 + \frac{q^2 k_F^2}{m^2}}}{2\pi \left(q^2 k_F^2 + q_0^2 m^2\right)^2}. \quad \text{(4.9)}$$

Plugging this expansion into the definition of the susceptibility, we find that the correction to the zero field susceptibility due to this RPA diagram is

$$\Delta \chi = -\frac{1}{\beta} \sum_{q_0} \int \frac{dq}{(2\pi)^2} \frac{2A(q)}{\Pi_0(q)}. \quad \text{(4.10)}$$

From the above functional forms of $A(q)$ and $\Pi_0(q)$, it is clear that $\Delta \chi > 0$. Thus the
RPA correction to the gauge field gives rise to an additional paramagnetic contribution to the total susceptibility. When the gauge field is gapped after pairing, this correction is reduced. This is consistent with the measured drop that is seen experimentally.

An alternate way of calculating the spin susceptibility would be to dress the spin-spin correlation function with the gauge field propagator from Eq. 4.4. From this one could calculate the susceptibility explicitly. These two methods are the same because given the free energy RPA diagrams, taking each derivative with respect to magnetic field is equivalent to adding a spin-flip vertex. By writing down all the topologically inequivalent ways to add two spin-flip vertices, one generates the diagrams of the spin-spin correlation function. Kim et. al. calculated the density-density correlation function for small $q$ and found that the singular portions coming the self-energy and vertex corrections cancel and that there are only analytic corrections. [57] This result applies equally to the spin-spin correlation function. Our calculation corresponds to calculating the numerical value of the nonsingular part of this correction.

We now proceed to calculate the numerical value of the shift in the susceptibility in this RPA approximation for the gauge propagator. From the derived forms of $\Pi_0(q)$ and $A(q)$, we see that the integrand of Eq. 4.10 increases as $q$ increases. Thus to calculate a numerical value we need to introduce a cutoff. In the derivation of the polarization bubble in Eq. 4.4, we assumed that $q < k_F$. Thus we let the energy integration go from zero to infinity and cutoff the momentum integral at something of order $k_F$. In the standard calculation of the density-density polarization bubble for fermions in two-dimensions [58], one finds that the polarization bubbles dies off sharply as a square root for $q > 2k_F$ and is relatively flat inside the Fermi surface. Thus in order to compare to experiment, we take the cutoff to be $2k_F$. We write the paramagnetic correction at the RPA level in terms of the 2-D Pauli paramagnetic susceptibility for a spin 1/2 free fermion system, $\chi_0 = m/\pi$, where $m$ is the effective mass of the spinons. For this cutoff, the extra paramagnetic contribution is $\Delta \chi \sim 0.42 \chi_0$. This number, however, is strongly dependent on the cutoff as seen in Fig. 4-2.

We introduce the gapping of the gauge field due to spinon pairing. Calling the
gap energy $E_g$, once the spinons begin to pair, $\Pi(q)$ is shifted by this energy and as a result the denominator of the integrand of Eq. 4.10 becomes $\Pi_0(q) + E_g$. As the temperature decreases $E_g$ rises and the paramagnetic correction falls. In Fig. 4-2, we plot $\Delta \chi(E_g)$, the extra paramagnetic contribution due to these RPA diagrams, for different values of the cutoff.

We now consider the effect of the short range interaction on this calculation. We work perturbatively in $U$, the strength of this interaction in order to determine if such an interaction can enhance the size of the shift in the susceptibility. Continuing to work using the RPA, we need to consider the free energy diagrams that contain both the gauge field and the short range interaction. To lowest order in $U$ there are four diagrams that contribute to the propagator by adding corrections to the spinon bubble $\Pi(q)$. These diagrams are shown in Fig. 4-3. The top two diagrams are the standard Hartree and Fock corrections to the spinon propagator. These two are clearly related by an exchange. One can also see that the bottom two diagrams in Fig. 4-3 are also related to each other via an exchange.

First we consider the bottom two diagrams. We denote the correction to the total polarization from the vertex correction diagram (Fig. 4-3c) as $\Pi_c$ and from its associated exchange diagram (Fig. 4-3d) as $\Pi_d$. In order to calculate the free energy, we close these diagrams with the propagator calculated from the bare spinon bubble

---

**Figure 4-2:** $\Delta \chi$ in units of $\chi_0$ as a function of the pairing gap $E_g$ ins units of $\epsilon_F$. The solid, dotted, and dashed lines are for cutoffs 1, 1.5, and $2k_F$. 

---
Figure 4-3: The dressed spin bubble diagrams that are the lowest order corrections in the short range interaction, $U$, to the gauge propagator.

\[ D(q) = \Pi(q)^{-1}. \]

We find that

\[
\Pi_c(q) = \int dk dk' G(k)G(k+q)G(k'+q) \times \frac{[k \cdot k' - (k \cdot \hat{q})(k' \cdot \hat{q})]}{m^2} U(k-k'),
\]

\[ (4.11) \]

\[
\Pi_d(q) = \int dk dk' G(k)G(k+q)G(k'+q) \times \frac{[k \cdot k' - (k \cdot \hat{q})(k' \cdot \hat{q})]}{m^2} U(q).
\]

\[ (4.12) \]

Assuming, for simplicity, that $U(q)$ is independent of $q$, it is clear that for both diagrams the integral over $\theta_{kq}$, the angle between $k$ and $q$, is odd and thus gives zero. This is because unlike in Eq. 4.4 there is now only one power of $k$ from the vertex. We note that even without the assumption of $U$ being momentum independent $\Pi_d$ is zero, but that the assumption is necessary for $\Pi_c$.

The short range interaction can also dress the spinon propagator with Hartree-Fock corrections. Instead of evaluating these diagrams explicitly, we use the Dyson equation to calculate the dressed spinon propagator for a given spin, $\tilde{G}_\sigma$. The Hartree term, diagram Fig. 4-3b, gives a self energy $Un$ where $n$ is the total density of spinons.
The Fock term, diagram Fig. 4-3a, gives a self energy $U n_\sigma$. Thus we have

$$\tilde{G}_\sigma = \frac{1}{i\omega - \xi_k^\sigma - U n + U n_\sigma}. \quad (4.13)$$

The total spinon density does not depend on magnetic field, thus the Hartree term contributes a field independent shift to the chemical potential which does not effect the susceptibility and thus is dropped. Applying a magnetic field does shift the density of a particular spin to $n_\sigma(H) = n_\sigma(0) + \frac{dn}{d\mu} \delta \mu_\sigma$, where $\delta \mu_\sigma = \pm 2\mu_B H$ for up and down spins respectively and $\frac{dn}{d\mu} = \frac{m}{2\pi}$ is the standard 2-D density of states. Thus,

$$\tilde{G}_\sigma = \frac{1}{i\omega - (\epsilon_k - (\mu + \delta \mu_\sigma) - U(n_\sigma(0) + \frac{dn}{d\mu} \delta \mu_\sigma))}. \quad (4.14)$$

Again, dropping a shift in the chemical potential, this dressed spinon propagator is the same as the undressed one except that when a magnetic field $H$ is applied it responds to an effective field $\tilde{H} = H (1 + \frac{U m}{2\pi})$.

The gauge-field correction to the susceptibility including the short-range interaction to lowest order $\tilde{\chi}$ is thus

$$\tilde{\chi} = -\frac{\partial^2 F}{\partial H^2} = \left(\frac{\partial \tilde{H}}{\partial H}\right)^2 \chi \quad (4.15)$$

$$= \left(1 + \frac{U m}{2\pi}\right)^2 \chi, \quad (4.16)$$

where $\chi$ is the paramagnetic correction from Eq. 4.10. Thus for $U > 0$, we see that including the short range interaction diagrams enhances the extra paramagnetic term and thus leads to a larger drop in the susceptibility as the pairing gap opens.

In conclusion, we have shown that the proposed Amperean pairing of a spinon Fermi surface coupled to a $U(1)$ gauge field is consistent with the experiments performed on the candidate material $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$. In particular, the unconventional pairing of spinons on the same side of the Fermi surface allows for a non-zero $T = 0$ susceptibility despite the opening of a gap. Also by calculating the effect of the gauge field on the paramagnetic susceptibility, we found a drop in the
susceptibility as the gauge field becomes gapped due to pairing. This is consistent with the drop seen in the experiments. However, since the contribution to the susceptibility comes from the gauge field carrying large momentum, the result is sensitive to the cut-off and the exact numerical factor cannot be trusted. Our goal is rather to show as a matter of principle that there is a large paramagnetic contribution to the susceptibility that is suppressed by the onset of pairing.

As a special acknowledgement for this chapter, we thank Y. Nakazawa and K. Kanoda for sharing their data from $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ experiments prior to publication.
Chapter 5

Conclusion

In this thesis, we have studied transport properties in the vicinity of the Mott insulator. In the most common cases the Mott insulating phase is magnetically ordered and thus its properties are determined by the theory of spin waves which are well-understood. However, here we have studied two possible nearby phases that can occur when the system is hole-doped or when $U/t$ is such that the system is near the metal-insulator transition.

Using the VMC technique, we studied the physics of the Gutzwiller projected d-wave BCS quasiparticle as a function of hole doping concentration. We chose to study this particular state because of recent work establishing the Gutzwiller projected d-wave BCS ground state as a good starting point for understanding the physics of the cuprate superconductors. In particular, we calculated the renormalization of the current carried by a quasiparticle from its unprojected value. Then using a phenomological theory for nodal d-wave excitations we related this renormalization to experimental results and found good agreement. We also considered the spectral weight both as a function of doping and its dependence on wave vector $k$. Finally we considered the effects on the above quantities of perturbatively relaxing the strong coupling limit.

In the second half of this thesis, we studied a particular spin-liquid state described by a spinon Fermi surface coupled to a $U(1)$ gauge field. The presence of spin-liquid phases in real materials or even realistic Hamiltonians is an important question that
has yet to be fully explored. In this work, the particular spin-liquid is derived from the slave-particle method applied to the Hubbard model. We justify its use through comparison to experimental results on the recently discovered organic compound $\kappa$-(BEDT-TTF)$_2$-$\text{Cu}_2(\text{CN})_3$. Many of the measured quantities for this compound indicate Fermi surface physics, while the system remains a charge insulator. In this work we calculated the temperature dependence of the transport properties. The results differ from the standard metal and thus if measured could provide further evidence that this compound is described the this particular spin-liquid. We also investigated the static spin susceptibility and showed that the experimental results are consistent with this model when the additional effect of possible spinon pairing near the Fermi surface is taken into consideration. Overall, we hope to further establish that this organic compound is the first experimentally realized spin-liquid state in dimension greater than one.
Appendix A

Derivation of $\Pi(q)$

In this appendix, we present the details of the calculation of the gauge field propagator generated by the bare spinon bubble, Eq. 4.2. We define $\Pi(q) = \Pi_a(q) + \Pi_b(q)$, where the two one-loop diagrams that contribute are shown in Fig. A-1.

We start with the diagram in Fig. A-1a. Thus

$$\Pi_a(q) = \frac{2}{\beta} \sum_{k_0} \int \frac{d^2 k}{(2\pi)^2} G \left(k + \frac{q}{2}\right) G \left(k - \frac{q}{2}\right) \left| \frac{k \times \mathbf{q}}{m} \right|^2,$$  \hspace{1cm} (A.1)

where the extra factor of two came from the spin summation. Just as in the standard calculation of the polarization bubble we do the Matsubara sum first and get

$$\Pi_a(q) = -2 \int \frac{d k d \theta}{(2\pi)^2} k \left( \frac{f(\xi_{k+\frac{q}{2}}) - f(\xi_{k-\frac{q}{2}})}{i q_0 + \frac{k q}{m}} \right) \frac{k^2 \sin^2(\theta)}{m^2},$$ \hspace{1cm} (A.2)

where $\xi_k = \epsilon_k - \mu$, $\epsilon_k$ being the spinon dispersion relation and $\mu$ the Fermi energy. If $|q| < k_F$ then the difference of the two Fermi functions is only nonzero for a region of

![Diagram A-1a](image)

(a)

![Diagram A-1b](image)

(b)

Figure A-1: The one loop corrections to the bare gauge propagator.
length \( q \cos(\theta) \) around \( k_F \). Assuming that \( q \) is much smaller than \( k_F \), the \( k \) integration is just replaced by \( k = k_F \). We now calculate the real and imaginary parts of \( \Pi(q) \) and find

\[
\Pi_1^1(q) = \frac{-k_F^3}{2\pi^2 m^2} \int_0^{2\pi} \frac{v_F q^2 \cos^2(\theta) \sin^2(\theta)}{q_0^2 + v_F^2 q^2 \cos^2(\theta)} \quad (A.3)
\]

\[
\Pi_2^2(q) = \frac{-k_F^3}{2\pi^2 m^2} \int_0^{2\pi} \frac{-q_0 q \cos(\theta) \sin(\theta)}{q_0^2 + v_F^2 q^2 \cos^2(\theta)} . \quad (A.4)
\]

Doing these integrals, we find that the imaginary part is zero and that the real part gives,

\[
\Pi_a(q) = \frac{-k_F^2}{2\pi m} - \frac{m}{2\pi q^2} \left[ 2q_0^2 - 2|q_0| \sqrt{v_F^2 q^2 + q_0^2} \right] . \quad (A.5)
\]

This gives the dominate correction for small \( q \) for the non-static polarization bubble. For the static part of the polarization bubble, \( q_0 = 0 \), this \( \frac{1}{q^2} \) term vanishes, so we have to relax the approximation to the difference of the Fermi functions in order to get the \( q \) dependence in the static case. We now write

\[
\xi_{k \pm \frac{q}{2}} = \xi_k + \Delta_{\pm}, \quad (A.6)
\]

where \( \Delta_{\pm} = \pm \frac{k q}{2m} + \frac{q^2}{8m} \). We Taylor expand each distribution function in \( \Delta_{\pm} \). We work to third order in \( \Delta_{\pm} \) in order to generate all the terms up to order \( q^2 \). Dropping all higher powers of \( q \), we find that in the static limit, \( q_0 = 0 \),

\[
\Pi_a(q) = -\frac{1}{2\pi^2} \int d^2 k \frac{k^2 \sin^2(\theta)}{m^2} \times \\
\left[ n'(\xi_k) + \frac{q^2}{8m} n''(\xi_k) + \frac{k^2 q^2}{96 m^2} n'''(\xi_k) \right] . \quad (A.7)
\]

Which gives

\[
\Pi_a(q) = -\frac{1}{\pi} \left[ \frac{k_F^2}{2m} - \frac{q^2}{12m} \right] . \quad (A.8)
\]

We now compute the effect of the diagram shown in Fig. A-1b. The spinon loop
here just gives a density. So that this diagram evaluates to

$$\Pi_b(q) = \frac{-2}{m}(-n) = \frac{k_F^2}{2\pi m}$$

(A.9)

Putting Eq. A.5, Eq. A.8 and Eq. A.9 together, we get that

$$\Pi(q) = \frac{\gamma v_F |q_0|}{\sqrt{v_F^2 q^2 + q_0^2}} + \chi_d q^2$$

(A.10)

where $\gamma = \frac{k_F}{m}$ and $\chi_d = \frac{1}{12\pi}$.  

Taking the limit $q_0 \ll v_F q$, we recover the result from earlier papers $\Pi(q) = \gamma |q_0| \frac{1}{|q_0|} + \chi_d q^2$. [13, 34] Note that the actually value of $\chi_d$ differs from [13] by a factor of two because in that paper, there is a factor of two error in the form of the 2-D Landau diamagnetic susceptibility that gives rise to $\chi_d$. 

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Bibliography


[52] Y. Nakazawa et al., unpublished.