Slave particle study of the strongly correlated electrons

by

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Abstract

Until three decades ago, our understanding of the condensed matter systems were based on two frameworks developed by Russian physicist Lev Landau: his theory of phase transition, and Fermi liquids. The Landau theory of phase transition and the Fermi liquid theory together, can successfully explain a wide range of phenomena from ferromagnetism and anti-ferromagnetism to the conventional superconductivity. However, in the last thirty years, many experiments including the fractional quantum Hall effect (QHE) have revolutionized our view of nature. For a system of electrons that is subject to a very strong interactions and/or strong correlations between electrons, these two frameworks may break down. There many phases of matter, e.g. spin liquids, that do not break any classical symmetry, but are separated by phase transition. These states has the so called topological order. Also, many of these states do not follow predictions of the Fermi liquid theory and have many exotic behaviors. A rather powerful technique to handle with these issues is the slave particle method. In the first part of this thesis, using a more general slave particle method we study the strongly correlated Hubbard model, whose ground state may represent a Fermi liquid state at two spatial dimensions. We study the phase diagram of this model and show that the gapped spin liquid can be realized on the both honeycomb and square lattices, within mean-field. We also investigate the effective low energy theory of these states. Some of them are subject to compact gauge fluctuations. We study instanton effect in them and show that instanton proliferation can destabilize some of them.

Another interesting problem in which we are interested in is the copper based high temperature superconductors (HTSC). The parent state of cuprates materials (undoped case) is a Mott insulator whose ground state is proposed to be a spin liquid. Upon doping, many exotic phases appear, from high temperature superconductivity to the pseudogap phase with disjoint Fermi segments (Fermi arcs) instead of a closed Fermi surface, or the strange metal phase where the Fermi liquid theory breaks down and exhibits very unusual transport properties. The isotope effect in these materials is also very different from that of conventional superconductors. In the second part of this thesis we study the above mentioned problem in detail and explain them by appealing to the slave particle method.

Thesis Supervisor: Xiao-Gang Wen
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Chapter 1

Introduction

1.1 Background and Motivation

Until three decades ago, our understanding of the condensed matter systems were based on two frameworks developed by Russian physicist Lev Landau: his theory of phase transition, and Fermi liquids. According to the Landau paradigm of phase transition, every physical phase of matter can be characterized by symmetry breaking. Landau paradigm of phase transition states that any phase transition can be associated with a symmetry breaking. Therefore two states of matter with different symmetries belong to two different phases and we cannot smoothly transform one to another without phase transition. Within this picture, the ground state possesses a subgroup H of the symmetry group of the Hamiltonian G and the broken symmetry can be described through an order parameter. Therefore, every phase is classified by the set of (G, H). The second building block of the conventional condensed matter systems, is the Landau Fermi liquid theory. This framework is based on the notion of quasiparticles. In this theory, it is assumed that there is a one to one correspondence between the interacting fermion system with a noninteracting fermion systems and low energy excitations can be described as free fermionic quasiparticles. It is also based on the validity of the perturbation theory even when the interaction is very strong and much larger than the level spacing. So we can achieve the groundstate of the interacting system through turning on the interactions between fermions in the noninteracting system adiabatically. After a long enough time, the groundstate of the noninteracting system evolves to the groundstate of the interacting one. Since quasiparticles in the former case are fermions, the excitations of the interacting fermion system are expected to be described by fermionic quasiparticles as well and they follow Fermi-Dirac statistics. Therefore the overlap between the wavefunction of quasiparticles in the interacting system with free fermions in the non-interacting system is nonzero and quasiparticles carry the same quantum numbers as in the noninteracting system.

The Landau theory of phase transition and Fermi liquid theory together, can successfully explain a wide range of phenomena from ferromagnetism and anti-ferromagnetism to the conventional superconductivity. However, in the last thirty years, many experiments including the fractional quantum Hall effect (QHE) have revolutionized our view of nature. There are many phases in the nature that are indistinguishable in terms of symmetries and the system has to undergo a phase transition to transform from one phase to another one with exactly the same (G, H). Additionally, the concept of well defined quasiparticles breaks down in many systems including Mott insulator, spin liquids and the strange metal phase of the high temperature superconductors. In all of these examples, an electron experiences a very strong interactions and/or strong correlations with other electrons in the system. So the single quasiparticle picture cannot be applied in these cases and we have to develop a new approaches to such systems. This field has been extensively studied during last thirty years, but there are still many open problems that need intense effort. For example, the stability and classification of the spin liquid phases which are proposed to be the ground state of some frustrated quantum magnets, has not been fully understood yet. For instance, the staggered flux phase on the square lattice is a very interesting phase, but its stability is under question. On the other hands, spin liquids do not break any symmetry down to lowest temperatures, while they can exist in many topologically different phases and they belong to different topological orders. For such exotic phase we need a complete theory to classify every phase in the nature, because the Landau paradigm of phase transitions is incapable of distinguishing these phases, based on symmetry concerns. Moreover, many of spin liquids are subject to strong gauge interactions and it is important to understand how gauge interactions modify the meanfield results.

A very rich playground for these problems is the copper based high temperature superconductors (HTSC). The parent state of cuprates materials (undoped case) is a Mott insulator whose ground state is proposed to be a spin liquid. Upon doping, many exotic phases appear, from high temperature superconductivity to the pseudogap phase with disjoint Fermi segments (Fermi arcs) instead of a closed Fermi surface, or the strange metal phase where the Fermi liquid theory breaks down and exhibits very unusual transport properties. Among these phases, the superconducting state is more conventional, even though its underlying pairing mechanism is still under debate. In one hand, it originates from a Mott insulator with strong magnetic interactions, and exhibits many unusual behaviors and has a rather high transition temperature. On the other hand, the the notion of quasi particles is applicable up to some extent, or the isotope effect has been observed in HTSC, although it is very different from conventional superconductors. In addition to these phenomena, the existence of microscopic inhomogeneities, e.g. charge and spin stipe orders should also be considered. As of now, there is no comprehensive theory capturing the physics of different parts of phase diagram.

1.2 Slave particle theory

In strongly correlated electron systems, perturbation theory breaks down due to strong interaction and/or strong correlation between particles. For example, in the large U/t Hubbard model, the expectation value of the kinetic term is much smaller than the onsite Coulomb repulsion and as a result the interaction term cannot be regarded as a perturbation to the kinetic energy. Because of the large charge gap, it is very costly to create two electrons at the same site. If we exclude the happening of such doubly occupied sites in the low energy description of the system, we obtain the $t - J$ model as an effective Hamiltonian for spin fluctuations, however electron operators are different from their usual representation. The reason is that we have to project the Hilbert space to the non-doubly occupancy subspace and electron operators should not mix it with the rest of Hilbert space. So we have to use the following transformation

$$c_{i,\sigma}^{\dagger} \rightarrow \tilde{c}_{i\sigma}^{\dagger} = (1 - n_{i,-\sigma})\, c_{i,\sigma}^{\dagger}. \tag{1.2.1}$$

It can be easily checked that anticommutation relation $\tilde{c}_{i,\sigma}$ operator is different from real electrons. It is actually very difficult to use these projected operators. A brilliant idea is to consider empty states as a state occupied by a "slave boson" dubbed as "holon", and the projected spin σelectron operator removes this slave boson and creates a "slave fermion" with spin σ dubbed as "spinon" at that site. Therefore

$$\tilde{c}^{\dagger}_{i,\sigma} = f^{\dagger}_{i,\sigma} h_i, \tag{1.2.2}$$

where $f^{\dagger}_{i,\sigma}$ creates a spin σ spinon and $h^{\dagger}_i$ creates a holon. This identity should be considered with the following local constraint on the number of slave particles

$$n^f_{i,\uparrow} + n^f_{i,\downarrow} + n^h_i = 1. \tag{1.2.3}$$

The above constraint implements the non-doubly occupancy constraint and as a result, the effective Hamiltonian (in this case the $t - J$ Hamiltonian) in terms of new slave particles, is mathematically equivalent to its original form. The advantage of the slave particle method is that, although it does not solve the problem, using this approach, we can study the model Hamiltonian in a systematic way and we can apply many standard techniques such as perturbation theory to the problem. Within meanfield theory, many exotic topological phases, e.g. spin liquids, emerge using the slave particle method and the projective symmetry group (PGS) study of these meanfield state has lead to the classification of topological orders beyond Landau paradigm. Many of these states have non-Fermi liquid behavior, *e.g* their electric conductance can be different from the T^2 behavior of Fermi liquids at low temperature or in some there is no Fermi surface and no coherent and well defined quasiparticle description of the low energy theory.

1.3 Mott insulator versus band insulator

Now let us consider a system of atoms with periodic lattice structure and one electron (in the conduction band) per site, i.e. the half-filling case. According to the Fermi liquid theory we can find a correspondence between this system and a noninteracting one which can be studied by band theory. Band theory of solids predicts that in the absence of symmetry breaking, the ground-state should exhibit metallic behavior. The reason is that the chance of having neighboring sites where only one of them contains electron with spin σ is nonzero and nothing prevents the electron from hopping. Exclusion principle only bans hopping of an spin σ electron to its neighbor which has a similar electron. So charged quasiparticles can hop and we obtain a conducting state. Therefore we expect metallic behavior from band theory. This theory predicts insulating behavior for the filled case, where there are two electrons per site. The reason is that electrons cannot hop due to Pauli exclusion principle. There is for certain one electron with the same spin on the neighboring sites and therefore the electron cannot hop to that site. Another example is a half filled system with broken translation symmetry. In this case, the Brillouin zone reduces to half of its original size, and we obtain two bands. In the presence of translation symmetry breaking, a nonzero gap opens up between two bands. Since the system is at half filling, the lower band is fully occupied by quasiparticles at $T = 0$, while the upper band is empty. Because of the nonzero gap, there is now low energy excitations and the response function for frequencies less than gap vanishes. So we obtain an insulating system. This is called a band insulator, because the argument presented was based on band theory.

In 1949, N. Mott introduced another kind of insulator which cannot be described by band theory. Mott insulators have one electron per atom, and the ground state preserves all lattice symmetries, so according to the band theory should be a conducting state. It is however an insulator, not because of Pauli exclusion principle, but due to the strong onsite Coulomb repulsion between electrons. This is the case in compounds of transition metals whose valence electrons occupy d or f states. These states are much more localized than s or p states and therefore the Coulomb interaction between two electrons on d or f is much stronger. Because of this tremendous repulsion, electrons tend to repel each other and the most economical state has exactly one electron per site. When the onsite Coulomb repulsion energy U is much larger than hopping energy t, hopping is very costly and as a result the wavefunction of electrons localizes at their sites and electrons do not hop up to the first order approximation. In other words, charge excitation is gapped, so charge cannot transfer through the system and we obtain an insulating phase at half filling without symmetry breaking.

1.4 Generalized slave particle method

In 1963, J. Hubbard introduced his model Hamiltonian as the simplest model for Mott transition. This model has two parts, the kinetic part that describes the itinerant (waveness) nature of electrons, and short range potential energy part that represents the onsite

Coulomb repulsion. The Hubbard model in its simplest form contains only nearest neighbor hopping and is written as

$$H = U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - t \sum_{<i,j>,\sigma} C^\dagger_{i,\sigma} C_{j,\sigma} + H.c. \ , \tag{1.4.4}$$

where $C_{i,\sigma}$ is the annihilation operator of an electron with spin σ at site i, $\hat{n}_{i,\sigma} = C^\dagger_{i,\sigma} C_{i,\sigma}$ is the number operator of that electron and $< i, j >$ means that sites i and j are nearest neighbors of each other.

To study the Mott transition in the Hubbard model, we need a slave particle method that not only allows magnetic fluctuations, but also contains charge fluctuations. In Eq. 1.2.2, we used a redefinition of projected electron operators in terms of spinons and holons. At half filling, holon is absent, because for any empty state, there should exist a doubly occupied state. So the recipe in Eq. 1.2.2 does not contain charge fluctuation at half filling, and we need to take "doublon" slave bosons that represents states with two electrons (doubly occupied states) into consideration. It is easy to check that following decomposition

$$C_{i,\sigma} = f^\dagger_{i,\sigma} h_i + \sigma f_{i,-\sigma} d^\dagger_i, \tag{1.4.5}$$

where $d^\dagger_i$ creates a doublon, along with the following physical constraint

$$n^f_{i,\uparrow} + n^f_{i,\downarrow} + n^h_i + n^d_i = 1, \tag{1.4.6}$$

represent unprojected electron operators and has the right anticommutation relations. This more general slave particle method can be employed to study the strongly correlated Hubbard model and investigate the Mott transition in it, which is the subject of chapters 3,4 and 5.

1.5 Physics of high Tc

Identifying the underlying mechanism of the high temperature superconductivity in cuprates is one of the most challenging and outstanding problems in theoretical physics. Even quarter of a century after the first report of high temperature superconductor by Bednorz and Muller in 1986, there is still no general consensus on the pairing mechanism of the superconductivity in these materials. So far, many theories have been developed to explain the exotic properties of cuprates, but they can explain only a limited number of experiments and suffer from several limitations. One of the popular proposals is the preformed Cooper pairs scenario that was first proposed by P.W. Anderson. This theory can successfully explain many basic properties of cuprates but not all of them. This framework is based on strong correlation and it does not incorporate phonons in the pairing mechanism. On the other hand, many experiments have been reported indicating the importance of phonon mechanism such as the oxygen isotope effect on both the transition temperature of superconductivity and the London penetration depth. The reported isotope effect on T_c is very different from that of the conventional superconductors. For example, the BCS theory, which is based on phonon mediated attractive interaction, can explain the universal isotope effect on the transition temperature of conventional superconductors, but it predicts no isotope effect on the London penetration depth. In cuprates however, not only has the isotope effect been reported for both of these quantities, the isotope exponents also decrease as doping increases. More importantly the isotope effect on T_c on the overdoped cuprates is very small and negligible. These experiments indicate the importance of understanding the electron-phonon interaction in the strongly correlated regime, to unravel the mystery of cuprates. Therefore, to have a better understanding of the high T_c problem, the relation of the electron phonon interaction and the strong correlation remains to be solved.

Apart from the above mentioned difficulties of the Anderson theory, there are many difficulties in implementing his idea. So far, several techniques have been developed to implement Anderson's idea. One of the most successful ones is the $U(1)$ slave boson method. This method is based on the spin charge separation in the resonating valence bond (RVB) states. Although this approach achieves a phase diagram similar to the observed phase diagram of cuprates, it suffers from some serious problems. For example in the superconducting phase, this method predicts two kinds of vortices. The cheaper one is h/ec, and the other one is $h/2ec$. Experimentally only the latter one has been observed, and the first one has never been reported thus far which, although the $U(1)$ slave boson predicts its existence and its stability. Another important limitation which should be mentioned is the calculation of the linear T coefficient of the superfluid density. Slave boson gives a doping squared behavior (x^2, x is doping), however, experimentally, it has a weak dependence on the doping percentage.

These problems should be resolved in a consistent way. There are also many other important phenomena which are to be addressed in any comprehensive theory. Two of these are the linear temperature resistivity of the strange metal phase and the existence of the Fermi arcs in the pseudo-gap phase. Fermi liquid theory predicts T^2 dependence of resistivity in a metallic phase since their lifetime is proportional to $1/\epsilon^2$ (ϵ is the excitation energy of quasi-particles). Therefore linear temperature resistivity means a non-Fermi liquid whose quasi-particles have a decay rate proportional to their energy. This means we do not have sharp quasi-particles in this phase. The theory of such phases are called marginal Fermi liquid. Slave boson method has been applied to this phase but it has not been able to explain the observed behavior correctly so far. On the other hand photoemission experiments show Fermi arcs(locus of gapless excitations) instead of Fermi pockets or Fermi surface. This is a very remarkable observation, because, we always obtain a closed Fermi surface using standard techniques.

These limitations and difficulties motivate us to look for a more refined formalism and a more general framework, capable of explaining the physics of the high-temperature superconductors on a more solid basis. In last three chapters, we address all of the mentioned issues and try to explain them within Anderson idea of preformed Cooper pairs and through $U(1)$ slave boson method. We emphasize on the importance of electron phonon interaction and argue that it is possible to explain the observed unusual isotope effect and resolve other limitations in these materials within slave boson approach by slightly modifying the standard framework of Anderson theory. So it is necessary to take electron phonon interaction in the presence of strong correlations into consideration in order to reconcile Anderson theory with experimental observations and resolve the limitations of the $U(1)$ slave boson method.

Eq. 1.2.2 is applied to the projected electron operator, where does not allow double occupation. We can use the idea of the slave particle approach to decompose the unprojected electron operator as well.

1.6 Statement of the problem

We would like to establish a framework based on a generalized slave particle approach to study strongly the Mott metal-insulator transition in the Hubbard model on different lattice, and investigate various properties of meanfield states, in particular their stability. Among tens of possibilities for the meanfield state, many of them are spin liquid, i.e. do not break any lattice symmetry down to lowest temperatures. The low energy theory of spin liquids is usually coupled to a compact gauge filed and we have to deal with this problem to obtain reliable physical results. We want to study when these gauge fluctuations are gapless, and when they are not. In case of gapless gauge fluctuations, instanton proliferation becomes possible due to the compactness of the gauge field. Instanton proliferation changes the properties of the meanfield state drastically. It is important to study this problem in detail and determine the fate of meanfield state.

Recently, the Hubbard model on the honeycomb lattice has been studied using the quantum Monte Carlo (QMC) method. For moderate values of U/t, a gapped state has been reported that does not break any symmetry. We would like to see whether our formalism can realize such a gapped spin liquid phase or not. We are also interested in the possibility of such phases on other lattices, e.g. square lattice and in other phases, e.g. staggered flux phase. In previous studies and in the absence of charge fluctuations, this possibility was ruled for the staggered flux phase, using arguments based on symmetry considerations. Here we use the more general slave particle approach and reexamine their arguments by allowing charge fluctuations.

We also would like to take a journey from half filling and study the physics of doped cuprates within slave boson approach. We are interested in studying the physics of the strange metal and the pseudogap phases. Both states exhibit non-Fermi liquid behaviors and have unusual properties. Another problem in which we are interested is how to deal with electron phonon interaction in the presence of strong correlations. This is a nontrivial problem, because the electron phonon interaction in the presence of strong correlations has a very different behavior and its effect on the properties of high Tc cuprates is very different from its effect on conventional superconductors. Understanding this problem is crucial in the phenomenology of high temperature superconductivity in cuprates. The ultimate goal is to take electron phonon interaction in the presence of strong correlations into account appropriately, in order to explain a wider range of experiments within Anderson idea of superconductivity. In other words, we want to show that the strong correlation physics is the primary cause and the major deriving force of the high temperature superconductivity in cuprates and the phonon mediated attraction is a secondary effect. Therefore, phonon related problems should be addressed in a more fundamental attack line.

1.7 Outline

In this thesis, we are going to address the above mentioned problems within the slave particle approach. In the first few chapters, we limit ourselves to the half filling case and study the properties of the strongly correlated Hubbard model on honeycomb and square lattices. The thesis is organized as follows.

In chapter two, we present a brief introduction to the slave particle method and review standard techniques and known methods for dealing with the systems we are going to study. In chapter three, we discuss different aspects of the more general slave particle approach. We derive the phase diagram of the Hubbard model on the honeycomb lattice using this framework. We discuss the possibility of stable gapped spin liquids on the honeycomb lattice. In chapter four, we focus on the low energy effective theory of the spin liquid obtained in chapter three and discuss the confinement/defonfinement problem in detail. We present a method to calculate different quantum numbers of instanton operators. These quantum numbers determine the fate of the spin liquid phase. In chapter five, the physics of the gapped staggered flux phase is discussed. We follow the method presented in chapter four to compute the transformation properties of the instanton operator under the different symmetries of the square lattice, to determine the fate of this phase. It is shown that the gapped staggered flux phase is not stable and the resulting phase breaks translation and some other symmetries of the square lattice.

In the last three chapters, we apply the $U(1)$ slave boson method to study the physics of the doped cuprates. In chapter six, we investigate the gauge theory of the doped Mott insulator in the strange metal and the pseudogap phases. It is discussed that the linear temperature resistivity of the strange metal phase and the observation of Fermi arcs in the pseudogap phase can be successfully explained by calculating the self energy and the scattering rate of quasiparticles. In chapter seven, we generalize Anderson theory of high Tc by taking phonons into account. We present a cooperative electronic and phononic mechanism for the high temperature superconductivity in cuprates. It is shown than within this generalized framework, we can resolve several limitations of the $U(1)$ slave boson theory. In chapter eight, we investigate the gauge theory of the doped Mott insulator in the strange metal and the pseudogap phases. It is discussed that the linear temperature resistivity of the strange metal phase and the observation of Fermi arcs in the pseudogap phase can be successfully explained by calculating the self energy and the scattering rate of quasiparticles.

Chapter 2

A brief review of previous studies

In this chapter we present important results of previous studies for the Hubbard and t-J models. We start from the meanfield study of the weakly correlated Hubbard model at half filling on the square lattice. This method obtains the anti-ferromagnetic order for any positive U, and therefore the ground-state breaks the translation symmetry. As a result the system is insulator at half filling. Then we review properties of the Hubbard model at large U limit and present the derivation of the t-J model. We also discuss the gauge theory of the strongly correlated systems.

2.1 Small U-limit of the Hubbard model

In 1949, N. Mott introduced another kind of insulator which cannot be described by band theory. Mott insulators have one electron per atom, that according to the band theory should be metallic. It is insulator not because of Pauli exclusion principle, but due to the strong onsite Coulomb repulsion between electrons. This is the case in compounds of transition metals whose valence electrons occupy d or f states. These states are much more localized than s or p states and therefore the Coulomb interaction between two electrons on d or f is much stronger. Because of this tremendous repulsion, electrons tend to repel each other and the most economical state has exactly one electron per site. When the onsite Coulomb repulsion energy U is much larger than hopping energy t, hopping is very costly and as a result the wavefunction of electrons localize on their sites as do not hop up to the first approximation. In 1963, J. Hubbard introduced his model Hamiltonian as the simplest model for Mott transition. The Hamiltonian has two parts, the kinetic part that describes the itinerant (wave-ness) nature of electrons and short range potential energy part that represents the onsite Coulomb repulsion. Hubbard model in its simplest form contains only nearest neighbor hopping and is written as

$$H = U\sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} - t\sum_{<i,j>,\sigma} C^{\dagger}_{i,\sigma}C_{j,\sigma} + H.c. \,, \tag{2.1.1}$$

where $C_{i,\sigma}$ is the annihilation operator of an electron with spin σ at site i, $\hat{n}_{i,\sigma} = C^{\dagger}_{i,\sigma}C_{i,\sigma}$ is the number operator of that electron and $< i,j >$ means that sites i and j are nearest neighbors of each other. For small U/t ratios, the kinetic term is dominant and we can study the above Hamiltonian using standard methods, for instance through perturbation theory.

Now let us we study the properties of the Hubbard model at half filling on the square lattice. The interaction term can be written in term of the spin operator and we have

$$Un_{i,\uparrow}n_{i,\downarrow} = -\frac{2U}{3}\vec{S}_i.\vec{S}_i + \frac{n_{i,\uparrow}+n_{i,\downarrow}}{2}. \tag{2.1.2}$$

We can ignore the last term, since $\sum_{i,\sigma} n_{i,\sigma} = N$ is a constant number and we can drop it with out losing any physics. Within the path integral formulation we can use the Hubbard-Stratonovic transformation to obtain the following action

$$\exp\left(\frac{2U}{3}\int d\tau S_i.S_i\right) = \int D\phi_i^a \exp\left(-U\int d\tau \,\left(\frac{3}{8}\vec{\phi}_i.\vec{\phi}_i - \vec{\phi}_i.\vec{S}_i\right)\right). \tag{2.1.3}$$

The advantage of this method is that we replaced the U-term which was bilinear in terms of spin operator with a linear one. We can appeal to the saddle point approximation to simplify this integral further. By varying the action with respect to ϕ_i field, we obtain $\phi_i^a = \frac{4}{3}\langle S_i^a\rangle$. Then we can expand the Hamiltonian around this point and obtain a systematic perturbative expansion. Since in the classical action, we expect staggered magnetization along some direction, i.e. $\vec{S}_i = m(-1)^{i_x+i_y}\hat{n}$ (m is called Néel order parameter). $\hat{n}$ can be any direction, but after symmetry breaking, the system picks up only one direction. We choose it to be $\hat{z}$ direction. So we have

$$H_{\text{eff}} = -\frac{4mU}{3}\sum_{i,\sigma}(-)^{i_x+i_y}\sigma n_{i,\sigma} - t\sum_{<i,j>,\sigma} C^{\dagger}_{i,\sigma}C_{j,\sigma} + H.c. \; . \tag{2.1.4}$$

Because of $(-)^{i_x+i_y}$ we lose translation symmetry and we now use the reduced Brillouin zone (BZ) whose boundary is defined as

$$|k_x| + |k_y| \leq \pi \tag{2.1.5}$$

The area of this new BZ is $2\pi^2$ which is half if the translation symmetric case. Going to the momentum space we obtain the following effective Hamiltonian for small $U-$Hubbard model on the square lattice

$$H_{eff} = \sum_{k,\sigma}\left[C^{\dagger}_{k,\sigma},\ C_{k+Q}\right]\begin{bmatrix} t_k & \frac{3Um}{4}\sigma \\ \frac{3Um}{4}\sigma & -t_k \end{bmatrix}\begin{bmatrix} C_{k,\sigma} \\ C_{k+Q,\sigma} \end{bmatrix},$$

$$t_k = -2t\left(\cos k_x + \cos k_y\right), \qquad \vec{Q} = (\pi, \pi)\,. \tag{2.1.6}$$

The energy eigenvalues are

$$E_{k,\sigma} = \pm\sqrt{\left(\frac{3Um}{4}\right)^2 + t_k^2}. \tag{2.1.7}$$

So there is a finite gap equal to $E_g = \left|\frac{3Um}{4}\right|$. At half filling the lower band (the band with negative sign) is filled and therefore we have an insulating phase. We can use either self consistent equation of $m = (-)^{i_x+i_y}\left\langle S^3_i\right\rangle$ or energy minimization obtain the optimum value for m. It can be shown that at small U-limit (but positive) we have [27]

$$m \sim e^{-\#\frac{t}{U}}, \tag{2.1.8}$$

up to the first order and therefore only at $U = 0$, m is zero and above $U = 0$, the groundstate exhibits antiferromagnetic behavior and the Néel order parameter is nonzero. So the Hubbard model on square lattice does not show metallic behavior for positive U, and has an anti-ferromagnetic groundstate at least for small U/t limit.

2.2 Derivation of t-J model

In this section we follow the method by J. Spalek for the derivation of the t-J model [72, 59]In the*strong correlation* limit of the Hubbard model where $U \gg zt$, there is a small probability for double occupancy. So we assume there is no charge fluctuation in the system. In the next section we argue that this assumption is misleading in some cases. We now want to use this assumption to derive t-J model as an effective Hamiltonian describing the physics of all states without double occupation. To derive t-J model in a rigorous way, we first define P_0 that projects the Hilbert space into a subspace without double occupation. Similarly $P_N = 1 - P_0$ projects to the rest of Hilbert space. At half filling, the number of empty sites is equal to the number of doubly occupied sites. Therefore, the absence of double occupation leads to the absence of empty sites at half filling. Hilbert space contains four states per site. For each spin we have occupied and occupied state. Therefore we have $|1\rangle_i = |0, \uparrow\rangle_i |0, \downarrow\rangle_i$, $|2\rangle_i = |1, \uparrow\rangle_i |0, \downarrow\rangle_i$, $|3\rangle_i = |0, \uparrow\rangle_i |1, \downarrow\rangle_i$ and $|4\rangle_i = |1, \uparrow\rangle_i |1, \downarrow\rangle_i$. From the definition of P_0 we have $P_0 |4\rangle_i = 0$. Since $(1 - \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}) |4\rangle_i = 0$, so we can identify P_0 with

$$P_0 = \prod_i (1 - \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}) \,. \tag{2.2.9}$$

It is easy to check that $P_0 P_N = P_N P_0 = 0$ while $P_0^2 = P_0$ and $P_N^2 = P_N$. Now let us consider the following equation for the groundstate of the Hubbard model

$$H\Psi = E\Psi. \tag{2.2.10}$$

We are interested in finding a Hamiltonian whose groundstate is $P_0\Psi$ and has the same ground state energy E as the Hubbard model. Therefore we have

$$H_{eff}P_0\Psi = EP_0\Psi. \tag{2.2.11}$$

To achieve our goal, we use the fact that $P_0 + P_N = 1$. So we have

$$H\left(P_0 + P_N\right)\Psi = E\left(P_0 + P_N\right)\Psi. \tag{2.2.12}$$

Multiplying both sides of the above equation by P_N and using the fact that $P_N P_0 = 0$, $P_0^2 = P_0$ and $P_N^2 = P_N$, we have

$$P_N H\left(P_0^2 + P_N^2\right)\Psi = EP_N\Psi. \tag{2.2.13}$$

Rearranging this equation we have

$$\left(P_N H P_N - E\right)P_N\Psi = \left(P_N H P_0\right)P_0\Psi. \tag{2.2.14}$$

Therefore

$$P_N\Psi = \frac{1}{P_N H P_N - E}\left(P_N H P_0\right)P_0\Psi. \tag{2.2.15}$$

Let us plug in the above expression for $P_N\Psi$ in Eq. 2.2.12

$$\left[H - (H - E)\frac{1}{P_N H P_N - E}\left(P_N H P_0\right)\right]P_0\Psi = EP_0\Psi \tag{2.2.16}$$

Using ${P_0}^2 = P_0$ and $P_N^2 = P_N$ one further time and comparing the above equation with Eq. 2.2.11, we obtain the following

$$H_{eff} = P_0HP_0 - (P_0HP_N - E)\frac{1}{P_NHP_N - E}(P_NHP_0) \tag{2.2.17}$$

We divide Hubbard model in two parts. The kinetic part H_K that mobilizes electrons and potential part H_U which represents the onsite Coulomb repulsion.

$$H = H_K + H_U \tag{2.2.18}$$

$$H_K = -t\sum_{<i,j>,\sigma} C^{\dagger}_{i,\sigma}C_{j,\sigma} \tag{2.2.19}$$

$$H_U = U\sum_i n_{i,\uparrow}n_{i,\downarrow} \tag{2.2.20}$$

When H_K acts on $P_0\Psi$, at half filling, it creates one doubly occupied and another empty site. The resulting state is no longer an eigenstate of P_0 operator. Therefore at half filling we have $P_0H_KP_0 = 0$. On the other hand, $n_{j,\uparrow}n_{j,\downarrow}\prod_i(1 - \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}) = 0$, so $H_UP_0 = P_0H = 0$ and therefore we have

$$P_0HP_0 = 0. \tag{2.2.21}$$

$$P_0HP_N = P_0H_KP_N \tag{2.2.22}$$

$$P_NHP_0 = P_NH_KP_0 \tag{2.2.23}$$

As we discussed after acting H_K on $P_0\Psi$ we obtain an state with one double occupancy. Therefore it the potential energy of this state is U and we have $P_NH_UP_N = U$. $P_NH_KP_N - E$ is of order hopping integral times coordinate number of lattice, i.e. $-zt$ and therefore in $U \gg zt$ limit is negligible compared to $P_NH_UP_N$. So we can replace $(P_NHP_N - E)^{-1}$ by $1/U$ up to the first order of zt/U. So we have the following expression for the effective Hamiltonian up to the first order of approximation

$$H_{eff} = -\frac{P_0H_K^2P_0}{U}, \tag{2.2.24}$$

where we have used $P_N H_K P_0 = (P_N + P_0) H_K P_0 = H_K P_0$. Now we only need to simplify H_K^2. We have

$$H_K^2 = t^2 P_0 \sum_{<i,j>,<m,n>,\alpha,\beta} C_{i,\alpha}^\dagger C_{j,\alpha} C_{m,\beta}^\dagger C_{n,\beta} P_0 \tag{2.2.25}$$

Since H_K, creates a doubly occupied site, the second H_K has to remove this state and therefore we have $i = m$ and $j = n$. And we have

$$H_K^2 = t^2 P_0 \sum_{<i,j>,\alpha,\beta} C_{i,\alpha}^\dagger C_{i,\beta} C_{j,\alpha} C_{j,\beta}^\dagger P_0 \tag{2.2.26}$$

Since $\sum_{k=1,2,3} \sigma_{\alpha,\beta}^k \sigma_{\mu,\nu}^k = 2\delta_{\alpha,\nu}\delta_{\beta,\nu}$, where σ^k is $k-$th Pauli matrix, we have the following identities

$$C_{i,\alpha}^\dagger C_{i,\beta} = \delta_{\alpha,\beta} \frac{n_{i,\uparrow} + n_{i,\downarrow}}{2} + \vec{S}_i.\vec{\sigma}_{\beta,\alpha} \tag{2.2.27}$$

$$C_{j,\alpha} C_{j,\beta}^\dagger = \delta_{\alpha,\beta} \left(1 - \frac{n_{j,\uparrow} + n_{j,\downarrow}}{2}\right) - \vec{S}_j.\vec{\sigma}_{\alpha,\beta}, \tag{2.2.28}$$

in which we have defined

$$S_i^k = \frac{1}{2} \sum_{\alpha,\beta} C_{i,\alpha}^\dagger \sigma_{\alpha,\beta}^k C_{i,\beta}. \tag{2.2.29}$$

At half filling $n_{i,\uparrow} + n_{i,\downarrow} = 1$, so we have

$$H_K^2 = t^2 P_0 \sum_{<i,j>,\alpha,\beta} \left(\frac{\delta_{\alpha,\beta}}{2} + \vec{S}_i.\vec{\sigma}_{\beta,\alpha}\right) \left(\frac{\delta_{\alpha,\beta}}{2} - \vec{S}_j.\vec{\sigma}_{\alpha,\beta}\right) P_0 \tag{2.2.30}$$

$$H_K^2 = t^2 P_0 \sum_{<i,j} \mathrm{Tr} \left\{ \left(\frac{1}{2} + \sum_m S_i^m \sigma^m\right) \left(\frac{1}{2} - \sum_n S_j^n \sigma^n\right) \right\} P_0 \tag{2.2.31}$$

$$H_K^2 = t^2 P_0 \sum_{<i,j} \left(\frac{1}{2} - 2\vec{S}_i.\vec{S}_j\right) P_0, \tag{2.2.32}$$

where we have used $\mathrm{Tr}(\sigma^m) = 0$ and $\mathrm{Tr}(\sigma^m \sigma^n) = 2\delta_{m,n}$. Since spin operator does not change the number of electrons, we can remove P_0 from the above equation and we eventually achieve the following effective Hamiltonian for the strongly correlated Hubbard model at half filling

$$H_{eff} = \frac{t^2}{U} \sum_{<i,j>} \left(\vec{S}_i . \vec{S}_j - \frac{1}{4} \right), \tag{2.2.33}$$

which is nothing but Heisenberg Hamiltonian. So far we assumed half filling. Away from half-filling we can follow the same procedure and we obtain

$$H_{t-J} = -t \sum_{<i,j>,\sigma} P_0 C^{\dagger}_{i,\sigma} C_{j,\sigma} P_0 + J \sum_{<i,j>} \left(\vec{S}_i . \vec{S}_j - \frac{n_i n_j}{4} \right), \tag{2.2.34}$$

where $J = \frac{2t^2}{U}$. This effective Hamiltonian is the sum of the constrained (projected) hopping model (t model), and the Heisenberg model (J model). So it is called $t - J$ model which includes both hopping and antiferromagnetic exchange interaction of projected electrons.

2.3 Introduction to slave-boson method for t-J model

In derivation of the t-J model, we assumed no double occupancy in the many body wavefunction. For large U/t ratio, the charge gap is of order U and therefore we can keep states with at most one electron per site. To derive the standard $U(1)$ slave boson approach, it should be noted that P_0 operator which projects the Hilbert space into no-doubly occupancy, allows only hopping of electrons to the neighboring empty sites. Any other hopping process involves going away from projected Hilbert space. So we have

$$P_0 C^{\dagger}_{i,\uparrow} C_{j,\uparrow} P_0 = (1 - n_{i,\downarrow}) C^{\dagger}_{i,\uparrow} C_{j,\uparrow} (1 - n_{j,\downarrow}) \tag{2.3.35}$$

$$P_0 C^{\dagger}_{i,\downarrow} C_{j,\downarrow} P_0 = (1 - n_{i,\uparrow}) C^{\dagger}_{i,\downarrow} C_{j,\downarrow} (1 - n_{j,\uparrow}). \tag{2.3.36}$$

So we can rewrite the t-J model as

$$H_{t-J} = -t \sum_{<i,j>,\sigma} \tilde{C}^{\dagger}_{i,\sigma}\tilde{C}_{j,\sigma}P_0 + J \sum_{<i,j>} \left(\vec{S}_i.\vec{S}_j - \frac{n_i n_j}{4}\right), \tag{2.3.37}$$

where we have used the following notation

$$\tilde{C}_{i,\sigma} = (1 - n_{i,-\sigma})\, C_{i,\sigma}. \tag{2.3.38}$$

It is easy to check that projected electrons ($\tilde{C}_{i,\sigma}$) do not follow onsite fermionic anti-commutation relations. For example we have

$$\left\{\tilde{C}^{\dagger}_{i,\alpha}, \tilde{C}_{i,\alpha}\right\} = \delta_{i,j}\left(1 - C^{\dagger}_{i,-\alpha}C_{i,-\alpha}\right) \tag{2.3.39}$$

$$\left\{\tilde{C}^{\dagger}_{i,\uparrow}, \tilde{C}_{i,\downarrow}\right\} = \delta_{i,j}C^{\dagger}_{i,\uparrow}C_{i,\downarrow}. \tag{2.3.40}$$

It is now cleat that projected electron are operators are not fermions and this is the reason why the Hubbard model is highly nontrivial despite its simple form. Using "tilde" operators, naturally implements the no-doubly occupancy constraint. The effective Hamiltonian in Eq. 2.3.37 does not violate this constraint as well, provided we start from an allowed state which is eigenstate of P_0 operator, i.e. satisfies the no-doubly occupancy which is

$$n_{i,\uparrow}n_{i,\downarrow} = 0, \tag{2.3.41}$$

for every site. Since this constraint in nonlinear in terms of electron operators, its implementation is difficult. Note that it is equivalent to the following inequality constraint

$$n_{i,\uparrow} + n_{i,\downarrow} \leq 1. \tag{2.3.42}$$

From classical mechanics, we know that implementing inequality constraints is difficult. Now we use a trick to turn the above inequality as an equality. To do so, we introduce a "slave" boson h_i which fills all empty sites [15]. We assume this auxiliary particle carries no spin. So we have

$$n_{i,\uparrow} + n_{i,\downarrow} + n_{i,h} = 1. \tag{2.3.43}$$

Now we can easily implement the above equality constraint using Lagrange multiplier method. So whenever we annihilate an electron and as a result we obtain an empty site, a slave boson should occupy that site. On the other hand, whenever an electron wants to occupies a state empty of electrons but with one slave boson, that site is no longer empty and therefore there is no for having a slave boson there. These together leads us to write the following

$$\tilde{C}_{i,\sigma} = (1 - n_{i,-\sigma})\, C_{i,\sigma} = f_{i,\sigma} h_i^\dagger, \tag{2.3.44}$$

in which we have assumed that $f_{i,\sigma}$ is fermion and h_i is boson. The slave fermion $f_{i,\sigma}$ is dubbed as "spinon" and slave boson h_i as holon. We can interpret the above relation as fractionalization of the projected electron. It is a composite operator whose spin is carried by spinon and holon carries its charge [1]. The constraint in Eq. 2.3.43 can be written in terms of new slave particles. We have

$$f_{i,\uparrow}^\dagger f_{i,\uparrow} + f_{i,\downarrow}^\dagger f_{i,\downarrow} + h_i^\dagger h_i = 1. \tag{2.3.45}$$

From this constraint it is obvious that slave particles are hard core fermion and bosons. For example two spinon with opposite spins cannot occupy the same site, however it is allowed by Pauli exclusion principle. There is actually an infinite onsite repulsion between slave particles. So despite its simple form, using slave particles does not solve the problem, because we still have to deal with non-doubly occupancy constraint (we have more of it now!) . It only make the original problem more tractable.

Spin operator in terms of new slave particle becomes

[1] Attaching charge to holon (slave boson particle) is a convention. We can also attach it to spinon without any problem. It can even be distributed between spinon and holon provided $e_h - e_s = e$, where e_h is the electric charge of holon and e_s is that of spinon.

$$S_i^m = \tilde{C}^\dagger_{i,\alpha}\sigma^m_{\alpha,\beta}\tilde{C}_{i,\beta} = n_i^h f^\dagger_{i,\alpha}\sigma^m_{\alpha,\beta}f_{i,\beta} = f^\dagger_{i,\alpha}\sigma^m_{\alpha,\beta}f_{i,\beta}, \tag{2.3.46}$$

where in the last step we have used the hardcoreness of slave particles. Similarly, electrons number operator $n_{i,\uparrow} + n_{i,\downarrow}$, can be written only in terms of spinons and we have $n_i = n^f_{i,\uparrow} + n^f_{i,\downarrow}$. Now We are able to transform the t-J model in its new form in terms of slave particles

$$H_{t-J} = -t \sum_{<i,j>,\sigma} f^\dagger_{i,\sigma}f_{j,\sigma}h^\dagger_j h_i + J\sum_{<i,j>}\left(S_i.S_j - \frac{n_i n_j}{4}\right), \tag{2.3.47}$$

along with the constraint in Eq. 2.3.45. So far there were no approximation in our journey from the original t-J model in Eq. 2.2.34 to Eq. 2.3.51. As it can be seen from the above equation, even the hopping term is nonlinear and involves interaction between spinons and holons. To have a better insight of the problem and use a more systematic approach to exploit approximations for the t-J model, we appeal to the path integral formalism. We have

$$\begin{aligned}
P &= \int Df^\dagger Df Dh^\dagger Dh\; e^{iS} = \int Df^\dagger Df Dh^\dagger Dh\; e^{-\int d\tau L} \\
L &= f^\dagger_{i,\sigma}\frac{\partial}{\partial\tau}f_{i,\sigma} + h^\dagger_i\frac{\partial}{\partial\tau}h_i + i\lambda_i g_i + H \\
g_i &= f^\dagger_{i,\uparrow}f_{i,\uparrow} + f^\dagger_{i,\downarrow}f_{i,\downarrow} + h^\dagger_i h_i - 1.
\end{aligned} \tag{2.3.48}$$

Integration over auxiliary λ_i field leads to the physical constraint in Eq. 2.3.45. This field serves as Lagrange multiplier. Now let us define the following notations

$$\hat{\chi}^f_{i,j} = \sum_\sigma f^\dagger_{i,\sigma}f_{j,\sigma} \tag{2.3.49}$$

$$\hat{\chi}^h_{i,j} = h^\dagger_i h_j \tag{2.3.50}$$

So the t-J Hamiltonian is

$$H_{t-J} = -t \sum_{<i,j>} \hat{\chi}^{f}_{i,j}\hat{\chi}^{h}_{j,i} + J \sum_{<i,j>} \left(S_i.S_j - \frac{n_i n_j}{4}\right), \quad (2.3.51)$$

Now let us focus on the first term. To decouple spinons from holons at the mean field level we first use the extended Hubbard Stratonovic transformation

$$e^{i\epsilon\hat{\chi}^{f}_{i,j}\hat{\chi}^{h}_{j,i}} = N \int \mathcal{D}m^{h}_{i,j}\mathcal{D}m^{f}_{i,j} e^{i\epsilon\left[\hat{\chi}^{f}_{i,j}m^{h}_{j,i}+\hat{\chi}^{h}_{j,i}m^{f}_{i,j}-m^{f}_{i,j}m^{h}_{j,i}\right]} \quad (2.3.52)$$

$$m^{f,h}_{j,i} = m^{f,h}_{i,j}, \quad (2.3.53)$$

where N is renormalization constant. Using the saddle point approximation for $m^{f}_{i,j}$, $m^{h}_{i,j}$ and λ_i fields, we can ignore fluctuations around classical minimum and replace the above path integral with the following

$$e^{i\epsilon\hat{\chi}^{f}_{i,j}\hat{\chi}^{h}_{j,i}} \simeq e^{i\epsilon\left[\hat{\chi}^{f}_{i,j}\left\langle m^{h}_{j,i}\right\rangle+\hat{\chi}^{h}_{j,i}\left\langle m^{f}_{i,j}\right\rangle-\left\langle m^{f}_{i,j}\right\rangle\left\langle m^{h}_{j,i}\right\rangle\right]} \quad (2.3.54)$$

$$e^{i\hat{\lambda}_i g_i} \simeq e^{-\lambda_0 g_i} \quad (2.3.55)$$

$$\left\langle m^{f,h}_{j,i}\right\rangle = \left\langle \hat{\chi}^{f,h}_{i,j}\right\rangle \quad (2.3.56)$$

$$\left\langle \hat{\lambda}_i\right\rangle = i\lambda_0 \quad (2.3.57)$$

From now on by $\chi^{f,h}_{i,j}$ we mean $\left\langle \hat{\chi}^{f,h}_{i,j}\right\rangle$. For Heisenberg term we can use a similar method and we have

$$\begin{aligned} J\sum_{i,j} S_i.S_j = &-J_1 \sum_{<i,j>,\sigma} \chi^{f}_{i,j} f^{\dagger}_{i,\sigma} f_{j,\sigma} - J_2 \sum_{<i,j>,\sigma} \Delta^{f}_{i,j} f^{\dagger}_{i,\sigma} f^{\dagger}_{j,\sigma} + J_3 \sum_{<i,j>} f^{\dagger}_{i,\alpha} \vec{S}_j.\vec{\sigma}_{\alpha,\beta} f_{i,\beta} \\ &+H.c. + J_1 \sum_{i,j,\sigma} \chi^{f}_{i,j}\chi^{f}_{j,i} + J_1 \sum_{i,j,\sigma} \Delta^{f}_{i,j}\Delta^{f\,\dagger}_{i,j} - J_3 \sum_{<i,j>} f^{\dagger}_{i,\alpha} \vec{S}_j.\vec{\sigma}_{\alpha,\beta} f_{i,\beta} + \text{classical fields} \end{aligned} \quad (2.3.58)$$

where there is an ambiguity in choosing J_1, J_2, J_3. Within Hubbard stratonovic method this ambiguity cannot be resolved. So we can decouple $S_i.S_j$ into a linear combination of direct $(f^{\dagger}_i f_j)$, exchange $(f^{\dagger}_i f_j)$, and pairing terms $(f^{\dagger}_i f^{\dagger}_j)$, In Ref. [76], a method has been presented to resolve this problem. It has been argued that an appropriate choice is $J_1 = J_2 = \frac{3}{8}$ and $J_3 = \frac{1}{2}$, provided $\langle S_i\rangle = 0$.

Using the above approximation we have

$$\mathcal{L}_{eff} = f^{\dagger}_{i,\uparrow}\frac{\partial}{\partial\tau}f_{i,\uparrow} + f^{\dagger}_{i,\downarrow}\frac{\partial}{\partial\tau}f_{i,\downarrow} + h^{\dagger}_{i}\frac{\partial}{\partial\tau}h_i + H_{eff}. \tag{2.3.59}$$

where

$$\begin{aligned} H_{eff} = \quad & -t\sum_{<i,j>,\sigma}\chi^{h}_{j,i}f^{\dagger}_{i,\sigma}f_{j,\sigma} - t\sum_{<i,j>}\chi^{f}_{j,i}h^{\dagger}_{i}h_j \\ & -J_1\sum_{<i,j>,\sigma}\chi^{f}_{i,j}f^{\dagger}_{i,\sigma}f_{j,\sigma} - J_2\sum_{<i,j>,\sigma}\Delta^{f}_{i,j}f^{\dagger}_{i,\sigma}f^{\dagger}_{j,\sigma} + J_3\sum_{<i,j>}f^{\dagger}_{i,\alpha}\vec{S}_j.\vec{\sigma}_{\alpha,\beta}f_{i,\beta} \\ & -\lambda_0\sum_{i}\left(f^{\dagger}_{i,\uparrow}f_{i,\uparrow} + f^{\dagger}_{i,\downarrow}f_{i,\downarrow} + h^{\dagger}_{i}h_i - 1\right) + \text{classical terms.} \end{aligned} \tag{2.3.60}$$

In the above approximation for the $t-J$ model, since we implement the physical constraint in Eq. 2.3.45 only in average, the approximation can be dangerous and results of mean-field theory untrustful. Additionally, , the fluctuations of $\chi^{f,h}_{i,j}$ fields should be taken into consideration. The fluctuations of the magnitude of these fields is gapped but their phase fluctuation is gapless (Goldstone modes). In the following it will be turned out that the phase of $\chi^{h,f}_{i,j}$ fields is tied up with the fluctuations of λ_i field which implements the constraint, in time. To have a better insight of the situation lets consider the following local $U(1)$ gauge transformations on slave particles

$$h_i \rightarrow e^{i\theta_i}h_i \tag{2.3.61}$$

$$f_{i,\sigma} \rightarrow e^{i\theta_i}f_{i,\sigma}. \tag{2.3.62}$$

It is obvious that the projected electron operator is invariant under these transformations.

$$\tilde{C}_{i,\sigma} = f_{i,\sigma}h^{\dagger}_{i} \rightarrow \tilde{C}_{i,\sigma}. \tag{2.3.63}$$

The constraint is also invariant. So the original $t-J$ Lagrangian is invariant under local gauge transformation as well This fact should be somehow reflected in the meanfield state as well. Therefore $\chi_{i,j}$ and λ_i fields should transform in the following way

$$\chi_{i,j}^{f,h} \to e^{i(\theta_i - \theta_j)} \chi_{i,j}^{f,h} \tag{2.3.64}$$

$$\lambda_i \to \lambda_i - \partial_\tau \theta_i. \tag{2.3.65}$$

Using the above relations, it can be checked that when $\delta_{i,j}^f = 0$, the meanfield Lagrangian in Eq. 2.3.59 is also gauge invariant. Now let us use the following notations

$$\chi_{i,j} = |\chi_{i,j}| \, e^{i\vec{a}_{i,j}} \tag{2.3.66}$$

$$a_0(i) = \lambda_i. \tag{2.3.67}$$

So we have

$$h_i \to e^{i\theta_i} h_i \tag{2.3.68}$$

$$f_{i,\sigma} \to e^{i\theta_i} f_{i,\sigma} \tag{2.3.69}$$

$$a_{i,j} \to a_{i,j} + (\theta_i - \theta_j) \tag{2.3.70}$$

$$a_0(i) \to A_0(i) - \partial_\tau \theta_i. \tag{2.3.71}$$

So the $A^\mu(i)$ field defined in the following way, is the vector potential of a compact gauge field.

$$\mu = 1, 2: \qquad a_\mu(i) = a_{i,i+\hat{e}_\mu}, \qquad \hat{e}_1 = \hat{x}, \qquad \hat{e}_2 = \hat{y}. \tag{2.3.72}$$

$$\mu = 0: \qquad a_0(i) = \lambda_i. \tag{2.3.73}$$

Compactness originates from the definition of $a_{i,j}$ field. $a_{i,j}$ is identified with $a_{i,j} + 2\pi$, because only $e^{ia_{i,j}}$ is physical. Therefore

$$a_{i,j} \sim a_{i,j} + 2\pi. \tag{2.3.74}$$

The vector potential is therefore defined on a circle with radius one instead of an infinite line. Although meanfield calculations are rather simple, the study of compact gauge fluctuations makes the problem difficult. We have two situations. In one regime the gauge fluctuations are weak so we can ignore the compact nature of the gauge field and approximate it with a non-compact $U(1)$ gauge field with gaussian fluctuations. This is called the deconfined phase. In the second regime, gauge fluctuations are strong and we cannot ignore the compactness of the gauge field. This is called the confined phase. In chapters four and five we discuss more about the properties of this phase.

2.4 Properties of the t-J model at Half filling

At half filling we have only spinons and there is no holon in the half filled t-J model and we have particle hole symmetry on bipartite lattices. Let us focus on square lattice for now. Particle hole symmetry imposes $\lambda_0 = 0$ constraint. Let us assume that there is staggered magnetization, i.e. the Néel order parameter is zero. Within meanfield we have

$$H = \quad -J_1 \sum_{<i,j>,\sigma} \chi^f_{i,j} f^\dagger_{i,\sigma} f_{j,\sigma} - J_2 \sum_{<i,j>,\sigma} \Delta^f_{i,j} f^\dagger_{i,\sigma} f^\dagger_{j,\sigma} + H.c. + \text{classical terms} \tag{2.4.75}$$

This model has been studied extensively in literature. One possible phase is the d-wave state. In this state $2J_1\chi^f_{i,j} = \chi_0$, $2J_2\Delta^f_{i,i\pm\hat{x}} = \Delta_0$ and $2J_2\Delta^f_{i,i\pm\hat{y}} = -\Delta_0$. We can rewrite the Hamiltonian in the Momentum space and we have

$$H = \sum_k \left[f^\dagger_{k,\uparrow}, f_{-k,\downarrow} \right] \begin{bmatrix} -\chi_0 \left(\cos\left(k_x\right) + \cos\left(k_y\right)\right) & -\Delta_0 \left(\cos\left(k_x\right) - \cos\left(k_y\right)\right) \\ -\Delta_0 \left(\cos\left(k_x\right) - \cos\left(k_y\right)\right) & +\chi_0 \left(\cos\left(k_x\right) + \cos\left(k_y\right)\right) \end{bmatrix} \begin{bmatrix} f_{k,\uparrow} \\ f^\dagger_{-k,\downarrow} \end{bmatrix} \tag{2.4.76}$$

With energy excitations

$$E_k = \sqrt{\chi_0^2 \left(\cos\left(k_x\right) + \cos\left(k_y\right)\right)^2 + \Delta_0^2 \left(\cos\left(k_x\right) - \cos\left(k_y\right)\right)^2}. \tag{2.4.77}$$

The energy spectrum is gapless at four inequivalent points in the Brillouin zone which are $\vec{k} = \frac{\pi}{2}\left(\pm, \pm\right)$. Around these points we can expand the energy and we obtain massless dirac cones with energy $E_Q = \sqrt{Q_+^2 + Q_-^2}$, where $Q_+ = \chi_0 (q_x + q_y)$ and $Q_- = \Delta_0 (q_x - q_y)$.

Now let us consider a state where $\chi^f_{i,j} = \chi_0 \exp\left(i(-)^{i_x+j_y}\Phi\right)$ where $\tan\Phi = \chi_0/\Delta 0$, and $\Delta^f_{i,j} = 0$. If we go around a plaquette defined by i, $i+\hat{x}$, $i+\hat{x}+\hat{y}$ and $i+\hat{y}$, we obtain a staggered pattern of $\pm 4\Phi$ phases. This state is called the staggered flux phase. This phase has exactly the energy spectrum as in the Eq. 2.4.77. In fact this property is not accidental. It is due to a hidden $SU(2)$ symmetry in the t-J model at half filling. To see this more explicitly let us consider the following operator

$$\psi_i = \begin{bmatrix} C_{i,\uparrow} & C_{i,\downarrow} \\ C^\dagger_{i,\downarrow} & -C^\dagger_{i,\uparrow} \end{bmatrix}. \tag{2.4.78}$$

The Heisenberg interaction can be written in terms of this new operator as

$$H = (J/16)\sum_{i,j} \left(\psi_i^\dagger \psi_i \sigma^T\right) \cdot \left(\psi_j^\dagger \psi_j \sigma^T\right). \tag{2.4.79}$$

It is obviously invariant under global $SU(2)$ transformations of the $\psi_i \to \psi_i g_{2\times 2}$. It is also invariant under local $SU(2)$ gauge transformations as $\psi_i \to [h_{2\times 2}]_i \psi_i$. So the Heisenberg model is invariant under

$$\psi_i \to h_i \psi_i g, \tag{2.4.80}$$

transformations. Going back to the slave particle language, it corresponds to the following local $SU(2)$ particle-hole transformation

$$f_{i,\uparrow} \to \alpha_i f_{i,\uparrow} + \beta_i f^\dagger_{i,\downarrow}, \tag{2.4.81}$$

$$f_{i,\downarrow} \to -\beta_i^* f_{i,\uparrow} + \alpha^* f^\dagger_{i,\downarrow}. \tag{2.4.82}$$

Using an appropriate $SU(2)$ transformation we can map the staggered flux ansatz to the d-wave ansatz, and these two states become gauge equivalent.

2.5 Projective symmetry group(PSG) of the Model

A projective symmetry group (PSG) is a property of an ansatz. It is formed by all of the transformations that keep the ansatz unchanged. Each transformation (or each element in the PSG) can be written as a combination of a symmetry transformation U (such as translation) and a gauge transformation G_U. The invariance of the ansatz under its PSG can be expressed as follows:

$$G_U U\left(u_{ij}\right) = u_{ij} \tag{2.5.83}$$

$U\left(u_{ij}\right) \equiv u_{U(i),U(j)}$, $G_U\left(u_{ij}\right) \equiv G_U\left(i\right) u_{ij} G_U^{\dagger}\left(j\right)$, $G_U\left(i\right) \in U\left(1\right)$, for each $G_U U \in PSG$.

Every PSG contains a special subgroup, which will be called the invariant gauge group (IGG). The IGG (denoted by g) for an ansatz is formed by all of the pure gauge transformations that leave the ansatz unchanged.

$$g = \left\{W_i | W_i u_{ij} W_j^{\dagger} = u_{ij}, W_i \in U(1)\right\} \tag{2.5.84}$$

If we want to relate the IGG to a symmetry transformation, then the associated transformation is simply the identity symmetry transformation.

If the IGG is non-trivial, then for a fixed symmetry transformation U, there can be many gauge transformations G_U such that G_U will leave the ansatz unchanged. If G_U is in the PSG of u_{ij}, then GG_U will also be in the PSG if and only if $G \in g$. Thus for each symmetry transformation U, the different choices of G_U have a one-to-one correspondence with the elements in the IGG. From the above definition, we see that the PSG, the IGG, and the symmetry group (SG) of an ansatz are related as follows:

$$SG = PSG/IGG$$

This relation tells us that a PSG is a projective representation or an extension of the symmetry group.[2]

[2]More generally, we say that a group PSG is an extension of a group SG if the group PSG contains a

Therefore, however the meanfield ansatz may break some symmetries of the lattice, its meanfield state can preserve all symmetries. For example let us consider translation in the $\hat{x}$ direction. The meanfield state $|\psi\rangle$ may break this symmetry, but the transformed wavefunction $|\psi'\rangle$ can be gauge equivalent to the untransformed, i.e. $|\psi'\rangle = \prod_i G_i |\psi\rangle$. Since all gauge equivalent wavefunctions correspond to the same physical state after projection, these two states are not physically distinguishable. Therefore the physical state (projected wavefunction) does not break the lattice symmetry. Similarly we can argue that under any symmetry operation, if the transformed wavefunction is gauge equivalent to the untransformed one, the physical wavefunction preserves that symmetry. The topological orders of that physical state is represented by the symmetry properties of the corresponding meanfield Hamiltonian. Therefore we can classify physical states by the set of gauge transformations needed for each symmetry operation. For example let us consider the staggered flux phase. If we translate this state in the $\hat{x}$ direction for instance, the meanfield ansatz changes as

$$\chi^f_{i,j} = \chi_0 \exp\left(i(-)^{i_x+j_y}\Phi\right) \to \chi^f_{i+\hat{x},j+\hat{x}} = \chi_0 \exp\left(i(-)^{i_x+1+j_y}\Phi\right) = {\chi^f_{i,j}}^*. \tag{2.5.85}$$

However we can use the following gauge transformation

$$\begin{pmatrix} f_{i,\uparrow} \\ f^\dagger_{i,\downarrow} \end{pmatrix} \to G_{T_x}(i) \begin{pmatrix} f_{i,\downarrow} \\ f^\dagger_{i,\downarrow} \end{pmatrix}, \tag{2.5.86}$$

where

$$G_{T_x}(i) = i\,(-)^{i_x+i_y}\,\tau^1, \tag{2.5.87}$$

where τ^1 is the first Pauli matrix, it goes back to $\chi^f_{i,j}$. Therefore the ansatz and as a result the meanfield Hamiltonian is invariant under $G_{T_x}T_x$ not T_x. Similarly it can be shown that the ansatz is invariant under $G_{T_y}T_y$ (translation in the $\hat{y}$ direction),$G_{P_x}P_x$ (parity under x axis where $(x,y) \to (-x,y)$),$G_{P_y}P_x$ (parity under y axis where $(x,y) \to (x,-y)$),$G_{P_{xy}}P_{xy}$ (reflection under x=y line where $(x,y) \to (y,x)$) and $G_T T$ (time reversal operator where $t \to -t$) is invariant where

normal subgroup IGG such that PSG/IGG=SG.

$$G_{T_y}(i) = i(-)^{i_x+i_y}\tau^1, \qquad G_{P_x}(i) = G_{P_y}(i) = \tau^0$$
$$G_{P_{xy}}(i) = i(-)^{i_x+i_y}\tau^1, \qquad G_T(i) = \tau^0 \tag{2.5.88}$$

Chapter 3

Phase diagram of the Hubbard model on honeycomb lattice

In this chapter we study the phase diagram of the Hubbard model on honeycomb lattice. We start from the non-interacting tight binding model which is a good approximation for some physical systems, e.g. graphene. At half-filling we obtain semi-metallic phase whose Fermi surface shrinks to two isolated points in the Brillouin zone. The energy spectrum near these two points is linear in momentum and can be approximated as two Dirac cones. Using this approach, we develop an effective continuum model describing this phase. Then we consider small U-limit of the Hubbard model. We discuss that for small U/t ratios, the onsite Coulomb repulsion is irrelevant in the renormalization group sense and the semi-metal phase is robust and stable against weak and short ranged interactions. For moderate values of U/t, we use rotor slave particle approach to study this phase. For higher values of U, Mott transition into insulating phase is expected. To study this phase transition, we generalize the slave-particle technique to study the phase diagram of the strongly correlated Hubbard model on honeycomb lattice which may contain charge fluctuations. For large U, we have antiferromagnetic order phase. As we decrease U below $U_{c2} \simeq 3t$, the system undergoes a first order phase transition into a gapped spin rotation invariant phase. Within meanfield theory, this state preserves all symmetries of the lattice and exhibits the staggered compact $U(1)$ gauge fluctuations. Because of the compactness of the gauge field, we expect instanton proliferation a therefore a confined phase in $2+1D$. Under a semiclassical approximation of the slave-particle approach, we find that such phase breaks the translation symmetry, the time reversal and the lattice rotation symmetry. However, beyond the semiclassical approximation, a Z_2 spin liquid that does not break any lattice symmetry is also possible.

3.1 Introduction

Hubbard model[30, 27] is believed to describe the physics of many strongly correlated systems e.g., Mott insulator[58, 31] and high temperature superconductors[13, 8, 46]. It is the simplest model one can write capturing the strong correlation physics. So far many theoretical[26, 50] and numerical techniques[56, 21, 51] have been developed to study this model. Among them is the slave particle[92, 19, 49, 68] theory which was motivated by the RVB state first introduced by P.W. Anderson[7]. One of the interesting phases that have been studied and is strongly supported by the slave particle approach is the Z_2 spin liquid phase[64, 83, 84] which does not show any long range order down to zero temperature. Unfortunately this phase has not been experimentally verified but recently Meng *et al*[56] have studied the Hubbard model on honeycomb lattice at half filling using the quantum Monte Carlo (QMC) method and have reported the existence of a spin liquid phase for a range of U/t. Fortunately QMC does not have sign problem on bipartite lattices at half filling so we can trust its results. For small U-limit they have reported the semi-metallic phase. At $U_{c1} \sim 3.5t$ they have seen a phase transition to the spin liquid with nonzero spin excitation gap (gapped spin liquid). At U_{c1} the charge gap opens up and therefore this transition point is associated with the Mott metal-insulator transition. For a larger value of $U_{c2} \sim 4.3t$ they have obtained the anti-Ferromagnetic (AF) order in which the charge gap is still nonzero but the spin excitation is the gapless Goldstone mode.

In this chapter, we generalized the slave-particle method[92, 46] to capture charge fluctuations[49] to study the Hubbard model on honeycomb lattice. we have obtained a similar phase diagram (see Fig. 3-1 and 3-2) as in [56] but with different numerical values for U_{c1} and U_{c2}. We obtained a superconducting phase (instead of the semi-metal phase) for small U/t and a AF phase for large U/t. At the meanfield level, our phase between U_{c1} and U_{c2} is a spin liquid with finite charge/spin gap that do not break any symmetry. However, the meanfield state is unstable. Under a semiclassical approximation, we show that phase between U_{c1} and U_{c2} is a charge/spin gapped state that breaks translation and lattice rotation symmetry but not spin rotation symmetry. On the other hand, in the presence of the

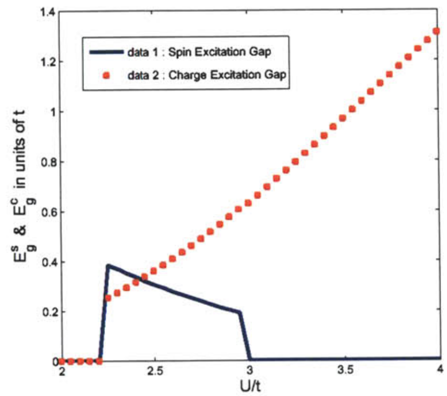

Figure 3-1: **Spin and charge excitation gap.**— Spin excitation gap (blue line) and charge excitation gap (red dots)

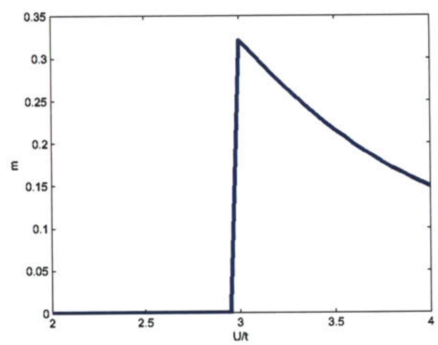

Figure 3-2: **Néel order parameter.**— Staggered magnetization, m $((-)^i\ S_z(i))$, as a function of $\frac{U}{t}$. There is a phase transition to the antiferromagnetic order at $U/t = 3$.

second neighbor hopping, the meanfield state may become a Z_2 spin liquid state[64, 83, 84] that does not break any symmetry and has finite charge/spin gaps. All phase transitions are first order which agrees with experiments[31].

We would like to point out that the slave-rotor method is the other method to include charge fluctuations which give rise to a nodal spin liquid between $1.68t < U < 1.74t$. The slave-rotor method is more reliable for small U/t and gives rise to the correct semi-metal phase. Our method is quite unreliable at small U/t and gives rise to a (wrong) superconducting state.

In the large U/t limit, the Hubbard model can be approximated by the Heisenberg model and we expect strong AF order in it. This model has been extensively studied by different methods [57, 81, 52, 62, 63, 20, 89]. Here we use a different approach to study the antiferromagnetic phase. It is shown that the spin/chrage gapped phase has an instability towards antiferromagnetism.

3.2 RG flow of small-U Hubbard model on honeycomb lattice

Let us consider the tight binding model on the honeycomb lattice at half filling. Since the unit cell contains two atoms, we label electronic operators by sublattice indices A and B, $C^{\dagger}_{i,A,\sigma}$ creates one spin σ electron on sublattice A and $C^{\dagger}_{i,B,\sigma}$ creates a spin σ electron on sublattice B. The tight binding Hamiltonian with only nearest neighbor is defined as

$$H = -t \sum_{<i,j>,\sigma} C^{\dagger}_{i,A,\sigma} C_{i,B,\sigma} + H.c. \ . \tag{3.2.1}$$

Consider the Fourier transform of electronic operators defined as follow

$$\begin{aligned} C^{\dagger}_{k,A,\sigma} &= \frac{1}{\sqrt{N}} \sum_i \exp\left(ik.R_i\right) C^{\dagger}_{i,A,\sigma}, \\ C^{\dagger}_{k,B,\sigma} &= \frac{1}{\sqrt{N}} \sum_i \exp\left(ik.R_i\right) C^{\dagger}_{i,B,\sigma}, \end{aligned} \tag{3.2.2}$$

where N is the number of sites on sublattice A. The Hamiltonian in this basis is

$$H = \sum_{k,\sigma} \left[C^{\dagger}_{k,A,\sigma}, C^{\dagger}_{k,B,\sigma}\right] \begin{bmatrix} 0 & t_k \\ t^*_k & 0 \end{bmatrix} \begin{bmatrix} C_{k,A,\sigma} \\ C_{k,B,\sigma} \end{bmatrix}, \tag{3.2.3}$$

where t_k is defined as

$$t_k = \sum_{i=1,2,3} e^{ik.b_i} = e^{ik_y} + 2e^{\frac{ik_y}{2}} \cos\frac{\sqrt{3}k_x}{2}. \tag{3.2.4}$$

The energy spectrum of this system is

$$E_k = \pm |t_k| = \pm \sqrt{1 + 4\cos\frac{3k_y}{2}\cos\frac{\sqrt{3}k_x}{2} + 4\cos^2\frac{\sqrt{3}k_x}{2}}\,. \tag{3.2.5}$$

At half filling the chemical potential is zero at $T = 0$. So we should fill all negative bands. From the band structure it can be seen that we have two inequivalent gapless points in the Brillouin zone, corresponding to

$$K = \frac{4\pi}{3\sqrt{3}}(1,0)\,, \qquad K' = \frac{4\pi}{3\sqrt{3}}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right). \tag{3.2.6}$$

Since we have obtained isolated Fermi points instead of a closed Fermi surface, the ground-state is "semi-metal". The Hamiltonian can be expanded around these points and we obtain

$$\vec{k} = \vec{K} + \vec{q}: \qquad t_{K+q} = -\frac{3t}{2}\left(-q_x + iq_y\right) \qquad H_{K+q} = v_F q_x \sigma^1 + v_F q_y \sigma^2 \tag{3.2.7}$$

$$\vec{k} = \vec{K'} + \vec{q}: \qquad t_{K'+q} = -\frac{3t}{2}\left(q_x + iq_y\right) \qquad H_{K'+q} = -v_F q_x \sigma^1 + v_F q_y \sigma^2, \tag{3.2.8}$$

where v_F is the fermi velocity of low energy excitations. In the remainder of this section $\mu = A, B$ denotes the sublattice index and $\nu = K, K'$ denotes valley index. Now let us use the following continuum wavefunctions defined as

$$\psi_{\nu,\mu,\sigma}(\vec{r}) = \sqrt{\frac{2}{L_1 L_2}} \int d^2\vec{r}\; e^{-iq.r} C_{\nu+q,\mu,\sigma}, \tag{3.2.9}$$

where $L_{1,2}$ is the length of the system in the x and y directions. The continuum Hamiltonian can be written in terms of these wavefunction and we have

$$H = -iv_F \int d^2\vec{r}\; \psi^\dagger(r)\left(\mu^3 \otimes \nu^1 \otimes \sigma^0 \partial_x + \mu^0 \otimes \nu^2 \otimes \sigma^0 \partial_y\right)\psi(r)\,. \tag{3.2.10}$$

From the above expression we can construct Lagrangian and using $S = \int dtL$ definition of action, we have

$$S = i \int d^2\vec{r}dt \ \psi^\dagger(r) \left(\partial_t - v_F \mu^3 \otimes \nu^1 \otimes \sigma^0 \partial_x + v_F \mu^0 \otimes \nu^2 \otimes \sigma^0 \partial_y \right) \psi(r) . \quad (3.2.11)$$

Now we want to investigate properties of this phase under renormalization group (RG) flow. Since action is invariant under $x \to e^{-l}x$, $y \to e^{-l}y$ and $t \to e^{-l}t$ transformations, we conclude that wavefunction should changes as $\psi \to e^{+l}\psi$. Now let us add the onsite $U \sum_{i,\tau} n_{i,\mu,\uparrow} n_{i,\mu,\downarrow}$ term to the tight binding Hamiltonian to obtain the Hubbard model. For small U/t limit which is connected to the $U = 0$ case, the tight binding model is a good starting point. We can replace $n_{i,\mu,\sigma}$ by $\psi^\dagger \frac{1+\mu\mu^3}{2} \frac{1+\sigma\sigma^3}{2} \psi$ within the continuum approximation. So we have:

$$\delta S \sim U \int d^2\vec{r}dt \ \psi^\dagger(r) \frac{1+\sigma^3}{2} \psi(r) \psi^\dagger(r) \frac{1-\sigma^3}{2} \psi(r) . \quad (3.2.12)$$

Since we already showed that under RG flow $\psi \to e^{+l}\psi$, we conclude that

$$U \to e^{-l}U. \quad (3.2.13)$$

So the onsite term is an irrelevant perturbation and does not gap out the system. As a result the semi-metal phase is robust for small U/t limit of the Hubbard model on the honeycomb lattice. Any other short range interaction can be replaced by a similar quartic term as in Eq. 3.2.12 and is therefore an irrelevant perturbation.

3.3 Intermediated U/t limit of the Hubbard Model

3.3.1 Introduction to the Rotor Slave Boson Method

In slave rotor model, electron operator is decomposed in to parts. The first part creates spin and the second one creates charge of spin. The spin is attached to a fermionic object while charge is attached to a quantum rotor. In rotor model, the L_z and X operators are defined in the following way

$$L_i = i\partial_{\theta_i}, \qquad X_i^\dagger = e^{i\theta_i}. \tag{3.3.14}$$

L_i can be viewed as number operator, while $X_i^\dagger$ is creation operator. To see this more explicitly, note that $|l\rangle_i = \exp(il\theta_i)$ is an eigenstate of L_i with quantum number equal to l. By acting $X_i^\dagger = e^{i\theta_i}$, l changes to $l+1$. So X_i is the creation operator for L_i eigenstates. Now let us identify L_i operator with the fluctuations of electric charge at site i. So l runs from to $-1, 0, +1$. -1 corresponds to the doubly occupied state, 0 to a state with only one electron and $+1$ corresponds to the empty state at site i. On the other hand, let us consider $f_{i,\sigma}^\dagger$ operator which creates a neutral spin σ fermion at site i. Therefore $f_{i,\sigma}^\dagger X_i^\dagger$ creates a neutral spin σ fermion and adds one quantum of electric charge at site i. So we can identify this operator with the electron creation operator at site i and we have

$$C_{i,\sigma} = f_{i,\sigma} X_i. \tag{3.3.15}$$

It should be noted that for doubly occupied site $L_i = 1 - f_{i,\uparrow}^\dagger f_{i,\uparrow} - f_{i,\downarrow}^\dagger f_{i,\downarrow} = -1$. For singly occupied sites $L_i = 1 - f_{i,\uparrow}^\dagger f_{i,\uparrow} - f_{i,\downarrow}^\dagger f_{i,\downarrow} = 0$ and for empty site $L_i = 1 - f_{i,\uparrow}^\dagger f_{i,\uparrow} - f_{i,\downarrow}^\dagger f_{i,\downarrow} = +1$. So for physical states we have to implement the following constraint at each site

$$L_i = 1 - f_{i,\uparrow}^\dagger f_{i,\uparrow} - f_{i,\downarrow}^\dagger f_{i,\downarrow}. \tag{3.3.16}$$

At half filling, $\sum_i n_{i,\uparrow} n_{i,\downarrow} = \sum_i n_{i,\uparrow} \frac{n_{i,\downarrow} + (1-n_{i,\uparrow})(1-n_{i,\downarrow})}{2}$. On the other hand, $\frac{n_{i,\downarrow} + (1-n_{i,\uparrow})(1-n_{i,\downarrow})}{2} = L_i^2$. So the Hubbard model can be written in terms of slave particles as follows

$$H = U \sum_i L_i^2 - t \sum_{<i,j>,\sigma} f_{i,\sigma}^\dagger f_{j,\sigma} X_i^\dagger X_j. \tag{3.3.17}$$

The above Hamiltonian should be considered along with the local constraint in Eq. 3.3.16. To implement the constraint we can use the Feynman path integral formulation, with the following action

$$S = \int_0^\beta d\tau \left[\sum_{i,\sigma} f_{i,\sigma}^\dagger \left(\frac{\partial}{\partial\tau} + ih_i \right) f_{i,\sigma} + \frac{1}{2U} \sum_i (\partial_\tau \theta_i + h_i)^2 \right.$$
$$\left. -t \sum_{<i,j>,\sigma} \left(f_{i,\sigma}^\dagger f_{j,\sigma} e^{i(\theta_i - \theta_j)} \right) - i \sum_i h_i \right], \tag{3.3.18}$$

in which we have used h_i field to implement the local constraint in Eq. 3.3.16. Integration over h_i leads to the constraint. The above action has been studied by several authors. S.S. Lee and P.A. [49] Lee have developed a $U(1)$ gauge theory for this model. They have studied the phase diagram of the Hubbard model on honeycomb lattice and triangular lattice within slave rotor formalism. On the honeycomb lattice and for the nearest neighbor hopping Hubbard model, below the phase transition the excitation energy for slave rotors is gapless, while it is gapped above Mott transition. *"For nearest neighbor hopping, the fermion dispersion is characterized by 2 inequivalent Dirac cones at the Brillouin zone corner. On the insulating side of the Mott transition, the rotor is again gapped and the problem reduces to* $2N$ *Dirac cones coupled to a compact* $U(1)$ *gauge field with* $N = 2$*".*

3.4 Strongly correlated Hubbard Model

3.4.1 Anderson Zou Slave Particle Method

The Hubbard model is defined as the following:

$$H = U \sum_i n_{i,\uparrow} n_{i,\downarrow} - t \sum_{\langle i,j \rangle,\sigma} C_{j\sigma}^\dagger C_{i\sigma} + h.c. \tag{3.4.19}$$

Here $\langle i,j \rangle$ means site j is one of the nearest neighbors of site i. We know that Hilbert space of Hubbard Hamiltonian has four sates per site. $|0_f\rangle_i, |\uparrow\rangle_i, |\downarrow\rangle_i, |\uparrow\downarrow\rangle_i$. Let's name each state as follows: $|\text{holon}\rangle_i = h_i^\dagger |\text{vac}\rangle_i = |0\rangle_i$, $|\text{spin up spinon}\rangle_i = f_{i,\uparrow}^\dagger |\text{vac}\rangle_i = |\uparrow\rangle_i$, $|\text{spin down spinon}\rangle_i = f_{i,\downarrow}^\dagger |\text{vac}\rangle_i = |\downarrow\rangle_i$, $|\text{doublon}\rangle_i = d_i^\dagger |\text{vac}\rangle_i = |\uparrow\downarrow\rangle_i$ in which $|\text{vac}\rangle$ is the vacuum, an unphysical state which contains no slave particles even holons. Using this picture we can rewrite the electron creation operator as

$$C_{i,\sigma}^{\dagger} = f_{i,\sigma}^{\dagger} h_i + \sigma\, d_i^{\dagger} f_{i,-\sigma} = \begin{bmatrix} h_i & d_i^{\dagger} \end{bmatrix} \begin{bmatrix} f_{i,\sigma}^{\dagger} \\ \sigma f_{i,-\sigma} \end{bmatrix}. \tag{3.4.20}$$

It should be mentioned that the physical Hilbert space contains only four states: empty state (holon), one electron (spinon) and two electrons (doublon) on each site. So we always have one and only one slave particle on each site. So we conclude that we should put the local constraint

$$n_i^h + n_{i,\uparrow}^f + n_{i,\downarrow}^f + n_i^d = 1, \tag{3.4.21}$$

to get rid of redundant states. This is the physical constraint which should be satisfied on every site. We could also obtain this result by noting that the electron operators are fermion and should satisfy the anticommutation relations. From the definition of $C_{i,\sigma}^{\dagger}$ it is obvious that it is invariant under the following U(1) gauge transformations (We require h_i and d_i to remain bosonic operators i.e., preserve their statistics after transformation, otherwise we would have SU(2) gauge invariance. However at $U = \infty$ we have only fermions and only in that case we have SU(2) gauge symmetry).

$$f_{i,\sigma} \to e^{-i\theta} f_{i,\sigma}, \qquad h_i \to e^{-i\theta} h_i, \qquad d_i \to e^{-i\theta} d_i. \tag{3.4.22}$$

It is worth noting the above equation tells that all the slave particles carry the same charge under the internal U(1) gauge. Since the constraint as well as the Hubbard Hamiltonian are gauge invariant, so is the action of the Hubbard model.

In terms of new slave particles, the Hubbard Hamiltonian can be written as:

$$H = \sum U d_i^{\dagger} d_i - t \sum_{\langle i,j \rangle} \left(\chi_{i,j}^f \chi_{j,i}^b + \Delta_{i,j}^{f\dagger} \Delta_{i,j}^b + h.c. \right) \tag{3.4.23}$$

In which we have used these notations $\chi_{i,j}^f = \sum_\sigma f_{i,\sigma}^{\dagger} f_{j,\sigma}$, $\chi_{i,j}^b = h_i^{\dagger} h_j - d_i^{\dagger} d_j$, $\Delta_{i,j}^f = \sum_\sigma \sigma f_{-\sigma,i} f_{j,\sigma}$, $\Delta_{i,j}^b = d_i h_j + h_i d_j$. To implement the constraint we appeal to the path integral and the Lagrange multiplier methods, in which we use the following identity

$$\int \mathcal{D}\lambda e^{i\int d\vec{r}\lambda_{\vec{r}}\mathcal{O}_{\vec{\nabla}}} = \delta\left(\mathcal{O}_{\vec{\nabla}}\right). \tag{3.4.24}$$

where $\lambda_{\vec{r}}$ field serves as the Lagrange multiplier in the classical mechanics. So we have

$$\begin{aligned}
\mathcal{P} &= \int \mathcal{D}f^{\dagger}\mathcal{D}f\mathcal{D}h^{\dagger}\mathcal{D}h\mathcal{D}d^{\dagger}\mathcal{D}d\; e^{-\int d\tau\mathcal{L}} \\
\mathcal{L} &= f^{\dagger}_{i,\sigma}\frac{\partial}{\partial\tau}f_{i,\sigma} + d^{\dagger}_{i}\frac{\partial}{\partial\tau}d_i + h^{\dagger}_{i}\frac{\partial}{\partial\tau}h_i + i\lambda_i g_i + H, \\
g_i &= f^{\dagger}_{i,\uparrow}f_{i,\uparrow} + f^{\dagger}_{i,\downarrow}f_{i,\downarrow} + h^{\dagger}_{i}h_i + d^{\dagger}_{i}d_i - 1.
\end{aligned} \tag{3.4.25}$$

The above motivates us to define the effective Hamiltonian as $H_{eff} = H + i\sum_i \lambda_i g_i$. Now by using the Hubbard-Stratonovic transformation we can decouple spinons from [hard-core] bosons at the mean field level. To do so we just replace $\chi_{i,j}$ and other operators with their average. For translational invariant systems we can assume: $\langle\chi_{i,j}\rangle = \langle\chi_{i-j}\rangle$ and so on. From now on χ stands for the average of χ operators and so on. Moreover $\langle i\lambda_i\rangle = \lambda_0$. By these assumptions we can obtain unknown parameters in the effective Hamiltonian from self-consistency equations. Now, let us focus on the effective Hamiltonian of bosons. As long as Δ_f is nonzero, the pairing between holons and doublons is nonzero, and they form bound state. Using the Bogoliubov transformation we can show that the ground-state wave-function of bosons is a paired state which is completely symmetric between holons and doublons. Therefore, as long as this state represents the ground, we have $\left\langle h^{\dagger}_{k,A}h_{k,B}\right\rangle = \left\langle d^{\dagger}_{k,A}d_{k,B}\right\rangle$, and as a result: $\chi_b = \left\langle h^{\dagger}_{i,A}h_{j,B} - d^{\dagger}_{i,A}d_{j,B}\right\rangle = 0$. Spinons cannot hop in this case and the system is insulator. Self-consistent equations show that $\chi_f = 0$ as well and therefore the following Hamiltonians describe the low energy theory of this phase:

$$H_f^{A,B} = \sum_k \begin{bmatrix} f^{\dagger}_{k,A,\uparrow} & f_{-k,B,\downarrow} \end{bmatrix} \begin{bmatrix} -\lambda_0 & -t\Delta^b_k \\ -t\Delta^b_k & +\lambda_0 \end{bmatrix} \begin{bmatrix} f_{k,A,\uparrow} \\ f^{\dagger}_{-k,B,\downarrow} \end{bmatrix} \tag{3.4.26}$$

$$H_b^{A,B} = \sum_k \begin{bmatrix} d^{\dagger}_{k,A} & h_{-k,B} \end{bmatrix} \begin{bmatrix} U-\lambda_0 & -t\Delta^f_k \\ -t\Delta^f_k & -\lambda_0 \end{bmatrix} \begin{bmatrix} d_{k,A} \\ h^{\dagger}_{-k,B} \end{bmatrix} \tag{3.4.27}$$

where $\Delta^{f,b}\left(\vec{k}\right) = \sum_{\delta}\Delta^{f,b}_{\vec{\delta}}\, e^{i\vec{k}.\vec{\delta}}$ and $\vec{\delta}$ connects two nearest neighbors. We have similar equations for $H_f^{B,A}$ and $H_b^{B,A}$. Using the Bogoliubov transformation we can diagonalize the above Hamiltonians. The energy excitation for spinons is

$$E_k^f = \sqrt{\lambda_0^2 + (t\Delta_k^b)^2}. \tag{3.4.28}$$

For bosonic part we obtain

$$E_b^{\pm,k} = + \pm \frac{U}{2} + \sqrt{\left(\frac{U - 2\lambda_0}{2}\right)^2 - \left(t\Delta_k^f\right)^2}. \tag{3.4.29}$$

At half filling, in order to excite a charge we need to annihilate two spinons and create a pair of holon-doublon. So we can define the charge excitation gap as the sum of the excitation energy of a holon and a doublon. When the charge gap is nonzero then the paired holon-doublon state is stable because exciting quasi-particles on top of this state costs energy. For this state, the charge gap is $E_c^g = \min E_b^{+,k} + \min E_b^{-,k} = 2\sqrt{\left(\frac{U-2\lambda_0}{2}\right)^2 - (3t\Delta^f)^2}$. Therefore, as long as $U - 2\lambda_0 > 6t\Delta_f$, charge gap is finite and we are in the insulating phase.

On the other hand, when the charge gap closes, the paired holon-doublon state becomes unstable and free holons and doublons proliferate. In this state, doublons and holons condense independently (single boson condensation) such that $\langle d_{i,A}\rangle = -\langle d_{i,B}\rangle$ and $\langle h_{i,A}\rangle = \langle h_{i,B}\rangle$, and therefore $\chi_b = 2\langle h_{i,A}\rangle^2 = 2n_h \neq 0$, therefore spinons can hop freely and the ground state is no longer an insulator. Since doublons condense at sublattice A and B with opposite signs, we show that $\Delta_b = 0$ and as a result $\Delta_f = 0$. we relate the onset of single boson condensation, i.e. the critical point below which charge gap closes, to the Mott transition. It should be mentioned that $\chi_{f,b}$ as well as $\Delta_{b,f}$ jump at this point, so we obtain a first order phase transition in this way, which is consistent with experiments. We like to point out that since $d^\dagger h$ operator that carries $2e$ electric charge, condenses in this state, we indeed obtain a superconducting state instead of a semi-metallic phase.

The ground state of H_{MF} is the tensor product of $|g\rangle_f$ and $|g\rangle_b$. But because of the constraint on the physical states, at each lattice site there should be only and only one slave particle. Thus we need to put a projection operator P_G behind the ground state to impose the constraint exactly[23]. In our calculations we relax this constraint for simplicity. So in general the ground state has the following form.

$$|g\rangle = P_G \, |g\rangle_b \, |g\rangle_f \tag{3.4.30}$$

3.5 Phase diagram

In the following subsections we discuss the three phases that we have obtained from the slave particle method.

3.5.1 Superconducting phase

Now let us approach the Mott transition point from below i.e. from superconducting side. In this phase both Δ_f and Δ_b are zero and therefore the charge excitation gap as well as the spin excitation gap vanishes. Gapless charge excitation implies : $\min E^b_{h,k} + \min E^b_{d,k} = U - 2\lambda - 6\chi_f = 0$. This condition can be satisfied up to $U_{c1} = 2\lambda + 6t\chi_f = 2.2t$. At this point the Mott transition happens. In terms of physical electrons, we obtain an s-wave superconducting state with gapless charge and spin excitations. The pairing order parameter changes sign under parity and 60 degrees rotation and transforms trivially under all other symmetry transformations. It should be mentioned that at small U limit, the Bose gas of holons and doublons becomes very dense and there is strong interaction between them. So the mean-field results are unreliable in this regime and the superconducting state is a fake result. However, our method captures two important right features of the system below the phase transition, because we obtain zero spin excitation energy as well as zero charge excitation energy.

3.5.2 Charge/spin gapped phase

For $U > U_{c1}$ we have $\chi_b = 0$. So the quasi-particle weight of spinons are zero and they cannot hop since for any i and j arbitrary sites: $\left\langle f^\dagger_{j,\sigma} f_{i,\sigma} \right\rangle = 0$. Therefore this state is like a superconductor with infinite carrier's mass $m \sim \frac{1}{t\chi_b} \to \infty$. Now let us find U_{c1}. To do so we assume that: $\Delta_{f,b}\left(\vec{\delta}\right) = \Delta_{f,b}$. So we have $\Delta_{f,b}\left(\vec{k}\right) = \Delta_{f,b}\eta(\vec{k})$, where $\eta(\vec{k}) = e^{ik_y} + 2e^{-i\frac{k_y}{2}} cos\frac{\sqrt{3}}{2}k_x$ and therefore the energy spectrum of spinons and bosons are $\sqrt{\lambda^2 + |t\Delta_b(k)|^2}$ and $\pm U/2 + \sqrt{(U/2-\lambda)^2 - |t\Delta_f(k)|^2}$ respectively. From the energy dispersion of bosons, one can read that the charge gap closes when $U_{c1} = 2\lambda + 6t\Delta_f$. Our numerical results show that near the phase transition, $\Delta_f \simeq .5$ and $\lambda \simeq -.4$ and the Mott transition occurs at $U_{c1}/t = 2.2$. For large U/t limit: $\Delta_f \to .53$, $\Delta_b \sim \frac{t}{U}$, $\lambda \sim (\frac{t}{U})^3 Ln\frac{t}{U}$ and $n_b \sim \Delta_b^2 \sim (\frac{t}{U})^2$. It is clear from the energy spectrum of spinons that in the spin liquid phase, there is a gap in their spectrum equal to: $E_g^f = |\lambda|$. Note that in the spin-charge separation picture, the physics of spin is determined by that of spinons. Therefore the spin excitation gap is also $E_g^s = |\lambda|$.

Now let us focus on the gauge theory of this phase. In this phase the effective action of spinons is of the following forms:

$$\begin{aligned} H_s = \quad & \lambda \sum_{i,\sigma,\tau} f^\dagger_{i,\tau,\sigma} f_{i,\tau,\sigma} \\ & -t \sum_{<i,j>,\sigma,\tau} \Delta_b\left(i,j\right)\sigma f^\dagger_{i,A,\sigma} f^\dagger_{j,B,-\sigma} + h.c. \end{aligned} \tag{3.5.31}$$

Now if we transform operators as: $f_{i,A,\sigma} \to e^{i\alpha} f_{i,A,\sigma}$ and $f_{i,B,\sigma} \to e^{-i\alpha} f_{i,B,\sigma}$ for any arbitrary phase α, i.e. assuming a staggered global gauge transformation, then the effective Hamiltonian does not change. Therefore the invariant gauge group (IGG) of the Hamiltonian is the staggered $U(1)$. The reason is that there is no hopping term due to the nonzero charge gap and the gauge transformation of two neighboring sites have opposite phases, the total phase change of the pairing term becomes zero and therefore gauge fluctuations are described by staggered compact $U(1)$ instead of compact $U(1)$ gauge theory. This is equivalent to assuming positive unit charge on sublattice A and negative unit charge on sublattice B for slave particles under the internal gauge transformation.

So, at mean field level, the charge/spin gapped phase has a neutral spinless $U(1)$ gapless mode as its only low energy excitations. However, it is well known that $U(1)$ theory in 2+1D is confined due to instanton effects. So let us assume that the $U(1)$ fluctuations are weak and use the semiclassical approach to study the $U(1)$ confined phase where the $U(1)$ mode is gapped. In the next chapter we show that these instanton operators, $e^{i\theta}$ (in the dual XY model), carry a non-trivial crystal momentum. Also, under 60 degree lattice rotation and time reversal, an instanton is changed to an anti-instanton, $e^{i\theta} \to e^{-i\theta}$. The instantons carry trivial quantum numbers for other symmetries. However, a triple instanton operator $\cos(3\theta)$ carries trivial quantum numbers for all symmetries. This allows us to conclude that the neutral spinless $U(1)$ mode is described by $L = \frac{1}{2g}(\partial\theta)^2 + K\cos(3\theta)$. In the semiclassical limit (the small g limit), $\langle e^{i\theta} \rangle \neq 0$ and we obtain a phase that breaks the translation, the time reversal and the $60°$ rotation symmetries, but not spin rotation symmetry [78].

We like to point out that in the presence of second neighbor hopping in the Hubbard model the charge/spin gapped phase can be spin liquid that do not break translation, parity, 60 degree lattice rotation, and spin rotation symmetries. It is because we can break the staggered compact $U(1)$ gauge symmetry down to a Z_2 one by Anderson-Higgs mechanism. If we add second neighbor hopping to the Hubbard model, within slave particle approach, this term generates pairing terms of the form $f^{\dagger}_{i,\tau,\sigma} f^{\dagger}_{j,\tau,-\sigma}$, i.e. it induces the same sublattice pairing and the Hamiltonian is no longer invariant under the staggered global $U(1)$ gauge transformation. In this case the staggered compact $U(1)$ gauge symmetry is broken down to a Z_2 gauge symmetry. The $U(1)$ gauge fluctuations are gapped and thus our mean filed state is stable and we can trust our meanfield results. Therefore we obtain a spin liquid phase.

3.5.3 Antiferromagnetic phase

In this part we show that the charge/spin gapped phase is unstable towards antiferromagnetic order above $U_{c2} = 3t$. To obtain Neel order in the t-J model we simply assume that $\left\langle \vec{S}_{z,A} \right\rangle = -\left\langle \vec{S}_{z,B} \right\rangle = m$. But how can one implement this idea in the Hubbard model within slave particle approach? In the Neel order phase, translation symmetry is broken and there is an asymmetric situation between sublattice A and B. For example we can obtain a antiferromagnetic phase by assuming $\Delta_{1,f} = \langle f_{j,B,\downarrow} f_{i,A,\uparrow} \rangle \neq \langle f_{j,A,\downarrow} f_{i,B,\uparrow} \rangle = \Delta_{2,f}$. This assumption simply means that the chance of finding a spin-up spinon on sublattice A and another spin-down spinon on sublattice B is more than finding the opposite one, so this method introduces staggered sublattice magnetization and leads to the Neel order. If there is a Neel order in the system then the chance of creating one holon-doublon pair from annihilating a spin-up spinon on sublattice A and a spin-down spinon on sublattice B is more than the other process. Therefore the excitation energy of spinons for up-spin on A and down-spin on B is $E^1_f(k) = \sqrt{\lambda^2 + |t\Delta_{1,b}(k)|^2}$ while for down-spin on A and up-spin on B is $E^2_f(k) = \sqrt{\lambda^2 + |t\Delta_{2,b}(k)|^2}$. On the other hand, since we are not interested in CDW, we need a symmetric situation between sublattices A and B for the charge sector. So the energy excitation of bosons is $E_b(k) = \sqrt{(U/2 - \lambda)^2 - |t\Delta_f(k)|^2}$. Using these assumptions we lead to the following self-consistency equations:

$$\Delta_{1,f} = \frac{t}{N_s}\sum_k \frac{|\eta(k)|^2\Delta_{1,b}}{E_{1,f}(k)} \tag{3.5.32}$$

$$\Delta_{2,f} = \frac{t}{N_s}\sum_k \frac{|\eta(k)|^2\Delta_{2,b}}{E_{2,f}(k)} \tag{3.5.33}$$

$$\Delta_f = \Delta_{1,f} + \Delta_{2,f} \tag{3.5.34}$$

$$\frac{\Delta_{1,b}\Delta_{1,f} + \Delta_{2,b}\Delta_{2,f}}{\Delta_{1,f} + \Delta_{2,f}} = \frac{t}{N_s}\sum_k \frac{|\eta(k)|^2\Delta_f}{E_b(k)} \tag{3.5.35}$$

By solving the above equations we find that above $U_{c2} = 3t$, $m \neq 0$. So we conclude that for $U > U_{c2}$ we obtain AF order. It is interesting that in this phase, the gap of spinons is very small and negligible (for example at U=4, it is -2×10^{-7}). So in this phase we can assume that spinons are massless quasi-particles.

To conclude this chapter, we have used a generalized slave particle method to derive the phase diagram of the Hubbard model at half filling on the honeycomb lattice. Within the mean field approximation we can decouple fermions from bosons to achieve the effective Hamiltonian that describes the low energy physics of the system. The physics of the Mott transition is discussed and it turns out to be a first order phase transition. It is shown that the phase transition occurs when the charge gap opens up. Above the critical point, within meanfield theory we obtain a spin liquid phase. But after including gauge fluctuations of the emergent spin liquid and investigating the instanton effect, we argue that this phase is unstable and we finally obtain a spin/charge gapped phase that breaks the translation symmetry. For large U limit, a new approach to study antiferromagnetic phase within the slave particle picture has been developed. It is shown that the gapped spin liquid phase has an instability towards antiferromagnetism.

Chapter 4

Gauge theory of the Hubbard Model on the honeycomb lattice and its instanton effect

In this chapter we investigate possible spin disordered phase in the Hubbard model on the honeycomb lattice. Using a slave-particle theory that include the charge fluctuations, we find a meanfield spin disordered phase in a range of on-site repulsion U. The spin disordered state is described by gapped fermions coupled to compact U(1) gauge field. We study the confinement/deconfinement problem of the U(1) gauge theory due to the instantons proliferation. We calculate all allowed instanton terms and compute their quantum numbers. It is shown that the meanfield spin disordered phase is unstable. The instantons proliferation induce a translation symmetry breaking.

4.1 Introduction

In previous chapter, we studied the phase diagram of the Hubbard model on the honeycomb lattice (see Fig. 3-1 and 3-2) using the generalized slave-particle technique [92, 19, 49, 68] which include charge fluctuations. Within meanfield approximation, we found a Mott phase transition to the insulating phase at $U_{c1} \simeq 2.2t$ above which charge gap opens up and we obtained the gapped spin liquid phase (spin/charge gapped phase). There is also another phase transition between the spin liquid and the anti-ferromagnetic order phases at $U_{c2} \simeq 3t$. In this phase, in contrast to the the gapped spin liquid phase, the mass of spinons is very small and negligible. In the case of nearest neighbor hopping Hubbard model, which is a bipartite system, the gauge theory of our meanfield spin liquid phase is the compact staggered U(1). In this phase, all excitations are gapped except gauge fluctuations. These results are within mean-field and due to the compactness of the U(1) lattice gauge theory, stability of such mean-field states are under question. In compact $U(1)$ gauge theories, instanton (anti-instanton) configurations are allowed and when they proliferate, spinons become confined and the results of the mean-field are no longer valid. Therefore studying the fate of this gapped spin liquid is necessary.

In this chapter we find that instanton configurations are relevant. instantons have nonzero fugacity and we do obtain a confined phase. More importantly, instanton operators carry a non-trivial crystal momentum. Also, under 60 degree lattice rotation and parity, an instanton is changed to an anti-instanton. However, the instantons carry trivial quantum numbers for other symmetries. Since a triple instanton carries trivial quantum numbers for all symmetries, so triple instanton can proliferate which leads to a confined phase. Since single instanton carries non-trivial crystal momentum, this allows us to conclude that the $U(1)$ confined phase is a phase that break translation symmetry but not spin rotation symmetry. Therefore we finally obtain an insulating phase at half filling that breaks the lattice translation symmetry! On the other hand, in the presence of second neighbor hopping in the Hubbard model the charge/spin gapped phase can be spin liquid that do not break translation, parity, 60 degree lattice rotation, and spin rotation symmetries.

4.2 Symmetry transformations on the honeycomb lattice

Since the unit cell of the honeycomb lattice has two sites in it, and we can label them by A and B or $s = 0, 1$, any lattice point can be represented as $\vec{R} = x_1\vec{a}_1 + x_2\vec{a}_2 + s\hat{y} \equiv (x_1, x_2, s)$, where $\vec{a}_1 = \sqrt{3}a\,(1,0)$ (a is the lattice spacing between A and B atoms), $\vec{a}_2 = \sqrt{3}a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$ and s takes 0 and 1 values. The basis vectors of the reciprocal lattice are $\vec{G}_1 = \frac{4\pi}{3a}\left(\frac{\sqrt{3}}{2}, 1\right)$ and $\vec{G}_2 = \frac{4\pi}{3a}\,(0,1)$ (see Fig. 4-1). Type A atoms are connected to type B atoms by the following three vectors: $\vec{b}_1 = a\,(0,1)$, $\vec{b}_2 = a\left(\frac{\sqrt{3}}{2}, \frac{-1}{2}\right)$ and $\vec{b}_3 = a\left(\frac{-\sqrt{3}}{2}, \frac{-1}{2}\right)$. Honeycomb lattice is invariant under five symmetry transformations: time reversal, parity ($\sigma : (x,y) \to (x,-y)$), 60 degree rotation ($C_6$), translation along $\vec{a}_1$ and $\vec{a}_2$ (T_1 and T_2). It is easy to

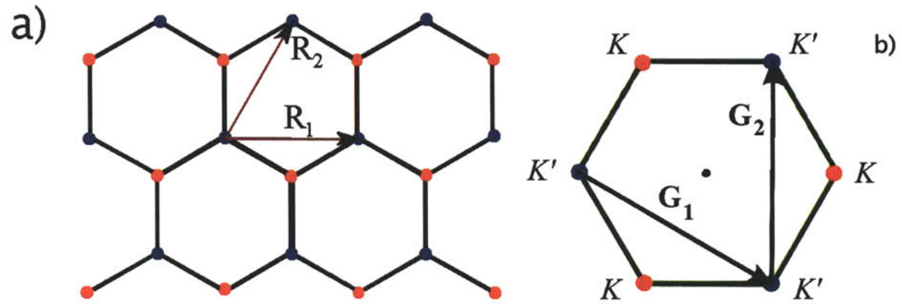

Figure 4-1: **Lattice structure of the honeycomb lattice.**— Honeycomb lattice and basis vectors of reciprocal lattice. (a), Honeycomb lattice in real space. Blue dots represent atoms on sublattice A and the red dots represent atoms on sublattice B. $\vec{R}_1$ and $\vec{R}_2$ are basis vectors of the honeycomb lattice. (b), Brillouin zone. $\vec{G}_1$ and $\vec{G}_2$ are basis vectors of reciprocal lattice. In the absence of λ, energy dispersion has two inequivalent nodal points at $\vec{K}$ and $\vec{K}'$. It is clear form this figure that under C_6 (60 degrees rotation) $K \to K'$ and $K' \to K$, while they do not change under parity σ.

check these symmetry operations act on the lattice as the following:

$$T_1 : \quad (x_1, x_2, s) \quad \to \quad (x_1 + 1, x_2, s) \tag{4.2.1}$$

$$T_2 : \quad (x_1, x_2, s) \quad \to \quad (x_1, x_2 + 1, s) \tag{4.2.2}$$

$$T : \quad (x_1, x_2, s) \quad \to \quad (x_1, x_2, s) \tag{4.2.3}$$

$$\sigma : \quad (x_1, x_2, s) \quad \to \quad (x_1 + x_2, -x_2, 1 - s) \tag{4.2.4}$$

$$C_6 : \quad (x_1, x_2, s) \quad \to \quad (1 - s - x_2, x_1 + x_2 + s - 1, 1 - s)\,. \tag{4.2.5}$$

4.3 Method

In the Anderson-Zou slave particle method, electron operators are represented as:

$$C^\dagger_{i,\sigma} = f^\dagger_{i,\sigma} h_i + \sigma\, d^\dagger_i f_{i,-\sigma} = [\ h_i \quad d^\dagger_i\ ] \begin{bmatrix} f^\dagger_{i,\sigma} \\ \sigma f_{i,-\sigma} \end{bmatrix}, \tag{4.3.6}$$

where $f^\dagger_{i,\sigma}$ creates a state with a single electron on it (a spinon), $h^\dagger_i$ creates a state with no charge on it (a holon), and $d^\dagger_i$ creates a state with two electron on site i (a doublon). It should be mentioned that the physical Hilbert space contains only four states: empty state (holon), one electron (spinon) and two electrons (doublon) on each site. So we always have one and only one slave particle on each site. So we conclude that we should put the local constraint

$n_i^h + n_{i,\uparrow}^f + n_{i,\downarrow}^f + n_i^d = 1$, to get rid of redundant states. This is the physical constraint which should be satisfied on every site. We could also obtain this result by noting that the electron operators are fermion and should satisfy the anticommutation relations. From the definition of $C_{i,\sigma}^\dagger$ it is obvious that it is invariant under U(1) gauge transformation (We require h_i and d_i to remain bosonic operators i.e., preserve their statistics after transformation, otherwise we would have SU(2) gauge invariance. However at $U = \infty$ we have only fermions and only in that case we have SU(2) gauge symmetry). It is worth noting that all the slave particles carry the same charge under the internal U(1) gauge. Since the above constraint and as a result the Hubbard Hamiltonian are also gauge invariant, so is the action of the Hubbard model.

Using this slave technique the Hubbard Hamiltonian can be rewritten as the following:

$$\begin{aligned} H = \quad & \sum U d_i^\dagger d_i - t \sum_{<i,j>} \left(\chi_{i,j}^f \chi_{j,i}^b + \Delta_{i,j}^{f\dagger} \Delta_{i,j}^b + h.c. \right) \\ & + \lambda (f_{i,\uparrow}^\dagger f_{i,\uparrow} + f_{i,\downarrow}^\dagger f_{i,\downarrow} + h_i^\dagger h_i + d_i^\dagger d_i - 1), \end{aligned} \tag{4.3.7}$$

in which we have used these notations $\chi_{i,j}^f = \sum_\sigma f_{i,\sigma}^\dagger f_{j,\sigma}$, $\chi_{i,j}^b = h_i^\dagger h_j - d_i^\dagger d_j$, $\Delta_{i,j}^f = \sum_\sigma \sigma f_{-\sigma,i} f_{j,\sigma}$, $\Delta_{i,j}^b = d_i h_j + h_i d_j$. Within mean field and by using Hubbard-Stratonovic we can decouple spinons and bosons and obtain a mean field state. In our numerical studies we have obtained three phases. At small U/t limit we obtain a semi-metallic phase. At large U/t limit we obtain AF order and for moderate values of U/t we obtain a spin liquid phase.

4.4 Instanton proliferation and confinement

Now let us focus on the spin liquid phase. In this phase: $\chi_{i,j}^{f,h} = 0$. Therefore the effective Hamiltonian of spinons in this phase is of the following forms:

$$H_s = \lambda \sum_{i,\sigma,\tau} f_{i,\tau,\sigma}^\dagger f_{i,\tau,\sigma} - t \sum_{<i,j>,\sigma,\tau} \Delta_b (i,j) \, \sigma f_{i,A,\sigma}^\dagger f_{j,B,-\sigma}^\dagger + h.c. \,. \tag{4.4.8}$$

Now let us use the following ansatz: $\Delta_b \left(\vec{\delta}\right) = \Delta_b$. So we have $\Delta_b \left(\vec{k}\right) = \Delta_f \eta(\vec{k})$, where $\eta(\vec{k}) = e^{-ik_y} + 2e^{+i\frac{k_y}{2}} cos\frac{\sqrt{3}}{2}k_x$ is the structure factor of the honeycomb lattice. Therefore the energy spectrum of spinons are: $\sqrt{\lambda^2 + |t\Delta_b\,(k)|^2}$. From the energy spectrum we see that spinons are gapped. But what if we include the effect of instantons? To answer this important question, we first study the gauge theory of this mean-field state.

In the above effective Hamiltonian we transform operators as: $f_{i,A,\sigma} \to e^{i\alpha} f_{i,A,\sigma}$ and $f_{i,B,\sigma} \to e^{-i\alpha} f_{i,B,\sigma}$ for any arbitrary phase α, i.e. assuming a staggered global gauge transformation, then the effective Hamiltonian does not change. Therefore the IGG of the Hamiltonian is staggered $U(1)$. The reason is that there is no hopping term due to the non-zero charge gap and the if we the gauge transformation of two neighboring sites have opposite phases, the total phase change of the pairing term becomes zero and therefore gauge fluctuations are described by staggered compact $U(1)$ instead of compact $U(1)$ gauge theory. This is equivalent to assuming have positive unit charge on sublattice A and negative unit charge on sublattice B for slave particles under the internal gauge transformation. So, at mean field level, the charge/spin gapped phase has a neutral spinless $U(1)$ gapless mode as its only low energy excitations. However, it is well known that $U(1)$ theory in 2+1D is confined due to instanton effects. So in the latter part of this chapter, we will assume that the $U(1)$ fluctuations are weak and use the semiclassical approach to study the $U(1)$ confined phase where the $U(1)$ mode is gapped.

We like to remark that it is possible to break this staggered compact $U(1)$ down to a Z_2 [53, 87, 75, 44, 66] one by Anderson-Higgs mechanism. If we add second neighbor hopping to the Hubbard model, within slave boson this term generate pairing terms of the form $f^{\dagger}_{i,\tau,\sigma} f^{\dagger}_{j,\tau,-\sigma}$, i.e. it induces the same sublattice pairing and the Hamiltonian is no longer invariant under the staggered global $U(1)$ gauge transformation. In this case gauge fluctuations are gapped and thus our mean filed state is stable and we can trust our results. Therefore for this case spin liquid phase is physical. On the frustrated lattices like the triangular lattice the gauge theory is Z_2 because we cannot dive the lattice in two sublattices, A and B.

It is useful to do particle hole transformation on sublattice B, so that we can see the gauge theory of the transformed Hamiltonian manifestly:

$$H_s = \sum_{i,\sigma,\tau} \lambda \left(f^{\dagger}_{i,A,\sigma} f_{i,A,\sigma} - F^{\dagger}_{i,B,\sigma} F_{i,B,\sigma} \right) - t \sum_{i,\vec{\delta},\sigma,\tau} \Delta_b \left(i,j\right) \sigma f^{\dagger}_{i,A,\sigma} F_{j,B,-\sigma} + h.c. \; . \quad (4.4.9)$$

In the absence of λ energy band of spinons has two nodal points around $\vec{K} = \frac{4\pi}{3\sqrt{3}a}(1,0)$

and $\vec{K'} = \frac{4\pi}{3\sqrt{3}a}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$ (see Fig. 4-1).If we expand the η_k around these two points we have:

$$\eta\left(K+\vec{q}\right) = \frac{3a}{2}\left(-q_x + iq_y\right) \qquad (4.4.10)$$

$$\eta\left(K'+\vec{q}\right) = \frac{3a}{2}\left(q_x + iq_y\right), \qquad (4.4.11)$$

where $\vec{q} = (q_x, q_y)$. So we have 8 flavors of spinons depending on their physical spin degree of freedom, sublattice index, and wether their momentum is around K or K'. Therefore we define the 8 component spinor as:

$$\Psi^{\dagger}(x) = \left(f^{\dagger}_{A,K,\uparrow}(x), F^{\dagger}_{B,K,\uparrow}(x), f^{\dagger}_{A,K,\downarrow}(x), F^{\dagger}_{B,K,\downarrow}(x), f^{\dagger}_{A,K',\uparrow}(x), F^{\dagger}_{B,K',\uparrow}(x), f^{\dagger}_{A,K',\uparrow}(x), F^{\dagger}_{B,K',\uparrow}(x)\right) \qquad (4.4.12)$$

Using the linearized Hamiltonian around K and K' it is straightforward to show that the continuum model can be written as:

$$H = \int d^2x\ \Psi^{\dagger}(x)\left[\lambda\mu^3 \otimes \tau^0 \otimes \nu^0 - i\frac{3a}{2}\Delta_b\partial_x\mu^1 \otimes \tau^0 \otimes \nu^3 - i\frac{3a}{2}\Delta_b\partial_y\mu^2 \otimes \tau^0 \otimes \nu^0\right]\Psi(x) \qquad (4.4.13)$$

where μ^a (a =0,1,2,3) are Pauli matrices acting on the sublattice indices, τ^b are Pauli matrices acting on the physical spin, and ν^c are Pauli matrices that act on the valley indices. It is known that if filled band has a nontrivial total Chern number, then instanton effects can be ignored, since the nontrivial Chern number lead to a Chern-Simons term for the $U(1)$ gauge field. So we need to calculate the Chern number of the filled band.

We will calculate the Chern number through the Dirac nodes. Each Dirac node contribute $\pm 1/2$ Chern numbers (see appendix), and each filled band have an even number of Dirac nodes. So adding the contribution from all the Dirac nodes, we obtain an integer Chern number for the filled band.

Let us consider the following two by two Dirac theory:

$$H = \int d^2x\ \psi^{\dagger}(x)\left[m\sigma^3 + \frac{3a}{2}\Delta_b\psi^{\dagger}(x)\left(-i\sigma^1\partial_x + i\sigma^2\partial_y\right)\right]\psi(x), \qquad (4.4.14)$$

where σ^i are Pauli matrices. The mass of the above Hamiltonian is by definition m. It has been shown that each massive Dirac cone with mass m has $C = \frac{m}{2|m|}$ nontrivial Chern number [34, 35]. Now let us consider following Hamiltonian:

$$H=\int d^{2}x\ \psi^{\dagger}\left(x\right)\left[m\sigma^{3}+\frac{3a}{2}\Delta_{b}\left(-i\sigma^{1}\partial_{x}-i\sigma^{2}\partial_{y}\right)\right]\psi\left(x\right). \tag{4.4.15}$$

If we us the following transformation: $\psi\rightarrow\psi'=\sigma^{1}\psi$, then the above Hamiltonian can be rearranged as the following:

$$H=\int d^{2}x\ \psi'^{\dagger}\left(x\right)\left[-m\sigma^{3}+\frac{3a}{2}\Delta_{b}\left(-i\sigma^{1}\partial_{x}+i\sigma^{2}\partial_{y}\right)\right]\psi'\left(x\right). \tag{4.4.16}$$

Therefore the mass of this Hamiltonian is $-m$, and therefore it has $C=-\frac{m}{2|m|}$ nontrivial Chern number.

Using the above arguments it can be shown that the mass of the two Dirac cones at $\vec{k}=\vec{K}$ is $\lambda<0$ and they contribute $C=-\frac{1}{2}$ Chern number. The mass of the two other Dirac cones at $\vec{k}=\vec{K}'$ is $-\lambda>0$ and they contribute $C=\frac{1}{2}$ Chern number. Therefore the total Chern number of our theory is $2\times-1/2+2\times1/2=0$. So the coefficient of the Chern-Simon action is zero, and it does not constraint the proliferation of instantons.

On the other hand since we have a massive Dirac theory, instant-instanton correlation function at large distances DOES NOT decay exponentially. Therefore nothing prevents instantons from proliferation. They will proliferate and gap out the gauge particles. So the $U(1)$ gauge theory is in the confined phase. Now we should compute the quantum numbers[22, 5, 88, 9, 10, 43] of instantons, in order to understand the symmetry properties of the $U(1)$ confined phase. To do so let us first derive the instanton operators.

Since instantons (instantons) in the presence of the Chern-Simon action with chern number C, create C fermions, therefore the instanton operator creates $2\times-1/2=-1$ fermions at $\vec{k}=\vec{K}$ (i.e. annihilates 1 fermion at $\vec{K}$), and creates $2\times1/2=1$ fermions at $\vec{k}=\vec{K}'$. Therefore, we obtain many different possibilities for the instanton operators, which include:

$$\phi_1 = f^\dagger_{A,\uparrow,K'} f_{A,\uparrow,K} \tag{4.4.17}$$

$$\phi_2 = F^\dagger_{B,\uparrow,K'} f_{A,\uparrow,K} = f_{B,\downarrow,K} f_{A,\uparrow,K} \tag{4.4.18}$$

$$\phi_3 = f^\dagger_{A,\downarrow,K'} f_{A,\uparrow,K} \tag{4.4.19}$$

$$\phi_4 = F^\dagger_{B,\downarrow,K'} f_{A,\uparrow,K} = f_{B,\uparrow,K} f_{A,\uparrow,K} \tag{4.4.20}$$

$$\phi_5 = f^\dagger_{A,\uparrow,K'} F_{B,\uparrow,K} = f^\dagger_{A,\uparrow,K'} f^\dagger_{B,\downarrow,K'} \tag{4.4.21}$$

$$\phi_6 = F^\dagger_{B,\uparrow,K'} F_{B,\uparrow,K} = f_{B,\downarrow,K} f^\dagger_{B,\downarrow,K'} \tag{4.4.22}$$

$$\phi_7 = f^\dagger_{A,\downarrow,K'} F_{B,\uparrow,K} = f^\dagger_{A,\downarrow,K'} f^\dagger_{B,\downarrow,K'} \tag{4.4.23}$$

$$\phi_8 = F^\dagger_{B,\downarrow,K'} F_{B,\uparrow,K} = f_{B,\uparrow,K} f^\dagger_{B,\downarrow,K'} \tag{4.4.24}$$

$$\phi_9 = f^\dagger_{A,\uparrow,K'} f_{A,\downarrow,K} \tag{4.4.25}$$

$$\phi_{10} = F^\dagger_{B,\uparrow,K'} f_{A,\downarrow,K} = f_{B,\downarrow,K} f_{A,\downarrow,K} \tag{4.4.26}$$

$$\phi_{11} = f^\dagger_{A,\downarrow,K'} f_{A,\downarrow,K} \tag{4.4.27}$$

$$\phi_{12} = F^\dagger_{B,\downarrow,K'} f_{A,\downarrow,K} = f_{B,\uparrow,K} f_{A,\downarrow,K} \tag{4.4.28}$$

$$\phi_{13} = f^\dagger_{A,\uparrow,K'} F_{B,\downarrow,K} = f^\dagger_{A,\uparrow,K'} f^\dagger_{B,\uparrow,K'} \tag{4.4.29}$$

$$\phi_{14} = F^\dagger_{B,\uparrow,K'} F_{B,\downarrow,K} = f_{B,\downarrow,K} f^\dagger_{B,\uparrow,K'} \tag{4.4.30}$$

$$\phi_{15} = f^\dagger_{A,\downarrow,K'} F_{B,\downarrow,K} = f^\dagger_{A,\downarrow,K'} f^\dagger_{B,\uparrow,K'} \tag{4.4.31}$$

$$\phi_{16} = F^\dagger_{B,\downarrow,K'} F_{B,\downarrow,K} = f_{B,\uparrow,K} f^\dagger_{B,\uparrow,K'}. \tag{4.4.32}$$

It is obvious that all the above operators carry nonzero crystal momentum which is equal to $\vec{K}' - \vec{K}$. Since the microscopic Hubbard Hamiltonian does not break translation symmetry, therefore the single instanton operator cannot appear in the path integral. On the other hand since $3\left(\vec{K}' - \vec{K}\right) \equiv (0,0)$, triple-instanton is not forbidden and will appear in the path integral. So the the path integral contain a triple-instanton gas, which will cause a confinement of the $U(1)$ theory.

	T_1	T_2	T	σ	C_6
$f_{A,\alpha,K}(x)$	$e^{i\frac{4\pi}{3}} f_{B,\alpha,K}(T_1 x)$	$e^{i\frac{2\pi}{3}} f_{B,\alpha,K}(T_2 x)$	$\alpha f_{A,-\alpha,K'}(x)$	$f_{B,\alpha,K}(\sigma x)$	$f_{B,\alpha,K'}(C_6 x)$
$f_{B,\alpha,K}(x)$	$e^{i\frac{4\pi}{3}} f_{A,\alpha,K}(T_1 x)$	$e^{i\frac{2\pi}{3}} f_{A,\alpha,K}(T_2 x)$	$\alpha f_{B,-\alpha,K'}(x)$	$f_{A,\alpha,K}(\sigma x)$	$f_{A,\alpha,K'}(C_6 x)$
$f_{A,\alpha,K'}(x)$	$e^{i\frac{2\pi}{3}} f_{B,\alpha,K'}(T_1 x)$	$e^{i\frac{4\pi}{3}} f_{B,\alpha,K'}(T_2 x)$	$\alpha f_{A,-\alpha,K}(x)$	$f_{B,\alpha,K'}(\sigma x)$	$f_{B,\alpha,K}(C_6 x)$
$f_{B,\alpha,K'}(x)$	$e^{i\frac{2\pi}{3}} f_{A,\alpha,K'}(T_1 x)$	$e^{i\frac{4\pi}{3}} f_{A,\alpha,K'}(T_2 x)$	$\alpha f_{B,-\alpha,K}(x)$	$f_{A,\alpha,K'}(\sigma x)$	$f_{A,\alpha,K}(C_6 x)$

Table 4.1: Symmetry transformation rules of spinon operators under translation, time reversal, parity and $\pi/3$ rotation.

4.5 Quantum number of instantons

Now we like to compute other nontrivial quantum numbers of the above instanton operators. To do so, let us first comment on the transformation of the continuum wavefunction. Using transformation rules in Table 1, we obtain following relations:

$$\textit{Physical spin rotation around z axis by angle } \theta : S_z\Psi \quad \to e^{i\theta\tau^3/2}\Psi(x).$$

$$\textit{Physical spin rotation around y axis. by angle } \theta : S_y\Psi \quad \to e^{i\theta\mu^3\otimes\tau^2/2}\Psi(x).$$

$$\textit{Translation } T_1 \ : T_1\Psi \quad \to e^{-i\frac{2\pi}{3}}\Psi(x').$$

$$\textit{Translation } T_2 \ : T_2\Psi \quad \to e^{+i\frac{2\pi}{3}}\Psi(x').$$

$$\textit{Time reversal } : T\Psi \quad \to i\tau^2\otimes\nu^1\Psi(x').$$

$$\textit{Parity } : \sigma\Psi \quad \to \mu^1\otimes\tau^1\otimes\nu^0\Psi^\dagger(x').$$

$$C_6 \ : C_6\Psi \quad \to \mu^1\otimes\tau^1\otimes\nu^1\Psi^\dagger(x').$$

where x' is the transformed x under each symmetry transformations.

4.5.1 Symmetry transformations on instanton operators

Using symmetry transformation of continuum wavefunction, we can read the corresponding transformation of monopole operators. Under $\pi/3$ rotation (C_6) we have:

$$C_6 \quad : \quad \phi_i \to -\phi^\dagger_{17-i}. \tag{4.5.33}$$

Parity operator σ where takes y to $-y$ acts on monopole operators as following:

$$\phi_1 \to -\phi_{16}, \qquad \phi_2 \to -\phi_{12}, \qquad \phi_3 \to -\phi_8, \qquad \phi_4 \to -\phi_4 \tag{4.5.34}$$
$$\phi_5 \to -\phi_{15}, \qquad \phi_6 \to -\phi_{11}, \qquad \phi_7 \to -\phi_7, \qquad \phi_8 \to -\phi_3 \tag{4.5.35}$$
$$\phi_9 \to -\phi_{14}, \qquad \phi_{10} \to -\phi_{10}, \qquad \phi_{11} \to -\phi_6, \qquad \phi_{12} \to -\phi_2 \tag{4.5.36}$$
$$\phi_{13} \to -\phi_{13}, \qquad \phi_{14} \to -\phi_9, \qquad \phi_{15} \to -\phi_5, \qquad \phi_{16} \to -\phi_1. \tag{4.5.37}$$

Under time reversal T we have

$$\phi_1 \to +\phi^\dagger_{11}, \qquad \phi_2 \to -\phi^\dagger_{15}, \qquad \phi_3 \to -\phi^\dagger_3, \qquad \phi_4 \to +\phi^\dagger_7 \tag{4.5.38}$$
$$\phi_5 \to -\phi^\dagger_{12}, \qquad \phi_6 \to +\phi^\dagger_{16}, \qquad \phi_7 \to +\phi^\dagger_4, \qquad \phi_8 \to -\phi^\dagger_8 \tag{4.5.39}$$
$$\phi_9 \to -\phi^\dagger_9, \qquad \phi_{10} \to +\phi^\dagger_{13}, \qquad \phi_{11} \to +\phi^\dagger_1, \qquad \phi_{12} \to -\phi^\dagger_5 \tag{4.5.40}$$
$$\phi_{13} \to +\phi^\dagger_{10}, \qquad \phi_{14} \to -\phi^\dagger_{14}, \qquad \phi_{15} \to -\phi^\dagger_2, \qquad \phi_{16} \to +\phi^\dagger_6. \tag{4.5.41}$$

Monopole operators transform under translation along $\vec{R}_1$ as

$$T_1 \quad : \quad \phi_k \to \exp\left(i\frac{2\pi}{3}\right)\phi_k. \tag{4.5.42}$$

Similarly for translation along $\vec{R}_2$ we have

$$T_2 \quad : \quad \phi_k \to \exp\left(-i\frac{2\pi}{3}\right)\phi_k. \tag{4.5.43}$$

And finally rotation around z axis by θ angle:

$$\phi_1 \to \phi_1, \qquad \phi_2 \to \phi_2, \qquad \phi_3 \to \exp(i\theta)\,\phi_3, \qquad \phi_4 \to \exp(i\theta)\,\phi_4 \quad (4.5.44)$$

$$\phi_5 \to \phi_5, \qquad \phi_6 \to \phi_6, \qquad \phi_7 \to \exp(i\theta)\,\phi_7, \qquad \phi_8 \to \exp(i\theta)\,\phi_8 \quad (4.5.45)$$

$$\phi_9 \to \exp(-i\theta)\,\phi_9, \qquad \phi_{10} \to \exp(-i\theta)\,\phi_{10}, \quad \phi_{11} \to \phi_{11}, \qquad \phi_{12} \to \phi_{12} \quad (4.5.46)$$

$$\phi_{13} \to \exp(-i\theta)\,\phi_{13}, \qquad \phi_{14} \to \exp(-i\theta)\,\phi_{14}, \quad \phi_{15} \to \phi_{15}, \qquad \phi_{16} \to \phi_{16}. \quad (4.5.47)$$

The instanton operators should have the same symmetry as the microscopic Hamiltonian and therefore they carry trivial quantum numbers. Using the above transformations, it is easy to see The following term is invariant under all transformations:

$$\delta\mathcal{L} = g \int d^2x \left(\phi^3(x) + \phi^{\dagger 3}(x)\right), \tag{4.5.48}$$

where ϕ is defined as the following:

$$\begin{aligned} \phi &= \phi_2 - \phi_{12} + \phi_5 - \phi_{15} && (4.5.49) \\ &= f_{B,\downarrow,K} f_{A,\uparrow,K} - f_{B,\uparrow,K} f_{A,\downarrow,K} + f^\dagger_{A,\uparrow,K'} f^\dagger_{B,\downarrow,K'} - f^\dagger_{A,\downarrow,K'} f^\dagger_{B,\uparrow,K'}. && (4.5.50) \end{aligned}$$

This operator has the following symmetry properties:

$$\begin{aligned} \sigma: &\quad \phi \;\to\; \phi && (4.5.51) \\ T: &\quad \phi \;\to\; \phi^\dagger && (4.5.52) \\ C_6: &\quad \phi \;\to\; \phi^\dagger && (4.5.53) \\ T_1: &\quad \phi \;\to\; \exp\left(-i\frac{2\pi}{3}\right)\phi && (4.5.54) \\ T_2: &\quad \phi \;\to\; \exp\left(+i\frac{2\pi}{3}\right)\phi. && (4.5.55) \end{aligned}$$

It can be easily checked that ϕ operator is also invariant under rotation x and y axes.

4.6 Discussion and conclusion

We have found a triple-instanton operator that has all symmetries of the microscopic Hamiltonian. Therefore this term is relevant and has a non-zero fugacity. Because of

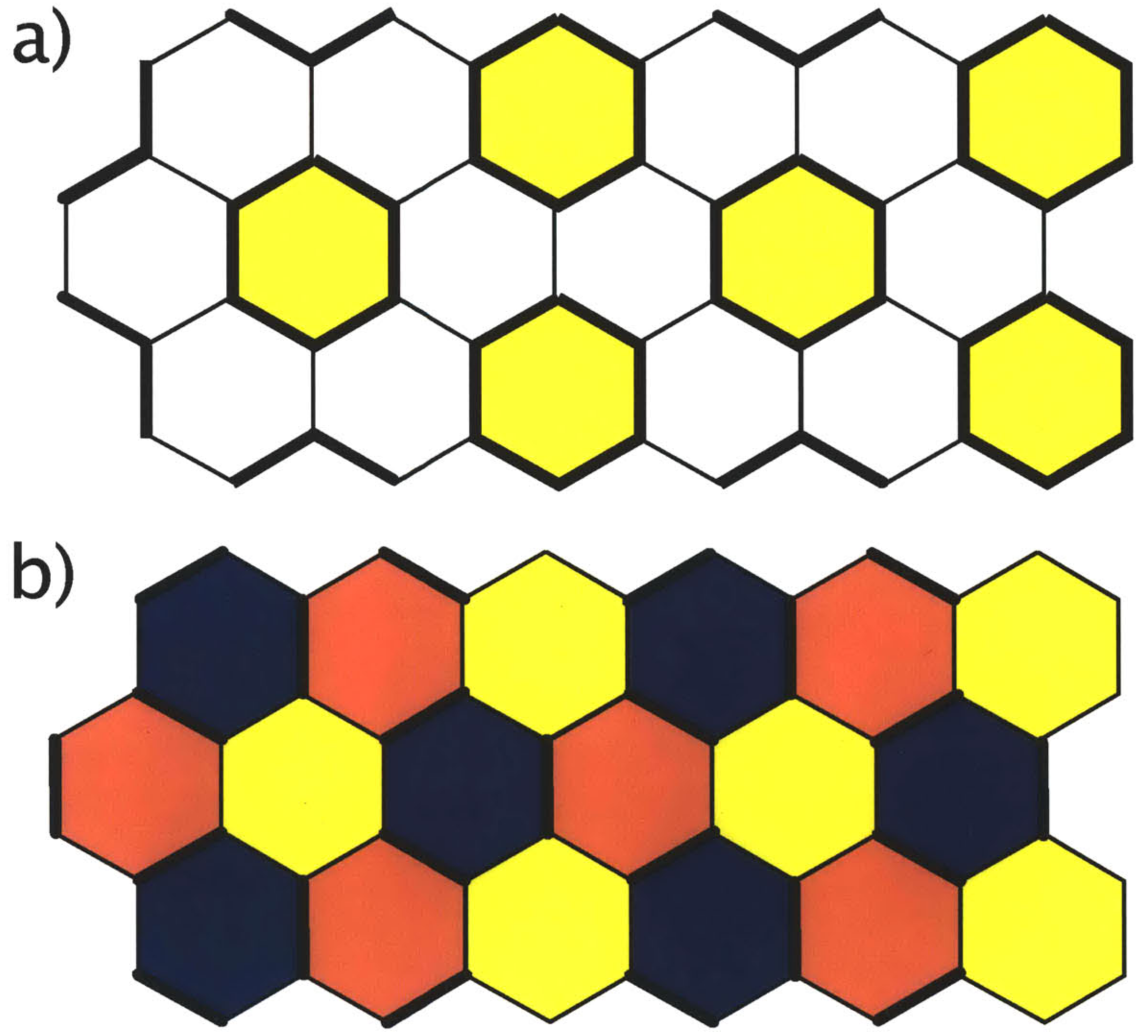

Figure 4-2: **Possible groundstates of the Hubbard model on the honeycomb lattice.** Two possible valence bond solid (VBS) states in honeycomb lattice that break the translation symmetry. Bold line indicates the stronger bonds and narrow line the weaker links. The bond operator in our case corresponds to the exchange energy i.e. $\Delta_b(i,j)$. $\vec{R}'_1 = 3\vec{R}_1$ and $\vec{R}'_2 = \vec{R}_1 + \vec{R}_2$ are new basis vectors of the lattice. The area of the unit cell is three times bigger than the translation symmetric case and contains six atoms in it. (a), Honeycomb lattice with broken translation symmetry, while C_6 and time reversal symmetries are unbroken. This phase corresponds to $\theta = 0$. θ can correspond to the flux of the hexagon. (b), Honeycomb lattice with broken translation, C_6 rotation and time reversal symmetry (center of rotation is yellow hexagons). This state corresponds to $\theta = \frac{2\pi}{3}$. The phase with $\theta = -\frac{2\pi}{3}$ is related to this by C_6 or T. From this figure it is clear that in this case C_6 breaks down to C_3.

instanton proliferation, the U(1) gauge fluctuations are now gapped out. On the other hand, since single instanton operator carries nonzero crystal momentum, the translation symmetry breaks spontaneously. To have a better insight of the situation, we can use the duality between $U(1)$ gauge theory and the nonlinear sigma model. If we identify ϕ operator with $\exp(i\theta)$, then $g\left(\phi^3(x) + \phi^{\dagger 3}(x)\right) = 2g\cos(3\theta)$. The $U(1)$ gauge theory with triple-instantons can be described by the following dual theory:

$$L = \frac{m}{2}\dot{\theta}^2 - \frac{\rho}{2}(\nabla\theta)^2 + 2g\cos(3\theta). \tag{4.6.56}$$

Therefore T and C_6 transformation are equivalent to $\theta \to -\theta$, σ is trivial and T_1 and T_2 are equivalent to $\theta \to \theta - \frac{2\pi}{3}$ and $\theta \to \theta + \frac{2\pi}{3}$ respectively. This model has three inequivalent ground states determined for $\theta \in \left\{0, \frac{2\pi}{3}, \frac{4\pi}{3}\right\}$ (see Fig. 4-2). Therefore the ground-state degeneracy of our model is also three. This happens because we lose the translation symmetry along $\vec{a}_1$ and $\vec{a}_2$ direction. The reason is that ϕ operator carries nonzero crystal momentum. But it is easy to show that ϕ is invariant under T_1^3 and T_1T_2 transformation. So the basis vectors of the new lattice are $\vec{R}_1' = (3,0) = 3\vec{R}_1$ and $\vec{R}_2' = (1,1) = \vec{R}_1 + \vec{R}_2$. The area of the unit cell is three times bigger and it contains six atoms in it.

In summary, if we treat the U(1) gauge field as a semi-classical field (i.e.Gaussian approximation), by analogy to the nonlinear sigma model, instantons proliferate, gauge field gaps out and lattice symmetry spontaneously breaks. What we finally obtain is a band insulator instead of a spin liquid phase. We want to mention that if gauge fluctuations are strong, other possibilities may happen. Among them, the Z_2 spin liquid is of more interest. This phase can be obtained if strong gauge fluctuations generate hopping term to the nearest site or a nonzero pairing amplitude to the second neighboring site. The presence of any of these two terms breaks U(1) down to Z_2 gauge theory which is stable.

4.7 APPENDIX: Hall conductance of an insulator

Conducting fermionic systems possess Fermi surface as a locus of gapless excitations. So if we couple these systems to an external electromagnetic field, low energy excitations is allowed and the system responses by exciting particle-holes across the Fermi surface (in some cases, *e.g. in honeycomb lattice*, Fermi point). For insulator the valence band is fully occupied by fermions and there is no Fermi surface and as a result there is finite gap for particle-hole excitation. Due to the absence of low energy excitations, the imaginary part of response function is zero for $\omega \leq E_g$, where E_g is the minimum energy gap.

Now we want to couple such an insulating state to the electromagnetic field. As a result, the Lagrangian of the system is

$$L\left(f, f^{\dagger}\right) + L_{\text{gauge}}\left(A_{\mu}\right), \tag{4.7.57}$$

where A_{μ} is the electromagnetic gauge potential. The first part is the lagrangian for interacting fermions in the presence of the external electromagnetic field and the second part is the Lagrangian for the electromagnetic field itself. The first part is assumed to be invariant under the following gauge transformation

$$f\left(x^{\mu}\right) \rightarrow e^{i\phi\left(x^{\mu}\right)} c\left(x^{\mu}\right), \qquad A_{\mu} \rightarrow A_{\mu} + \partial_{\mu}\phi\left(x^{\mu}\right). \tag{4.7.58}$$

We can obtain an effective action only in terms of gauge field by integrating out fermions. Since the electromagnetic is couple minimally to fermions, i.e. is coupled to their current, upon integrating fermion we obtain an effective Lagrangian in terms of current-current correlation function of fermion as follows

$$\begin{aligned} L_{\text{eff}}\left(A_{\mu}\right) &= L_{\text{gauge}}\left(A_{\mu}\right) + \delta L_{\text{eff}}\left(A_{\mu}\right) \\ \delta L_{\text{eff}}\left(A_{\mu}\right) &= -\frac{1}{2}\int dx dx' \; A_{\mu}\left(x\right) P^{\mu\nu}\left(x - x'\right) A_{\nu}\left(x'\right), \end{aligned} \tag{4.7.59}$$

where $P^{\mu\nu}\left(x - x'\right)$ is the current-current correlation function. Since the original Lagrangian in Eq. 4.7.57 is gauge invariant, $\delta L_{\text{eff}}\left(A_{\mu}\right)$ should be gauge invariant as well. Electric and magnetic fields are the only local function of A_{μ} which are invariant. So $\delta L_{\text{eff}}\left(A_{\mu}\right)$ contains the following term

$$\delta L_{\text{eff},1} = -\frac{1}{2}\left(B_i \chi^{ij} B_j + E_i p^{ij} E_j\right). \tag{4.7.60}$$

In $2+1$ dimension, δL_{eff} may also contain the following Chern-Simons term

$$\delta L_{\text{eff},2} = \frac{K}{4\pi} A_\mu \partial_\nu A_\lambda \epsilon^{\mu\nu\lambda}, \tag{4.7.61}$$

where $\mu, \nu, \lambda = 0, 1, 2$ and $\epsilon^{\mu\nu\lambda}$ is the fully antisymmetric tensor. Although this field cannot be written in terms of the electric and magnetic fields, it is invariant under gauge transformation, since after

$$A_\mu \to A_\mu + \partial_\mu \phi, \tag{4.7.62}$$

the Chern-Simons action changes as follows

$$S_{C-S} = \int_V \delta L_{\text{eff},2} \to S + \oint_{S=\partial V} dS_\mu \phi \frac{K}{4\pi} \partial_\nu A_\lambda \epsilon^{\mu\nu\lambda}, \tag{4.7.63}$$

where V is the space-time volume and S is its boundary. For closed space-time that does not have boundary, the surface integral vanishes and therefore the Chern-Simons action is gauge invariant on such systems. By varying the Chern-Simons action respect to the gauge potential we can obtain the linear response current as follows

$$J_x = \frac{K}{2\pi} E_y, \qquad J_y = -\frac{K}{2\pi} E_x, \qquad \rho = \frac{K}{2\pi} B, \tag{4.7.64}$$

where ρ is the change in the density of fermions. From the above relations we see that $\frac{K}{2\pi}$ is the offdiagonal conductivity of the system. To compute K explicitly, we consider the following gauge field configurations

$$A_1 = \frac{\theta_1(t)}{L_1}, \qquad A_2 = \frac{\theta_2(t)}{L_2}, \qquad A_0 = 0, \tag{4.7.65}$$

where $L_{1,2}$ is the size of the system in the x and y directions. $\delta L_{\text{eff}} = \delta L_{\text{eff},2} + \delta L_{\text{eff},1}$ in terms of these new variables becomes

$$\delta L_{\text{eff}} = \frac{K}{4\pi}\theta_i\dot{\theta}_j\epsilon^{ij} + \dot{\theta}_i p^{ij}\dot{\theta}_j. \tag{4.7.66}$$

This can be viewed as the Lagrangian of a particle whose coordinates are θ_1 and θ_2. Therefore the above Lagrangian describes the motion of a particle in 2 spatial dimension in a uniform magnetic field.

$$\begin{aligned} &\delta L_{\text{eff}} = a_i(\theta)\dot{\theta}_i + \dot{\theta}_i p^{ij}\dot{\theta}_j, \\ &a_1 = -\frac{K}{4\pi}\theta_2, \qquad a_2 = \frac{K}{4\pi}\theta_1\dot{\theta}_2, \qquad b = \partial_{\theta_1}a_2 - \partial_{\theta_2}a_1 = \frac{K}{4\pi}. \end{aligned} \tag{4.7.67}$$

It can be shown that $\theta_i \sim \theta_i + 2\pi$, therefore the above Lagrangian in fact describes the motion a particle on a torus T^2. It should be noted that $\oint \delta L_{eff}$ is the action for the adiabatic evolution of $|\theta(t)\rangle$. So it should be related to the Berry phase and therefore

$$\oint \delta L_{eff} = \oint dt \frac{K}{4\pi}\theta_i\dot{\theta}_j\epsilon^{ij} = \oint i\langle\theta(t)|\frac{d}{dt}|\theta(t)\rangle. \tag{4.7.68}$$

If we go around the lattice, i.e. using $(0,0)\to(\pi,0)$, $(\pi,0)\to(\pi,\pi)$, $(\pi,\pi)\to(0,\pi)$ and $(0,\pi)\to(0,0)$ (let us call this path C), we have

$$\oint dt \frac{K}{4\pi}\theta_i\dot{\theta}_j\epsilon^{ij} = \frac{K}{4\pi}\times 2 \times \text{Area of loop } C = 2\pi K. \tag{4.7.69}$$

So we have

$$K = \frac{1}{2\pi}\oint_C dt\,\langle\theta(t)|\,i\partial_\theta\,|\theta(t)\rangle. \tag{4.7.70}$$

Now let us consider the Hamiltonian of a Band insulator. In real space, (in some cases after some transformations) it can be written in the following way

$$H=\sum_{i,j} f_i^\dagger t_{ij} f_j=\sum_k f_k^\dagger M\left(k\right) f_k, \tag{4.7.71}$$

where f_i has n components, and t_{ij} is an $n\times n$ matrix that depends only on $i-j$ and $M\left(k\right)$ is the Fourier transform of t_{ij}. After turning on the electromagnetic field, the Hamiltonian changes and we have

$$H'=\sum_{i,j} f_i^\dagger t_{ij} e^{iA.(i-j)} f_j=\sum_k f_k^\dagger M^\theta\left(k\right) f_k. \tag{4.7.72}$$

We can diagonalize $M^\theta\left(k\right)$ matrix to obtain eigenvectors $\psi^\theta_{a,k}$ where $a=1,...,n$, labels ath eigenvector. Now we identify $|\theta\rangle$ with the filled lowest band, i.e.

$$|\theta\rangle=\otimes_k\left|\psi^\theta_{1,k}\right\rangle. \tag{4.7.73}$$

Using Eq. 4.7.70, we can calculate the Hall conductance of this insulator. The following identity can be easily verified

$$\begin{aligned}K &= \frac{1}{2\pi}\oint_{C_k} dk.\psi^\dagger_{1,k} i\partial_k\psi_{1,k}\\ &= \frac{1}{2\pi}\int d^2k\; i\left[\left(\partial_{k_x}\psi^\dagger_{1,k}\right)\left(\partial_{k_y}\psi_{1,k}\right)-\left(\partial_{k_y}\psi^\dagger_{1,k}\right)\left(\partial_{k_x}\psi_{1,k}\right)\right],\end{aligned} \tag{4.7.74}$$

where C_k is a loop around each momentum. For example let us consider the following Dirac Hamiltonian

$$H=-\sum_k \psi_k^\dagger\left(m\sigma^3+\eta_1 k_x\sigma^1+\eta_2 k_y\sigma^2\right)\psi_k=-\sum_k \psi_k^\dagger \vec{B}_k.\vec{\sigma}\psi_k. \tag{4.7.75}$$

The above Hamiltonian for each k, is mathematically equivalent to the Hamiltonian of a spin in the presence of $\vec{B}_k$. For $\left(\eta_1 k_x\right)^2+\left(\eta_2 k_y\right)^2\ll m^2$, the pseudo-magnetic field B_k is in the $m\hat{z}$ direction, while for $\left(\eta_1 k_x\right)^2+\left(\eta_2 k_y\right)^2\gg m^2$ it is in the $x-y$ plane. So by changing $\vec{k}$ and as a result changing $\vec{B}_k$ we span Half of a sphere, i.e. $\pm 2\pi$ solid angel. The sign of angel, depends on $\alpha = \text{sgn}\,(m\eta_1\eta_2)$, because when $\alpha > 0$, B_k evolves counterclockwise and therefore we span $+2\pi$ solid angel and when $\alpha > 0$, B_k evolves clockwise and therefore we span -2π solid angel. Berry phase is related to the solid angel in the following way

$$\theta_B = \frac{\Omega}{2} = \text{sgn}\,(m\eta_1\eta_2)\,\pi. \tag{4.7.76}$$

From Eqs. 4.7.74 and 4.7.76, we have $K = \frac{1}{2\pi}\text{sgn}\,(m\eta_1\eta_2)\,\pi$. So the Chern number of a massive Dirac band is

$$K = \frac{1}{2}\text{sgn}\,(m\eta_1\eta_2)\,. \tag{4.7.77}$$

Chapter 5

Fate of π-flux state in Hubbard model on square lattice

In this chapter we investigate the fate of the π-flux spin liquid phase in a Hubbard model on the square lattice. We argue that, in the $U \to \infty$ limit, such a spin liquid are a gapless spin liquid described by QCD3 with massless Dirac fermions coupled to an $SU(2)$ gauge theory. For finite U, we use a generalized slave particle approach to the strongly correlated Hubbard model that allows charge fluctuations in addition to the spin fluctuations. The generalized slave particle approach has only an $U(1)$ gauge symmetry. In this case, we find that, a mass term for the Dirac fermion is allowed that respect all the symmetries and the $U(1)$ gauge symmetry. Therefore, the π-flux spin liquid phase have an instability to open an energy gap when there are charge fluctuations. The gapped π-flux contain strong $U(1)$ gauge field fluctuations which is confining. By calculating the $U(1)$ gauge instanton quantum number, we argue that such a gapped π-flux phase breaks the translation symmetry and correspond to some kind of valance bond solid.

5.1 Introduction

The slave-particle approach is a quite effective approach to study quantum spin liquid phases [85, 79]. In particular, within an $SU(2)$ slave-particle approach for the Heisenberg model, the π-flux phase is a very interesting gapless spin liquid[1, 2, 25, 24, 6, 41, 82]. The low energy effective theory of the π-flux phase is described by QCD3 with massless Dirac fermions coupled to an $SU(2)$ gauge theory. It was argued that the masslessness of the Dirac fermions is protected by symmetry within the Heisenberg model[85, 46]. In this chapter, we study the π-flux phase in the Hubbard model. We used a generalized slave-particle construction that allows both spin and charge fluctuations. The generalized slave-particle approach also has a π-flux phase with massless Dirac fermions. However, such a π-flux phase now only has a $U(1)$ gauge symmetry. We show that, in this case, a mass term of the Dirac fermions can be generated without breaking any lattice symmetry and the $U(1)$ gauge symmetry. This suggests that, in the presence of charge fluctuations, the gapless π-flux phase is unstable. The charge fluctuations will open an energy gap for π-flux phase.

The gapped π-flux spin liquid contain a $U(1)$ gauge field which fluctuates strongly. One way to include the strong $U(1)$ gauge fluctuation is to project the mean-field slave particle state to physical spin states. We find that after projection, the projected physical spin wave function does not break the translation symmetry on even by even lattice and have a zero crystal momentum. However, such a result does not necessarily imply that the translation symmetry is unbroken. It may simply means that a particular superposition of the degenerate ground states of the gapped π-flux phase does not break the translation symmetry.

To understand the symmetry properties of the gapped π-flux phase, we need to understand the dynamics of the $U(1)$ gauge field. Because of the compactness of the gauge theory, instanton configurations are allowed. We study the confinement/deconfinement problem of the $U(1)$ gauge theory due to the instantons proliferation. In particular, we studied in detail the symmetry properties of the instanton operators using field theory. We find that the instanton operators always carry a crystal momentum (π, π). This suggests that the gapped π-flux phase break the translation symmetry and corresponds to some kind of valence bond solid. We also perform some direct numerical calculations of the crystal momentum quantum number of the instantons on lattice. The numerical result is consistent with the field theory result.

5.2 Slave-particle approach with charge fluctuations

In the Anderson-Zou slave particle method for strongly correlated Hubbard model, the electron operators are represented as:

$$C^{\dagger}_{i,\sigma} = f^{\dagger}_{i,\sigma} h_i + \sigma\, d^{\dagger}_i f_{i,-\sigma} = \left[\begin{array}{cc} h_i & d^{\dagger}_i \end{array}\right] \left[\begin{array}{c} f^{\dagger}_{i,\sigma} \\ \sigma f_{i,-\sigma} \end{array}\right] \tag{5.2.1}$$

where $f^{\dagger}_{i,\sigma}$ creates a state with a single electron on it (a spinon), $h^{\dagger}_i$ creates a state with no charge on it (a holon), and $d^{\dagger}_i$ creates a state with two electron on site i (a doublon). It should be mentioned that the physical Hilbert space contains only four states: empty state (holon), one electron (spinon) and two electrons (doublon) on each site. So we always have one and only one slave particle on each site. So we conclude that we should put the local constraint $n^h_i + n^f_{i,\uparrow} + n^f_{i,\downarrow} + n^d_i = 1$, to get rid of redundant states. This is the physical constraint which should be satisfied on every site. We could also obtain this result by noting that the electron operators are fermion and should satisfy the anticommutation relations. From the definition of $C^{\dagger}_{i,\sigma}$ it is obvious that it is invariant under U(1) gauge transformation (We require h_i and d_i to remain bosonic operators i.e., preserve their statistics after transformation, otherwise we would have SU(2) gauge invariance. However at $U = \infty$ we have only fermions and only in that case we have SU(2) gauge symmetry). It is worth noting that all the slave particles carry the same charge under the internal U(1) gauge. Since the above constraint and as a result the Hubbard Hamiltonian are also gauge invariant, so is the action of the Hubbard model.

Using this slave technique the Hubbard Hamiltonian can be rewritten as the following:

$$\begin{aligned} H = \quad & \sum U d^{\dagger}_i d_i - t \sum_{<i,j>} \left(\chi^f_{i,j} \chi^b_{j,i} + \Delta^{f\dagger}_{i,j} \Delta^b_{i,j} + h.c. \right) \\ & + \lambda (f^{\dagger}_{i,\uparrow} f_{i,\uparrow} + f^{\dagger}_{i,\downarrow} f_{i,\downarrow} + h^{\dagger}_i h_i + d^{\dagger}_i d_i - 1) \end{aligned} \tag{5.2.2}$$

In which we have used these notations $\chi^f_{i,j} = \sum_\sigma f^{\dagger}_{i,\sigma} f_{j,\sigma}$, $\chi^b_{i,j} = h^{\dagger}_i h_j - d^{\dagger}_i d_j$, $\Delta^f_{i,j} = \sum_\sigma \sigma f_{-\sigma,i} f_{j,\sigma}$, $\Delta^b_{i,j} = d_i h_j + h_i d_j$. Within mean field and by using Hubbard-Stratonovic we can decouple spinons and bosons and obtain a mean field state. In our numerical studies we have obtained three phases. At large U/t limit we obtain AF order and for moderate values of U/t we obtain a meanfield spin liquid phase. From now on we choose $t = 1$.

Now let us focus on the meanfield spin liquid phase. In this phase: $\chi_{i,j}^{f,h} = 0$. Therefore the effective Hamiltonian of spinons in this phase is of the following forms

$$H_s = -\lambda \sum_{i,\sigma,\mu} f_{i,\mu,\sigma}^{\dagger} f_{i,\mu,\sigma} - \sum_{<i,j>,\sigma} \Delta_b(i,j)\, \sigma f_{i,A,\sigma}^{\dagger} f_{j,B,-\sigma}^{\dagger} + H.c. \tag{5.2.3}$$

where $\mu = \{A, B\}$. But what if we include the effect of instantons? To answer this important question, we first study the gauge theory of this mean-field state.

In the above effective Hamiltonian we transform operators as: $f_{i,A,\sigma} \to e^{i\alpha} f_{i,A,\sigma}$ and $f_{i,B,\sigma} \to e^{-i\alpha} f_{i,B,\sigma}$ for any arbitrary phase α, i.e. assuming a staggered global gauge transformation, then the effective Hamiltonian does not change. Therefore the invariant gauge group (IGG) of the Hamiltonian is staggered $U(1)$. The reason is that there is no hopping term due to the non-zero charge gap and the if the gauge transformation of two neighboring sites have opposite phases, the total phase change of the pairing term cancels out. Therefore gauge fluctuations are described by staggered compact $U(1)$ instead of compact $U(1)$ gauge theory. This is equivalent to assuming we have positive unit charge on sublattice A and negative unit charge on sublattice B for slave particles under the internal gauge transformation. So, at mean field level, the above charge/spin gapped phase has a neutral spinless $U(1)$ gapless mode as its only low energy excitations. However, it is well known that $U(1)$ theory in 2+1D is confined due to instanton effects. So let us assume that the $U(1)$ fluctuations are weak and use the semiclassical approach to study the $U(1)$ confined phase where the $U(1)$ mode is gapped.

It is possible to break this staggered compact $U(1)$ down to a Z_2 one by Anderson-Higgs mechanism. If we add second neighbor hopping to the Hubbard model, within slave boson this term generate pairing terms of the form $f_{i,\mu,\sigma}^{\dagger} f_{j,\mu,-\sigma}^{\dagger}$, i.e. it induces the same sublattice pairing and the Hamiltonian is no longer invariant under the staggered global $U(1)$ gauge transformation. In this case gauge fluctuations are gapped and thus our mean filed state is stable and we can trust our results. Therefore for this case spin liquid phase is physical. On the frustrated lattices like the triangular lattice the gauge theory is Z_2 because we cannot dive the lattice in two sublattices, A and B.

Let us define the spinon doublet operator as on the A and B sublattice as

$$\psi_i = \begin{pmatrix} f_{i,\uparrow} \\ f_{i,\downarrow}^\dagger \end{pmatrix}. \tag{5.2.4}$$

The meanfield Hamiltonian of spinons in the insulating phase can be written as

$$H = \sum_{i,j} \psi_i^\dagger U_{i,j} \psi_i + H.c. \tag{5.2.5}$$

where $U_{i,j} = u_{i,j}^\alpha \tau^\alpha$, where $\alpha = 0, .., 3$ and τ^i are Pauli matrices. Here $u_{i,j}^0$ is imaginary and $u_{i,j}^{1,2,3}$ are real in order to have the spin rotation symmetry. The λ term becomes $U_{i,i} = -\lambda\tau^3$. It can be easily checked that the mass term does not break any symmetry and opens up gap in spinon excitation energy.

In the absence of charge fluctuations and at half filling, the number of spinons at each site is exactly one. This can be implemented in average by choosing $\lambda = 0$. On the other hand, if we allow charge fluctuations, number of spinons is no longer necessarily equal to one due to the presence of holons and doublons. Therefore $\lambda < 0$ to make sure that there are other slave particles than spinons. One may wonder whether this term breaks the particle-hole symmetry at half-filling or not. The answer is no. Because the mass term of spinons is originated from the following term

$$\lambda \left(f_{i,\uparrow}^\dagger f_{i,\uparrow} + f_{i,\downarrow}^\dagger f_{i,\downarrow} + h_i^\dagger h_i + d_i^\dagger d_i - 1 \right) = \frac{1}{2}\lambda \sum_\sigma \left(C_{i,\sigma}^\dagger C_{i,\sigma} + C_{i,\sigma} C_{i,\sigma}^\dagger - 1 \right) \tag{5.2.6}$$

which is obviously particle-hole symmetric. In terms of electron operators this term is zero, though in the slave particle approach, we have to keep it in order to kill unphysical states.

To summarize, non-zero charge fluctuations generate a non-zero λ. A non-zero λ in general gaps the spinon excitations at mean-field level.

5.3 Mean-field ansatz and its symmetry for gapped π-flux phase

Let us consider a concrete example described by the following ansatz

$$\begin{aligned} &U_{i,i+\hat{x}} = -(-)^{i_y}\Delta_b\tau^1, \qquad U_{i,i+\hat{y}} = -\Delta_b\tau^1, \qquad U_{i,i} = -\lambda\tau^3, \\ &\Delta_b(i,i+\hat{x}) = (-)^{i_y}\Delta_b, \qquad \Delta_b(i,i+\hat{y}) = \Delta_b. \end{aligned} \tag{5.3.7}$$

When $\lambda = 0$ the above ansatz describe the gapless π-flux state. The ansatz is invariant under the following symmetry transformations followed by the corresponding $U(1)$ gauge transformations $G_{T_x}T_x$, $G_{T_y}T_y$, $G_{P_x}P_x$, $G_{P_y}P_y$, $G_{P_{xy}}P_{xy}$, and $G_T T$. Here the symmetry transformations are two translations $T_x : i \to i+\hat{x}$, $T_y : i \to i+\hat{y}$, three parities $P_x : (i_x, i_y) \to (-i_x, i_y)$, $P_y : (i_x, i_y) \to (i_x, -i_y)$, $P_{xy} : (i_x, i_y) \to (i_y, i_x)$, and a time reversal $T : f_{i,\sigma} \to \sigma f_{i,-\sigma}$. We find

$$G_{T_x} = 1, \quad G_{T_y} = (-1)^{i_x}, \quad G_{P_x} = 1, \quad G_{P_y} = 1, \quad G_{P_{xy}} = (-1)^{i_x i_y}, \quad G_T = 1. \tag{5.3.8}$$

So the ansatz (5.3.7) does not break any symmetry. The ansatz is invariant under any gauge transformation of the form $G_0(i) = \exp\left(i\,(-)^{i_x+i_y}\,\theta\tau_3\right)$.

The above ansatz, represents the gapped π-flux phase. To see this more explicitly, we only need to divide the square lattice into sublattice A and B and do particle hole transformation only on sublattice B. So we have

$$i \in A \quad \Psi_i = \begin{pmatrix} f_{i,\uparrow} \\ f^\dagger_{i,\downarrow} \end{pmatrix}, \qquad i \in B \quad \Psi_i = \begin{pmatrix} F_{i,\uparrow} \\ F^\dagger_{i,\downarrow} \end{pmatrix} = \begin{pmatrix} f^\dagger_{i,\downarrow} \\ f_{i,\uparrow} \end{pmatrix}. \tag{5.3.9}$$

Now let us rewrite the meanfield Hamiltonian in terms of new operators. We have

$$H_s = -\lambda\sum_i (-)^{i_x+i_y}\Psi_i^\dagger\tau^3\Psi_i - \Delta_b\sum_i\left[(-)^{i_y}\Psi_i^\dagger\Psi_{i+\hat{x}} + \Psi_i^\dagger\Psi_{i+\hat{y}} + H.c.\right] \tag{5.3.10}$$

For $\lambda = 0$, we recover the conventional π-flux state, and for nonzero λ we achieve the gapped π-flux state. The above Hamiltonian is clearly invariant under the global $U(1)$ gauge transformations. The $U(1)$ gauge transformation for the transformed spinon operators is equivalent to the staggered $U(1)$ gauge transformation of the original spinon operators. It is worth mentioning that we can similarly obtain the gapped staggered flux phase by choosing

$$\Delta_b\left(i,i+\hat{x}\right)=\exp\left(i(-)^{i_y}\frac{\phi}{2}\right)\Delta_b \quad , \quad \Delta_b\left(i,i+\hat{y}\right)=\Delta_b \tag{5.3.11}$$

which represents the staggered ϕ flux phase with $E_g = 2\,|\lambda|$ gap.

Now let us consider the meanfield Hamiltonian in Eq. 5.2.3 using ansatz 5.3.7. To find energy spectrum of the π-flux Hamiltonian, we use the following notations:

$$f_{k,A,\sigma}=\sum_i \exp\left(ik.R_i\right) f_{i,\sigma}, \quad i_x+i_y=2m \tag{5.3.12}$$

$$F_{k,B,\sigma}=\sum_i \exp\left(ik.R_i\right) F_{i,\sigma}=\sum_i \exp\left(ik.R_i\right) f^{\dagger}_{i,-\sigma}, \quad i_x+i_y=2m+1 \tag{5.3.13}$$

Using these operators we can rewrite Hamiltonian in Eq 5.3.10 in the momentum space as

$$H_\sigma=\sum_{\vec{k}} \Psi^{\dagger}_{k,\sigma}\left[-\lambda\sigma^0\otimes\sigma^3-2\sigma\Delta_b\cos\left(k_x\right)\sigma^1\otimes\sigma^1-2\sigma\Delta_b\cos\left(k_y\right)\sigma^3\otimes\sigma^1\right]\Psi_{k,\sigma} \tag{5.3.14}$$

$$\Psi_{k,\sigma}=\left(f_{k,A,\sigma}\ ,\ F_{k,B,\sigma}\ ,\ f_{k+\vec{Q},A,\sigma}\ ,\ F_{k+\vec{Q},B,\sigma}\right)^T. \tag{5.3.15}$$

where $\vec{Q}=(0,\pi)$and $\vec{k}$ is in the reduced Brillouin zone defined as

$$0\le k_x\le\pi \quad , \quad 0\le k_y\le\pi. \tag{5.3.16}$$

For later purposes we need to transform $\Psi_{k,\sigma}$ in the following way to make the Hamiltonian block diagonal.

$$\Psi_{k,\sigma} \to U_k \Psi_{k,\sigma} \tag{5.3.17}$$

$$[U_k]_{4\times 4} = \begin{pmatrix} u_k \exp\left(i\frac{\sigma^3}{2}\theta_k\right) & -v_k \exp\left(-i\frac{\sigma^3}{2}\theta_k\right) \\ v_k \exp\left(i\frac{\sigma^3}{2}\theta_k\right) & u_k \exp\left(-i\frac{\sigma^3}{2}\theta_k\right) \end{pmatrix} \tag{5.3.18}$$

$$u_k = \mathrm{sgn}\left(\cos\left(k_y\right)\right)\sqrt{\frac{1}{2}\left(1+\cos\theta_k\right)} \tag{5.3.19}$$

$$v_k = \sqrt{\frac{1}{2}\left(1-\cos\theta_k\right)} \tag{5.3.20}$$

$$\cos\left(\theta_k\right) = \frac{\cos\left(k_y\right)}{\sqrt{\cos^2\left(k_x\right)+\cos^2\left(k_y\right)}}, \tag{5.3.21}$$

after which the Hamiltonian becomes

$$H_\sigma = \sum_{\vec{k}} \tilde{\Psi}^\dagger_{k,\sigma}\left[-\lambda\gamma^0 + 2\sigma\Delta_b\cos\left(k_x\right)\gamma^1 - 2\sigma\Delta_b\cos\left(k_y\right)\gamma^2\right]\tilde{\Psi}_{k,\sigma} \tag{5.3.22}$$

$$\tilde{\Psi}_{k,\sigma} = \left(\tilde{f}_{k,1,A,\sigma}\ ,\ \tilde{F}_{k,1,B,\sigma}\ ,\ \tilde{f}_{k,2,A,\sigma}\ ,\ \tilde{F}_{k,2,B,\sigma}\right)^T \tag{5.3.23}$$

$$\tilde{f}_{k,1,A,\sigma} = \exp\left(+i\frac{\theta_k}{2}\right)\left[u_k f_{k,A,\sigma} + v_k f_{k+\vec{Q},A\sigma}\right] \tag{5.3.24}$$

$$\tilde{F}_{k,1,B,\sigma} = \exp\left(-i\frac{\theta_k}{2}\right)\left[u_k F_{k,B,\sigma} + v_k F_{k+\vec{Q},B,\sigma}\right] \tag{5.3.25}$$

$$\tilde{f}_{k,2,A,\sigma} = \exp\left(+i\frac{\theta_k}{2}\right)\left[u_k f_{k+\vec{Q},A,\sigma} - v_k f_{k,A,\sigma}\right] \tag{5.3.26}$$

$$\tilde{F}_{k,2,B,\sigma} = \exp\left(-i\frac{\theta_k}{2}\right)\left[u_k F_{k+\vec{Q},B,\sigma} - v_k F_{k,B,\sigma}\right], \tag{5.3.27}$$

where $\gamma^0 = \sigma^0 \otimes \sigma^3$, $\gamma^1 = \sigma^3 \otimes \sigma^1$ and $\gamma^2 = \sigma^0 \otimes \sigma^2$ are Dirac matrices. The energy dispersion relation of this Hamiltonian is

$$E_{k,\sigma} = \pm\sqrt{\lambda^2 + 4\Delta_b^2\left(\cos^2\left(k_x\right)+\cos^2\left(k_y\right)\right)}. \tag{5.3.28}$$

From the above expression, the energy gap in the spectrum is $E_g = 2\lambda$. The energy dispersion has a minimum at

$$\vec{K} = \left(\frac{\pi}{2}, \frac{\pi}{2}\right). \tag{5.3.29}$$

We can expand the Hamiltonian around this momentum after which we obtain a massive

Dirac Hamiltonian. We have

$$H_{K,\sigma} = \sum_{\vec{q}} \tilde{\Psi}^{\dagger}_{K+q,\sigma} \left[-\lambda\gamma^0 - \sigma\Delta_b q_x \gamma^1 + 2\sigma\Delta_b q_y \gamma^2\right] \tilde{\Psi}_{K+q,\sigma} \tag{5.3.30}$$

$$\tilde{\Psi}_{K+q,\sigma} = \left(\tilde{f}_{K+q,1,A,\sigma}\ ,\ \tilde{F}_{K+q,1,B,\sigma}\ ,\ \tilde{f}_{K+q,2,A,\sigma}\ ,\ \tilde{F}_{K+q,2,B,\sigma}\right)^T. \tag{5.3.31}$$

with dispersion

$$E_{q,\sigma} = \pm\sqrt{\lambda^2 + 4\Delta_b^2\left(k_x^2 + k_y^2\right)}. \tag{5.3.32}$$

Since the Chern number is a topological number, we can deform the block diagonal Hamiltonian smoothly without changing this number, provided it remains block diagonal. So we can drop $\exp\left(\pm i\frac{\sigma^3}{2}\theta_k\right)$ factor in the definition of U_k. Now Let us define continuum wavefunction in the following way

$$\tilde{\Psi}_{\sigma}(\vec{x}) = \int d^2q \exp(i\vec{q}.\vec{x})\, \tilde{\Psi}_{K,\sigma}(\vec{q}) \tag{5.3.33}$$

$$\tilde{\Psi}_{\sigma}(\vec{x}) = \left(\tilde{f}_{A,1,\sigma}(\vec{x})\ ,\ \tilde{F}_{B,1,\sigma}(\vec{x})\ ,\ \tilde{f}_{A,2,\sigma}(\vec{x})\ ,\ \tilde{F}_{B,2,\sigma}(\vec{x})\right)^T. \tag{5.3.34}$$

$$\tilde{f}_{A,1,\sigma}(\vec{x}) = \ e^{-i\vec{K}.\vec{x}}\bar{C}_{A,+,\sigma}(x) + e^{-i(\vec{K}+\vec{Q}).\vec{x}}\bar{C}_{A,-,\sigma} \tag{5.3.35}$$

$$\tilde{f}_{B,1,\sigma}(\vec{x}) = \ e^{-i\vec{K}.\vec{x}}\bar{C}_{B,+,\sigma}(x) + e^{-i(\vec{K}+\vec{Q}).\vec{x}}\bar{C}_{B,-,\sigma} \tag{5.3.36}$$

$$\tilde{f}_{A,2,\sigma}(\vec{x}) = -e^{-i\vec{K}.\vec{x}}\bar{C}_{A,-,\sigma}(x) + e^{-i(\vec{K}+\vec{Q}).\vec{x}}\bar{C}_{A,+,\sigma} \tag{5.3.37}$$

$$\tilde{f}_{B,2,\sigma}(\vec{x}) = -e^{-i\vec{K}.\vec{x}}\bar{C}_{B,-,\sigma}(x) + e^{-i(\vec{K}+\vec{Q}).\vec{x}}\bar{C}_{B,+,\sigma}, \tag{5.3.38}$$

in which we have used the following notations

$$\bar{C}_{A,+,\sigma}(x) = \sum_k u_k \exp\left(i\vec{k}.\vec{x}\right) f_{k,A,\sigma} \tag{5.3.39}$$

$$\bar{C}_{A,-,\sigma}(x) = \sum_k v_k \exp\left(i\vec{k}.\vec{x}\right) f_{k,A,\sigma} \tag{5.3.40}$$

$$\bar{C}_{B,+,\sigma}(x) = \sum_k u_k \exp\left(i\vec{k}.\vec{x}\right) F_{k,B,\sigma} \tag{5.3.41}$$

$$\bar{C}_{B,-,\sigma}(x) = \sum_k v_k \exp\left(i\vec{k}.\vec{x}\right) F_{k,B,\sigma}. \tag{5.3.42}$$

	$G_{T_x}T_x$	$G_{T_y}T_y$	$G_{P_y}P_y$	$G_{P_y}P_y$	$G_{P_{xy}}P_{xy}$	$G_T T$
$\tilde{f}_{A,1,\sigma}$	$i\tilde{f}_{B,1,\sigma}$	$i\tilde{f}_{B,2,\sigma}$	$e^{i\pi x_2}\tilde{f}_{A,1,\sigma}$	$e^{i\pi x_1}\tilde{f}_{A,1,\sigma}$	$e^{i\pi x_1}\tilde{f}_{A,1,\sigma}$	$\sigma e^{i\pi x_2}\tilde{f}_{A,1,-\sigma}(x)$
$\tilde{f}_{B,1,\sigma}$	$i\tilde{f}_{A,1,\sigma}$	$i\tilde{f}_{B,2,\sigma}$	$e^{i\pi x_2}\tilde{f}_{B,1,\sigma}$	$e^{i\pi x_1}\tilde{f}_{B,1,\sigma}$	$\tilde{f}_{B,1,\sigma}$	$\sigma e^{i\pi x_2}\tilde{f}_{B,2,-\sigma}(x)$
$\tilde{f}_{A,2,\sigma}$	$i\tilde{f}_{B,2,\sigma}$	$i\tilde{f}_{B,2,\sigma}$	$e^{i\pi x_2}\tilde{f}_{A,2,\sigma}$	$e^{i\pi x_1}\tilde{f}_{A,2,\sigma}$	$e^{i\pi x_1}\tilde{f}_{A,2,\sigma}$	$\sigma e^{i\pi x_2}\tilde{f}_{A,2,-\sigma}(x)$
$\tilde{f}_{B,2,\sigma}$	$i\tilde{f}_{A,2,\sigma}$	$i\tilde{f}_{B,2,\sigma}$	$e^{i\pi x_2}\tilde{f}_{B,2,\sigma}$	$e^{i\pi x_1}\tilde{f}_{B,2,\sigma}$	$\tilde{f}_{B,2,\sigma}$	$\sigma e^{i\pi x_2}\tilde{f}_{B,2,-\sigma}(x)$

Table 5.1: Symmetry transformation rules of spinon operators in the staggered flux phase.

	$G_{T_x}T_x$	$G_{T_y}T_y$	$G_{P_y}P_y$	$G_{P_y}P_y$	$G_{P_{xy}}P_{xy}$	$G_T T$
ϕ_1	$-\phi_2^\dagger$	$-\phi_1$	$e^{i\pi\left(x_2'-x_2\right)}\phi_1$	$e^{i\pi\left(x_1'-x_1\right)}\phi_1$	$e^{i\pi x_1}\phi_1$	$\sigma e^{i\pi\left(x_2-x_2'\right)}\phi_1(x)$
ϕ_2	$-\phi_1^\dagger$	$-\phi_2$	$e^{i\pi\left(x_2'-x_2\right)}\phi_2$	$e^{i\pi\left(x_1'-x_1\right)}\phi_2$	$e^{i\pi x_1}\phi_2$	$\sigma e^{i\pi\left(x_2-x_2'\right)}\phi_2(x)$
ϕ_3	$-\phi_4^\dagger$	$-\phi_3$	$e^{i\pi\left(x_2'-x_2\right)}\phi_3$	$e^{i\pi\left(x_1'-x_1\right)}\phi_3$	$e^{i\pi\left(x_1-x_1'\right)}\phi_3$	$\sigma e^{i\pi\left(x_2-x_2'\right)}\phi_1(x)$
ϕ_4	$-\phi_3^\dagger$	$-\phi_4$	$e^{i\pi\left(x_2'-x_2\right)}\phi_4$	$e^{i\pi\left(x_1'-x_1\right)}\phi_4$	ϕ_4	$\sigma e^{i\pi\left(x_2-x_2'\right)}\phi_1(x)$

Table 5.2: Symmetry transformation rules of monopole operators.

Using the above definitions we achieve the two following continuum Dirac models

$$\tilde{H}_\sigma = \tilde{H}_{1,\sigma} \oplus + \tilde{H}_{2,\sigma} \tag{5.3.43}$$

$$\tilde{H}_{1,\sigma} = \int d^2 \tilde{\Psi}^\dagger_{1,\sigma}(x)\left[-\lambda\sigma_3 - 2i\sigma\Delta_b\partial_x\sigma_2 - 2i\sigma\Delta_b\partial_y\sigma_1\right]\tilde{\Psi}_{1,\sigma}(x) \tag{5.3.44}$$

$$\tilde{H}_{2,\sigma} = \int d^2 \tilde{\Psi}^\dagger_{2,\sigma}(x)\left[-\lambda\sigma_3 - 2i\sigma\Delta_b\partial_{\sim}\sigma_2 + 2i\sigma\Delta_b\partial_{\cdot\cdot}\sigma_1\right]\tilde{\Psi}_{2,\sigma}(x) \tag{5.3.45}$$

$$\tilde{\Psi}^\dagger_{1,\sigma}(x) = \left(\tilde{f}_{A,1,\sigma}(x), \tilde{F}_{B,1,\sigma}(x)\right)^T \tag{5.3.46}$$

$$\tilde{\Psi}^\dagger_{2,\sigma}(x) = \left(\tilde{f}_{A,2,\sigma}(x), \tilde{F}_{B,2,\sigma}(x)\right)^T. \tag{5.3.47}$$

5.4 Quantum number of instantons

Now we should compute other nontrivial quantum numbers of the above instanton operators. To do so, let us first comment on the transformation of the continuum wave-function, we have:

5.4.1 Symmetry transformations on instanton operators

We are now ready to study instanton effect. From now on we closely follow our method presented in Ref. [80] to calculate quantum numbers of instanton operator and its transformation properties. An instanton by definition adds 2π internal $U(1)$ gauge flux to the system. Because of nonzero Hall conductance of Dirac cones, this nonzero flux can induce charge transfer between the above two Dirac cones. We only need to compute the Hall conductance of each band. To evaluate Hall conductance of the above bands we consider the following 2×2 Dirac Hamiltonian

$$H = \int d^2x \psi^\dagger (\vec{x}) \left(m\sigma_3 + i\eta_1 |t_1| \partial_x \sigma_1 + i\eta_2 |t_2| \partial_y \sigma_2 \right) \psi (\vec{x}), \tag{5.4.48}$$

where η_i can be +1 or -1, and $\sigma^{1,2,3}$ are Pauli matrices. The Hall conductance for this system is known to be $\sigma_{xy} = \frac{C}{2\pi}$, where

$$C = \frac{1}{2} \text{sgn} (m\eta_1\eta_2), \tag{5.4.49}$$

is the Chern number of the energy band. Using this equation, we can read the Chern number and therefore the Hall conductance of each band. Noting the fact that $\lambda < 0$, We have

$$C_{1,\sigma} = +\frac{1}{2} \tag{5.4.50}$$

$$C_{2,\sigma} = -\frac{1}{2} \tag{5.4.51}$$

Since Chern number of each band is independent of spin, after each instanton configuration, its magnetic flux induces $2 \times \frac{-1}{2} = -1$ fermions at the first band and $2 \times \frac{1}{2}$ at the second band. Therefore each instanton annihilates 1 fermion from the first band and creates 1 fermion on the second band. So there is a charge transfer between two bands. Using this argument the monopole operator can be written as a linear combination of following operators

$$\begin{array}{llll} \tilde{f}^\dagger_{A,1,\sigma}(x)\, \tilde{f}_{A,2,\sigma'}(x) & , & \tilde{F}^\dagger_{B,1,\sigma}(x)\, \tilde{F}_{B,2,\sigma'}(x) & , \\ \tilde{f}^\dagger_{A,1,\sigma}(x)\, \tilde{F}_{B,2,\sigma'}(x) & , & \tilde{F}^\dagger_{B,1,\sigma}(x)\, \tilde{f}_{A,2,\sigma'}(x) & \end{array} \tag{5.4.52}$$

Since monopole operator should be invariant under spin rotation around z axis, we have to choose $\sigma' = \sigma$. Now let us go back to untransformed spinon operators by using $\tilde{f}_{B,\sigma} = \tilde{F}^\dagger_{B,-\sigma}$. So the monopole operator is a linear combination of following operators

$$\lim_{x\to x'} \tilde{f}^{\dagger}_{A,1,\sigma}(x')\,\tilde{f}_{A,2,\sigma}(x)\ ,\ \lim_{x\to x'} \tilde{f}_{B,1,-\sigma}(x')\,\tilde{f}^{\dagger}_{B,2,-\sigma}(x)$$
$$\lim_{x\to x'} \tilde{f}^{\dagger}_{A,1,\sigma}(x)\,\tilde{f}^{\dagger}_{B,2,-\sigma}(x')\ ,\ \lim_{x\to x'} \tilde{f}_{B,1,-\sigma}(x')\,\tilde{f}_{A,2,\sigma}(x) \tag{5.4.53}$$

Now let us consider the following operators that are invariant under all spin rotation operators

$$\phi_1(x) = \lim_{x\to x'} \tilde{f}^{\dagger}_{A,1,\uparrow}(x)\,\tilde{f}^{\dagger}_{B,2,\downarrow}(x') - \tilde{f}^{\dagger}_{A,1,\downarrow}(x)\,\tilde{f}^{\dagger}_{B,2,\uparrow}(x') \tag{5.4.54}$$
$$\phi_2(x) = \lim_{x\to x'} \tilde{f}_{B,1,\downarrow}(x)\,\tilde{f}_{A,2,\uparrow}(x) - \tilde{f}_{B,1,\uparrow}(x')\,\tilde{f}^{\dagger}_{A,2,\downarrow}(x') \tag{5.4.55}$$
$$\phi_3(x) = \lim_{x\to x'} \tilde{f}^{\dagger}_{A,1,\uparrow}(x)\,\tilde{f}_{A,2,\uparrow}(x') + \tilde{f}^{\dagger}_{A,1,\downarrow}(x)\,\tilde{f}_{A,2,\downarrow}(x') \tag{5.4.56}$$
$$\phi_4(x) = \lim_{x\to x'} \tilde{f}_{B,1,\uparrow}(x)\,\tilde{f}^{\dagger}_{B,2,\uparrow}(x') + \tilde{f}_{B,1,\downarrow}(x)\,\tilde{f}^{\dagger}_{B,2,\downarrow}(x') \tag{5.4.57}$$

It should be noted that although all of the above operators are odd under $G_{T_y}T_y$. So every instanton term breaks the translation symmetry in the y direction. In order for the instanton operator to be a relevant perturbation, it should have all symmetries of the meanfield Hamiltonian. Since we have obtained spin liquid phase within meanfield calculation and spin liquids respect all lattice symmetries by definition, we should find a combination of the above operators that is invariant under all symmetries of the meanfield Hamiltonians. It is easy to check that the following instanton term has the desired property.

$$\delta\mathcal{L}_1 = \frac{\chi}{2}\int d^2\vec{x}\left(\hat{\phi}_3^2(x) + \hat{\phi}_4^2(x) + H.c.\right) \tag{5.4.58}$$
$$\delta\mathcal{L}_2 = \frac{1}{2}\sum_{\mu=\pm,\nu=\pm} g_{\mu,\nu}\int d^2\vec{x}\left((\phi_1+\mu\phi_2) + \nu\left(\phi_1^{\dagger}+\mu\phi_2^{\dagger}\right)\right)^2 \tag{5.4.59}$$

Using symmetry considerations, it can be shown that there is no other allowed instanton operator and the above terms are the only relevant perturbations.

5.4.2 Discussion and conclusion

We have found a double-instanton operator that has all symmetries of the microscopic Hamiltonian. Therefore this term is relevant and has a non-zero fugacity. Because of the instanton proliferation, the U(1) gauge fluctuations are now gapped out. On the other hand, since single instanton operator carries nonzero crystal momentum in the x direction, the translation symmetry breaks spontaneously. To have a better insight of the situation, we can appeal to the duality between $U(1)$ gauge theory and the nonlinear sigma model. If we identify $\frac{g}{2}\left(\phi_i^2(x)+\phi_i^{\dagger 2}(x)\right)=g\cos(2\theta)$, then we have a dual description of the $U(1)$ gauge theory with instanton:

$$L=\frac{m}{2}\dot{\theta}^2-\frac{\kappa}{2}(\nabla\theta)^2+g\cos(2\theta) \tag{5.4.60}$$

If g is not very small, we are n the phase $<\theta>=0$. In such a phase $<\phi_i>\neq 0$. Since all ϕ_i carry a crystal momentum (π,π), so the $<\phi_i>\neq 0$ phase at least break the translation symmetry. Therefore we conclude that the π-flux spin liquid phase is not stable after including instanton effects. We would like to point out that the basis vectors of the resulting state are $(1,1)$ and $(1,-1)$, because the symmetry between A and B sublattices is spontaneously broken due to instanton effect. The area of the unit cell is two times bigger and it contains two atoms in it.

In summary, if we treat the U(1) gauge field as a semi-classical field (i.e.Gaussian approximation), by analogy to the nonlinear sigma model, instantons proliferate, gauge field gaps out and lattice symmetry spontaneously breaks. What we finally obtain is a band insulator with a nonzero gap for spin and charge excitations, instead of a spin liquid phase. We want to mention that if gauge fluctuations are strong, other possibilities may happen. Among them, the Z_2 spin liquid is of more interest. This phase can be obtained if strong gauge fluctuations generate a hopping term to the nearest site or a nonzero pairing amplitude to the second neighboring site. The presence of any of these two terms breaks U(1) down to Z_2 gauge theory whose gauge fluctuations are gapped and therefore is stable.

5.5 Numerical results

We have studied the effect of instantons numerically. We start from the meanfield Hamiltonian of the gapped π-flux state. Then we add a single instanton to the system and measure the crystal momentum of the resulting many body wavefunction. Because of the nonzero gap the problem is well-defined. For gapless case there is an ambiguity in occupying zero mode states. In our case we fill all negative state energies with no

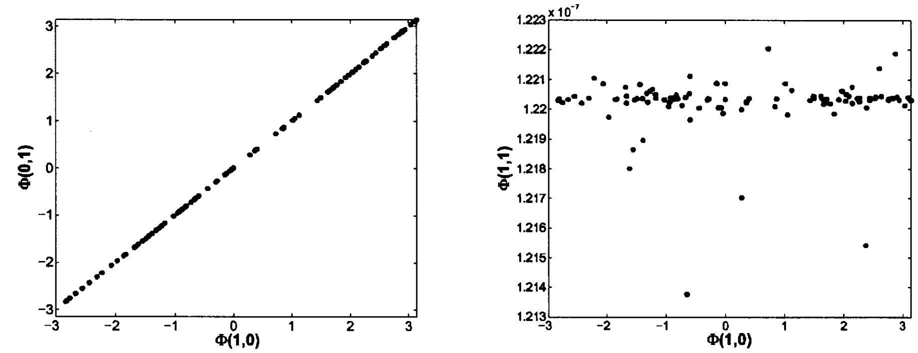

Figure 5-1: **Crystal momentum.**— Phase change of the many body wavefunction for 100 samples. $\exp(i\Phi(\vec{m})) = \frac{\Psi\left(\vec{R}_1+\vec{m},\ldots,\vec{R}_i+\vec{R}_1+\vec{m},\ldots,\vec{R}_N+\vec{R}_1+\vec{m}\right)}{\Psi\left(\vec{R}_1,\ldots,\vec{R}_i,\ldots,\vec{R}_N\right)}$. Wavefunction is invariant after T_xT_y, $T_xT_y^{-1}$, while acquires nonzero phase after T_x and T_y. (a), $\Phi(\hat{x}) = \Phi(\hat{y})$, which implies $\Psi\left(\vec{R}_i + \hat{y} - \hat{x}\right) = \Psi\left(\vec{R}_i\right)$. The value of Φ however is very sample dependent. (b), while $\Phi(\hat{x})$ can be anything, $\Phi(\hat{x}+\hat{y}) = 0$, which reflects the periodicity of many body wavefunction by $\hat{x}+\hat{y}$.

ambiguity. We can find the average number of spinons per lattice site and we obtain $\left\langle f_{i,\uparrow}^{\dagger} f_{i,\uparrow} + f_{i,\downarrow}^{\dagger} f_{i,\downarrow}\right\rangle = n_f < 1$. Because the Hamiltonian in Eq. 5.2.3 contains pairing, the ground state is superposition of many configurations with different number of spinons. According to the weak law of large numbers, in thermodynamic limit, the most probable configurations contain n_f spinons per site. So we generate a random configuration that has n_f fermions per site. We can easily compute the many body wavefunction in real space corresponding to this configuration by evaluating the Slater determinant. Then we translate this configuration by one lattice in the x or y direction followed by the corresponding G_{T_x} and G_{T_y} gauge transformations. We see that the wavefunction does not change in this case. So in the absence of instantons, groundstate carries no crystal momentum.

Then we add an instanton to the system by adding a quantum flux of magnetic field 2π to the lattice. We investigated the evolution of instanton and we saw that we can safely assume the resulting magnetic flux is uniform. Due to nonzero magnetic flux, the phase of the hopping amplitude changes as $\Delta_b(i,j) \to \Delta_b(i,j)\exp\left(i\int_{x_i}^{x_j}\vec{A}.\vec{dl}\right)$, where $\nabla\times A = B$ is the magnetic field of instanton. Again, we generate a random configuration and evaluate the many body wavefunction. Then we translate that configuration and we evaluate the new many body wavefunction. Absolute value of wavefunction never changes. Its phase however changes if we translate in the $\hat{x}$ or $\hat{y}$ directions. This phase vanishes if we translate the system in $\hat{x}+\hat{y}$, $\hat{x}-\hat{y}$, $2\hat{x}$ and $2\hat{y}$ directions. We have presented the results for 100 samples in Fig 3-1. It shows that $\Psi\left(\vec{R}_1+\hat{x},..!.,\vec{R}_i+\hat{x},...,\vec{R}_N+\hat{x}\right)=\exp\left(i\Phi\left(1,0\right)\right)\Psi\left(\vec{R}_1,...,\vec{R}_i,...,\vec{R}_N\right)$, $\Psi\left(\vec{R}_1+\hat{x},...,\vec{R}_i+\hat{x},...,\vec{R}_N+\hat{x}\right)=\Psi\left(\vec{R}_1+\hat{y},...,\vec{R}_i+\hat{y},...,\vec{R}_N+\hat{y}\right)$, and $\Psi\left(\vec{R}_1+\hat{x}+\hat{y},...,\vec{R}_i+\hat{x}+\hat{y},...,\vec{R}_N+\hat{x}+\hat{y}\right)=\Psi\left(\vec{R}_1,...,\vec{R}_i,...,\vec{R}_N\right)$, where Ψ is many body wavefunction. These relations implies that the many body wavefunction is invariant under T_xT_y but not T_x or T_y. Therefore after taking the effect of instantons into consideration, the lattice symmetry breaks spontaneously and the new basis vectors are $(1,1)$ and $(1,-1)$. Unit cell doubles and Brillouin zone reduces by a factor of $1/2$. So our numerical calculation verifies our theoretical prediction.

5.6 APPENDEX: Self-consistent equations and the uniform RVB state

For the uniform RVB, $\chi_{i,j}^{f,b}=0$ and $\Delta_{i,j}^{f,b}=\Delta^{f,b}$=constant. We also assume that $\lambda_i=\lambda$=constant. By solving the following self-consistent equations, we can obtain the phase diagram of the meanfield state. The values of $\Delta^{f,b}$ and λ can give us a hint about physics of the Hubbard model at large U-limit. We can also compute the average number of slave particle and in particular the number of doublons using them. We have the following self-consistent equations

$$\Delta^f=\frac{1}{N_s}\sum_k\langle f_{-k,\downarrow}f_{k,\uparrow}\rangle\left(\cos[k_x]-\cos[k_y]\right). \tag{5.6.61}$$

$$\Delta^b=\frac{1}{N_s}\sum_k\langle h_{-k}d_k\rangle\left(\cos[k_x]-\cos[k_y]\right). \tag{5.6.62}$$

$$\Delta^f=\frac{1}{N_s}\sum_{k,\sigma}\left\langle f_{k,\sigma}^\dagger f_{k,\sigma}\right\rangle\left(\cos[k_x]+\cos[k_y]\right). \tag{5.6.63}$$

$$\Delta^f=\frac{1}{N_s}\sum_k\left\langle h_k^\dagger h_k-d_k^\dagger d_k\right\rangle\left(\cos[k_x]+\cos[k_y]\right). \tag{5.6.64}$$

$$\frac{1}{N_s}\sum_k\left\langle h_k^\dagger h_k-d_k^\dagger d_k\right\rangle=x. \tag{5.6.65}$$

$$\frac{1}{N_s}\sum_k\left\langle f_{k,\uparrow}^\dagger f_{k,\uparrow}+f_{k,\downarrow}^\dagger f_{k,\downarrow}+h_k^\dagger h_k+d_k^\dagger d_k\right\rangle=1. \tag{5.6.66}$$

At $T = 0$ we have

$$\langle f_{-k,\downarrow} f_{k,\uparrow} \rangle = -|u_k v_k| = -\frac{t\Delta_b \left|\cos[k_x] - \cos[k_y]\right|}{E_k^f}. \tag{5.6.67}$$

$$\left\langle f_{k,\uparrow}^\dagger f_{k,\uparrow} \right\rangle = \left\langle f_{-k,\downarrow}^\dagger f_{-k,\downarrow} \right\rangle = |v_k|^2,$$
$$= \frac{1}{2} + \frac{\lambda + \mu + 2t\chi_b \left(\cos[k_x] + \cos[k_y]\right)}{2E_k^f}. \tag{5.6.68}$$

$$\langle h_{-k} d_k \rangle = \frac{2t\Delta_f \left|\cos[k_x] - \cos[k_y]\right|}{E_{1,k}^b + E_{2,k}^b}. \tag{5.6.69}$$

$$\left\langle h_k^\dagger h_k \right\rangle = \left\langle d_k^\dagger d_k \right\rangle = |\beta_k|^2,$$
$$= -\frac{1}{2} + \frac{U - 2\lambda - 2\mu}{4E_k^f}. \tag{5.6.70}$$

Let us use the following approximations

$$y = 2\left(\cos[k_x] - \cos[k_y]\right). \tag{5.6.71}$$

$$E_k^f = \sqrt{(\lambda)^2 + (t\Delta_b y)^2}. \tag{5.6.72}$$

$$E_{1,k}^b + E_{2,k}^b = \sqrt{(U - 2\lambda)^2 - (2t\Delta_f y)^2}. \tag{5.6.73}$$

$$\frac{1}{N_s}\sum_k \to \frac{1}{(2\pi)^2}\int d^2\vec{k} \simeq \frac{1}{8}\int_{-4}^{+4} dy. \tag{5.6.74}$$

Using the above assumptions we can rewrite the above self-consistent equations as

$$\frac{\Delta_f}{t\Delta_b} = \frac{1}{32}\int_{-4}^{+4} \frac{y^2}{\sqrt{(\lambda)^2 + (t\Delta_b y)^2}} dy. \tag{5.6.75}$$

$$\frac{\Delta_b}{t\Delta_f} = \frac{1}{16}\int_{-4}^{+4} \frac{y^2}{\sqrt{(U - 2\lambda)^2 - (2t\Delta_f y)^2}} dy. \tag{5.6.76}$$

$$n_f - 1 = \frac{1}{8}\int_{-4}^{+4} \frac{\lambda}{\sqrt{(\lambda)^2 + (t\Delta_b y)^2}} dy. \tag{5.6.77}$$

$$n_b + 1 = \frac{1}{8}\int_{-4}^{+4} \frac{U - 2\lambda}{\sqrt{(U - 2\lambda)^2 - (2t\Delta_f y)^2}} dy \tag{5.6.78}$$

By using the following integrals we have

$$\int \frac{dz}{\sqrt{1+z^2}} = Ln\left(z + \sqrt{1+z^2}\right) \tag{5.6.79}$$

$$\int \frac{z^2 dz}{\sqrt{1+z^2}} = \frac{z\sqrt{1+z^2} - \ln\left(z+\sqrt{1+z^2}\right)}{2} \tag{5.6.80}$$

$$\int \frac{dz}{\sqrt{1-z^2}} = \sin^{-1}(y) \tag{5.6.81}$$

$$\int \frac{z^2 dz}{\sqrt{1-z^2}} = \frac{1}{2}\left(\sin^{-1}(z) - z\sqrt{1-z^2}\right) \tag{5.6.82}$$

So we have

$$\Delta_f = \frac{X_1\sqrt{1+X_1^2} - Ln\left(X_1 + \sqrt{1+X_1^2}\right)}{2X_1^2}. \tag{5.6.83}$$

$$\Delta_b = \frac{\sin^{-1}(X_2) - X_2\sqrt{1-X_2^2}}{2X_2^2}. \tag{5.6.84}$$

$$n_f - 1 = -n_b = \frac{-1}{X_1}\ln\left(X_1 + \sqrt{1+X_1^2}\right). \tag{5.6.85}$$

$$n_b + 1 = 2 - n_f = \frac{1}{X_2}\sin^{-1}(X_2). \tag{5.6.86}$$

$$X_1 = \frac{4t\Delta_b}{|\lambda|} \quad X_2 = \frac{8t\Delta_f}{U - 2\lambda}. \tag{5.6.87}$$

If we assume $X_1 \gg 1$ and $X_2 \ll 1$ i.e.; for $U \gg U_c$ we can simplify the above equations and we will get

$\lambda \leq 0.$

$$\Delta_f = \frac{1}{2} - \frac{Ln(X_1)}{X_1^2}. \tag{5.6.88}$$

$$\Delta_b = \frac{X_2}{3} \simeq \frac{4t}{3U}. \tag{5.6.89}$$

$$n_f = 1 - \frac{Ln(2X_1)}{X_1} = 1 - \frac{|\lambda|}{8t\Delta_b} Ln\left(\frac{4t\Delta_b}{|\lambda|}\right). \tag{5.6.90}$$

$$n_b = \frac{X_2^2}{6} \simeq \frac{8}{3}\left(\frac{t}{U}\right)^2. \tag{5.6.91}$$

$$n_b + n_f = 1 \Rightarrow \frac{Ln(2X_1)}{2X_1} = \frac{4}{3}\left(\frac{t}{U}\right)^2. \tag{5.6.92}$$

We see that the number of doublons scales with $\left(\frac{t}{U}\right)^2$, and Δ_b with $\frac{t}{U}$. λ scales with $t\left(\frac{t}{U}\right)^3/\left(\ln\left(t/U\right)\right)$ and is very small at large U.

Chapter 6

Self-consistent calculation of the single particle scattering rate in high Tc cuprates

The linear temperature dependence of the resistivity above the optimal doping is a longstanding problem in the field of high temperature superconductivity in cuprates. In this chapter, we investigate the effect of gauge fluctuations on the momentum relaxation time and the transport scattering rate within the slave boson method. We use a more general slave treatment to resolve the ambiguity of decomposing the Heisenberg exchange term. We conclude that this term should be decomposed only in the Cooper channel. This results in the spinon mass inversely proportional to the doping. It is showed that solving the equation for the transport scattering rate self-consistently, we find a crossover temperature above which we obtain the linear temperature dependence of the electrical resistivity as well as the single particle scattering rate. It is also shown that this linear temperature dependence of the scattering rate in the pseudogap region explains the existence of the Fermi arcs with a length that linearly varies with temperature.

6.1 Introduction

It has been emphasized by many authors that the physics of high temperature superconductivity in cuprates [13] should be viewed as a doped Mott insulator [8, 46, 69]. This proximity to the Mott insulating phase at half filling, sheds some light on the underlying pairing mechanism of the superconductivity. One of the useful and rather successful treatments of the doped Mott insulator is the slave particle method [15, 92, 79]. It is well-known that this method results in the emergent internal gauge field that is strongly coupled to slave particles. Indeed it is the dressed slave particles by gauge bosons that is physical and observable.

Since slave particles are strongly interacting with gauge bosons, the effect of gauge interactions on the physical properties of electrons should be taken into consideration in any realistic model. This effect has been extensively studied in the past three decades. For example, Ioffe and Larkin [32] have studied how the physical properties of electrons, e.g. their electrical conductivity, are related to the corresponding properties of slave particle, in the presence of the gauge field. Also, many authors [47, 69] have studied the effect of gauge fluctuations on the transport properties of electrons. Here we follow their method but with two modifications. First of all, we argue that the mass of spinons is inversely proportional to the doping, instead of being almost independent of it. As a result, the Fermi velocity of electrons should scale with doping outside the superconducting phase. The second difference is that we solve equations self-consistently. We show that either a simple scaling argument or exact numerical calculation, results in the transport scattering time that is linear in T above a crossover temperature, T^* that scales with the doping.

6.2 Linear temperature dependence of the resistivity

From the Fermi liquid theory we expect T^2 dependence for the electrical resistivity. This reflects the stability of this phase at low temperatures. On the other hand, in the normal state above the optimal doping (strange metal phase of the hole doped cuprates), the resistivity exhibits a linear dependence on temperature instead of the expected parabolic dependence [13, 46, 16]. For temperatures comparable to the Debye temperature and higher, this linear dependence can be explained through electron phonon interaction. The Debye temperature is several hundred Kelvin while this behavior remains down to much smaller temperatures. So this is a fundamental issue that cannot be explained only through simple electron phonon interaction. In slave boson approach, holons and spinons are strongly interacting with the internal gauge field. One popular notion is that this interaction can

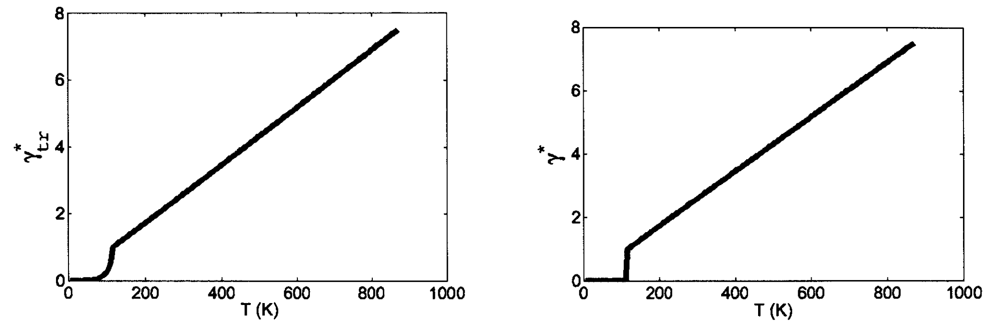

Figure 6-1: **Scattering rate.**— Self-consistent calculation of the transport scattering rate γ_{tr} and momentum relaxation scattering rate γ versus temperature in the absence of external magnetic field. We assume that Cooper pairs are killed so we can study the crossover between the Fermi liquid and the strange metal phases. At low enough temperatures, holon gas condenses and we obtain FL phase. At high enough temperatures, we obtain linear temperature dependence for γ_{tr} and γ signaling the strange metal phase. (a), Reduced inverse transport lifetime $\gamma^*_{tr} = \frac{\gamma_{tr}(T)}{\gamma_{tr}(T^*)}$ at $x = 0.15$. Temperature is in units of Kelvin. Below the crossover temperature $T^* \sim 100K$, holons undergo Bose Einstein condensation and we obtain Fermi liquid behavior, $\gamma_{tr} \sim T^2$. Above T^*, we obtain marginal non-Fermi liquid with $\gamma_{tr} \sim T$. Interestingly T^* scales with doping x, like the BEC transition temperature of the holon gas. (b), Reduced inverse momentum relaxation time $\gamma^* = \frac{\gamma(T)}{\gamma(T^*)}$ at $x = 0.15$.

explain the desired behavior. By calculating the self energy of electrons due to scattering off the gauge field at finite temperature, we can compute the transport lifetime, as well as the momentum and energy relaxation time of quasiparticles resistivity.

Some authors have studied the effect of gauge fluctuations on the transport properties of cuprates, and they find $T^{4/3}$ temperature dependence for the resistivity [47, 69]. Here we closely follow their method, but with two important differences. First of all they assume the mass of spinons has a weak dependence on the doping and is inversely proportional to the exchange energy J. Using the more general Anderson-Zou slave boson method [92, 79], we obtain a different behavior. In this method, the spinon mass is inversely proportional to the doping. This for instance means that the Fermi velocity outside the superconducting phase e.g. in the Fermi liquid phase, is proportional to the doping. The doping dependence of the spinon mass should be observed in the density of states at Fermi level. The second difference is that the problem should be solved self-consistently. In the rest of this chapter, we have provided the details of calculation and we have presented an integral expression for the transport scattering rate γ_{tr} that depends on itself. If we keep γ_{tr} inside the integral, along with the assumption $1/m_s^* \sim x$, we obtain a temperature scale T^* above which we find linear temperature resistivity. Surprisingly T^* scales with doping x, the same behavior that we expect for the crossover temperature between the Fermi liquid and strange metal phases. Below this temperature scale, holons condense and we recover the results of the Fermi liquid theory [70]. We have solved the self-consistent equation for γ_{tr} and we verify T^2 behavior for the resistivity at low temperatures in the Fermi liquid phase and linear temperature resistivity above T^* in the strange metal phase. Fig. 1 summarizes our result.

6.3 Method

Hubbard model is the simplest model that captures the physics of the Mott insulators. The Hamiltonian of the Hubbard model is defined as,

$$H = U \sum_i n_{i,\uparrow} n_{i,\downarrow} - t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{j\sigma} c_{i\sigma} + h.c. \tag{6.3.1}$$

Here $\langle i, j \rangle$ means site j is one of the nearest neighbors of site i.

Now let us employ a more general slave boson approach to the Hubbard model [69, 92, 79]. In this approach an electron operator decomposes in the following way

$$c_{i,\sigma} = f_{i,\sigma} h^\dagger_i + \sigma f^\dagger_{i,-\sigma} d_i. \tag{6.3.2}$$

where $f^\dagger_{i,\sigma}$ is spinon creation operator (assumed to be fermion), $h^\dagger_i$ is holon creation operator and $d^\dagger_i$ is doublon creation operator. We assume spinons are fermions and obey Fermi Dirac statistics and are electrically neutral, while holons and doublons are bosons and have $+e$ and $-e$ electric charges respectively. Spin σ spinon corresponds to a site with only one electron with spin up, holon represents an empty site and doublon corresponds to a doubly occupied site. As it is clear from the above definition, electron operator is invariant an under internal compact U(1) gauge transformations (i.e. if we multiply each creation operator by a local phase $exp(i\theta_i)$), provided all slave particles carry the same internal gauge charge(i.e. θ_i is the same for all slave particles at site i). Note that we must keep the bosonic statistics of holons and doublons after gauge transformation, otherwise we had SU(2) gauge freedom. In order to have fermionic statistics for electron operator, we have to implement $f^\dagger_{i,\uparrow} f_{i,\uparrow} + f^\dagger_{i,\downarrow} f_{i,\downarrow} + h^\dagger_i h_i + d^\dagger_i d_i = 1$ constraint at each site. On the other hand, doping implies $\left\langle h^\dagger_i h_i - d^\dagger_i d_i \right\rangle = x$ constraint.

Since in the Mott insulator where onsite Coulomb repulsion is very large ($U \ll t$), the double occupancy is very costly, and these states can be removed in the low energy studies of cuprates. In other words, for large U/t limit of the Hubbard model, charge excitation gap is of order U and therefore we can integrate out doublons to obtain an effective action for spinon and holons. This process provides a systematic way to recover the t-J model and naturally reduces to the famous slave boson theory of the t-J model.

In the t-J model, there is at most one electron at each site. To implement this constraint in the slave boson method, as we discussed before, empty states are treated as the charged bosonic particles, dubbed as holon. So we can take the non-doubly occupancy constraint by using the Lagrange multiplier method. The physical Hilbert space, contains three states at each site, occupied state with spin up or down and unoccupied state (empty sites). However, the Hilbert space of the slave boson method is much larger as we can have as many holons per site as we want and the constraint is implemented only in average. Therefore the meanfield description of the slave boson method is incomplete and redundant. In the next section, it is shown that this redundancy is responsible for the emergent $U(1)$ gauge field. Although at the beginning there is no kinetic term for the gauge field, upon renormalization and by integrating out the slave particles, this term will be generated and the gauge field will have its own dynamics in that case. Slave particles are interacting strongly with this gauge field and their scattering off gauge potential gives them a finite lifetime. The single particle scattering rate is computed in section VI and we show that it is results in a transport scattering rate that is linear in temperature.

One ambiguity in the t-J model is how to decompose the exchange term $JS_i.S_j$, where S_i is the spin operator. Most authors, decompose this term in direct and Cooper channels symmetrically. Within meanfield approximation, they rewrite $J\sum_{i,j} S_i.S_j$ as

$$
\begin{aligned}
&-3/8J \sum_{i,j,\sigma} \left\langle \chi^f_{i,j} \right\rangle f^\dagger_{i,\sigma} f_{j,\sigma} + h.c. \\
&-3/8J \sum_{i,j,\sigma} \left\langle \Delta^f_{i,j} \right\rangle \sigma f^\dagger_{i,\sigma} f^\dagger_{j,-\sigma} + h.c.
\end{aligned}
$$

$$+3/8J\sum_{i,j}\left(\left|\left\langle\chi^f_{i,j}\right\rangle\right|^2+\left|\left\langle\Delta^f_{i,j}\right\rangle\right|^2\right), \tag{6.3.3}$$

where $\chi^f_{i,j}=\sum_\sigma f^\dagger_{i,\sigma}f_{j,\sigma}$ and $\Delta^f_{i,j}=\sum_\sigma \sigma f_{-\sigma,i}f_{j,\sigma}$. At small dopings, the above hopping implies $1/m^* \sim J\chi_{i,j}$ which has a weak dependence on the doping. However, if we use the more general slave boson approach, it resolves the above mentioned ambiguity and we have only one choice. In this formalism, the exchange term only decomposes in the Cooper channel. Using the Eq. [2], within the meanfield approximation, the Hubbard model can be rewritten as

$$H=\sum Ud^\dagger_i d_i - t\sum_{\langle i,j\rangle}\left(\chi^s_{i,j}\chi^b_{j,i}+\Delta^s_{i,j}\Delta^b_{i,j}+h.c.\right), \tag{6.3.4}$$

in which we have used these notations $\chi^b_{i,j}=h^\dagger_i h_j - d^\dagger_i d_j$ and $\Delta^b_{i,j}=d_i h_j + h_i d_j$. By integrating out doublons, it can be shown that $\langle\chi_b\rangle\sim x$, and $\langle\Delta_b\rangle\sim t/U$. $\Delta^s_{i,j}\Delta^b_{i,j}$ represents the exchange term and after integrating out doublons it decouples only in the Cooper channel (we replace the exchange term by $\left\langle\Delta^b_{i,j}\right\rangle\Delta^s_{i,j}\sim\frac{t}{U}f^\dagger f^\dagger+H.c.$ form). Therefore the hopping term for spinons is $-t\langle\chi_b\rangle\sum_{i,j}f^\dagger_{i,\sigma}f_{j,\sigma}$ and as results they have a mass $1/m^*_s\sim 2tx$. As we approach the half filling (undoped material), the effective mass of spinons diverges signalling the metal-Mott insulator phase transition.

So we end up at the the t-J model starting from the large U limit of the Hubbard model. It is believed that the t-J model captures the essential physics of the strongly correlated systems. This model is defined as the following

$$H_{t-J}=-t\sum_{\langle i,j\rangle,\sigma}P_G c^\dagger_{i,\sigma}c_{j,\sigma}P_G + J\sum_{i,j}\hat{S}_i.\hat{S}_j, \tag{6.3.5}$$

where P_G is the Gutzwiller projection operator that removes doubly occupied states. Within the slave boson formalism, after removing doubly occupied states, electrons can be decomposed as $c^\dagger_{i,\sigma}=f^\dagger_{i,\sigma}h_i$ along with the physical constraint on each site: $h^\dagger_i h_i+\sum_\sigma f^\dagger_{i,\sigma}f_{i,\sigma}=1$ which implements the Gutzwiller projection. Whenever $c^\dagger_{i,\sigma}$ acts on an empty site, it annihilates one holon and creates a spinon with spin σ. We cannot act further on the resulting state by $c^\dagger_{i,-\sigma}$, since this operator has to kill a holon, but there is no holon anymore at that site. If we act $c_{i,\sigma}$ on a site that contains a spinon with spin σ, the operators annihilates the spinon and creates a holon at that site. So by acting projected electron operator we always annihilate one type of slave particle and create another one and therefore the number of slave particles at each site is conserved. Now we can rewrite the t-J model in terms of the new slave particles. Within meanfield approximation and by using Hubbard-Stratonovic transformation, we can decouple spinons (spin sector) from holons (charge sector) and we obtain the following effective Hamiltonians for each sector

$$H_h = -\sum_{<i,j>} t\chi_s h_i^\dagger h_j - \sum_i \mu_h h_i^\dagger h_i. \tag{6.3.6}$$

$$\begin{aligned} H_s = &- \sum_{<i,j>,\sigma} t\chi_h f_{i,\sigma}^\dagger f_{j,\sigma} - \sum_{i,\sigma} \mu_s f_{i,\sigma}^\dagger f_{i,\sigma}, \\ &- \sum_{<i,j>} (J/2)\, \Delta_s(i,j) \left(f_{i,\uparrow}^\dagger f_{j,\downarrow}^\dagger - f_{i,\downarrow}^\dagger f_{j,\uparrow}^\dagger \right) + h.c., \end{aligned} \tag{6.3.7}$$

where the following notations have been used

$$\chi_h = \left\langle h_{i+\vec{\delta}}^\dagger h_i \right\rangle. \tag{6.3.8}$$

$$\chi_s = \left\langle \sum_\sigma f_{i+\vec{\delta},\sigma}^\dagger f_{i,\sigma} \right\rangle. \tag{6.3.9}$$

$$\Delta_s(i,j) = \frac{1}{2} \left\langle f_{i,\uparrow}^\dagger f_{j,\downarrow}^\dagger - f_{i,\downarrow}^\dagger f_{j,\uparrow}^\dagger \right\rangle. \tag{6.3.10}$$

At low temperatures, most of holons occupy the groundstate with momentum $k = 0$, therefore $\chi_h \sim x$. This model has been extensively studied in the literature and it is well known that this model leads to the d-wave pairing symmetry for spinons [46], i.e. $\Delta_s(\pm\hat{x}) = \Delta_s$ and $\Delta_s(\pm\hat{y}) = -\Delta_s$.

6.4 Single particle scattering rate

Now, we discuss the effect of gauge fluctuations on the transport properties of cuprates in the strange metal phase. Here we closely follow the method used by Lee and Nagaosa [47] and a more recent approach by Senthil and Lee [69].

In the continuum approximation, the hopping part of the action of spinons and holons are written as

$$\int dxdt f_{\sigma}^{\dagger}(x)\left(-i\partial_t - \nabla^2/2m_s^* - \mu_s\right) f_{\sigma}(x),$$
$$+\int dxdt h^{\dagger}(x)\left(-i\partial_t - \nabla^2/2m_h^* - \mu_h\right) h(x). \tag{6.4.11}$$

As we pointed out before, the slave boson formalism has U(1) gauge theory. Under the gauge transformation, $f_{i,\sigma} \to e^{i\theta_i} f_{i,\sigma}$ and $h_i \to e^{i\theta_i} h_i$. So $\chi_{i,j}^{s,h} \to e^{i(\theta_j-\theta_i)}\chi_{i,j}^{s,h}$. If we define $a_{\vec{\delta}}(i)$ as $\chi_{i,j} = |\chi_{i,j}| e^{ia_{\vec{\delta}}(i)}$, where $\vec{\delta} = \vec{R}_i - \vec{R}_j$, we have $a_{\vec{\delta}}(i) \to a_{\vec{\delta}}(i) + \theta_j - \theta_i$. This implies that in the continuum model, $a_{\mu}(x) \to a_{\mu}(x) - \partial_{\mu}\theta(x)$. Therefore we should add modify the continuum model in the following way to obtain a gauge invariant model

$$\int dxdt f_{\sigma}^{\dagger}(x)\left(-iD_t - D_i^2/2m_s^* - \mu_s\right) f_{\sigma}(x)$$
$$+\int dxdt h^{\dagger}(x)\left(-iD_t - D_i^2/2m_h^* - \mu_h\right) h(x), \tag{6.4.12}$$

where $D_{\mu} = \partial_{\mu} - ie_{int}a_{\mu}/c$, where e_{int} is the internal gauge charge. We scale a_{μ} so that $e_{int} = e$.

To obtain an effective action for gauge particles we can integrate out spinons and holons. By expanding D_{μ} in terms of ∂_{μ} and a_{μ}, it is clear that in the continuum model, the vector potential is minimally coupled to matter field, i.e. the gauge field is coupled to the current carried by quasiparticles and we have the following interaction between gauge field and spinons

$$e\int dxdt J_s^{\mu}(x,t)\, a_{\mu}(x,t), \tag{6.4.13}$$

where $a^{\mu} = (\phi, a_x, a_y)$ and $J^{\mu} = (n, J_x, J_y)$, where $n_s = f^{\dagger}f$, $\vec{J}_s = if^{\dagger}\left(\vec{\nabla}/2m_s\right)f + H.c.$. We have a similar term for holons. Now we use the gauge freedom to set $\phi = 0$ and choose the Coulomb gauge $\vec{\nabla}.\vec{a} = 0$. Up to the second order perturbation theory the above interaction terms leads to an following effective action for the gauge field proportional to the following form,

$$\int dxd\tau dx'd\tau' a_i(x,\tau)\left\langle J^i(x,\tau), J^j(x',\tau')\right\rangle a_j(x,t). \tag{6.4.14}$$

This is only the contribution coming from paramagnetic response. There is a similar contribution from the diamagnetic part. Lee and Nagaosa have studied this problem in detail. Following their method, we can find the gauge field propagator $D_{\mu,\nu}(r,\tau) = \langle T_\tau a_\mu(r,\tau) a_\mu(r',0)\rangle$. it can be shown that the gauge field propagator can be written as $D_{ij}(q) = (\Pi_s + \Pi_h)^{-1}_{ij}$, where

$$\Pi_s^{ij} = -\left\langle T_\tau\left[J_s^i(r,\tau) J_s^j(0,0) - \delta_{ij} n_s \delta(r)\delta(\tau)\right]\right\rangle, \tag{6.4.15}$$

and similarly for Π_h^{ij}. In the Coulomb gauge the spatial part of the gauge field is transverse and can be written as

$$D_{ij}(q,\omega) = \left(\delta_{ij} - q_i q_j/q^2\right) D^T(q,\omega), \tag{6.4.16}$$

where we have defined $D^T(q,\omega)$ as

$$D^T(q,\omega) = \left[\Pi_s^T(q,\omega) + \Pi_h^T(q,\omega)\right]^{-1}. \tag{6.4.17}$$

For small q and ω we can use the following approximation

$$\Pi_s^T(q,\omega) = i\omega\sigma_s^T(q,\omega) - \chi_s^D q^2 - \rho_{s,c}(T), \tag{6.4.18}$$

where σ_s^T is the transverse conductivity and χ_s^D is the Landau diamagnetic susceptibility of the spinon system, which equals $1/24\pi m_s$ in 2D fermion systems. $\rho_{s,c}$ is the condensation fraction of the spinon system in the paired state and in the normal state it is zero. Similarly for holons we have

$$\Pi_s^T(q,\omega) = i|\omega|\sigma_h^T(q,\omega) - \chi_h^D q^2 - m_h\rho_{h,c}(T) \tag{6.4.19}$$

where $\chi_h^D = n(0)/48\pi m_s$ in which $n(0)$ is the occupation number of the ground state and $\rho_{h,c}$ is the superfluid density of holons, which is zero in the strange metal phase as well as the pseudogap phase. We see that the propagator of the gauge field that determines the transport scattering rate of spinons, depends on the optical conductivity of spinons. On the other hand, optical conductivity itself depends on the transport scattering rate, since we have $\sigma_s(q,\omega) = v_F k_F/\sqrt{4\gamma_{tr}^2 + v_F^2 q^2}$. If we neglect γ_{tr} in the $\sigma_s(q,\omega)$, we recover the results of the Ref. [47], except that since the spinon mass is much larger in our case, the crossover temperature is smaller. In Ref. [47], Lee and Nagaosa have calculated the scattering rate of holons due to interaction with the gauge field and they report a linear temperature behavior above the BEC transition. They have also studied the transport scattering rate of spinons and they report $T^{4/3}$ in the strange metal phase, which is slightly different from the linear temperature behavior.

Now let us calculate the self energy of spinons due to their interaction with the gauge field. Then by looking at its imaginary part we can deduce the scattering rate. According to Senthil and Lee, up to the first order approximation, the self energy of spinons due to their scattering off the gauge field is described by the following expression

$$\begin{aligned} \Sigma''(K,\Omega=0) &= -\pi \int d\omega dq \left(v_F \times q\right)^2 D''(q,\omega), \\ &\times A(K-q,-\omega)\left(n_{BE}(\omega) + n_{FD}(\omega)\right), \end{aligned} \tag{6.4.20}$$

where n_{BE} and n_{FD} are Bose Einstein and Fermi-Dirac distribution functions respectively. Near the Fermi surface the above integral reduces to

$$\gamma = \pi v_F K_F \int d\omega \frac{1}{\sinh \beta\omega} \int dq D''(q,\omega), \tag{6.4.21}$$

where $D''(q,\omega) = Im\left(i\omega\sigma_{q,\omega}^T - \chi^D q^2 - \rho_c\right)^{-1}$ in which $\sigma = \sigma_s + \sigma_h$, $\chi^D = \chi_s^D + \chi_h^D$ and $\rho_c = \rho_{c,s} + \rho_{c,h}$. To compute γ_{tr} we should multiply $D''(q,\omega)$ by $\left(\frac{q}{K_F}\right)^2$. So we have

$$\gamma_{tr} = \pi v_F K_F \int d\omega \frac{1}{\sinh \beta\omega} \int dq \left(\frac{q}{K_F}\right)^2 D''(q,\omega). \tag{6.4.22}$$

Let us assume that $v_F \sim K_F/m_s^* \sim 2txK_F$ and at small dopings, $K_F \sim \pi$. When $q \ll \gamma_{tr}/v_F$, $\sigma_s(q,\omega) = v_F k_F/\gamma_{tr}$. On the other hand, in the absence of holon and spinon condensation, $\omega\sigma(q,\omega) \sim \chi^D q^2$, so $q \sim K_F \left(\frac{\omega}{2\gamma_{tr}}\right)^{1/2}$. Therefore the $q < q^* \sim \gamma_{tr}/v_F$ region contribution to the integral over q is of order $K_F(\gamma_{tr}/v_F)^{1/2}$. For q^* comparable to a fraction of π this is the leading order contribution. This corresponds to $\gamma^{tr}(T) \propto v_F \propto tx$. As long as this is satisfied we have

$$\gamma_{tr}^{3/2} \propto \pi v_F K_F^2 \int d\omega \frac{\omega^{1/2}}{\sinh \beta\omega}. \tag{6.4.23}$$

A simple scaling argument verifies that $\gamma_{tr} \sim T$ satisfies the above self-consistent equation for γ_{tr}. The crossover temperature can be found from $\gamma^{tr}(T^*) \sim v_F \propto tx$. Therefore $T^* \propto tx$, which is the expected behavior for the crossover temperature between the Fermi liquid phase and the strange metal phase.

Numerically, we solved this self-consistent equation exactly and we again we obtained linear T dependence of γ_{tr} above a temperature scale $T^*(x)$ that scales with doping x (see Fig. 6.2). On the other hand the BEC transition temperature of holons scales with doping as well. In summary, above a temperature scale comparable to the Bose Einstein transition temperature of holon gas, we obtain linear temperature transport scattering rate. It should be mentioned that the scattering rate of holons is linear in T even in the previous calculations [47]. To obtain the physical quantities from the corresponding quantities for spinons and holons, we should recombine them in a particular way, that is called Ioffe-Larkin formula. This formula tells us that the physical conductivity is related to that of holons and spinons in the following way $\sigma^{-1} = \sigma_s^{-1} + \sigma_h^{-1}$. For dc conductivity we have $\sigma = ne^2\tau_{tr}/m$ and $\tau_{tr} = 1/\gamma_{tr}$. Since the scattering rate of holons and spinons are both linear in T, the dc conductivity is is linear in temperature as well. In Fig. 1 we have presented our numerical results.

On the other hand, below the BEC transition temperature, $\rho_{c,h} \neq 0$. Numerically, we obtain T^2 behavior for the γ_{tr} in this phase, which is the right sign and is expected for the Fermi liquid phase.

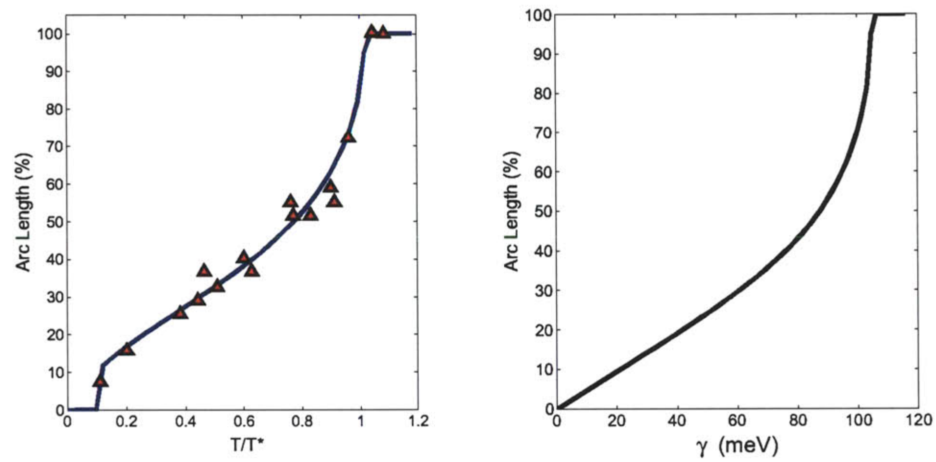

Figure 6-2: **Length of the Fermi arc.**— Length of the Fermi arc. In the pseudogap region, we obtain disjoint Fermi segments, at which excitations are gapless. The length of these segments increases with temperature and the scattering rate γ. (a), The length of the Fermi arc vs. normalized temperature (T/T^*). The blue line our theoretical calculation and red triangles are experimental data taken from Ref. [36]. Below the superconducting transition temperature T_c, the scattering rate γ is very small due to the condensation of quasiparticles. Therefore only very near nodal points we have gapless excitation. Above T_c, there is macroscopic condensation and the scattering rate varies linearly with temperature. As γ increases, the length of the Fermi arc increases. At T^*, we obtain closed Fermi surface. (b), The length of the Fermi arc vs. scattering rate γ. Below the superconducting transition temperature T_c, the scattering rate γ is very small due to the condensation of quasiparticles. Therefore only very near nodal points we have gapless excitation. Above T_c, there is macroscopic condensation and the scattering rate varies linearly with temperature. As γ increases, the length of the Fermi arc increases. At T^*, we obtain closed Fermi surface.

6.5 Observation of Fermi arcs

In the underdoped cuprates and above the superconducting region, the state of matter is very unusual. In one hand, it is a metallic phase, confirmed by transport experiments. On the other hand, there is no closed Fermi surface. Along some directions and segments of the Fermi surface, excitations are gapless, while on other directions, excitations are gapped [36, 60, 14]. c-axis transport measurements also show a gap in the excitations that implies a bound state of Fermions. It has been discussed by Norman *et al* [60] that if the scattering rate of quasiparticles γ varies linearly with temperature, one can explain the observations. As we discussed in the previous paragraph, gauge fluctuations can cause such a behavior. Some authors [14] have discussed that the electron phonon interaction may play an important role here and result in the linear T dependence of γ above some at high enough temperatures. Here we show that the interaction of slave particles with gauge bosons and the scattering of the quasiparticles from the d-wave potential results in such an exotic behavior. Using the method introduced in the previous section, we can compute the scattering rate of electrons in the superconducting region as well as the pseudogap phase. In the superconducting phase, the scattering rate is very small due to the condensation of both spinons and holons. In the pseudogap phase however, it is comparable to the pseudogap, varies linearly with T and cannot be neglected. In this region we assume that there is a local pairing potential that electrons scatter off. This assumption leads to the following expression for the electrons Green's function:

$$G(k,\omega)^{-1} = \omega - \epsilon_k + i\gamma - \frac{\Delta_k^2}{\omega + \epsilon_k + i\gamma}, \tag{6.5.24}$$

where, $\gamma(T)$ is the scattering rate at temperature T, energy of free quasiparticles. We have assumed d-wave pairing, i.e. $\Delta_k(T) = \Delta(T)(\cos(k_x) - \cos(k_y))$. Using the above expression we can compute the spectral function and from the position of its peak we can read the energy of interacting quasiparticles. When $\epsilon_k = 0$, it can be shown that as long as $\gamma > \sqrt{3}\Delta_k(T)$, the maximum is at $E = 0$ and as a result we have gapless excitations along that direction. At nodal points $\Delta_k = 0$ and we can always satisfy this equation at that point. Since $\gamma(T) \ll \Delta(T)$ in the superconducting phase, this condition is only satisfied very near nodal points and the length of Fermi arcs is negligible. If we parameterize Δ_k by the angle, we have $\Delta(\phi, T) = \Delta(T)\cos(2\phi)$, and nodal points are located at $\phi = \{\pm\pi/4, \pm3\pi/4\}$. Therefore the length of arc is $L(T) = 8\sin^{-1}\left(\gamma(T)/\sqrt{3}\Delta(T)\right)$. The crossover temperature of the pseudogap phase, T^*, can be found by solving $\gamma(T^*) = \sqrt{3}\Delta(T^*)$. Fig. 2 summarizes our results.

In conclusion, we reexamined the effect of gauge fluctuations on the single particle scattering rate. Using the mass of spinons proportional to the doping and doing a self-consistent calculation for the self-energy of quasiparticles scattering off the gauge field, we found the linear temperature dependent transport scattering rate of electrons above a crossover temperature that scales with the doping. Below this crossover temperature, we obtained T^2 behavior for the transport scattering rate that recovers the Fermi liquid behavior. We also found a scattering rate that is linear in T above the crossover temperature. We showed that the linear dependence of the scattering rate explains the existence of the Fermi arcs in the pseudogap phase. The success of our model emphasizes on the importance of including gauge fluctuations in understanding the underlying physics of cuprates. We predict that the Fermi velocity in the Fermi liquid phase varies linearly with the doping.

Chapter 7

Cooperative Electronic and Phononic Mechanism of the High Temperature Superconductivity in Cuprates

In conventional superconductors, phonons glue two electrons with opposite spins to form Cooper pairs and condensation of these pairs leads to the superconductivity. Identifying the underlying mechanism of the high temperature superconductivity in cuprates is among the most important problems in physics. Even quarter of a century after the first report of high temperature superconductor by Bednorz and Muller in 1986, there is still no general consensus on the pairing mechanism of superconductivity in these materials. So far, many theories have been developed to explain the exotic properties of cuprates, but they can explain only a limited number of experiments. In this article, we present a new pairing mechanism that incorporates both strong correlation and phonon mediated interaction on an equal footing to produce superconductivity. In this framework, strong correlation and anti-ferromagnetic interaction between electrons, create RVB pairs and phonons provide the phase coherence between these RVB pairs. Both of these are required in this approach to obtain the superconductivity. This approach resolves three limitations of the U(1) slave boson method. We achieve a better estimation of T_c, we only predict $\frac{h}{2ec}$ vortices and the linear T coefficient of the superfluid is not sensitive to the doping. This formalism provides a framework that connects Anderson's idea of preformed Cooper pairs and phonon based theories.

7.1 Introduction

One scenario for the high temperature superconductivity in cuprates [13] is the preformed Cooper pairs idea that was first proposed by Anderson [8]. This theory is based on the strong correlation effects and it does not incorporate phonons in the pairing mechanism. On the other hand, many experiments have been reported indicating the importance of electron phonon interaction in understanding the physics of high Tc cuprates, such as the oxygen isotope effect on both the transition temperature of superconductivity and the London penetration depth [77, 91, 39, 61, 90, 67].

Observation of the strong isotope effect in cuprates has led many authors to employ the strong limit of the electron phonon interaction as the primary cause of the superconductivity in these materials [3]. For example, some workers have applied bipolaron theory of superconductivity to the high temperature superconductivity problem. This theory requires the breakdown of the Migdal-Eliashberg theory and is based on the non-adiabatic limit of the electron phonon interaction, where phonons have a much larger energy than electrons. Experimentally, a typical energy of electrons is around the exchange energy $J \sim 130$ meV [46], while the energy of optical phonons is $40-70$ meV [33]. On the other hand, the breakdown of the Migdal-Eliashberg theory [54] in any phonon based theory is crucial, because isotope experiments in cuprates are very different from conventional superconductors that are explained by the BCS theory [11] and its generalization, i.e. Migdal-Eliashberg theory.

Some authors emphasize on the importance of the microscopic inhomogeneity, charge and spin stripes in understanding the mechanism of the superconductivity [18, 42]. The idea is that the phase segregation can save kinetic energy of holes and the exchange energy of spins. Stripe models are based on the competition between this phase and other states of matter. It is noteworthy that static stripes have been observed only in La_2SCuO_4 family near $x = \frac{1}{8}$, not in YBCO family, but dynamical stripes are expected even away from $x = \frac{1}{8}$ [45].

The idea of Anderson can be implemented using the slave particle method [46, 15, 47, 65, 79, 55]. The U(1) version of this method explains many basic properties of cuprates successfully. However, this method has several limitations. For example, the U(1) slave boson method overestimates the transition temperature of the superconducting state by an order of magnitude. Although in experiments only $\frac{h}{2ec}$ vortices have been observed, this method predicts another $\frac{h}{ec}$ vortices as well. For clean d-wave superconductors, the superfluid density decreases linearly with temperature up to the leading order. Experimentally the coefficient of this linear term is not very sensitive to the doping, while the U(1) slave boson treatment predicts a x^2 doping dependence, where x is the doping percentage. In this chapter we argue that phonons can mediate attractive interaction between holons and therefore we find a paired holon state. We show that this assumption resolves the three mentioned limitations of the U(1) slave boson approach.

Here we extend the Anderson theory of high Tc which is based on the resonating valence bond(RVB) state, by adding Holstein Hamiltonian such that the model Hamiltonian include the effect of electron phonon interaction. RVB state is the superposition of all possible singlet states between any two sites. The idea of RVB state can be quantified using the slave boson method, and naturally leads to the spin charge separation in two spatial dimensions. The low energy excitations of this state are described by the charged spinless quasiparticles which are called holon and are treated as bosons, and the neutral spin 1/2 quasiparticles which are called spinon and are treated as fermions. This can be implemented by writing the creation operator of physical electrons $c^{\dagger}_{i,\sigma}$ as the product of a fermionic operator $f^{\dagger}_{i,\sigma}$ and a bosonic operator h_i. Therefore $c^{\dagger}_{i,\sigma} = f^{\dagger}_{i,\sigma} h_i$. This assumption comes along with the nondoubly occupancy constraint due to very large onsite repulsion between electrons in cuprates. In terms of slave particles $f^{\dagger}_{i,\uparrow} f_{i,\uparrow} + f^{\dagger}_{i,\downarrow} f_{i,\downarrow} + h^{\dagger}_i h_i = 1$ at every site. Therefore at each site, we have either a holon or a spinon. Using this relation, the density of holon gas is set by doping x, and the density of spinons is equal to the density of electrons $1 - x$. Spinon pairing forms Cooper pairs in the system and holon condensation provides the phase coherence for these pairs and the superfluid density of the superconducting state is controlled by the condensation fraction of holons. Therefore, to obtain superconducting phase, both holon gas and spinon gas should condense. In case of spinons, we need a pairing mechanism due to their fermionic nature. Strong antiferromagnetic interactions in cuprates can result in such a pairing potential and as a result the transition temperature of spinon paired state is controlled by the exchange energy J which is quite large. This large gap in excitation spectrum of spinons is the origin of the pseudogap phenomenon in cuprates.

On the other hand, due to the bosonic nature of holons, they do not need a pairing mechanism and they can undergo Bose Einstein condensation(BEC). Although this can be in general true, we discuss in the following sections that the phenomenology of cuprates supports the holon pair condensation scenario. This assumption immediately resolves several limitations of the Anderson theory.

In order to pair holons, like in the BCS theory, we need a pairing mechanism. In our theory, electron phonon interaction can cause such a pairing instability. As we have shown in Ref. [77], this assumption can also explain the observed phonon experiments successfully. In summary in this framework spinons form RVB pairs and holons are also paired by phonons. Both of these are required for the superconductivity in cuprates.

This approach, gives a phase diagram similar to the phase diagram of the conventional U(1) slave boson treatment of the t-J model, except that the superconducting state has Z_2 gauge symmetry, and we obtain a better estimation of T_c, closer to the experimental data(see Fig. 7-1). We have also shown in Ref. [79], that at least at half filling, the antiferromagnetic order in the Hubbard model can be achieved by including a nonzero triplet component in the pairing amplitude besides the singlet component [79]. Now let us briefly comment on the experimental consequences of our theory. In appendix, we present more details and derive equations.

7.2 Better estimation of T_c

In the underdoped cuprates, both the slave boson theory and the phase fluctuation studies of superconductors [74] predict that the transition temperature of the superconducting state is controlled by the superfluid density. Using Ioffe-Larkin recombination formula (see Appendix C for derivations and discussions), it can be shown that at small dopings, the superfluid density is mostly determined by that of holons. Therefore T_c is determined by the BEC transition temperature T_{BEC}, of holon gas. In the single holon condensation theories we obtain $T^s_{\text{BEC}} = \frac{2\pi x}{m_h^*}$. Although this gives a good doping dependence, it is an order of magnitude higher than the superconducting transition temperature [48]. In the pair condensation scenario, we obtain the following expression for T_c (see Appendix B for

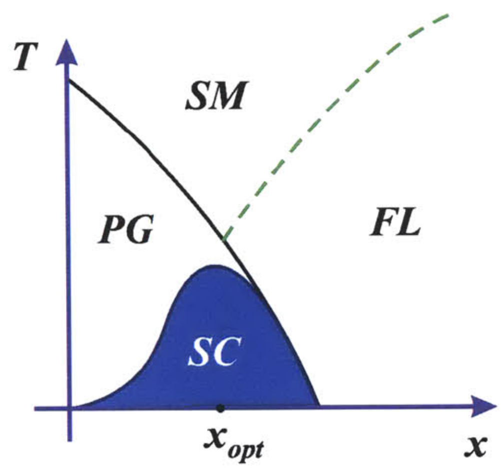

Figure 7-1: **Phase diagram.**— Schematic phase diagram of cuprates from our theory. x_{opt} is the optimal doping percentage which is typically around %15. It corresponds to the optimum transition temperature which is typically around 100 Kelvin. SC is the superconducting state in which we obtain spinon pair condensation and holon pair condensation. PG is the pseudogap phase where spinons are paired but holon gas in not condensed. FL is the Fermi liquid phase where we obtain single holon condensation but no spinon pair condensation. SM is the strange metal in which neither holons nor spinons condense. In this approach, spinons form RVB pairs due to anti-ferromagnetic interactions and holons are paired by phonons. Both of these are required to obtain the superconducting phase in cuprates. We have not shown AF order in this phase diagram, however we have shown in Ref. [79] that it can be achieved by adding a nonzero triplet component to the pairing amplitude near half filling.

derivation)

$$T^p_{\text{BEC}}\left(x,\tilde{V}\right)=\frac{T^s_{\text{BEC}}}{-\ln\left(2\tilde{V}N(0)\right)}. \tag{7.2.1}$$

where $\tilde{V}=V\Delta_s^2$, where $t\Delta_s$ is the pseudogap energy, is the renormalized coupling constant of the phonon mediated holon holon attraction, and $N(0)=\frac{m_h^*}{2\pi}$ is the density of states. In Ref. [77], we had to chose $V=12\frac{\omega_E}{t}$, where ω_E is the energy of optical phonons, to fit theory and experiment. In cuprates, $12\omega_E\sim t$ and therefore $\tilde{V}\sim\Delta_s^2\left(T_c\right)\ll 1$. Because of the extra factor in the denominator, T^p_{BEC} is much smaller than T^s_{BEC} and is closer to the experimental data.

7.3 Vortices

In the single holon condensation scenario, two kinds of vortices are allowed, $\frac{h}{2ec}$ and $\frac{h}{ec}$. Studies show that the energy of the latter is much smaller, so it should be more stable and visible in experiments. In experiments however, only $\frac{h}{2ec}$ vortices have been observed [46]. Absence of $\frac{h}{ec}$ vortices, challenges the assumption of single holon condensation in cuprates. In the holon pair condensation scenario we always obtain $\frac{h}{2ec}$ vortices from both $\langle hh\rangle$ or $\langle f_\uparrow f_\downarrow\rangle$ order parameters. This in fact reflects the Z_2 structure of our theory.

7.4 Linear T coefficient of the superfluid density

Another important limitation of the single holon condensation scenario, is the calculation of the linear temperature coefficient of the superfluid density. This scenario predicts a parabolic doping dependence behavior, while experimentally it has a weak dependence on the doping percentage [48, 86]. The reason is that within this assumption, the current carried by quasiparticles is $j=\alpha e v_F$, where v_F is the Fermi velocity of nodal quasiparticles and $\alpha\sim x$ (see Appendix D for details). Since holons are charged particles, they couple to both the external gauge field (A_{ext}), and the induced internal gauge field A_{int}. Within single holon condensation scenario and using Ioffe-Larkin formula, it can be shown that when both spinons and holons condense, we have $A_{int}\sim -xA_{ext}$. Since spinons are electrically neutral, they only couple to the internal gauge field and therefore they see $-xA_{ext}$, so their effective electric charge is $-xe$. Now we can estimate the value of α by computing the Green's function of real electrons. In the single holon condensation scenario, the diagonal part of the Green's does not respond to the gauge field, because it depends on $\langle h^\dagger \rangle \langle h \rangle$. Therefore only spinons couple to internal gauge field which is by factor of $-x$ smaller and this is why $\alpha = x$ in this case. In the pair condensation scheme, since $\langle h \rangle = 0$, the diagonal part of holons Green's function depends on $\left\langle h_j^\dagger h_i \right\rangle$. So it responds to the external as well as the internal gauge field. From convolution it can be checked that the real electrons respond to the whole external electromagnetic field and there quasiparticles have effective charge $-e$ (see Appendix D for details). So we obtain $\alpha = 1$ in this case, in consistent with the linear temperature coefficient of superfluid density measurements.

In Ref. [77], we have investigated the isotope effect on the superfluid density and the transition temperature of the superconducting phase by considering the effect of electron phonon interaction and have achieved a good agreement between theory and experiment.

It is worth mentioning that boson gas in a purely attractive potential is unstable. It collapses and phase separation happens in that case. However in our model, we deal with holons which are hardcore bosons, i.e. there is an infinite on-site repulsion between them. The phonon mediated attraction is also screened by the presence of spinons. These two can make the paired state of holons stable. We speculate that under some certain conditions, holons may become meta-stable and form stripes due to the phonon mediated attraction. Moreover as we mentioned earlier, the phase segregation saves the kinetic energy of holes and exchange energy of spinons. This can further stabilize stripe order phase. Therefore, the phonon mediated attraction between holons may enhance the stripe formation.

7.5 Conclusion

In this chapter, we have extended the Anderson theory of high Tc to take phonons into consideration. Phonons are engaged in the pairing mechanism by mediating attractive interaction between charged spinless quasiparticles (holons). This attraction destabilizes the single holon condensation state and gives rise to the paired holon state. Assuming the paired holon phase immediately resolves several limitations of the U(1) slave treatment of the Anderson theory. First of all, we achieve a better estimation of the superconducting transition temperature. Moreover, since both spinons and holons are paired, we only find $\frac{h}{2ec}$ vortices. Finally we showed that the effective electric charge of nodal quasiparticles is $-xe$ when we have single holon condensation, so they carry xev_F current, while the the effective electric charge of nodal quasiparticles is $-e$ and they carry ev_F when holons condense in pairs. We have shown that in the latter case, the linear temperature coefficient of the superfluid density is almost independent of doping, consistent with experimental observations.

APPENDICES

In the following, we provide detailed derivations of formulae in the main text concerning the expression for T_c, Ioffe-Larkin formula and Linear temperature coefficient of superfluid density. In Appendix A, we provide a brief introduction to the slave boson method. In Appendix B, we derive an expression for the transition temperature of the superconducting state. In Appendix C, we derive Ioffe Larkin formula which serves an a powerful tool in relating physical quantities to the corresponding properties of the slave particles. In Appendix D, we present an argument to calculate the linear temperature coefficient of the superfluid density.

APPENDIX A: METHOD

Let us start from the t-J model as our starting point. It is believed that this Hamiltonian captures the essential physics of the strongly correlated systems. We finally add the Holstein Hamiltonian to take the effect of electron phonon interaction into consideration. t-J model is defined as the following

$$H_{t-J} = -t \sum_{\langle i,j \rangle, \sigma} P_G c^{\dagger}_{i,\sigma} c_{j,\sigma} P_G + J \sum_{i,j} \hat{S}_i . \hat{S}_j, \tag{7.5.2}$$

where P_G is the Gutzwiller projection operator that removes doubly occupied states. Within the slave boson formalism, electrons can be decomposed as $c^{\dagger}_{i,\sigma} = f^{\dagger}_{i,\sigma} h_i$ along with the physical constraint on each site: $h^{\dagger}_i h_i + \sum_{\sigma} f^{\dagger}_{i,\sigma} f_{i,\sigma} = 1$ which implements the Gutzwiller projection. f particles are fermions and we call them spinon and h particles are bosons and we call them holon. Spinon corresponds to a state with only one electron and holon to an empty site. The definition of the projected electron operator along with the constraint, says that we have always one slave particle per site and two slave particles cannot sit on the same site. On the other hand, whenever $c^{\dagger}_{i,\sigma}$ acts on an empty site, it annihilates one holon and creates a spinon with spin σ. We cannot act further on the resulting state by $c^{\dagger}_{i,-\sigma}$, since this operator has to kill a holon, but there is no holon anymore at that site. If we act $c_{i,\sigma}$ on a site that contains a spinon with spin σ, the operators annihilates the spinon and creates a holon at that site. So by acting projected electron operator we always annihilate one type of slave particle and create another one and therefore the number of slave particles at each site is conserved. Now we can rewrite the t-J model in terms of the new slave particles. Within meanfield approximation and by using Hubbard-Stratonovic transformation, we can decouple spinons (spin sector) from holons (charge sector) and we obtain the following effective Hamiltonians for each sector

$$H_h = -\sum_{<i,j>} t\chi_s h_i^{\dagger} h_j - \sum_i \mu_h h_i^{\dagger} h_i. \tag{7.5.3}$$

$$\begin{aligned} H_s = &-\sum_{<i,j>,\sigma} t\chi_h f^{\dagger}_{i,\sigma} f_{j,\sigma} - \sum_{i,\sigma} \mu_s f^{\dagger}_{i,\sigma} f_{i,\sigma}, \\ &-\sum_{<i,j>} (J/2)\,\Delta_s(i,j)\left(f^{\dagger}_{i,\uparrow} f^{\dagger}_{j,\downarrow} - f^{\dagger}_{i,\downarrow} f^{\dagger}_{j,\uparrow}\right) + h.c., \end{aligned} \tag{7.5.4}$$

where the following notations have been used

$$\chi_h = \left\langle h^{\dagger}_{i+\vec{\delta}} h_i \right\rangle. \tag{7.5.5}$$

$$\chi_s = \left\langle \sum_{\sigma} f^{\dagger}_{i+\vec{\delta},\sigma} f_{i,\sigma} \right\rangle. \tag{7.5.6}$$

$$\Delta_s(i,j) = \frac{1}{2}\left\langle f^{\dagger}_{i,\uparrow} f^{\dagger}_{j,\downarrow} - f^{\dagger}_{i,\downarrow} f^{\dagger}_{j,\uparrow} \right\rangle. \tag{7.5.7}$$

At low temperatures, most of holons occupy the groundstate with momentum $k = 0$, therefore $\chi_h \sim x$. This model has been extensively studied in the literature and it is well known that this model leads to the d-wave pairing symmetry for spinons [46], i.e. $\Delta_s(\pm\hat{x}) = \Delta_s$ and $\Delta_s(\pm\hat{y}) = -\Delta_s$.

Now let us consider the electron-phonon interaction. Since the typical energy of electrons is around J and is much larger than ω_E, we can apply the BCS theory in our case. Within

BCS theory, electron phonon interaction, leads to the following pairing term:

$$-\sum_{k,k'} V_{k,k'} < c^{\dagger}_{k',\uparrow} c^{\dagger}_{-k',\downarrow} > c_{-k,\downarrow} c_{k,\uparrow}. \tag{7.5.8}$$

By translating the above term to the slave boson language in real space, and using the mean-field approximation, we can substitute $c_{i,\downarrow} c_{j,\uparrow} = f_{i,\downarrow} f_{j,\uparrow} h^{\dagger}_i h^{\dagger}_j$ by the following terms:

$$\Delta_h(i,j) f_{i,\downarrow} f_{j,\uparrow} + \Delta_s(i,j) h^{\dagger}_i h^{\dagger}_j - \Delta_s(i,j) \Delta_h(i,j), \tag{7.5.9}$$

where $\Delta_h(i,j) = \langle h_i h_j \rangle \sim x$ (doping). Now assuming a very short range interaction, we obtain the following effective interaction:

$$H'_{s-s} = -V\Delta_h^2 \sum_{<i,j>} \Delta_s(i,j) f^{\dagger}_{i,\uparrow} f^{\dagger}_{j,\downarrow} + h.c. \tag{7.5.10}$$

$$H'_{h-h} = -V\Delta_s^2 \sum_{<i,j>} \Delta_h(i,j) h^{\dagger}_i h^{\dagger}_j + h.c. \tag{7.5.11}$$

in which $V = \frac{\gamma_0^2}{M\omega_E^2}$ and γ_0 is the bare electron phonon interaction coupling constant, and ω_E is the energy of optical phonons. Let us assume that $V\Delta_h^2 \sim Vx^2 \ll J$, so we can neglect this phonon mediated pairing term and therefore, the d-Wave nature of the spinons does not change. From the above we see that the coupling constant of phonon mediated spinon spinon attraction is renormalized by Δ_h^2 factor and that of holons by Δ_s^2 due to strong correlation effects. It is easy to show that, $V \propto \gamma^2$, where γ is the electron phonon coupling constant. Therefore, we can interpret these renormalization factors as the renormalization of the coupling constant of spinon-phonon interaction to $\Delta_h \gamma_{k,q}$ and that of holon-phonon interaction to $\Delta_s \gamma_{k,q}$. In Appendix C, using Ioffe-Larkin recombination formula, we present another physical argument to justify this result. Now let us focus on the charge sector (holons). We have studied the effect of holon-phonon interaction on the holon mass in Ref. [77]. Since we treat charge sector as a Bose gas, we have shown the holon-phonon interaction is in the non-adiabatic limit and the small polaron picture can be applied. The mass of holons enhances by an exponential factor and we have: $m_h^*(T) = \frac{1}{2\chi_s(T)} = e^{g^2(T)} m_h$, where

$g^2(T) = \frac{V\Delta_s^2(T)}{\omega_E}$.

APPENDIX B: CALCULATION OF T_c

Taking the mentioned mass renormalization into account, the following continuum model describes the low energy physics of holons:

$$H_b = \sum_k (\epsilon_k + |\mu|)\, h_k^\dagger h_k - \tilde{V}\Delta_h \sum_k h_k^\dagger h_{-k} + h.c. \tag{7.5.12}$$

where $\epsilon_k = \frac{k^2}{2m_h^*}$, $\Delta_h = \sum_k h_k h_{-k}$, and $\tilde{V} = V\Delta_s^2$. It has been shown that in 2D, no matter how small $\tilde{V}$ is, we have a bound state of bosons and then the double condensation is energetically favorable. Using the Bogoliubov transformation, we can find the energy eigenvalue which is $E_k = \sqrt{(\epsilon_k + |\mu|)^2 - \left(\tilde{V}\Delta_h\right)^2}$ and the energy eigenvectors. On the other hand, we should choose μ such that $x = \frac{1}{N}\sum_k h_k^\dagger h_k$. The two mentioned constraints lead to the following self-consistency equations:

$$x = -\frac{1}{2} + \frac{1}{N}\sum_k \left(1 + 2n_{BE}(E_k, T)\right)\frac{\epsilon_k + |\mu|}{2E_k}. \tag{7.5.13}$$

$$\frac{2}{\tilde{V}} = \frac{1}{N}\sum_k \left(1 + 2n_{BE}(E_k, T)\right)\frac{1}{2E_k}, \tag{7.5.14}$$

in which $n_{BE}(E_k, T) = \frac{1}{\exp(E_k/T)-1}$ is the Bose Einstein distribution function. The first constraint can be solved exactly by $\frac{1}{N}\sum_k \to \frac{1}{2\pi}\int d\vec{k} = N(0)\int d\epsilon_k$, where $N(0) = \frac{2\pi}{m_h^*}$. After integration we obtain: $E_g = \sqrt{|\mu|^2 - \left(\tilde{V}\Delta_h\right)^2} = -2T\ln\left\{\frac{\sqrt{4+y^2}-y}{2}\right\}$ where $y = \exp\left(\frac{|\mu|-2T_0}{2T}\right)$ and $T_0 = \frac{2\pi x}{m_h^*}$. At $T = 0$ we always have $E_g = 0$ in consistent with Hugenholtz-Pines theorem. For small values of $\tilde{V}$, we have :

$$E_g(T) = T\exp\left(\frac{|\mu| - 2T_0}{2T}\right), \tag{7.5.15}$$

which is diminishing very rapidly and we can neglect it up to the first order approximation. Therefore, at small enough temperature energy excitations are sound-like an are of the form $E_k = ck$ where $c = \sqrt{\frac{|\mu|}{m_h^*}}$. At T_c^p, $\Delta_b = 0$ and therefore $E_k = \epsilon_k + |\mu|$ and $E_g = |\mu| =$

$T_c^p \exp\left(\frac{|\mu|-2T_0}{2T_c^p}\right) \simeq T_c^p \exp\left(-\frac{T_0}{T_c^p}\right)$. The second constraint can be written in the following way:

$$\frac{4}{N(0)\tilde{V}} = \int \frac{\coth\left(\frac{\epsilon+|\mu|}{2T_c^p}\right)}{\epsilon+|\mu|} d\epsilon. \tag{7.5.16}$$

$$\frac{4}{N(0)\tilde{V}} \simeq \int \frac{2T_c^p}{(\epsilon+|\mu|)^2} d\epsilon \simeq \frac{2T_c^p}{|\mu|} = 2\exp\left(\frac{T_0}{T_c^p}\right). \tag{7.5.17}$$

$$T_c^p = \frac{T_0}{-\ln 2N(0)\tilde{V}} = \frac{2\pi x}{-m_h^* \ln\left\{\frac{4\pi V \Delta_s^2}{m_h^*}\right\}}. \tag{7.5.18}$$

Using the paired state and assuming gapless excitations ($E_g = 0$), we can show that up to the first order, $\left\langle h_{i,t}^\dagger h_{j,0} \right\rangle = x_{pc}$, where x_{pc} is the ground-state macroscopic occupation number (condensation fraction), though $\langle h_{i,t} \rangle = 0$. If we replace every operator by minus itself the effective Hamiltonian and all order parameters remain the same, and therefore we have Z_2 gauge freedom and the low energy theory is described by a Z_2 gauge theory. As long as $T < T_c^p$, the condensation fraction is nonzero and $T = 0$, $x_{pc} = x$, where x is doping (number of holons).

APPENDIX C: IOFFE-LARKIN FORMULA

One important question that should be addressed is how to relate the physical quantities to the corresponding quantities of spinons and holons? For example, given the conductivity of spinons and holons, what is the conductivity of real electrons? To answer this question we should note two things. First of all, since at each site we should have one slave particle, therefore if one spinons hops from site i to site j, it should be accompanied by a hopping of one holons from site j to site i. So we conclude that the current carried by spinons is equal but opposite to the current carried by holons and they add up to zero. Since electron operator at site i with spin σ, is written in terms of slave particles as $c_{i,\sigma}^\dagger = f_{i,\sigma}^\dagger h_i$, it is invariant under U(1) gauge transformation, provided spinons and holons carry the same charge under this transformation. On the other hand, we assume spinons to be electrically neutral and assign $+e$ electric charge to holons (we could also assume neutral holons and assign $-e$ electric charge to spinons). By scaling the internal gauge field we can assume $e_{int} = e$. As we discussed we should satisfy the following constraint

$$\vec{J}_s + \vec{J}_h = 0. \tag{7.5.19}$$

Since only holons carry electric charge we have

$$\vec{J}_{ph} = \vec{J}_h = -\vec{J}_s. \tag{7.5.20}$$

Above two equations tells us that nonzero external gauge field (electromagnetic field) induces internal gauge field. Because we have

$$\vec{J}_s = e\sigma_s E_{int}. \tag{7.5.21}$$

$$\vec{J}_h = e\sigma_h \left(E_{ext} + E_{int}\right). \tag{7.5.22}$$

Solving Eq. 7.5

$$E_{int} = -\frac{\sigma_h}{\sigma_s + \sigma_h} E_{ext}. \tag{7.5.23}$$

and as a result $\vec{J}_{ph} = e\frac{\sigma_h \sigma_s}{\sigma_s + \sigma_h} E_{ext}$. Equivalently

$$\sigma_{ph} = \frac{\sigma_h \sigma_s}{\sigma_s + \sigma_h}. \tag{7.5.24}$$

Now let us consider two important cases. Fermi liquid phase and the Superconducting phase.

7.5.1 Fermi Liquid Phase

In the Fermi liquid (FL) phase, holons are condensed but spinons are not. So we have $\langle h \rangle \neq 0$ and $\Delta_s = 0$. Since in this case, $\sigma_h \gg \sigma_s$, we have $E_{int} \simeq -E_{ext}$, $\sigma_{ph} \simeq \sigma_s$, and $\vec{J}_{ph} \simeq e\sigma_s E_{ext}$. Now let us define the effective electric charge of spinons and holons as

$$\vec{J}_{ph} = -e_s\sigma_s E_{ext} = e_h\sigma_h E_{ext}. \tag{7.5.25}$$

Therefore in the Fermi liquid we have $e_s \simeq -e$ and therefore they have nonzero overlap with physical electrons and carry the same charge. On the other hand $e_h \simeq 0$ and we can safely assume that holons are electrically neutral in the FL phase. This can bee directly seen from $c^\dagger_{i,\sigma} \simeq \langle h \rangle f^\dagger_{i,\sigma}$. One important result of this argument is that in the absence of the pseudogap (i.e. when $\Delta_s = 0$), condensed holons do not couple to phonons, since phonons only couple to electrically charged quasiparticles. In other words, phonons create local electromagnetic field and this field induces another (internal) gauge field. Holons couple to the sum of these two fields. When $\Delta_s = 0$, but holons condense (i.e. at low enough temperatures) these two fields cancel out each other and as a result holons do not couple to phonons.

7.5.2 Superconducting Phase

In the superconducting (SC) phase , both holons and spinons are condensed. So we have $\Delta_h = \langle hh \rangle \neq 0$ and $\Delta_s \neq 0$. In this case, $\frac{\sigma_h}{\sigma_s} = \frac{\rho_{c,h}}{\rho_{c,s}}$, where $\rho_{c,h}$ and $\rho_{c,s}$ is the condensation fraction of holon and spinon gas respectively. At zero temperature all holons and spinons condense and therefore $\frac{\sigma_h}{\sigma_s} = \frac{x}{1-x}$ and we have $E_{int} \simeq -xE_{ext}$, $\sigma_{ph} \simeq x\sigma_s$, and $\vec{J}_{ph} \simeq xe\sigma_s E_{ext}$. We can compute the effective charge of spinons and holons and we obtain $e_s \simeq -xe$ and $e_h \simeq (1-x)\,e$ respectively. Therefore in the superconducting state, spinons only respond to the x fraction of the electromagnetic field. Since holons are effectively charged quasiparticles in this state, (or since the internal gauge field does not cancel out the local electromagnetic field of phonons completely) they couple to phonons. The larger pseudogap value, the stronger interaction between holons and phonons. This is an intuitive way to justify our recipe for renormalization of the electron phonon coupling constant from the brae value γ, to the effective value $\Delta_s\gamma$. Using this expression and since Δ_s decreases with doping, we can easily explain why the isotope effect is a decreasing function of doping as well. Moreover, in the overdoped region, $\Delta_s = 0$ at the transition temperature and therefore holons do not interact with phonons and as a result we do not expect isotope effect on the T_c. However at $T = 0$, $\Delta_s \neq 0$ even in the overdoped region and the mass of holons enhances in an isotope dependent way and this explains the nonvanishing isotope effect on the superfluid density and the London penetration depth in this region.

APPENDIX D: LINEAR T COEFFICIENT OF THE SUPERFLUID DENSITY

Another important limitation of the single holon condensation scenario, is the calculation of the linear temperature coefficient of the superfluid density. This scenario predicts a parabolic doping dependence behavior, while experimentally it has a weak dependence on the doping percentage [48, 86]. The reason is that within this assumption, the current carried by quasiparticles is $j = \alpha e v_F$, where v_F is the Fermi velocity of nodal quasiparticles and $\alpha \sim x$. Lee and Wen have shown that the linear temperature dependence of a d-Wave superconductor is given by the following expression

$$\frac{\rho_s(T)}{m} = \frac{x}{m} - \frac{2\ln 2}{\pi}\alpha^2 \left(\frac{v_F}{v_2}\right) T. \tag{7.5.26}$$

where v_2 is the velocity of the d-wave SC quasiparticles in the direction perpendicular to v_F. Now let us give a simple argument on how to compute α. Since holons are charged particles, they couple to both the external gauge field (A_{ext}), and the induced internal gauge field A_{int}. Within single holon condensation scenario and using Ioffe-Larkin formula, it can be shown that when both spinons and holons condense, we have $A_{int} \sim -xA_{ext}$. Since spinons are electrically neutral, they only couple to the internal gauge field and therefore they see $-xA_{ext}$, so their effective electric charge is $-xe$. Now we can estimate the value of α by computing the Green's function of real electrons. Green's function can be calculated by convoluting the Green's function of holons with that of spinons. Within the single holon condensation scenario $g_e(k + eA_{ex}/c, \omega) = x_c g_s(k + eA_{int}/c, \omega)$, where x_c is the condensation fraction of holon gas. This expression means that the physical quasiparticles only response to the induced internal field $A_{int} \sim -xA_{ext}$, and therefore their effective electric charge is $-xe$. Therefore they carry xev_F current and this leads to $\alpha = x$. On the other hand, in the double condensation scenario, as it has been discussed by Lee and Wen [48, 86], we have $g_e(k + eA_{ext}/c, \omega) = x_{pc} g_s(k + eA_{ext}/c, \omega)$. Therefore, in this case, quasiparticles see the whole external field and we obtain $\alpha = 1$ in consistent with the linear temperature coefficient of superfluid density measurements. Let us do more serious calculations now. In the pair condensed scenario, since $x_{pc}(T)$ holons per lattice site condense at the ground state with energy E_g (which we showed before is exponentially small), we can write the diagonal part of the holons Green's function as

$$ig_h(k,\omega) = x_{pc}\delta(k)\,\delta(\omega - E_g) + i\tilde{g}_h(k,\omega). \tag{7.5.27}$$

where $\tilde{g}_h$ denotes the uncondensed part of the system. The Green's function of spinons is

$$ig_s(k,\omega) = \frac{|u_k|^2}{\omega + E_{s,k} - i0^+} - \frac{|v_k|^2}{\omega - E_{s,k} - i0^+}. \tag{7.5.28}$$

$$i\Delta_s(k,\omega) = \frac{u_k v_k}{\omega + E_{s,k} - i0^+} - \frac{u_k v_k}{\omega - E_{s,k} - i0^+}. \tag{7.5.29}$$

Now let us choose the Coulomb gauge in which $A_0 = 0$ and $\nabla.\vec{A} = 0$. Since holons are charged quasiparticles, they couple to the both internal and external gauge fields. Since we have assumed pair condensation, the diagonal part of Green's function responds to the gauge fields and we have

$$ig_{A,h}(k,\omega) = g_h(k - e(A_{int} + A_{ext})/c, \omega). \tag{7.5.30}$$

In the presence of the gauge field only the diagonal part of the spinons Green's function responds to the gauge field and the off-diagonal part does not change. Since spinons are electrically neutral, they only couple to the internal gauge field

$$g_{A,s}(k,\omega) = g_s(k - eA_{int}/c, \omega) \tag{7.5.31}$$

From $c^\dagger_{i,\sigma} = f^\dagger_{i,\sigma} h_i$ it can be read that the Green's function of the real electrons is related to the Green's function of holons and spinons by convolution.

$$g_{A,e}(k,\omega) = i\int \frac{d^2Q\,d\Omega}{(2\pi)^3} g_{A,s}(k+Q, \omega+\Omega)\, g_{A,h}(Q,\Omega). \tag{7.5.32}$$

Let us separate the coherent and incoherent parts of the Green's function $g_e(k,\omega) = g_e^{coh}(k,\omega) + g_e^{inc}(k,\omega)$. For the coherent part we immediately conclude

$$g_{A,e}^{coh}(k,\omega) = g_e^{coh}(k + eA_{ext}/c, \omega), \tag{7.5.33}$$

which clearly implies that the effective charge of quasiparticles is $-e$ and therefore they carry ev_F current, not xev_F. So we conclude that in the pair condensation scenario, quasiparticles carry the whole current and therefore $\alpha = 1$ in this case.

In the single condensation scenario, the diagonal part of the holons Green's function is also $ig_h(k,\omega) = |\langle h\rangle|^2 \delta(k)\delta(\omega) + i\tilde{g}_h(k,\omega)$. However the first term does not respond to the gauge field, like the offdiagonal part of the electrons Green's function and we have $ig_{A,h}(k,\omega) = |\langle h\rangle|^2 \delta(k)\delta(\omega) + i\tilde{g}_h(k - e(A_{int} + A_{ext})/c, \omega)$. After convolution it can be verified that the coherent part of the real electrons Green's function is $g_{A,e}^{coh}(k,\omega) = g_e^{coh}(k - eA_{int}/c, \omega)$. In the previous section we showed that in the SC state and at very low temperatures, $A_{int} \simeq -xA_{ext}$, so we have $g_{A,e}^{coh}(k,\omega) = g_e^{coh}(k + xeA_{ext}/c, \omega)$. This results $\alpha = x$ and therefore quasiparticles carry only x fraction of the ev_F current. So the single holon condensation scenario gives x^2 dependence for the linear temperature dependence of the superfluid density, which is far from experimental observations.

Chapter 8

Isotope effect on T_c and the superfluid density of high-temperature superconductors

In this chapter, the oxygen isotope effect (OIE) in cuprates is studied. We introduce a simple model that can explain experiments both qualitatively and quantitatively. In this theory, isotope substitution only affects the superfluid density, but not the pseudo-gap. Within the spin-charge separation picture, we argue that the spinon-phonon interaction is in the adiabatic limit, and therefore within the Migdal-Eliashberg theory, there is no isotope effect in the spinon mass renormalization. On the other hand, we show that the holon-phonon interaction is in the non-adiabatic limit. Therefore, the small polaron picture is applicable and there is a large mass enhancement in an isotope-dependent way. Our theory explains why upon $^{16}O/^{18}O$ substitution, the superconducting transition temperature changes only in underdoped cuprates, while there is no considerable OIE at the optimal doped as well as the overdoped cuprates. Additionally, in contrast to the conventional superconductors, we obtain OIE on the superfluid density for whole superconducting region in agreement with the experimental observations.

8.1 Introduction

Finding the underlying mechanism of the high temperature superconductivity in cuprates [13] is one of the most challenging and outstanding problems in theoretical physics. Observation of strong isotope effect on both the transition temperature and the superfluid density in cuprates [91, 39, 61, 90], indicates the importance of the electron-phonon interaction in understanding the physics of high Tc [67, 12]. Experiments show strong OIE on T_c only in underdoped cuprates (see Fig. 8-1), while there is no considerable OIE in overdoped cuprates. On the other hand OIE on the London penetration depth ($\lambda_{ab}(0)$) (in-plane penetration depth) has been reported for both sides [28, 37, 73, 40]. In both cases the isotope exponent decreases as we approach the optimal doping from the underdoped side. There is also an unusual correlation between isotope effect on T_c and $\lambda_{ab}(0)$ [38](See Fig. 2). It is impossible to explain such effects using BCS theory [11] or its extensions such as Migdal-Eliashberg [54] theory. The reason is that within BCS theory which is based on the adiabatic electron-phonon approximation [39], the isotope exponent of T_c which is defined as $\alpha = -\frac{M}{T_c}\frac{\Delta T_c}{\Delta M}$, is around 1/2 [11]. On the other hand, the electron effective mass is $m^* = m(1+\lambda)$ [71], where λ is the dimensionless phonon mediated attraction coupling, and is isotope independent. Therefore, theories based on the adiabatic approximation, predict absence of the isotope effect on the superfluid density (n_s/m^*) which is inconsistent with experiments. Therefore, we have to look for other theories of superconductors. In this chapter we start from Anderson theory of high Tc [8] which is based on the strong correlation physics and the spin fluctuation pairing mechanism. This theory is very successful in explaining many aspects of cuprates but it does not take phonons into account. It is very important to explain the oxygen isotope effect within this successful theory. Here we use this general framework and then by adding electron phonon interaction, it is shown that the observed unusual isotope effects on T_c as well as $\lambda_{ab}(0)$ can be explained.

We start from t-J-Holstein model as our model Hamiltonian. In our model for simplicity, electrons are only coupled to a single Einstein phonon mode (ω_E). Then we use the spin-charge separation picture and we implement it by the slave boson method. Our idea is as follows: in underdoped cuprates, the superconducting transition temperature is controlled by the superfluid density (n_s/m^*), which is mostly determined by that of holons, in our theory. On the other hand in overdoped cuprates, T_c is controlled by the pseudo-gap

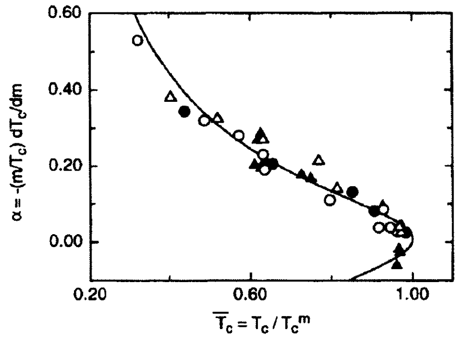

Figure 8-1: **Isotope effect on cuprates.**— Measured oxygen isotope coefficient of T_c (α) for doped YBCO as a function of the reduced transition temperature ($\bar{T}_c = T_c/T_{c,max}$) from different samples. After[3]

which is equal to pairing order parameter of spinons Δ_s in our theory. Electron-phonon interaction affects the superfluid by holon mass renormalization in an isotope-dependent way, while it does not affect the pseudo-gap much. In our theory, we argue that holons are strongly coupled to phonons and therefore, we are in the non-adiabatic limit, while spinons are weakly coupled to phonons and we should use the adiabatic limit calculation (Migdal-Eliashberg theory) for them. Therefore, $E_b \ll \omega_E \ll E_s$, where E_b and E_s are typical energies of holons and spinons respectively. It is also shown that in the presence of spinon pairing (pseudo-gap), the holon-phonon coupling constant,γ, renormalizes to $\Delta_s\gamma$. These facts together can explain the observed OIE on T_c as well as on $\lambda^{-2}(0) \propto \frac{n_s}{m_*}$.

8.2 Method

Let us start from the t-J[46, 47, 15] model which is defined as:

$$H_{t-J} = -t \sum_{\langle i,j \rangle,\sigma} P_G c^{\dagger}_{i,\sigma} c_{j,\sigma} P_G + J \sum_{i,j} \hat{S}_i . \hat{S}_j \tag{8.2.1}$$

where P_G is the Gutzwiller projection operator which removes doubly occupied states. Within the slave boson formalism, electrons can be decomposed as $c^{\dagger}_{i,\sigma} = f^{\dagger}_{i,\sigma} h_i$ along with the physical constraint on each site: $h^{\dagger}_i h_i + \sum_\sigma f^{\dagger}_{i,\sigma} f_{i,\sigma} = 1$ which implements the Gutzwiller projection. Now if we decouple spinons (spin sector) from holons (charge sector), we can write two following effective Hamiltonians for each sector:

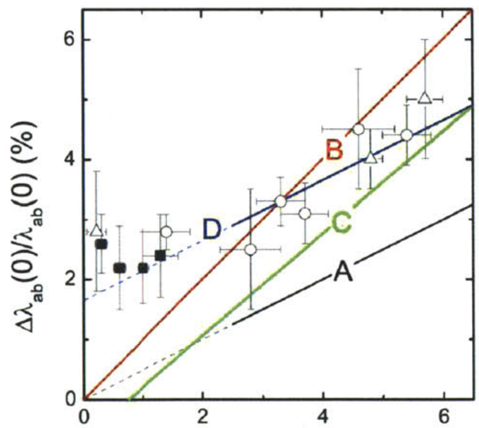

Figure 8-2: **Oxygen isotope effect on T_c vs the penetration depth.**— A color plot of the OIE shift $\Delta\lambda_{ab}(0)/\lambda_{ab}(0)$ versus the OIE shift $-\Delta T_c/T_c$ for $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$, $YBa_2Cu_4O_8$, and La_{2-x}SrxCuO$_4$. Squares are the μSR data obtained in the present study. Circles are bulk μSR data for $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ (Refs. 4 and 12) and LE μSR data for optimally doped $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ (Ref. 10). Triangles are torque magnetization and Meissner fraction data for La2-xSrxCuO4 (Refs. 6 and 9). Different lines are discussed in Ref. 13

$$H_h = -\sum_{<i,j>} t\chi_s h_i^\dagger h_j - \sum_i \mu_h h_i^\dagger h_i \tag{8.2.2}$$

$$\begin{aligned} H_s = \quad & -\sum_{<i,j>,\sigma} \left(t\chi_h + \tilde{J}\chi_s\right) f_{i,\sigma}^\dagger f_{j,\sigma} - \sum_{i,\sigma} \mu_s f_{i,\sigma}^\dagger f_{i,\sigma} \\ & -\sum_{<i,j>} 2\tilde{J}\Delta_s(i,j)\left(f_{i,\uparrow}^\dagger f_{j,\downarrow}^\dagger - f_{i,\downarrow}^\dagger f_{j,\uparrow}^\dagger\right) + h.c. \end{aligned} \tag{8.2.3}$$

where the following notations have been used:

$$\chi_h = \left\langle h_{i+\vec{\delta}}^\dagger h_i \right\rangle \simeq p \tag{8.2.4}$$

$$\chi_f = \left\langle \sum_\sigma f_{i+\vec{\delta},\sigma}^\dagger f_{i,\sigma} \right\rangle \tag{8.2.5}$$

$$\Delta_s(i,j) = \frac{1}{2}\left\langle f_{i,\uparrow}^\dagger f_{j,\downarrow}^\dagger - f_{i,\downarrow}^\dagger f_{j,\uparrow}^\dagger \right\rangle \tag{8.2.6}$$

Form the t-J model one may expect that $\tilde{J} = J/4$ but in literature it has been discussed that the best choice is $\tilde{J} = 3J/8$[46]. This model has been extensively studied in the literature and it is well known that this model leads to the d-wave pairing symmetry for spinons[46], i.e. $\Delta_s(\pm\hat{x}) = \Delta_s$ and $\Delta_s(\pm\hat{y}) = -\Delta_s$.

Now let us consider the electron-phonon interaction. Since the typical energy of electrons is around J and is much larger than ω_E, we can apply the BCS theory in our case. Within BCS theory, electron phonon interaction, leads to the following pairing term:

$$-\sum_{k,k'} V_{k,k'} < \tilde{c}^{\dagger}_{k',\uparrow}\tilde{c}^{\dagger}_{-k',\downarrow} > \tilde{c}_{-k,\downarrow}\tilde{c}_{k,\uparrow} \tag{8.2.7}$$

where $\tilde{c}_{k,\sigma}$ is the Fourier components of $P_G c_{i,\sigma} P_G = f_{i,\sigma} h_i^{\dagger}$. By translating the above term to the slave boson language in real space, and using the mean-field approximation, we can substitute $\tilde{c}_{i,\downarrow}\tilde{c}_{j,\uparrow} = f_{i,\downarrow} f_{j,\uparrow} h_i^{\dagger} h_j^{\dagger}$ by the following terms:

$$\Delta_h(i,j)\, f_{i,\downarrow} f_{j,\uparrow} + \Delta_s(i,j)\, h_i^{\dagger} h_j^{\dagger} - \Delta_s(i,j)\,\Delta_h(i,j) \tag{8.2.8}$$

where $\Delta_h(i,j) = \langle h_i h_j \rangle \sim p$ (doping). Now assuming a very short range interaction, we obtain the following effective interaction:

$$H'_{s-s} = -V\Delta_h^2 \sum_{<i,j>} \Delta_s(i,j)\, f^{\dagger}_{i,\uparrow} f^{\dagger}_{j,\downarrow} + h.c. \tag{8.2.9}$$

$$H'_{h-h} = -V\Delta_s^2 \sum_{<i,j>} \Delta_h h_i^{\dagger} h_j^{\dagger} + h.c. \tag{8.2.10}$$

Let us assume that $V\Delta_h^2 \sim Vp^2 \ll J$, so we can neglect this phonon mediated pairing term and therefore, the d-Wave nature of the spinons does not change. From the above we see that the coupling constant of phonon mediated spinon spinon attraction is renormalized by Δ_h^2 factor and that of holons by Δ_s^2 due to strong correlation effects. It is easy to show that, $V \propto \gamma^2$, where γ is the electron phonon coupling constant. Therefore, we can interpret these renormalization factors as the renormalization of the coupling constant of spinon-phonon interaction to $\Delta_h \gamma_{k,q}$ and that of holon-phonon interaction to $\Delta_s \gamma_{k,q}$. Therefore, we can substitute the electron phonon interaction term by sum the following two terms:

$$H_{s-ph} = \sum_{k,q} \frac{\Delta_h \gamma_{k,q}}{\omega_E \sqrt{2NM\omega_E}} \left(d_q + d_{-q}^\dagger\right) f_{k+q,\sigma}^\dagger f_{k,\sigma} \tag{8.2.11}$$

$$H_{h-ph} = \sum_{k,q} \frac{\Delta_s \gamma_{k,q}}{\omega_E \sqrt{2NM\omega_E}} \left(d_q + d_{-q}^\dagger\right) h_{k+q}^\dagger h_k \tag{8.2.12}$$

Now let us consider spinon-phonon interaction. The typical energy of spinons is around J. J is around 1500 Kelvin while the typical energy of optical phonons (ω_E) is a few hundred kelvin. Therefore, spinon-phonon interaction is in the adiabatic limit and therefore, we can apply Migdal-Eliashberg theory. In this regime the mass renormalizes as: $m^* = m(1+\lambda)$, where:

$$\lambda = 2 \int \frac{d\omega}{\omega} \alpha^2(\omega) F(\omega) \tag{8.2.13}$$

From our simple model it can be shown that $\lambda \propto \frac{1}{M\omega_E^2}$, and since $\omega_E \propto \frac{1}{\sqrt{M_{ion}}}$, λ is isotope independent. Therefore, oxygen isotope substitution does not enhance the effective mass of spinons. This agrees with experiment where there is no isotope effect on Fermi velocity by Laser ARPES, while there is shift in kink energy [33].

On the other hand, holons are hard-core bosons. They usually condense at the bottom of their energy band. So their effective band-width is much smaller than their actual band-width. To have a better idea, for the moment let us assume that they are fermions. In that case their Fermi energy will be around $4\chi_f tp$, where p is doping. Therefore, their effective bandwidth is at most of the order of $tp\chi_f$. Now if ω_E is larger than the typical kinetic energy of holons, the electron phonon interaction is in the non-adiabatic limit. In summary if $tp\chi_f \ll \omega_E \ll J$ then spinon-phonon interaction is in the adiabatic limit and holon-phonon interaction is in the non-adiabatic limit. For this limit it is easier to rewrite $H_h + H_{ph} + H_{h-ph}$ in the following way:

$$H = \quad -\sum_{<i,j>} t\chi_s h_i^\dagger h_j - \sum_i \mu_h h_i^\dagger h_i + \sum_q \omega_E d_q^\dagger d_q$$

$$+\frac{1}{\sqrt{2NM\omega_E}}\sum_{q,n,\sigma}\Delta_s\gamma_{n,q}h_n^\dagger h_n\left(d_{-q}^\dagger+d_q\right) \tag{8.2.14}$$

The above model has been extensively studied. In the non-adiabatic regime, we can use the results for a single polaron theory [4, 17]. Therefore, we can do the powerful Lang-Firsov transformation [29], i.e. $H \to \tilde{H} = e^{-S}He^{S}$ where: $S = \frac{1}{\omega_E \sqrt{2NM\omega_E}}\sum_{q,n}\gamma_{n,q}\Delta_s h_n^\dagger h_n\left(d_{-q}^\dagger - d_q\right)$. As an approximation let us assume that $<\gamma_{n,q}>=\gamma_0\frac{exp\left(iq.\vec{R}_n\right)}{\sqrt{N}}$. Doing Lang-Firsov transformation on h_i operators, we have: $e^{-S}h_ie^{S} = h_i\exp\left(\frac{\gamma_0\Delta_s\left(d_i^\dagger-d_i\right)}{\omega_E\sqrt{2NM\omega_E}}\right)$. If we replace the exponential factor by its average, we finally have:

$$\begin{aligned}\tilde{H} &= -\sum_{\vec{k}}\left(4t\tilde{\chi}_s\left(\cos k_x+\cos k_y\right)+\tilde{\mu}_h\right)h_k^\dagger h_k \\ &+\sum_q \omega_E\left(d_q^\dagger d_q+1/2\right) \\ &-4t\lambda_0\Delta_s^2(T)\sum_{q_1,q_2,q_3}h_{q_1}^\dagger h_{q_2}^\dagger h_{q_3}h_{-q_1-q_2-q_3}\end{aligned} \tag{8.2.15}$$

where, we have used the following notations:

$$\tilde{\chi}_s(T) = e^{-g^2(T)}\chi_s(T) \tag{8.2.16}$$

$$g^2(T) \simeq \frac{4t\gamma_0\Delta_s^2(T)}{\omega_E} \tag{8.2.17}$$

$$4t\lambda_0 = V = \frac{\gamma_0^2}{M\omega_E^2} \tag{8.2.18}$$

in which M is the ion mass. Now if we expand the energy of holons around $\vec{k}=0$ we have:

$$\epsilon_h(k) = \frac{k^2}{2m_h^*}-\mu_h^* \tag{8.2.19}$$

$$m_h^*(T) = \frac{1}{2\tilde{\chi}_s(T)} = e^{g^2(T)}m_h \tag{8.2.20}$$

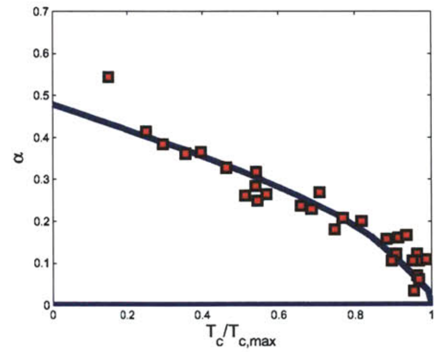

Figure 8-3: **Theoretical isotope effect on T_c vs experiment.**— The oxygen isotope effect on T_c (α) vs. $T_c/T_{c,max}$. Red square are the data extracted from Fig. 1 and the blue line is our theoretical calculation

Oxygen isotope effect on T_c

The oxygen isotope effect on T_c is determined by the α isotope exponent which is defined as:

$$\alpha = -\frac{M_O}{T_c}\frac{dT_c}{dM_O} = \frac{1}{2}\frac{\omega_E}{T_c}\frac{dT_c}{d\omega_E} \tag{8.2.21}$$

In the underdoped region, T_c is determined by the Bose-Einstein condensation (BEC) transition temperature of holons. If treat holons as a free 2D Bose gas, then the BEC transition temperature is:

$$T_c = T_{BEC} = \frac{2\pi tp}{m_h^*(T_c)} \tag{8.2.22}$$

Therefore, we have:

$$\alpha = -\frac{1}{2}\frac{\omega_E}{m_h^*(T_c)}\frac{dm_h^*(T_c)}{d\omega_E} \tag{8.2.23}$$

Since $m_h^* = e^{g_O^2} m_h$ and $g_O^2 \propto \frac{1}{\omega_E}$ we have:

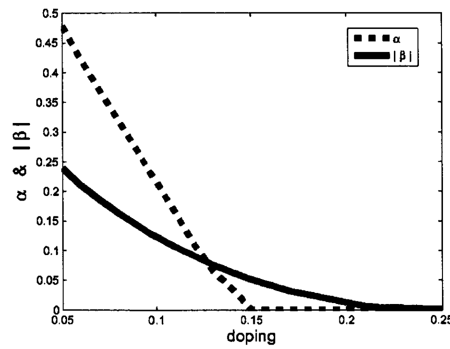

Figure 8-4: **Isotope effect on T_c and the penetration depth.**— The OIE on T_c, α (dashed blue line) and the OIE on the London penetration depth, $|\beta|$ (black line) versus doping.

$$\alpha = \frac{1}{2} g_O^2 \left(T_c\right) \tag{8.2.24}$$

From the definition of g^2, we have:

$$\alpha = \frac{2t\lambda_0 \Delta_s^2 \left(T_c\right)}{\omega_{O,E}} \tag{8.2.25}$$

Since $\Delta_s \left(T_c\right)$ is a decreasing function of doping and at the optimal doping it becomes very small, isotope exponent dies off as we approach the optimal doping and it finally becomes negligible. On the overdoped cuprates however, pseudo-gap controls T_c and as we discussed before, if $Vp^2 = 4t\lambda_0 p^2 \ll J$, electron phonon interaction does not affect pseudo-gap much and therefore, we do not expect isotope effect in overdoped side of the superconducting phase diagram. In our numerical calculation we have studied the phase diagram of the t-J for $J = t/3$. We have also chosen $\lambda_0 = 3\omega_E/t$ ratio. We obtain a very good fitting between our theoretical calculations and the experimental data (see Fig. 8-3).

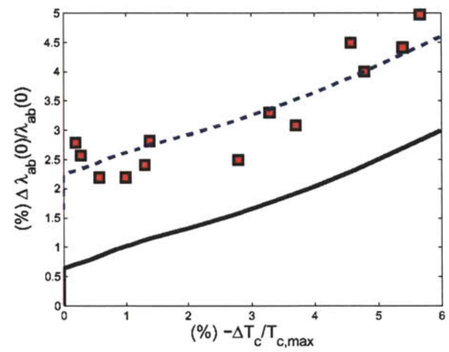

Figure 8-5: **Isotope effect: theory vs experiment.**— The OIE shift $\frac{\Delta\lambda_{ab}(0)}{\lambda_{ab}(0)}$ versus the OIE $-\frac{\Delta T_c}{T_c}$ (percent). Red squares are extracted data from Fig. 2. The black line is our theoretical calculation and the dashed blue line is the shifted black line. OIE on the thickness of the superconducting sheet can cause this shifting.

Oxygen isotope effect on the London penetration depth

The oxygen isotope effect on the superfluid density or equivalently on the London penetration depth, is defined as:

$$\beta = -\frac{M_O}{\lambda_{ab}}\frac{d\lambda_{ab}}{dM_O} = -\frac{1}{4}\frac{\omega_E}{\lambda_{ab}^{-2}}\frac{d\lambda_{ab}^{-2}}{d\omega_E} \tag{8.2.26}$$

According to the Ioffe-Larkin formula [32] the physical superfluid density is related to the superfluid density of spinons and holons in the following way:

$$\rho_{ph}^{-1} = \rho_h^{-1} + \rho_s^{-1} \tag{8.2.27}$$

Since condensation fraction of holons and spinons at zero temperature are p and $1-p$ respectively, and from $\rho = \frac{n_c}{m^*}$ we have:

$$\rho_{ph}^{-1}(0) = \frac{m_h^*}{p} + \frac{m_s^*}{1-p} \tag{8.2.28}$$

For small values of p, we have $\rho_{ph}(0) \simeq \frac{p}{m_h^*}$. On the other hand $\lambda_{ab}^{-2}(0) = \frac{4\pi e^2}{c^2}\rho_{ph}$. Therefore, we have:

$$\beta = \frac{1}{4}\frac{\omega_E}{m_h^*}\frac{dm_h^*}{d\omega_E} = -\frac{g^2(0)}{4} \tag{8.2.29}$$

Therefore, we have:

$$\beta(T=0) = -\frac{t\lambda_0\Delta_s^2(0)}{\omega_{O,E}} \tag{8.2.30}$$

For the whole superconducting region, $\Delta_s(T=0) > 0$, therefore, $|\beta|$ is always nonzero though it is a decreasing function of the doping. Despite the fact that both α and β depend on Δ_s^2 and we may expect $|\beta| = 0.5\alpha$, but we should note that they depend on Δ_s at two different temperatures (see Fig. 8-4 and 8-5). From Eqs. (26) and (31), we have: $|\beta|/\alpha = 0.5\left(\frac{\Delta_s(0)}{\Delta_s(T_c)}\right)^2 \geq 0.5$.

8.3 Discussion

Our theoretical curve for $\frac{\Delta\lambda_{ab}(0)}{\lambda_{ab}(0)}$ versus $-\frac{\Delta T_c}{T_c}$ has two important features. Firstly it has a nonzero inception since at the optimal doping, T_c does not change upon isotope substitution, but $\lambda_{ab}(0)$ does. Secondly it has the same slope(0.42) as the empirical data but our curve is shifted down by a constant amount (see Fig. 5). In literature the cause of this shift has been discussed [38]. One possible scenario is the change in the thickness of the superconducting sheet d_s, due to $^{16}O/^{18}O$ substitution. Note that the 2D density of holons is related to the 3D one by: $n_{2D} = n_{3D}d_s$. Thus $\lambda_{ab}^{-2} \propto \frac{n_{3D}d_s}{m_h^*}$ and finally we have: $\frac{\Delta\lambda_{ab}(0)}{\lambda_{ab}(0)} = 0.5\left(\frac{\Delta m_h^*}{m_h^*} - \frac{\Delta d_s}{d_s}\right)$. If we assume $0.5\frac{\Delta d_s}{d_s} = -1.6$ then our theoretical curve fits the experimental data very well. So our theory predicts OIE shift of the lattice spacing in the z direction.

We have studied the oxygen isotope effect in cuprates. We have shown that within the spin-charge separation formalism, the unusual isotope effect on T_c as well as the superfluid density can be explained by t-J-Holstein model. It is shown that $^{16}O/^{18}O$ substitution only affects the superfluid density and it does not affect the value of the pseudo-gap energy.

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