Numerical Studies of finite temperature properties of the t-J model

BY

SIU-KEUNG CHAN

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Dedication

This thesis is dedicated to my parents. Their encouragement and support are necessary for the completion of this thesis.
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Abstract

Using the technique of exact diagonalization, the whole spectrum of the Hamiltonian of the t – J model with one hole in clusters of 8 and 16 sites were obtained. Using group theory, translational and reflection symmetries in real space as well as spin inversion symmetry in spin space could be applied to reduce our matrix size. The static magnetic susceptibility, the dynamic spin-spin correlation and the spin-charge correlation of the above systems as a function of temperature were reported. A comparison between the result obtained by finite temperature Lanczos diagonalization (FTLD) and ours was made.
Chapter 1

Introduction

The \( t - J \) model is a quantum spin model proposed to describe the behavior of electronic spins in the CuO\(_2\) planes of high temperature superconductors. From the measurement of thermodynamical properties of high temperature superconductors, people generally believe that electronic spins on the CuO\(_2\) plane play a crucial role in the mechanism of superconductivity.

In this chapter, the historical background, structure and phase diagram of cuprates, and recent research are briefly reviewed. First, the development of superconductivity (SC) is briefly introduced. Then, the structures and electronic phase diagrams of two cuprate compounds, namely LSCO and YBCO, are described in more detail. Finally, some recent numerical studies on the \( t - J \) model are presented in order to make comparison with ours.

1.1 Historical Background

The story of SC began with the success in liquefying helium at 4K by Heike Kammerlingh Onnes in 1908. This brought scientists to explore nature in a low temperature regime. Three years later, Onnes was interested in the resistivity of pure metal mercury at low temperature. To his surprise, the resistance of mercury at about 4K dropped to almost zero and superconductivity was first discovered in 1911 [1].

In 1933, Walther Meissner and R. Ohsenfeld investigated the magnetic properties of a superconductor. They observed that the superconductor try to prevent external magnetic flux from penetrating into its interior. Magnetic induction inside the superconductor vanished, \( B_{int}=0 \) in contrast to a perfect conductor, \( \dot{B}_{int}=0 \). This phenomenon is known as the Meissner effect [2].
In 1935, F. London and H. London introduced the London Theory by modifying the Maxwell equations to account for the zero resistance and the Meissner effect in a superconductor [3]. This was the first attempt to explain superconductivity theoretically in a classical way by introducing a two-fluid concept. It assumes that in the superconducting phase, the current density are contributed by two kinds of electrons, namely normal electrons and superconducting electrons, $\vec{J} = \vec{J}_n + \vec{J}_s$. The former one obeys the Ohm’s law, $\vec{J}_n = \sigma \vec{E}$, where $\sigma$ is the conductivity and $\vec{E}$ is the electric field. The latter obeys the London’s equation, $\vec{J}_s = -\frac{1}{\mu \lambda_L} \vec{A}$, where $\lambda_L$ is a constant having the dimension of length and $\vec{A}$ is the vector potential [4].

In the 1950’s, researchers began to carry out experiments on different isotopes of a superconductor and noticed that the critical temperature was affected by the presence of isotopes. This led scientists to focus on electron-phonon interaction. At the same time, researchers performed a systematic search on superconductors among elements and binary alloys.

In 1950, Ginzberg and Landau introduced another remarkable theory, the Ginzberg-Landau theory. This was the first attempt to explain SC in a quantum mechanical way by introducing macroscopic wave function (or order parameter) to describe the behavior of superconducting electrons. The theory is based on the two fluid model. The electron density $\rho$ is composed of the normal and the superconducting electron densities, $\rho = \rho_n + \rho_s$. Then the current density is written as $\vec{J} = \rho_n \vec{v}_n + \rho_s \vec{v}_s$ where $\vec{v}_n$ and $\vec{v}_s$ are the velocities of the normal and superconducting electrons respectively. The normal component of current density $\rho_n \vec{v}_n$ results from a non-equilibrium distribution of quasi-particle excitations. The order parameter is introduced $\psi(\vec{r}) = |\psi| e^{i\chi(\vec{r})}$ with an amplitude $|\psi|$ and a phase $\chi(\vec{r})$. The superconducting electron density is proportional to $|\psi|^2$. And its velocity is given by $m^* \vec{v}_s = \vec{p}_s - (e^*/c) \vec{A}(\vec{r})$ where $\vec{p}_s = \hbar \nabla \chi(\vec{r})$. $m^*$ and $e^*$ are the effective mass and the effective charge of the quasi-particle respectively [5].

In 1957, Abrikosov worked out a particular solution from the Ginzberg-Landau theory that there exist certain kind of superconducting materials which allow
gradually decreasing penetration of an external magnetic flux. This kind of material is called Type II superconductors in contrast to the traditional Type I superconductors which spontaneously repel external magnetic flux below their critical temperatures.

In 1957, three genius named John Bardeen, Leon Cooper and Robert Schrieffer proposed a quantum mechanical microscopic theory to explain superconductivity [6]. Cooper proposed the existence of Cooper pairs, which are formed by two coupled electrons with opposite spins and momenta. If there exists an attractive potential between these two electrons, then they are energetically stable to form a bounded state above the Fermi surface [7]. Later, they found that the attractive potential is due to the virtual exchange of phonons. At the transition from normal to superconducting phase, the conduction band opens up an energy gap near the Fermi level. The superconducting ground state $\Psi_{sc}$ is below the energy gap. It is written as $\Psi_{sc} = \prod_{k}(u_{k} + v_{k}e^{i\chi_{k}}c^{+}_{k_{1}}c^{+}_{k_{2}})\mid 0 \rangle$ where $c^{+}$ is a creation operator. $\vec{k}$ is the wavevector and $\uparrow, \downarrow$ stand for spin-up and spin-down states respectively. The product $c^{+}_{k_{1}}c^{+}_{k_{2}}$ is to create a Cooper pair. $u_{k}$ is the amplitude of unoccupied states and $v_{k}$ is the amplitude of Cooper pairing states. They have a relationship, $|u_{k}|^2 + |v_{k}|^2 = 1$. $\chi_{k}$ is a phase. Note that if $\{\chi_{k}\}$ are all the same, the resulting wavefunction is the same as the Ginzburg-Landau's one. Cooper pairs behave like bosons and can condense to a low energy state without obeying the Pauli exclusion principle. The collective motion of Cooper pairs is like the superfluid in He$^3$ and the current continues to flow without any resistance. This results in superconductivity.

In 1960, Giaever discovered superconducting tunneling. In the next year, Kunzler realized that there are critical field and critical current density for the superconducting phase. In 1962, Josephson found that not a single electron having tunneling effect, but a pair of electrons. This is termed the Josephson effect, which can also be explained by the BCS theory. The story seems to come to an end and scientists didn’t expect a superconductor with a critical temperature higher than 30K [8].

However, in 1986 IBM scientists Geory Bednorz and Alex Müller carried out a
resistance measurement on a ceramic material containing La at low temperature. To their surprise, the ceramic material became superconducting at 34K [9, 10]. In 1987, P. Chu et al found another ceramic material YBCO which possesses a critical temperature at around 93K [11]. These discoveries opened a new chapter in condensed matter physics called High Temperature Superconductivity (HTSC). And scientists realized their insufficient knowledge in condensed matter physics.

In the past two decades, physicists around the world put much of their effort in understanding the mechanism of metal-insulator transition (MIT) of these new materials, i.e. the change of the electrical conductivity from metal to insulator as a function of external parameters, such as composition, pressure, strain or magnetic field [4]. In 1988, P.W. Anderson brilliantly pointed out that the new type of superconductivity is strongly related to the magnetism of the materials. And most research teams are working on the electron-magnon interaction rather than the traditional electron-phonon interaction as in the BCS theory. The HTSC is still a hit and challenging topic and plenty of papers were published on this subject. Some of its theoretical development will be discussed in the following sections.

1.2 Properties of Cuprate Superconductors

1.2.1 Structures

LSCO

Among all HTSC materials, La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) is the first discovered by Bednorz and Müller and it has a critical temperature of 34K. Electronic configurations of the lanthanum, strontium, copper and oxygen atoms are La:[Xe](5d)(6s)$^2$; Sr:[Kr](5s)$^2$; Cu:[Ar](3d)$^{10}$(4s)$^1$ and O:[He](2s)$^2$(2p)$^4$ respectively.

The crystal structure of LSCO is shown in Fig.1.1. It possesses a stacked structure of A-B-C layers. The upper layer is a copper oxide plane. In this plane, the Cu atoms form a square lattice, and each O atom is placed in the middle of two Cu atoms on every edge of the square lattice. The coordination number of a
Figure 1.1: Crystal structure of $\text{La}_{2-x}\text{Sr}_x\text{Cu}_3\text{O}_4$ (T phase) [12].

Cu atom is 4 and that of an O atom is two. Since the O atoms are not exactly lying in the same plane, each oxygen atom is predicted to be $sp^3$ hybridized. In order to have 4 bonding orbitals, each Cu atom has to excite two 3$d$ electrons to the 4$p$ empty orbitals and hybridized as $dsp^2$. This leaves an unpaired electron in 3$d$ orbital of each Cu atom. The second and the third layers are the lanthanum oxide layers having different orientations (Fig.1.1). These 3 layers continue to repeat themselves along the vertical axis to form a crystal. This kind of material is called perovskites.

On doping, divalent strontium atoms replace some trivalent lanthanum atoms. The difference in their valence attracts some unpaired electrons on the cuprate plane and leaves holes there. The distance between two successive layers is about 6Å (0.6nm) and the bond length of the Cu-O in the cuprate plane is about 1.9Å[16]. It is worth mentioning these in order to study the long-range magnetic order in this material.

**YBCO**

It is remarkable that $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (YBCO) has a critical temperature around 90K. Liquid nitrogen can be used as coolant to cool it below its critical temperature. This is much cheaper than using liquid helium as in conventional SC.

It also possesses a bit complicated structure compared with LSCO. The elec-
Figure 1.2: Crystal structure of YBCO (T phase) [13].
tronic configurations of yttrium, barium, copper and oxygen atoms are Y: [Kr](4d)(5s)²; Ba:[Xe](6s)²; Cu:[Ar](3d)¹⁰(4s)¹ and O:[He](2s)²(2p)⁴ respectively. As shown in Fig.1.2, two successive cuprate layers sandwiches two layers of barium oxide planes and there is a layer of copper oxide chains in the middle of the two barium oxide planes. The unit can be divided into conduction layers and charge reservoir layers. In between the conduction layers, there are some barium ions (Ba²⁺) to glue the layers. Therefore, the crystal is quite brittle.

Similar to LSCO, it is worth mentioning the dimension of the crystal structure in order to study its long-range antiferromagnetic (AF) order. The distance between two successive conduction cuprate layers is 3.2Å and the distance between those two sandwiching barium oxide planes and cuprate chains is approximately 8.2Å[16].

1.2.2 Phase diagrams

One common feature of HTSC materials is that they share a similar phase diagram. This diagram shows the phases at different temperature and doping level. On its left bottom corner(Fig.1.3-4), there is an antiferromagnetic (AF) phase bounded by the Neel temperature boundary. Doping introduces mobile holes to the cuprate plane and the long-range order of the AF phase is destroyed.

Upon doping, a HTSC material transits from an AF phase to a superconducting (SC) phase across a pseudogap phase at zero temperature. In the pseudogap region, the material possesses short-range AF order. But this order is completely destroyed in the SC phase. This is the reason why most theorists study HTSC in the direction of its magnetism. Note that there is an optimal doping level where the material has the highest critical temperature.

It is worth mentioning that HTSC materials are all Type II superconductors. They allow external magnetic flux to penetrate their interior a bit in the SC phase (Meissner effect). Fig.1.3 and Fig.1.4 show the phase diagrams of LSCO and YBCO respectively.
Figure 1.3: Phase diagram of La$_{2-x}$Sr$_x$CuO$_4$ [14].
Figure 1.4: Phase diagram of YBCO [15].
1.3 Present work

Due to the complexity of quantum many-body systems, there exists no exact analytic method to resolve the problems. Very often researchers have to resort to numerical methods.

At absolute zero, all physical system is in its ground state. However, the system may be in any excited state at finite temperature. Note that all experiments are carried out at finite temperature. In order to compare with experimental results, theoreticians should calculate finite temperature properties.

Jaklic and Prelovšik formulated their finite temperature Lanczos diagonalization (FTLD) in 1994 [18]. It is based on the Lanczos diagonalization plus random sampling. Although it is less demanding on computer resources, there is a loss of information induced by random sampling. Moreover it is uncontrollable. The more the iterations in Lanczos diagonalization, the more accurate the estimation of eigenvector. But this also forces the estimated eigenvector to approach the ground state. If a limitation is imposed to the number of iterations, the estimation of the eigenvector is inaccurate.

In this project, we use a brute force method to calculate some finite temperature properties of the $t - J$ model. Beside finite-size effect, all numerical results obtained are exact and no approximation is made in our calculation. Then our result is used to compare with other parties'.

In Chapter 2, two models for describing the HTSC materials are described. And in Chapter 3, the implementation of exact diagonalization is given. Some theoretical works on the magnetic susceptibility, dynamic structure factor and charge density correlation function are given in Chapter 4. Numerical results of the above quantities are discussed in Chapter 5 and the conclusions are given in Chapter 6.
Chapter 2

Spin Model

In this chapter, we discuss two microscopic Hamiltonians which are commonly used to describe the physics of HTSC materials. They are the Hubbard model and the $t - J$ model. The Hubbard model is formulated from the linear combination atomic orbital (LCAO) theory and the $t - J$ model is formulated as some holes moving in an AF spin background.

2.1 Hubbard model

It is generally believed that the occurrence of SC is strongly related to the cuprate plane. Thermodynamic properties of HTSC possess the characteristics of a two-dimension (2-D) system. It is remarkable that it brings physicists to study condensed matter physics in a lower dimension. Another observation is that the higher the density of cuprate planes in a unit cell, the higher the critical temperature. Some parts of the sample are acting as charge reservoirs, which are either adding or removing charge carriers to or from the planes [16].

![Diagram](image)

Figure 2.1: Interactions on a cuprate plane. $\epsilon_d$ and $\epsilon_p$ are the on-site energy contribution; $t^d_{ij}$ and $t^p_{ij}$, are the hopping integrals; $U_d$, $U_p$, and $U_{pd}$ are the on-site repulsions of $d$ orbital, $p$ orbital and $pd$ bonding orbital.
Based on the structures of HTSC materials, people began to develop some effective models based on the bondings of the 2-D copper oxide plane. From the first principle, a 3-bands Hubbard model was proposed from the LCAO theory and its parameters were obtained by band structure calculation [17]. The Hamiltonian is as follow:

\[
H_{\text{Hubbard}} = H_{3\text{band}}^0 + H_U,
\]

\[
H_{3\text{band}}^0 = \epsilon_d \sum_{i,\sigma} d_{i,\sigma}^\dagger d_{i,\sigma} + \epsilon_p \sum_{i,\sigma} p_{i,\sigma}^\dagger p_{i,\sigma}
+ \sum_{<i,j>\sigma} t^{ij}_{pd}(d_{i,\sigma}^\dagger p_{j,\sigma} + h.c.) + \sum_{<i,j>\sigma} t^i_{pp}(p_{i,\sigma}^\dagger p_{j,\sigma} + h.c.),
\]

\[
H_U = U_d \sum_i n_{i,\downarrow}^d n_{i,\uparrow}^d + U_p \sum_i n_{i,\downarrow}^p n_{i,\uparrow}^p + U_{pd} \sum_i n_{i,\downarrow}^p n_{i,\uparrow}^d,
\]  \hspace{1cm} (2.1)

where \(H_{3\text{band}}^0\) relates to hole interactions and \(H_U\) is a Coulomb repulsion term. The parameters, \(\epsilon_d, \epsilon_p, t^{ij}_{pd}, t^i_{pp}, U_d, U_p\) and \(U_{pd}\) are energy contributions due to different origins (Fig.2.1).

For the \(H_{3\text{band}}^0\) term, \(d_{i,\sigma}^\dagger\) and \(d_{i,\sigma}\) are creation and annihilation operators of a spin \(\sigma\) in the \(d\) orbital of the Cu atom at the \(i^{th}\) site. Similarly, \(p_{i,\sigma}^\dagger\) and \(p_{i,\sigma}\) are creation and annihilation operators of a spin \(\sigma\) in the \(p\) orbital of the O atom at the \(i^{th}\) site. This means that the parameters \(\epsilon_d\) and \(\epsilon_p\) are the on-site energy contributions. The product of operators, \(d_{i,\sigma}^\dagger p_{j,\sigma}\), is to allow a spin \(\sigma\) originally in the \(p\) orbital of the O atom at the \(j^{th}\) site to hop to the \(d\) orbital of the Cu atom at the \(i^{th}\) site; Likewise, the product of operators, \(p_{i,\sigma}^\dagger p_{j,\sigma}\), is to allow a spin \(\sigma\) originally in the \(p\) orbital of the O atom at the \(j^{th}\) site to hop to the \(p\) orbital of the O atom at the \(i^{th}\) site. Their Hermitian conjugates are the inverse operator of the corresponding hopping process. The summation, \(<i,j>,\), runs through all pairs of the nearest neighbors. It is obvious that the parameters \(t^{ij}_{pd}\) and \(t^i_{pp}\) are hopping integrals of the corresponding hopping respectively.

In the Coulomb repulsion term, \(H_U, n_{i,\uparrow}^d,\) and \(n_{i,\downarrow}^d\) are number operators of a up spin, \(\uparrow\), and of a down spin, \(\downarrow\), respectively in the \(d\) orbital of the Cu atom at the \(i^{th}\) site and the product of these operators, \(n_{i,\uparrow}^d n_{i,\downarrow}^d\), is to check double occupancy of the \(d\) orbital of the Cu atom at the \(i^{th}\) site. A similar interpretation applies
to the remaining parts of the Hamiltonian. But it is worth mentioning that the product $n_{i,i}^{p}n_{i,i}^{d}$, is to check double occupancy in the bonding orbital of a Cu-O bond. The parameters $U_d$, $U_p$, and $U_{pd}$ are the on-site repulsions of the $d$, $p$ and $pd$ bonding orbitals in the cuprate plane.

However, the 3-bands Hubbard model can be further reduced to be a 1-band Hubbard model by considering a square lattice of Cu atoms only. It is expressed as follow:

$$H_{Hubbard} = H_t + H_U,$$

$$H_t = -t \sum_{<i,j>\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{i\sigma} c_{j\sigma}^\dagger),$$

$$H_U = U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \quad \text{(2.2)}$$

where $H_t$ is the hole hopping term and $H_U$ is the Coulomb repulsion term. The parameter, $t$, is called the hopping integral. The operator, $c_{i\sigma}^\dagger$, is a creation operator of a spin, $\sigma$, at the $i^{th}$ site and $c_{i\sigma}$ is an annihilation operator of that spin at the $j^{th}$ site. The product of these 2 operators, $c_{i\sigma}^\dagger c_{j\sigma}$, allows a spin, $\sigma$, originally at the $j^{th}$ site to hop to the $i^{th}$ site. And its Hermitian conjugate, $c_{i\sigma} c_{j\sigma}^\dagger$, is an inverse operator of the above hopping process. The summation $<i,j>$ runs through all pairs of nearest neighbors.

In the Coulomb repulsion term, $H_U$, $n_{i,\uparrow}$ and $n_{i,\downarrow}$ are number operators of an up spin, $\uparrow$, and of a down spin, $\downarrow$, respectively at the $i^{th}$ site and the product of these operators, $n_{i,\uparrow} n_{i,\downarrow}$, is to check double occupancy of the $i^{th}$ site. The parameter $U$ is the on-site repulsion between two opposite spins at the same lattice point of the cuprate plane.

2.2 $t-J$ model

In 1988, Zhang and Rice proposed an effective Hamiltonian [26]. Their idea is that the hybridization on each square of O atoms strongly binds a hole to the central Cu$^{2+}$ to form a local singlet in the limit of strong Coulomb repulsion, $U >> t$. This Zhang-Rice singlet can be regarded as a hole hopping in an AF
background. The model is later called the \( t - J \) model. It models the physics of the cuprate plane under the condition of no double occupancy. Due to the infinitely strong on-site repulsion energy, \( U \) [25], it is energetically unfavorable for two spin-1/2 particles to occupy the same site.

The Hamiltonian of the \( t - J \) model is as follow:

\[
H_{t-J} = H_t + H_J,
\]

\[
H_t = -t \sum_{<i,j>} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \tilde{c}_{i\sigma} \tilde{c}_{j\sigma}^\dagger),
\]

\[
H_J = J \sum_{<i,j>} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_in_j),
\]

(2.3)

where \( H_t \) refers to a hole hopping term and \( H_J \) is a spin coupling term.

The parameter \( t \) is called the hopping integral and \( J \) is called the spin exchange integral. The operator \( \tilde{c}_{i\sigma}^\dagger \) is a creation operator of the spin, \( \sigma \), at the \( i^{th} \) site and \( \tilde{c}_{j\sigma} \) is an annihilation operator of the spin at the \( j^{th} \) site. The product of these operators, \( \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} \), is to allow the spin, \( \sigma \), originally at the \( j^{th} \) site to hop to the \( i^{th} \) site. And its Hermitian conjugate, \( \tilde{c}_{j\sigma} \tilde{c}_{i\sigma}^\dagger \), is the inverse operator of the hopping process. The summation, \( < i, j > \), runs through all the nearest neighbor pairs. It is worth mentioning that \( \tilde{c}_{i\sigma}^\dagger = c_{i\sigma}^\dagger (1 - n_{i,-\sigma}) \) where \( n_{i,-\sigma} \) is the number operator of an opposite spin, \(-\sigma\), at the \( i^{th} \) site. The projection operator \((1 - n_{i,-\sigma})\) imposes the constrain of no double occupancy to the model.

A positive value of \( J \) indicates that the spins prefers to anti-align. The operator, \( \vec{S}_i \), is a spin operator at the \( i^{th} \) site and the dot product, \( \vec{S}_i \cdot \vec{S}_j \), is a spin-coupling term between the spin at the \( i^{th} \) site and the spin at the \( j^{th} \) site. The summation \( < i, j > \) runs through all the nearest neighbor pairs. The operator, \( n_i \), is the number operator at the \( i^{th} \) site.

At half filling, every Cu atom has a spin and there is no hole in the plane. The hole hopping term can be dropped and the \( t - J \) model is reduced to the Heisenberg model plus a constant, \( H_{t-J} \rightarrow H_{\text{Heisenberg}} + \text{constant} \). The transport of charge is prevented by an energy gap of the order of Coulomb repulsion, \( U \).

This is a Mott-insulator, which is the undoped parent compound of all cuprate
superconductors.

However, noted that the superconductivity (SC) is in a lower energy regime and therefore most of theoretical studies published were using the ground state and some low-lying states for their calculation by reasonable approximation methods. In this project, our calculation was done by an exact diagonalization of the $t - J$ model on 2 clusters of different sizes.

2.3 Square lattices with periodic boundary conditions

The $t - J$ model describes the physics on the cuprate plane. However, ED is possible on small finite-size clusters only. It is because the computer resource is exhausted dramatically with a larger cluster. Several geometries have been investigated before [16]. Two clusters, which are employed in our calculation, are introduced in the following.

2.3.1 Square lattice with 8 sites

The square lattice with 8 sites is a square tilted at $45^\circ$. The real lattice (Fig.2.2a) and the reciprocal lattice (Fig.2.2b) are shown in Fig.2.2. Note that periodic

![Figure 2.2: Geometry of a square lattice with 8 sites: (a) the real lattice and (b) the reciprocal lattice.](image-url)
boundary conditions are applied so that those sites along the edges of the square are equivalent to their counterparts on the opposite edges. In the real lattice, there are 8 lattice points inside the cluster implying there are 8 translational symmetry operations and also there are 8 crystal momentum $\vec{k}$ inside the first Brillouin zone.

### 2.3.2 Square lattice with 16 sites

The real lattice (Fig.2.3a) and the reciprocal lattice (Fig.2.3b) of the square lattice with 16 sites are shown in Fig.2.3. Note that periodic boundary conditions are applied so that those sites along the edges of the square are equivalent to their counterparts on the opposite edges. In the real lattice, there are 16 lattice points inside the cluster implying there are 16 translation symmetry operations and also there are 16 crystal momentum $\vec{k}$ inside the first Brillouin zone.

![Figure 2.3: Geometry of a square lattice of 16 sites: (a) the real lattice and (b) the reciprocal lattice.](image)
Chapter 3

Methodology

In this chapter, exact diagonalization, group theory and programming technique employed in our project are discussed. Exact diagonalization is one of the numerical methods in solving the $t-J$ model. It returns the eigenenergy spectrum as well as their corresponding eigenvectors. However, this method requires a large amount of computer resources. So group theory of symmetry is used to divide and conquer a huge Hilbert space into several smaller subspaces which are diagonalized independently.

3.1 Exact Diagonalization

There are two major numerical methods in solving quantum many body systems. One is the quantum Monte Carlo method (QMC) and the other is exact diagonalization (ED). QMC is plagued by a negative sign effect, which arises from the antisymmetry of wave functions. However, ED has a disadvantage that it requires a large amount of memory to store a huge Hamiltonian matrix. So its calculation is limited to small finite-size clusters.

In 1994, J. Jaklic and P. Prelovsek introduced the finite temperature Lanczos diagonalization (FTLD) [18]. This method combines Lanczos diagonalization technique and random sampling to evaluate some thermodynamical properties and dynamical quantities of quantum many body systems. This can relieve the demand on computer resources. In contrast to ED, it is an approximation method to evaluate finite temperature quantities. Therefore, the ED is employed in our project.

In the process of finding the eigenvalues, $\lambda_i$, and their eigenvectors, $\tilde{\lambda}_i$, the basis vectors are transformed into another orthonormal basis set, i.e. $A = V^{-1}DV$
by a similarity transformation. $D$ is a diagonal matrix and its diagonal elements are the eigenvalues, $\lambda_i$, of $A$. $V$ is the corresponding eigenvector in the column form. Therefore, finding the eigenvalues and eigenvectors of $A$ is simply to transform the matrix, $A$, to a diagonal matrix, $D$, with a similarity transformation matrix, $V$. This is called diagonalization.

In a symmetric eigenvalue problem, $A\vec{x}_i = \lambda_i\vec{x}_i$, $A$ is either a real symmetric or complex Hermitian $n$-by-$n$ square matrix. The scalar, $\lambda_i$, is an eigenvalue and the nonzero column vector, $\vec{x}_i$, is the corresponding eigenvector.

In Lapack (linear algebra package), there is a subroutine to compute eigenvalues, $\lambda_i$, and, optionally, the corresponding eigenvectors, $\vec{x}_i$, for a given matrix $A$. The computation proceeds in the following two stages:

1. The matrix $A$ is reduced to real tridiagonal form $T$. If $A$ is real symmetric, its decomposition is $A = QTQ^T$ with $Q$ being orthogonal and $T$ being symmetric tridiagonal. If $A$ is complex Hermitian, the decomposition is $A = QTQ^H$ with $Q$ unitary and $T$, as before, real symmetric tridiagonal. This is called the Householder transformation.

2. Eigenvalues and eigenvectors of the real symmetric tridiagonal matrix $T$ are computed by QL factorization.

As the numbers of sites and holes of a cluster are specified, the total number of basis that spans the Hilbert space can be found analytically. The relation is given by the following formula:

$$\text{total number of basis} = nC_r \times 2^{(n-r)}, \quad (3.1)$$

where $n$ refers to a fixed number of sites and $r$ is a fixed number of holes. It is obvious that the first term, $nC_r$, is the multiplicity of placing the hole(s) randomly on lattice sites. And the second term, $2^{(n-r)}$, is the multiplicity of placing spin-up or spin-down particles on the remaining sites. By simple calculation, the size of different systems are obtained and summarized in Table 3.1:

There is about two million basis states in the largest cluster in our study. If the Hamiltonian matrix is defined on such a huge Hilbert space, both the physical
<table>
<thead>
<tr>
<th>Site</th>
<th>Hole</th>
<th>Total number of basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>* 8</td>
<td>0</td>
<td>256</td>
</tr>
<tr>
<td>* 8</td>
<td>1</td>
<td>1,024</td>
</tr>
<tr>
<td>* 8</td>
<td>2</td>
<td>1,792</td>
</tr>
<tr>
<td>* 16</td>
<td>0</td>
<td>65,536</td>
</tr>
<tr>
<td>* 16</td>
<td>1</td>
<td>524,288</td>
</tr>
<tr>
<td>* 16</td>
<td>2</td>
<td>1,966,080</td>
</tr>
<tr>
<td>18</td>
<td>0</td>
<td>262,144</td>
</tr>
<tr>
<td>18</td>
<td>1</td>
<td>2,359,296</td>
</tr>
</tbody>
</table>

Table 3.1: Basis number of different system (* indicated the systems to be discussed in this thesis.)

memory and the computational time required are unaffordable. It is because the memory required is proportional to the square of the total number of basis, $O(Basis\ number^2)$. And the computational time is proportional to the cube of the total number of basis, $O(Basis\ number^3)$.

Fortunately, a symmetry operation can help us to reduce our problem into diagonalizing several smaller matrices instead of a huge one. More symmetry properties of the model can be exploited to further divide the block matrices into even smaller ones.

### 3.2 Application of Symmetry Group

Symmetry is any operation which, when acting upon a physical system, does not alter its physical properties. In a mathematical sense, a symmetry operator, $\hat{A}$, commutes with the Hamiltonian $[\hat{H}, \hat{A}] = 0$, so that they share the same set of eigenstates. Also these commutation relation in quantum mechanics imply conservation laws.

$$\frac{d\langle \hat{A} \rangle}{dt} = \left\langle \frac{i}{\hbar} [\hat{H}, \hat{A}] + \frac{\partial \hat{A}}{\partial t} \right\rangle$$  \hspace{1cm} (3.2)

If $\hat{A}$ has no implicit dependence on time, $\frac{\partial \hat{A}}{\partial t}$ vanishes. Therefore,

$$\frac{d\langle \hat{A} \rangle}{dt} = \left\langle \frac{i}{\hbar} [\hat{H}, \hat{A}] \right\rangle$$  \hspace{1cm} (3.3)
In the case that $\hat{A}$ commutes with $\hat{H}$, the quantity, $\langle \hat{A} \rangle$, is constant in time and $A$ is called a constant of motion [19]. In the case of translational symmetry, the crystal momentum is conserved. In the cases of reflection and spin inversion symmetry, the parity and spin parity are the constants of motion respectively.

### 3.2.1 Translational Symmetry

There are three kinds of symmetry applicable to our systems. They are translational symmetry, reflection symmetry and spin inversion symmetry. Translational symmetry is the typical one in solid-state physics. Once a crystal is formed by putting basis atom(s)/molecule(s) on lattice points periodically, the crystal possesses this symmetry. The fundamental idea is based on the periodicity of the crystalline structure.

![Diagram](image.png)

Figure 3.1: 1-D spin chain with 4 spin-1/2 particles.

Consider an 1-D spin chain with four spin-1/2 particles placed on each site and with periodic boundary condition (Fig.5.1a). This geometry is equivalent to a ring with four spins (Fig.5.1b). A translation in the 1-D spin chain is equivalent to a rotation in the spin ring.

$$\hat{T}_{\bar{x}_j} |u_{\mathbf{g}}(x)\rangle = e^{i\bar{k} \cdot \bar{x}_j} |u_{\mathbf{g}}(x)\rangle,$$  \hspace{1cm} (3.4)

where $\bar{k}$ is a wave vector and $\bar{x}_j$ is a discrete displacement on the 1-D spin chain. The operation returns a phase as its eigenvalue. This is called the Bloch theorem and the eigenvector of the translational operator is called a Bloch State.
Applying a translational operation to the spin chain is simply to displace
the basis atom(s)/molecule(s) toward the right or left by an arbitrary integral
number of site(s). Therefore, it is clear that there are four distinct translational
operations in a 1-D spin chain with four sites namely, $\hat{T}_0$, $\hat{T}_1$, $\hat{T}_2$ and $\hat{T}_3$ where
the subscript is the index of the sites.

Further studying the nature of translational operators, $\hat{T}_0$ is an identity op-
erator, $\hat{I}$ which makes no change to the basis after the operation. Due to the
periodic boundary condition, $\hat{T}_0 = \hat{T}_4$, the product of the four operators is one
of them indeed, e.g. $\hat{T}_1 \hat{T}_2 = \hat{T}_3$. This is a closure relation. Moreover, for each
of these four operators, there exists an inverse operator to cancel its effect, e.g.
$\hat{T}_1 \hat{T}_3 = \hat{T}_4 = \hat{T}_0$. And it is obvious that the four operators obey the associative
law, i.e. $\hat{T}_1 (\hat{T}_2 \hat{T}_3) = (\hat{T}_1 \hat{T}_2) \hat{T}_3$.

In other word, these four translational operators form a group. A group is
defined to be a set whose elements obey the (1)Identity Law; (2)Closure Relation;
(3)Inverse Law and (4)Associative Law. Moreover, all translations also obey the
Commutative Law. This kind of groups is called Abelian groups.

In our study, the direct lattice is a square lattice with $4 \times 4$ sites. Since
the cluster has periodic boundary conditions in both $x$ and $y$ directions, two
groups of translations are available. They are $T_x = \{ \hat{T}_{x0}, \hat{T}_{x1}, \hat{T}_{x2}, \hat{T}_{x3} \}$ and $T_y = \{ \hat{T}_{y0}, \hat{T}_{y1}, \hat{T}_{y2}, \hat{T}_{y3} \}$. They can be combined to form a larger group, $T = T_x \otimes T_y$.
This is called the direct product of groups.

Therefore, sixteen distinct translational symmetry operations are available in
the $4 \times 4$ square lattice. The domain of the operators is defined on the real lattice.
Some states are said to be translational symmetry related when they can be
transformed into one another using one of these sixteen translational operators.

### 3.2.2 Reflection Symmetry

Besides translations, reflection operations can also be applied to the lattice. Once
a symmetry axis is defined, which is invariant under the reflection, the plane can
be reflected about the axis.
Figure 3.2: Reflection symmetry: (a) before reflection and (b) after reflection.

In the case of a 1-D spin chain with four sites, the symmetry axis can be defined to pass through site 1 (Fig.3.2). After reflection, the particle located on the reflection symmetry axis are invariant. In general, those particles which do not belong to this case will exchange their positions with their corresponding sites.

The reflection symmetry operators also form a group like its translational counterpart. There are only two operations available in the reflection symmetry group, namely \( \{ \hat{R}_0, \hat{R}_1 \} \). \( \hat{R}_0 \) is simply an Identity operator, \( \hat{I} \). \( \hat{R}_1 \) is reflecting the system once. Note that if the system is reflected twice, it will be restored to its original state, i.e. \( \hat{R}_1 \hat{R}_1 = \hat{I} \). Assume that,

\[
\hat{R}_1 |u(x)\rangle = \sigma |u(-x)\rangle.
\]

Then,

\[
\hat{R}_1 \hat{R}_1 |u(x)\rangle = \hat{R}_1 \sigma |u(-x)\rangle = \sigma^2 |u(x)\rangle.
\]

Therefore, under the condition that reflecting the system twice equal to identity, the possible values of \( \sigma \) are only \(-1, 1\). The phase, \( \sigma \), is called the parity.

In our system, there are three kinds of reflection possible. They are characterized by the orientation of the reflection symmetry axises, namely \( R_x \), \( R_y \) and \( R_d \) (as shown in Fig.5.3) and they form groups, i.e. \( R_x = \{ \hat{I}, \hat{R}_x \} \), \( R_y = \{ \hat{I}, \hat{R}_y \} \) and \( R_d = \{ \hat{I}, \hat{R}_d \} \).
3.2.3 Spin Inversion Symmetry

The spin inversion symmetry is the third kind of symmetry we use in our study. It is carried out in spin space and the consequences of this operation are: (1) spin-up particles become spin-down; (2) spin-down particles become spin-up; (3) hole has no change. If the system has equal number spin-up and spin-down particle in zero B-field, there is no preference direction in the spin space. Since the Hamiltonian of the $t - J$ model commutes with the spin inversion operator, the energy spectrum is unchanged under spin inversion.

Spin inversion operators also form a group. It consists of two operators i.e. identity and spin inversion, $\hat{R}_s = \{\hat{I}, \hat{R}_s\}$. It is mathematically the same as reflection symmetry groups $R_x$, $R_y$ and $R_d$, but with different physical meaning. As $\hat{R}_s^2 = \hat{I}$, $\hat{R}_s|u(x)\rangle = \sigma_s|u(x)\rangle$ where $\sigma_s$ is called spin parity and its allowed values are $\{-1, 1\}$.

There is another important point that the eigenvectors of the Hamiltonian can be transformed to be the simultaneous eigenvector of another observable, total spin, $\hat{S}_{\text{total}}^Z$. It can be shown that $[\hat{H}, \hat{S}_{\text{total}}^Z] = 0$. The advantage of using the eigenvectors of the total spin in the subspace $m_z = 0$ is that their multiplets on
other subspace can be obtained by applying the raising and lowering operator:

\[
\hat{S}^+_{\text{total}} = \sum_{j=1}^{N} \hat{S}^+_j, \\
\hat{S}^-_{\text{total}} = \sum_{j=1}^{N} \hat{S}^-_j.
\]  
(3.7)

In fact, it can be shown that \([\hat{H}, \hat{S}^z_{\text{total}}] = 0\). Therefore using the eigenvectors of the total spin, \(\hat{S}^z_{\text{total}}\), to span the Hilbert space of the \(t-J\) Hamiltonian in the subspace of \(m_z = 0\), the multiplicity of \((2S_{\text{total},z} + 1)\) can be used to determine the density of state of the system without performing any diagonalization on other subspaces of \(m_z \neq 0\).

### 3.3 Representation of basis

As an illustration, the simple 1-D spin-chain having four spin-1/2 particles (Fig.3.4) is used.

![Figure 3.4: Representation of basis in our programming](image)

Figure 3.4: Representation of basis in our programming : (a) actual spin configuration; (b) direct mapping; (c) reversed mapping and (d) decimal representation.

Note that every site is singly occupied by either a spin up or spin down particle (Fig.3.4a). A binary integer is sufficient to represent a spin state by using one bit to represent a site, “1” to represent spin-up and “0” to represent spin-down. By direct mapping, a spin configuration is converted to a binary integer(Fig.3.4b). However, due to the convention of representing a binary integer, the digits are rearranged in descending order (Fig.3.4c). Finally, a spin state can be mapped uniquely as a binary integer as well as a decimal integer(Fig.3.4d).
Upon doping, one of the spin-1/2 particles is removed from a site. This leaves a hole there. There are three kinds of possibilities for a single site, i.e. \(|\uparrow\rangle, |\downarrow\rangle\) or \(|0\rangle\). One bit is no longer sufficient to represent the spin state with doping. Then two bits are employed to solve this problem. In our project, the following convention is adopted:

\[
|0\rangle \quad \begin{array}{c|c}
\text{Up} & 1 \\
\text{Down} & 0 \\
\end{array} \rightarrow \begin{array}{c}
10100001 \\
161 \end{array}
\]

Figure 3.5: Representation with hole.

"1" is used to represent the existence of a spin particle, "0" stands for the absence of spin particle. To represent n sites, 2n bits are needed (Fig.3.5). The higher order half of the binary integer represents the existence of spin-up particles while the lower order half represents the existence of spin-down particles (Fig.3.5b). Finally, every spin state can be mapped uniquely to a binary integer as well as a decimal integer (Fig.3.5c).

The advantages of using this representation in programming are: (1) there exists a simple and systematic way to generate our basis; (2) the basis can be easily divided into certain subsets characterized by \(m_z\), the z-component of the total spin, \(\hat{S}_{\text{total}}\); (3) it is applicable to a system with any number of holes.

In the case of 2-D square plane lattice, a mapping is defined to transform the sites of a plane to a 1-D array. The difference between a 2-D problem and a 1-D problem is that there is one more degree of freedom in the 2-D case. Therefore, when neighbor interaction is considered, neighbor sites of a 2-D problem should be mapped carefully after it is relabeled to an 1-D array. After constructing the spin-states, they can be used as basis to build up our Hamiltonian matrix, \(\hat{H}\). However the Hilbert space is large.

Fortunately, the symmetry operations can help us to relieve the problem by dividing a huge Hilbert space into several smaller subspaces. Group theory makes
our project possible in the sense that more symmetry operations can be exploited to further divide the block matrix into smaller and smaller blocks (Appendix A).

The eigenstates of $\hat{S}_z^{\text{total}}$ (i.e. spin state) are used to construct the Hamiltonian matrix of the $t - J$ model. Since each eigenstate associates with an eigenvalue $\hat{S}_z^{\text{total}}|M_z\rangle = m_z|M_z\rangle$, therefore the basis can be grouped according to its $m_z$. Afterward, the non-zero elements of the Hamiltonian are located in the subspace spanned by the basis with the same $m_z$ and formed blocks along the diagonal of the huge matrix. Each block can be characterized by a good quantum number, $m_z$. It is possible because the $z$-component of the total spin is a constant of motion. The fundamental criterion is $[\hat{H}, \hat{S}_z^{\text{total}}] = 0$.

Using this scheme, the problem size is reduced. Originally, there is about two millions basis states (Table 3.1). After block diagonalizing, the size of the largest subspace is equal to $\frac{16!}{7!9!2!} = 411,840$. Although the problem size is reduced, it is still large in terms of the computational resources required.

Recalling the discussion of the previous section 3.2, the translational, reflection and spin-inversion symmetries can help us, i.e. Fig. 3.6.

![Figure 3.6: Schematic diagram of block diagonalization](image)

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The priority of our blocking scheme is: $\hat{S}_{total}^z \rightarrow \hat{T} \rightarrow \hat{R} \rightarrow \hat{R}_s$. After applying the translational group, $T$, the largest subspace is reduced to a size of about $\frac{1}{16 \cdot \frac{6!}{7! \cdot 1!}} = 25,740$. Each block of non-zero element possesses one more good quantum number as an identification, i.e. the crystal momentum, $\vec{k}$. It is also obvious that $[\hat{H}, \hat{T}] = 0$ and $[\hat{S}^z_{total}, \hat{T}] = 0$, i.e. energy and z-component of the total spin are conserved under translation due to the imposed periodic boundary conditions.

However, the reflection symmetry is implemented carefully in order to further block our matrix elements. In general, $[\hat{H}, \hat{R}] = 0$ and $[\hat{S}^z_{total}, \hat{R}] = 0$ but $[\hat{T}, \hat{R}] \neq 0$. Simultaneous eigenstates of $\hat{T}$ and $\hat{R}$ do not exist except when the reflection does not alter the crystal momentum of the translation. Finally, if the system possesses equal number of spin-up and spin-down, the spin inversion symmetry can be used to further divide the largest subspace $m_z = 0$, into smaller blocks.
Chapter 4

Static and Dynamical Properties

In this chapter, the physical significance of the static magnetic susceptibility, the dynamical spin-spin correlation function and the dynamical spin-charge correlation function are discussed. Some previous theoretical and experimental results are also summarized.

4.1 Static Magnetic Susceptibility

Spin configurations, $|n, m_z\rangle$, are used to span the Hilbert space where $n$ is the index of the spin configurations and $m_z$ is the $z$-component of the total spin of the state. The spin configurations are the eigenstates of the $z$-components of the total spin, $\hat{S}_{total}^z |n, m_z\rangle = m_z |n, m_z\rangle$ ($\hbar = 1$) where $\hat{S}_{total}^z = \sum_i \hat{S}_i^z$ and $i$ is the index of the sites. But they are not the eigenstates of the $t-J$ Hamiltonian. After diagonalization, the eigenstates, $|\phi_n, m_z\rangle$, of the $t-J$ Hamiltonian are obtained, i.e. $\hat{H}_{t-J} |\phi_n, m_z\rangle = E_n |\phi_n, m_z\rangle$. And they are linear combinations of the spin configuration in the subspace of the same $m_z$. Since the $z$-components of the total spin commutes with the Hamiltonian $[\hat{S}_{total}^z, \hat{H}_{t-J}] = 0$, $m_z$ of the system is a constant of motion.

The magnetic susceptibility $\chi$ is the response of the magnetic dipoles inside a material to an external field.

$$\chi(\tau) = \frac{1}{N} \lim_{B \to 0} \frac{\partial \langle M \rangle}{\partial B},$$  \hspace{1cm} (4.1)

where $M$ is the magnetization. $B$ is an external field. $\tau$ is equal to $k_B T$. $N$ is the number of sites. We take the direction of the external magnetic field as the $z$ axis. $\langle M_z \rangle$ is a thermal average of the $z$-component of magnetization, i.e.
\[ \langle M_z \rangle = \sum \frac{m_z e^{-H_j / \tau}}{\sum e^{-H_j / \tau}} \]. The summation runs through the index of all eigenstates of the Hamiltonian. And \( H = H_{t-J} - M \cdot B \) is the t-J model plus the interaction of magnetization with an external field. After some manipulation,

\[ \chi(\tau) = \frac{1}{N_\tau} \langle (m_z - \langle m_z \rangle)^2 \rangle = \frac{1}{N_\tau} [\langle m_z^2 \rangle - \langle m_z \rangle^2]. \] (4.2)

where \( \langle m_z^2 \rangle = \sum_n \frac{\sum_{\text{total}} |\phi_n, m_z \rangle e^{-E_n / \tau}}{\sum_n e^{-E_n / \tau}} \) and \( \langle m_z \rangle = \sum_n \frac{\sum_{\text{total}} |\phi_n, m_z \rangle e^{-E_n / \tau}}{\sum_n e^{-E_n / \tau}} \).

Note that \( \langle m_z \rangle^2 \) always vanishes because the cluster has an even number of sites. If the temperature \( \tau \) is greater than the width of the energy spectrum, the weight functions (i.e., Boltzmann factors) of each energy eigenstate approach one and each state is equally accessible. Under this condition, the quantity \( \langle (m_z - \langle m_z \rangle)^2 \rangle \) is a constant. As a consequence, the static magnetic susceptibility at high temperature is inversely proportional to the temperature.

However, it is not meaningful to study a system in a high temperature regime because superconductivity occurs in low temperature. Theoretically, the magnetization is only contributed by the ground state at absolute zero. As the temperature increases, the low-lying excited states begin to have a higher weight.

Fig.4.1-2 show the magnetic susceptibility of the \( t - J \) model on a square lattice with 16 site for 0, 2, 4, and 6 holes by exact calculation of low-lying states using the Lanczos method. They are at \( t/J=0.3 \) and \( t/J=0.5 \) respectively.[20] The curves demonstrate the typical shape of the magnetic susceptibility of AF materials. In contrary to that of ferromagnetic materials, there is a peak in the susceptibility. Above the temperature of the peak, the susceptibility drops gradually with increasing temperature. The figure also shows a spin gap in the low temperature region where the magnetization does not respond to an external field.

Fig.4.3 shows the uniform magnetic susceptibility of the \( t - J \) model on a 20 sites square lattice obtained with FTLM[21]. It demonstrates the effect of doping in the susceptibility. Using FTLD, Jaklic and Prelovsek obtained the
Figure 4.1: Uniform magnetic susceptibility of the $t-J$ model on a square lattice with 16 site for 0, 2, 4, and 6 holes by exact calculation of low-lying states with Lanczos method. $t/J=0.3$. [20]

Figure 4.2: Same as Fig.4.1 but at $t/J=0.5$. [20]
result that there is in general a peak at the temperature of $J$. Upon doping, the magnetic susceptibility increases at temperatures lower than $J$ and decreases at temperatures higher than $J$.

Fig. 4.4 is the experimental results of magnetic susceptibility of $La_{2-x}Sr_xCuO_{4-\delta}$ and $YBa_2Cu_3O_{6+x}$ measured at different temperatures [22, 23]. Note that the peak shifts towards lower temperature regime as the doping level increases.

### 4.2 Dynamical Spin-Spin Correlation Function

The dynamical spin-spin correlation function, $S(\vec{q}, \omega)$, is also called the dynamical structure factor. It is used to measure the dependence of spin components on each other. The expression is written as follow:

$$S(\vec{q}, \omega) = \sum_{m,n} e^{-E_m/\tau} |\langle \phi_m | S_{\vec{q}}^z | \phi_n \rangle|^2 \delta(\omega - E_m + E_n) / \sum_{m,n} e^{-E_m/\tau}, \quad (4.3)$$

where $\vec{q}$ is the momentum transfer and $\omega$ is the energy transfer. The summation runs through the index, $n$, and, $m$, in the ket space and the bra space respectively. The basis $|\phi_n\rangle$ and $|\phi_m\rangle$ are the eigenstates of the $t - J$ model and they
Figure 4.4: Magnetic susceptibility, $\chi$ vs. temperature for samples of La$_{2-x}$Sr$_x$CuO$_{4-y}$ and YBa$_2$Cu$_3$O$_{7-x}$.\textsuperscript{[22, 23]} In the upper figure, (I) and (II) refer to different oxygen compositions $y=0.0$ and 0.04 respectively.
are simultaneous eigenvector of the symmetry operator(s) and the Hamiltonian. 
$E_n$ and $E_m$ are the eigenenergies of $|\phi_n\rangle$ and $|\phi_m\rangle$ respectively. 
$S(\vec{q}, \omega)$ is directly related to the differential cross section of a neutron-scattering process in experiment (Appendix B).

The crucial operator, $S^z_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{q} \cdot \vec{r}_j} S^z_j$, is the $z$-component of the total spin operator in the k-space representation. This is the result of discrete Fourier transform of $S^z_j$ with $\frac{1}{\sqrt{N}}$ as normalization factor where $N$ is the number of sites and $j$ is the index of sites. Note that the spin-spin correlation function is an Equal-Time Correlation Function (ETCF) and it means that the quantity is measured at a specific time. As a consequence, there is an infinite frequency uncertainty. In equation 4.3, the $\delta$-function implies the correlation function is in its frequency-domain representation.

The $\delta$-function in equation 4.3 can be replaced by a Lorentzian function with a broadening factor, $\eta$. So that equation 4.3 becomes:

$$S(\vec{q}, \omega) = \sum_{m,n} e^{-E_m/\tau} |\langle \phi_m | S^z_{\vec{q}} | \phi_n \rangle|^2 \frac{\eta}{(\omega - E_m + E_n)^2 + \eta^2} \sum_{m,n} e^{-E_m/\tau}. \quad (4.4)$$

Note that eigenstates $\{|\phi_n\rangle\}$ and $\{|\phi_m\rangle\}$ are characterized by discrete value of $\vec{k}$s. The operator $S^z_{\vec{q}}$ alters the momentum of $|\phi_n\rangle$ and there is a selection rule that $\vec{k}_n - \vec{q} = \vec{k}_m$ where $\vec{k}_n$ is the momentum associated with the ket $|\phi_n\rangle$ and $\vec{k}_m$ is the momentum associated with the bra $|\phi_m\rangle$.

Fig 4.5 shows the spin-spin correlation function, $S(\vec{Q}, \omega)$, for a $4 \times 4$ cluster with 4 holes at zero temperature. Tohyama and Horsch did a calculation of different momentum transfer [24]. However, $\vec{Q} = (\pi, \pi)$ is the most interested as there is a profound peak. The characteristic peak for their result at $\vec{Q} = (\pi, \pi)$ is located at about $\omega=1.0t$.

Fig 4.6 also shows the spin-spin correlation at a fixed temperature, $T=0.2t$ at various dopings. Jaklic and Prelovsek used FTLD to get the above result at $\vec{Q} = (\pi, \pi)$ using a broadening factor of $\eta=0.07t$[29]. The result of 1 hole doping obtained with FTLD by Jaklic and Prelovsek and ours obtained with ED are under the same conditions. A fair comparison can be made.
Figure 4.5: $S(Q, \omega)$ of the $t - J$ model on a $4 \times 4$ cluster with four holes at zero temperature with $J=0.4t$ using ED.[24].

Figure 4.6: Dynamic spin structure factor, $S(Q, \omega)$, at fixed $T = 0.2 < J$ and different doping, $c_h$.[21]
4.3 Dynamical Spin-Charge Correlation Function

The dynamical spin-charge correlation function is used to measure the charge density component. The expression is written as follow:

$$N(\tilde{q}, \omega) = \sum_{m,n} e^{-E_m/\tau} |\langle \phi_m | N_{\tilde{q}} | \phi_n \rangle|^2 \frac{\delta(\omega - E_m + E_n)}{\sum_m e^{-E_m/\tau}},$$  

(4.5)

where $N_{\tilde{q}} = \frac{1}{N} \sum_i e^{i\tilde{q} \cdot \tau_i} (n_i - \bar{n})$. The expression of $N(\tilde{q}, \omega)$ is quite similar to $S(\tilde{q}, \omega)$. The only difference is the crucial operator $N_{\tilde{q}}$. $N_{\tilde{q}}$ is the result of a Fourier Transform where $n_j$ is an on-site occupation operator and $n$ is the average density of the whole system, e.g. for a 16 sites system with a single hole, the value of $n$ is equal to $\frac{15}{16}$.

In practical computation, the equation 4.5 is modified as follow:

$$N(\tilde{q}, \omega) = \sum_{m,n} e^{-E_m/\tau} |\langle \phi_m | N_{\tilde{q}} | \phi_n \rangle|^2 \frac{\eta}{(\omega - E_m + E_n)^2 + \eta^2} / \sum_m e^{-E_m/\tau}.$$  

(4.6)

However, it seems that it is difficult to probe the charge fluctuation by experiment. It is because the requirement of the incident particle must be charged and spinless in order to study spin-charge separation [24].

Fig. 4.7 shows the spin-charge correlation function, $N(\tilde{Q}, \omega)$, for a $4 \times 4$ cluster with 4 holes at zero temperature. Note that at the momentum transfer, $\tilde{Q} = (\pi, \pi)$, the spectrum is located at the frequency range from $\omega \sim 4.0t$ to $\sim 8.0t$.

Fig. 4.8 also shows the spin-charge correlation at $T=0.2t$, $J=0.4t$ and at two dopings obtained by Jaklic and Prelovsek [21]. This is similar to the results of Tohyama and Horsch [24]. At $\tilde{Q} = (\pi, \pi)$, most of the spectral weight is within the range $\omega \sim 4.0t$ to $\sim 8.0t$. There is no significant weight at $\omega < 4.0t$. 

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Figure 4.7: $N(Q, \omega)$ of the $t-J$ model on a $4 \times 4$ cluster with 4 holes at zero temperature with $J=0.4t$ using ED.[24].
Figure 4.8: Normalized density correlation spectra, $N(Q_\omega)/c_n$ at fixed $T/t = 0.2$ and $J/t = 0.4$ at two dopings: $c_n = 1/18$ and $c_n = 3/18$.[21]
Chapter 5

Result and Discussion

In this chapter, numerical results of the static magnetic susceptibility, the dynamical spin-spin correlation and the spin-charge correlation function of different clusters are reported. The finite-size effect can be observed by comparing the results of the 16-site and 8-site clusters.

5.1 Static magnetic susceptibility

![Graph of magnetic susceptibility](image)

Figure 5.1: Magnetic susceptibility of the $t-J$ model on a square lattice with 8 sites: $J = 0.4t$. 

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Fig. 5.1-3 show the magnetic susceptibility as a function of temperature. The vertical axis represents the magnetic susceptibility in arbitrary units and the horizontal axis is the temperature in units of \( t \). It is important to bear in mind that the experimental result of the spin coupling constant, \( J \), in HTSC was found to be between 1000K and 1500K[27]. And the parameter, \( t \), was obtained by microscopic calculation to be around 3\( J \)[28]. Therefore, it is reasonable to choose our parameter, \( J = 0.4t \). Note that \( t \) is around 3000K to 4500K.

In the study of the magnetic susceptibility using the 8-site cluster, the result of the undoped cluster and that of the 2-hole doped cluster are plotted in Fig.5.1. The result of the 1-hole doped cluster is plotted separately in Fig.5.2. Note that the two curves in Fig.5.1 have the same shape. In the low temperature region, the susceptibility vanishes and as the temperature increases, the susceptibility starts to rise to a peak and then drops gradually.

And the peak of the undoped cluster appears at the temperature 0.40\( t \) while the peak of the 2-hole doped cluster is at 0.20\( t \). Moreover, the former curve has a comparatively lower peak value. Below the temperature 0.60\( t \), the susceptibility of the 2-hole cluster is higher than that of the undoped one. But above the temperature, the response of the undoped one is higher than that of 2-hole one.

Fig.5.2 shows the magnetic susceptibility of the \( t-J \) model on an 1-hole doped cluster with 8 sites. Obviously, it is qualitatively different from the curves in Fig.5.1. The major difference between this system and the previous ones is that it has an odd number of spin-1/2 particles. The ground state of the system possesses a finite \( z \)-component of the total spin, \( m_z = 1/2 \) or \(-1/2 \). As mentioned before, the ground state dominates the characteristic at low temperature. Therefore, the system behaves like a free spin and it goes diverged as the temperature decreases because a non-zero spin fluctuation \( \langle m_z^2 \rangle \) is divided by a vanishing temperature.

The results of the magnetic susceptibility of the \( t-J \) model on a 16-site cluster at doping levels of 0%, 6.25% and 12.5% are plotted in Fig.5.3. The higher the doping, the larger the spin response and the larger the magnetic susceptibility. The free spin behavior is observed in the system with one hole.
Figure 5.2: Magnetic susceptibility of the $t - J$ model on a square lattice with 8 sites and 1 hole.

| Eigen-Energy | $|M_z|$ | $\vec{k}$       | $\sigma$(reflection) | Multiplicity |
|-------------|-------|-----------------|----------------------|-------------|
| -4.000000   | 0     | (0.0, 0.0)      | $1(R_d)$             | 1           |
| -3.600000   | 0     | ($\pi$, $\pi$) | $1(R_d)$             | 1           |
| -3.600000   | 1     | ($\pi$, $\pi$) | $1(R_d)$             | 2           |
| -2.800000   | 0     | ($\pi$, 0.0)   | $1(R_z)$             | 2           |

Table 5.1: Characteristics of low-lying states of the $t - J$ model on an 8-site cluster without doping.
Table 5.2: Characteristics of low-lying states of the $t-J$ model on an 8-site cluster with 1 hole.

| Eigen-Energy | $|M_z|$ | $\vec{k}$ | $\sigma$ (reflection) | Multiplicity |
|--------------|--------|----------|------------------------|--------------|
| -4.871563    | 1/2    | $(\pi, 0.0)$ | $1(R_x)$              | 4            |
| -4.871563    | 1/2    | $(\pi/2, \pi/2)$ | $1(R_d)$              | 8            |
| -4.708278    | 1/2    | $(\pi, 0.0)$ | $1(R_x)$              | 4            |
| -4.708278    | 1/2    | $(\pi/2, \pi/2)$ | $1(R_d)$              | 8            |

Table 5.3: Characteristics of low-lying states of the $t-J$ model on an 8-site cluster with 2 holes.

| Eigen-Energy | $|M_z|$ | $\vec{k}$ | $\sigma$ (reflection) | Multiplicity |
|--------------|--------|----------|------------------------|--------------|
| -5.903060    | 0      | $(\pi, \pi)$ | $1(R_d)$              | 1            |
| -5.903060    | 0      | $(0,0,0.0)$ | $1(R_d)$              | 3            |
| -5.844750    | 0      | $(\pi, \pi)$ | $-1(R_d)$             | 1            |
| -5.844750    | 0      | $(\pi, \pi)$ | $1(R_d)$              | 1            |

Figure 5.3: Magnetic susceptibility of the $t-J$ model on a square lattice with 16 sites: $J = 0.4t$. 

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The result obtained in the 8-site cluster is qualitatively different from that obtained in the 16-site cluster. The curve of the 2-hole system with 8 sites is higher than the undoped one in the lower temperature region and it is lower than the undoped one in the higher temperature region (Fig.5.1). Comparatively, the curve of the 2-hole system with 16 sites is higher than the undoped one throughout the whole temperature range we studied (Fig.5.3). It is obvious that the larger the cluster size, the more realistic is our calculation. But there is another tradeoff, i.e. the memory and the CPU time required. Refer to Table 4.1, the number of basis states increase exponentially as the system size increases.

<table>
<thead>
<tr>
<th>Eigen-Energy</th>
<th>( M_z )</th>
<th>( \vec{k} )</th>
<th>( \sigma(\text{reflection}) )</th>
<th>Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>-7.459954</td>
<td>0</td>
<td>((\pi, \pi))</td>
<td>(1(R_d))</td>
<td>1</td>
</tr>
<tr>
<td>-7.007075</td>
<td>0</td>
<td>((0.0, 0.0))</td>
<td>(1(R_d))</td>
<td>1</td>
</tr>
<tr>
<td>-7.007075</td>
<td>1</td>
<td>((0.0, 0.0))</td>
<td>(1(R_d))</td>
<td>2</td>
</tr>
<tr>
<td>-6.754577</td>
<td>0</td>
<td>((\pi, \pi/2))</td>
<td>(1(R_g))</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 5.4: Characteristics of low-lying states of the \( t - J \) model on a 16-site cluster without doping.

<table>
<thead>
<tr>
<th>Eigen-state</th>
<th>Eigen-Energy</th>
<th>( M_z )</th>
<th>( \vec{k} )</th>
<th>( \sigma(\text{reflection}) )</th>
<th>Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-9.013627</td>
<td>1/2</td>
<td>((\pi, 0.0))</td>
<td>(1(R_g))</td>
<td>4</td>
</tr>
<tr>
<td>0</td>
<td>-9.013627</td>
<td>1/2</td>
<td>((\pi/2, \pi/2))</td>
<td>(1(R_d))</td>
<td>8</td>
</tr>
<tr>
<td>1</td>
<td>-8.873333</td>
<td>1/2</td>
<td>((\pi/2, 0.0))</td>
<td>(1(R_g))</td>
<td>8</td>
</tr>
<tr>
<td>2</td>
<td>-8.752607</td>
<td>1/2</td>
<td>((\pi, \pi/2))</td>
<td>(1(R_g))</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>-8.705984</td>
<td>1/2</td>
<td>((\pi, 0.0))</td>
<td>(1(R_g))</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>-8.705984</td>
<td>1/2</td>
<td>((\pi/2, \pi/2))</td>
<td>(1(R_d))</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>-8.705984</td>
<td>3/2</td>
<td>((\pi, 0.0))</td>
<td>(1(R_g))</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>-8.705984</td>
<td>3/2</td>
<td>((\pi/2, \pi/2))</td>
<td>(1(R_d))</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 5.5: Characteristics of low-lying states of the \( t - J \) model on a 16-site cluster with 1 hole.

### 5.2 Dynamic spin-spin correlation function

For the sake of studying the effect of temperature, the dynamical spin-spin correlations at different temperatures are plotted in the same graph. Note that there
Figure 5.4: $S(q, \omega)$ of the system with 16 sites and 0 hole: $q = (\pi, \pi)$; $J = 0.40t$, $T = 0.10t$, $0.15t$ and $0.20t$; $\eta = 0.07t$. 
is a general tendency: the higher the temperature, the wider the spectrum. It is because higher temperature raises the possibility of accessing the higher excited states of the system, and the transition is no longer limited among the low-lying states. Therefore the spectrum is blurred by thermal agitation.

It is better to have a deeper understanding of the correlation function. Obviously, the energy transfer, $\omega$, gets involved in equation 4.3 through the delta function. Once the energy transfer is equal to the energy difference between the bra and ket, the matrix element does not vanish and a transition occurs. Therefore the locations of the peaks indicate the energies of all possible transitions in the scattering process.

Fig 5.4 shows the spectrum of $S(\vec{q} = (\pi, \pi), \omega)$ at different temperatures in a half-filled square lattice with 16 sites. The temperatures are $0.10t$, $0.15t$ and $0.20t$. At the temperature $0.10t$, the highest peak is located at about $\omega \approx J = 0.4t$. There is another small peak located at about $\omega \approx -J = -0.4t$. The positive energy transfer indicates the absorption of energy and the negative energy transfer indicates the release of energy. The highest peak reflects that most of the transition occurs in the energy gap roughly equal to $J$. At low temperature, most contribution come from the low-lying states. So the highest peak is exactly contributed by the excitation between the ground state and the first excited state. The energy gap between these two states is $\sim 0.45t$ (Table 5.4). Note that the crystal momentum of the ground state is $(\pi, \pi)$ and that of the first excited state is $(0, 0)$. The difference is exactly the momentum transfer, $\vec{q} = (\pi, \pi)$.

At the temperature $T = 0.15t$, the highest peak is lowered and the peak located at about $-J$ is raised. At the root of the highest peak, there is another small peak appearing in the right hand side. At the higher temperature, $T=0.20t$, the highest peak is further suppressed. On the other hand, the peaks located at $-0.45t$, $0$, and $0.70t$ are raised. The significance of the peak at $-0.45t$ is that there is more emission of energy from the first excited state to the ground state. The peak at 0 implies elastic collision of the system with the external probe. Finally, the peak at $0.70t$ indicates the transition from the ground state to the second excited state. The energy difference of these two states is more or less the
same as the energy transfer of this peak.

Figure 5.5: $S(q,\omega)$ of the system with 16 sites and 1 hole: $q = (\pi, \pi)$; $J = 0.40t$; $T = 0.10t$, 0.15$t$ and 0.20$t$; $\eta = 0.07t$.

Fig 5.5 shows the spectrum of $S(q = (\pi, \pi), \omega)$ at different temperatures in a square lattice with 16 sites and 1 hole. The temperatures are 0.10$t$, 0.15$t$ and 0.20$t$. At the temperature 0.10$t$, the highest peak is located at $\omega \approx 0.3t$. The second highest peak is located at $\omega \approx 0t$ and the third one is located at $\omega \approx 0.81t$. There is also a peak located at $\omega \approx -0.30t$. At the temperature 0.15$t$, the locations of the peak are the same. However, the peaks at 0.31$t$, 0 and 0.81$t$ are suppressed. On the other hand, the peak at $-0.30t$ is raised. At the higher temperature 0.20$t$, the peaks at 0.31$t$, 0 and 0.81$t$ are further suppressed; The peak at $-0.30t$ is raised. Note that there are peaks appearing at $\omega \approx 0.18t$ and 0.50$t$ at higher temperatures.

The peak located at 0.31$t$ corresponds to the transition from the ground state to the third excited state. The energy gap between these states are 0.31$t$. The
Figure 5.6: $S(q,\omega)$ of the system with 16 sites and 1 hole: $q = (\pi, \pi)$; $J = 0.40t$; $T = 0.10t$, 0.15t and 0.20t; $\eta=0.07t$ (enlarged).

larger weight indicates the large possibility of this transition due to the high degeneracy of the third excited state (Table 5.5). Also note that this transition satisfies the conservation of energy and momentum.

The second highest peak is located at $\omega \approx 0$. It reflects the elastic collision between the cluster and the external spin probe. Compared to the undoped system in Fig.5.4, it is obvious that the peak at 0 has a larger weight. It tells us that there exist some transitions and they don’t alter the energy of the system. From table 5.5, the degeneracy of the ground state is twelve and transitions occur among these twelve states. From the table 5.4, there is no degeneracy in the ground state of an undoped system. Therefore at $\omega \approx 0t$, the correlation function vanishes.

The third highest peak is located at $\omega \approx 0.81t$. This indicates a transition from the ground state to a higher excited state with an energy gap of 0.81t. But it doesn’t mean that there is no transition in between. Noted that the correlation function is non-zero from $\omega \approx 0.1t$ to 0.7t (Fig 5.6). Since the delta-function of the spin-spin correlation function is approximated by a Lorentian with a broadening factor, $\eta = 0.07t$, the value of the broadening factor is equivalent to the resolution of the spectrum. Some transitions in between 0.1t and 0.7t may be blurred by the low resolution (Fig.5.7-10).
Figure 5.7: $S(q, \omega)$ of the system with 16 sites and 1 hole: $q = (\pi, \pi); J = 0.40t; T = 0.05t$; $\eta = 0.003t$

Figure 5.8: $S(q, \omega)$ of the system with 16 sites and 1 hole: $q = (\pi, \pi); J = 0.40t; T = 0.10t$; $\eta = 0.003t$
Figure 5.9: $S(q, \omega)$ of the system with 16 sites and 1 hole: $\vec{q} = (\pi, \pi); \ J = 0.40t; \ T = 0.15t; \ \eta=0.003t$

Figure 5.10: $S(q, \omega)$ of the system with 16 sites and 1 hole: $\vec{q} = (\pi, \pi); \ J = 0.40t; \ T = 0.20t; \ \eta=0.003t$
5.3 Dynamic spin-charge correlation function

![Graphs showing N(\hat{q}, \omega) for different temperatures.]

Figure 5.11: \(N(\hat{q}, \omega)\) of the system with 16 sites and 0 hole: \(\hat{q} = (\pi, \pi)\); \(J = 0.40t\); \(T = 0.10t\), 0.15t and 0.20t; \(\eta = 0.07t\).

Fig 5.11 shows the spectrum of \(N(\hat{q} = (\pi, \pi), \omega)\) at different temperatures in a half-filled square lattice with 16 sites. The temperatures are 0.10t, 0.15t and 0.20t. At the temperature 0.10t, the highest peak is located at about \(\omega = 1.8t\). It is above 6000K and all materials are melted at that high temperature. There is another peak located at about \(\omega \approx 0.45t\). At low temperatures, contributions mainly come from the low-lying states. So the highest peak is mainly contributed by the excitation between the ground state and the first excited state. The energy difference between these two states is \(\sim 0.45t\) (Table 5.4). Note that the crystal momentum of the ground state is \((\pi, \pi)\) and that of the first excited state is \((0, 0)\). The difference is exactly the momentum transfer, \(\hat{q} = (\pi, \pi)\).

At the temperature \(T = 0.15t\), the highest peaks are lowered and peaks located
at about $-0.45t$ and 0 are raised. At the higher temperature, $T=0.20t$, the highest peaks are further suppressed. On the other hand, peaks located at $-0.45t$ and 0.0$t$ are raised. The peak at 0 implies elastic collision of the system with the external probe.

![Graph](image)

Figure 5.12: $N(q, \omega)$ of the system with 16 sites and 1 hole: $q = (\pi, \pi)$; $J = 0.40t$, $T = 0.10t$, 0.15$t$, and 0.20$t$; $\eta=0.07t$.

Fig 5.8 shows $N(q = (\pi, \pi), \omega)$ at different temperatures in a square lattice with 16 sites and 1 hole. The temperatures are 0.10$t$, 0.15$t$, and 0.20$t$. At the temperature, 0.10$t$, the highest peak is located at $\omega = 0$. The second highest peak is located at $\omega \approx 0.4t$. There is also no obvious peak located at negative $\omega$. At the temperature 0.15$t$, the locations of the peaks are the same. However, the peaks are suppressed. At the higher temperature 0.20$t$, the peaks are further suppressed.

Compared with other's result, there is a high peak at $\omega=0$ and a small peak at $\omega \approx 0.4t$. Beside the characteristic peaks, it is similar to the result obtained by
Jaklic and Prelovsek[21] using FTLD (Fig.4.8) and that obtained by Tohyama and Horsch[24] at zero temperature using ED (Fig.4.7). There is a broad spectrum located at $\omega \sim 4.0t$ to $\sim 8.0t$. 
Chapter 6

Conclusion

To summarize, we use exact diagonalization (ED) to obtain the whole energy spectrum of the $t - J$ model in two different square lattices: 8-site and 16-site clusters. The whole spectrum is essential in the evaluation of the finite-temperature properties. With the help of group theory, the huge Hilbert space is divided into smaller and smaller subspaces before being diagonalized.

The static magnetic susceptibility, the spin-spin correlation function and the spin-charge correlation function are calculated at different temperatures and various doping levels. The analysis of these quantities becomes clear with the help of the whole energy spectrum in contrast to the result obtained by finite temperature Lanczos diagonalization (FTLD).

Although the brute-force ED is very demanding on computer resources, it gives more information about the low-lying states and their degeneracy. FTLD combines the Lanczos diagonalization with random sampling. Compared to the result obtained by FTLD, more peaks are observed in the dynamical spin spin correlation function obtained by ED. It is worth implementing ED in studying quantum many-body system.

For the static magnetic susceptibility, the qualitative shape (Fig.5.1-3) generally agrees with the result obtained by Alcaraz using exact calculation of lower-lying states. For the dynamical spin spin correlation function of the cluster with 1 hole, the peaks locate at $0.3t$ and $0$ calculated by ED (Fig.5.6). In contrast, the highest peak obtained by FTLD locates at $\omega < 0.35t$ (Fig.4.6). For the dynamical spin charge correlation function, the broad spectrum locates in the range $4.0t \omega < 8.0t$ in both our result and that obtained by FLTD. However, ours shows some peaks at 0 and 0.4t.
The exact results of finite-temperature properties of the $t-J$ model on a square lattice with 8 sites and 16 sites are obtained by ED. They justify the results obtained by other approximation methods and a more detailed analysis can be done with the help of the whole energy spectrum.
Appendix A

Symmetry reduced basis

A.1 Construction of symmetry reduced basis set

Suppose \( \{ |n, m_z\rangle \} \) are the eigenstates of the z-component of the total spin operator:

\[
\hat{S}^z_{\text{total}} |n, m_z\rangle = m_z |n, m_z\rangle. \tag{A.1}
\]

where \( \hbar \) is taken as unity and \( n \) is an index of the spin configurations. Then the spin configurations can be divided into different subsets according to their \( m_z \) and form different subspaces characterized by \( m_z \).

Since \( [\hat{S}^z_{\text{total}}, \hat{H}_{t-J}] = 0 \), the Hamiltonian matrix can be constructed using the basis characterized by particular \( m_z \). After diagonalization, the basis becomes:

\[
\hat{H}_{t-J} |\phi_n, m_z\rangle = E_n |\phi_n, m_z\rangle, \tag{A.2}
\]

where \( E_n \) is the eigenenergy and \( |\phi_n, m_z\rangle \) is the eigenstate of the model. Similarly, the basis set can be further reduced by symmetry.

With translational symmetry, the set of spin configurations \( \{ |m_z\rangle \} \) can be divided into smaller subsets according to their momentum \( \vec{k} \) by forming Bloch states:

\[
|\vec{n}, m_z, \vec{k}\rangle = \frac{1}{N_k} \sum_j e^{-i\vec{k} \cdot \vec{r}_j} \hat{T}_j |n, m_z\rangle, \tag{A.3}
\]

With reflectional symmetry, the basis set can be further divided into smaller subsets according to their parity, \( \sigma \), i.e.

\[
|\vec{n}, m_z, \vec{k}, \sigma\rangle = \frac{1}{N_{k,\sigma}} \sum_j e^{-i\vec{k} \cdot \vec{r}_j} (\hat{I} + \sigma \hat{R}) \hat{T}_j |n, m_z\rangle. \tag{A.4}
\]
Spin inversion symmetry is only possible in the subspace \( m_z = 0 \). The Bloch state is modified as follow:

\[
|\tilde{n}, m_z, \tilde{k}, \sigma, \sigma_{\text{spin}} \rangle = \frac{1}{N_{\tilde{k}, \sigma, \sigma_{\text{spin}}}} \sum_j e^{-i\tilde{k} \cdot r_j} (\hat{I} + \sigma_{\text{spin}} \hat{R}_{\text{spin}})(\hat{I} + \sigma \hat{R}) \hat{T}_j |n, m_z \rangle.
\]

(A.5)

After constructing a symmetry reduced basis set, it is used to construct the Hamiltonian matrix. In the following, matrix elements in the reduced basis is discussed.

### A.2 Matrix element in a symmetry reduced basis set

Suppose \(|\tilde{m}\rangle\) and \(|\tilde{n}\rangle\) are two reduced basis and \(N_m\) and \(N_n\) are the normalization constants. We consider an operator, \(\hat{A}\):

\[
\hat{A}|m\rangle = a_m |l\rangle, \quad |l\rangle = \hat{S}_k^{-1}|n\rangle, \quad \text{where} \quad S_{ij} = R_i \otimes T_j.
\]

(A.6)

It follows:

\[
\hat{A}|\tilde{m}\rangle = \hat{A} \sum_l \phi_l \hat{S}_l |m\rangle
\]

\[
= \frac{a_m}{N_m} \sum_l \phi_l \hat{S}_l |l\rangle
\]

\[
= \frac{a_m}{N_m} \sum_l \phi_l \hat{S}_l [\hat{S}_k^{-1}|n\rangle]
\]

\[
= \frac{a_m}{N_m} \sum_l \phi_{k+l} \hat{S}_k \hat{S}_k^{-1} |n\rangle
\]

\[
= \frac{a_m}{N_m} N_n \phi_k |\tilde{n}\rangle.
\]

(A.7)

Therefore,

\[
\langle \tilde{n}|\hat{A}|\tilde{m}\rangle = a_m \frac{N_n}{N_m} \phi_k.
\]

(A.8)
Appendix B

Master formula for neutron scattering

Neutrons are used as a probe to detect the magnetic structure because it can be scattered from the magnetic moments associated with the unpaired electronic spins in magnetic samples. At the temperature of 300K, neutrons have a wavelength of 2Å (comparable to average interatomic distance in a solid) and energy of 25meV (a typical energy for collective excitations in solids). They are called thermal neutrons.

![Diagram of neutron scattering](image)

Figure B.1: (a) The picture of neutron scattering and (b) the vector diagram.

From the vector diagram of neutron scattering (Fig.B.1b),

$$Q^2 = k_0^2 + k_1^2 - 2k_1k_0\cos\phi.$$  

For a change in state of the sample from $\lambda_0$ to $\lambda_1$ and a possible change in incident neutron spin from $\sigma_0$ to $\sigma_1$,

Sample State : $\lambda_0 \rightarrow \lambda_1$

Neutron Spin : $\sigma_0 \rightarrow \sigma_1$

The differential cross section is given by the formula :

$$\left(\frac{d\sigma}{d\Omega}\right)_{k_0\sigma_0\lambda_0 \rightarrow k_1\sigma_1\lambda_1} = \frac{1}{N\Phi\Delta\Omega}W_{k_0\sigma_0\lambda_0 \rightarrow k_1\sigma_1\lambda_1},$$
where \( W_{k_0 \sigma_0 \lambda_0 \rightarrow k_1 \sigma_1 \lambda_1} \) is the rate of the transitions.

According to the Fermi’s Golden Rule:

\[
W_{k_0 \sigma_0 \lambda_0 \rightarrow k_1 \sigma_1 \lambda_1} = \frac{2\pi}{\hbar} |\langle k_1 \sigma_1 \lambda_1 | V | k_0 \sigma_0 \lambda_0 \rangle|^2 \rho_{k_1 \sigma_1} (E_1),
\]

where \( V \) is the interaction potential and \( \rho_{k_1 \sigma_1} (E_1) \) is the density of final scattering states per unit energy interval.

In a large box of volume \( V_o \),

\[\text{Incident neutron wavefunction : } \frac{1}{\sqrt{V_o}} e^{ik_0 \cdot \vec{r}} |\sigma_0\rangle,\]

\[\text{Scattered neutron wavefunction : } \frac{1}{\sqrt{V_o}} e^{ik_1 \cdot \vec{r}} |\sigma_1\rangle.\]

The number of states in an energy range \( dE_1 \) is

\[
\rho_{k_1 \sigma_1} (E_1) dE_1 = \frac{V_o}{8\pi^3} d\tau
= \frac{V_o}{8\pi^3} k_1^2 dk_1 \Delta \Omega,
\]

and \( dE_1 = \frac{\hbar^2 k_1 dk_1}{m} \). Therefore,

\[
\rho_{k_1 \sigma_1} (E_1) = \frac{V_o}{8\pi^3} \frac{mk_1}{\hbar^2} \Delta \Omega,
\]

and \( \Phi = \frac{1}{V_o} \bar{\Phi} = \frac{mk_0}{V_{om}} \). After some manipulation,

\[
\frac{d\sigma}{d\Omega} \left|_{k_0 \sigma_0 \lambda_0 \rightarrow k_1 \sigma_1 \lambda_1} \right. = \frac{1}{N} \frac{k_1}{k_0} \left( \frac{m}{2\pi \hbar^2} \right)^2 |\langle k_1 \sigma_1 \lambda_1 | V | k_0 \sigma_0 \lambda_0 \rangle|^2.
\]

Using the conservation of energy, \( E = E_0 - E_1 \) incorporated as \( \delta \)-function giving

\[
\frac{d^2 \sigma}{d\Omega dE} \left|_{k_0 \sigma_0 \lambda_0 \rightarrow k_1 \sigma_1 \lambda_1} \right. = \frac{1}{N} \frac{k_1}{k_0} \left( \frac{m}{2\pi \hbar^2} \right)^2 |\langle k_1 \sigma_1 \lambda_1 | V | k_0 \sigma_0 \lambda_0 \rangle|^2 \delta(E + E_1 - E_0).
\]

Finally, we sum over all the final states of the samples \( \lambda_1 \) and final polarization states of the neutron \( \sigma_1 \), and average over all the initial states \( \lambda_0 \) of the sample.
which occur with probability $p_{\lambda_0}$ and initial states of the neutron which occur with probability, $p_{\sigma_0}$.

\[
\left(\frac{d^2\sigma}{d\Omega dE}\right)_{k_0\sigma_0\lambda_0 \rightarrow k_1\sigma_1\lambda_1} = \frac{1}{N^2 k_0} \left(\frac{m}{2\pi\hbar^2}\right)^2 \sum_{\lambda_0\sigma_0} p_{\lambda_0} p_{\sigma_0} \times \sum_{\lambda_1\sigma_1} |\langle k_1\sigma_1\lambda_1 | V | k_0\sigma_0\lambda_0 \rangle|^2 \delta(E + E_1 - E_0).\]

This is called the “Master formula” for neutron scattering[30].
Bibliography


