

THE T-J MODEL AND SUPERCONDUCTIVITY

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(Received 26 May 2009; Revision Accepted 12, January 2010)

ABSTRACT

The t-J model written in terms of Hubbard operators is studied with a view to contributing to the search for the mechanism of high temperature superconductivity in the cuprates. The method of irreducible Green function is used to obtain the spectrum of quasiparticles excitation and d-wave pairing gap function.

KEY WORDS: Hubbard Operators, Superconductivity, Critical Temperature, Cuprates, t-J model.

INTRODUCTION

The epoch making discovery of the high temperature superconductivity ($\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$) or 214 by Bednorz and Muller (1986) soon led to a frenzy of activities towards finding a correct theory to explain the phenomenon. The Bardeen- cooper- Schrieffer (BCS) theory which describes the phonon- mediated low temperature ($T_c < 30$ k) superconductivity in lead and tin, for example, is inadequate for the Hi-Tc superconductors. The 214 system is a hole superconductor with the tetragonal La_2CuO_4 as a parent compound and unit cell dimensions $a=b=3.8\text{\AA}$, $c=13.2\text{\AA}$. The maximum value of the critical temperature of the 214 compound is about 40K.

The non- phononic mechanisms so far proposed to explain the Hi-Tc superconductivity are excitonic (Freeman et al., 1989), plasmonic (Kresin,1987), polaronic and bipolaronic (Martinez et al., (1991)), fractional statistics (Laughlin, 1989)

None of the above mechanisms is based on the nature of the cuprates which is magnetic. Perhaps that in the reason why their explanations of the superconductivity have had limited scope .

A proper theory and mechanism of superconductivity in the ceramic cuprates should take account of magnetism inherent in the compounds. For the (214) compound experiment have revealed strong antiferromagnetic (AF) correlation in the CuO plane (Masatoshi et al., 1998)

We start with the Hubbard Hamiltonian (Hubbard, 1963)

$$H = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} \dots\dots\dots(1.1)$$

where $c_{i\sigma}$, $c_{i\sigma}^+$ are the Fermi destruction and creation operators at site i and spin σ , $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ is the operator of the number of electrons in the state $i\sigma$, t_{ij} is the matrix element of the electron hopping from site to site, and U is the coulomb repulsion energy. The last term makes allowance for the Pauli principle, so that only two electrons with opposite spins can stay at a site of the lattice. Strong correlation between electrons will appear in a narrow band ($t < u$) making it expedient for U to appear in the zeroth approximation, while t is taken as a small perturbation. The arrows in the second term (1.1)

indicate the up and down directions of the electron spins.

The simple looking Hamiltonian (1.1) is very difficult to solve. The exact solution is available only in the one-dimensional case. It is reasonable to seek equivalent models in the strong coupling limit $U \gg t$. In this case the solution yields the so called t-J model. The essential constraint in the large U-limit is to remove the double occupancy. This can be achieved by using the (Schrieffer et al., (1966)) canonical transformation

$$H_{eff} = e^{is} H e^{-is} \\ = H + [is, H] + \frac{1}{2} [is, [is, H]] + \dots\dots\dots(1.2)$$

In that case the Hamiltonian (1.1) may be written in the form

$$H = T + V \dots\dots\dots(1.3)$$

where

$$T = t \sum_{ij,\sigma} I_{ij} c_{i\sigma}^+ c_{j\sigma} \dots\dots\dots(1.4)$$

$$V = U \sum_i n_{i\uparrow} n_{i\downarrow} \dots\dots\dots(1.5)$$

The factor $I_{ij} = 1$ for nearest neighbour and zero otherwise. We multiply (4) by $n_{i-\sigma} + h_{i-\sigma} = 1$ on the left and by $n_{j-\sigma} + h_{j-\sigma}$ on the right, where $h_{i-\sigma}$ is the hole and $n_{i-\sigma}$ the electron occupation numbers.

The followings are obtained

$$T_0 = t(n_{i-\sigma} c_{i\sigma}^+ c_{j\sigma} n_{j-\sigma} + h_{i-\sigma} c_{i\sigma}^+ c_{j\sigma} h_{j-\sigma}) \dots\dots\dots(1.6)$$

$$T_1 = t n_{i-\sigma} c_{i\sigma}^+ c_{j\sigma} h_{j-\sigma} \dots\dots\dots(1.7)$$

$$T_{-1} = t h_{i-\sigma} c_{i\sigma}^+ c_{j\sigma} n_{j-\sigma} \dots\dots\dots(1.8)$$

Here T_0 describes hopping between two doubly occupied sites (i,j)(first term) and two singly occupied sites (second term). T_1 increases the number of doubly occupied sites by 1, T_{-1} decreases the number of doubly occupied sites by 1. If we form the commutator $[V, T_1] = -uT_1$ and $[V, T_{-1}] = -u T_{-1}$; then we can choose

$$iS = u^{-1}(T_1 - T_{-1}) \dots\dots\dots(1.9)$$

Hence

$$H_{eff} = -t \sum_{ij,\sigma} h_{i-\sigma} c_{i\sigma}^+ c_{j\sigma} c_{j-\sigma} + \frac{4t^2}{u} \sum_{ij,\sigma} \left(S_i S_j - \frac{1}{4} n_i n_j \right) \dots\dots\dots(1.10)$$

where the spin of the lattice site is defined by

$$S_i = c_i^+ \frac{\sigma}{2} c_j \dots\dots\dots(1.11)$$

and σ is the Pauli matrices of the electron spin.

Usually eqn. (1.10) is written as

$$H_{t-J} = -t \sum_{ij,\sigma} h_{i-\sigma} c_{i\sigma}^+ c_{j\sigma} h_{j-\sigma} + J \sum_{ij,\sigma} \left(S_i S_j - \frac{1}{4} n_i n_j \right) \dots\dots\dots(1.12)$$

where the coupling constant

$$J = \frac{4t^2}{u} \dots\dots\dots(1.13)$$

Equation (1.12) represents the t-J model.

It should be noted that at half -filling, each site is occupied by one hole which makes the first term in (1.12) to vanish ,thus recovering the Heisenberg Hamiltonian for the antiferromagnetic (AF) lattice.

THE HUBBARD OPERATORS

The Hubbard or X-operator is defined as (Hubbard,1964)

$$X_i^{pq} = |i, p\rangle \langle i, q| \dots\dots\dots(2.1)$$

The operator X_i^{pq} changes the atomic state or configuration from q to p on the site i without affecting other sites. The states are listed as

$$(|p\rangle, \langle q|) = (|0\rangle, \langle 0|), (|+1\rangle, \langle +1|), (|-1\rangle, \langle -1|), (|2\rangle, \langle 2|) \dots \dots \dots (2.2)$$

The electron creation and annihilation operators are related to the X-operators by the expressions

$$c_\sigma = X^{0\sigma} + \sigma X^{\bar{\sigma}2}, c_\sigma^+ = X^{\sigma 0} + \sigma X^{2\bar{\sigma}} \dots \dots \dots (2.3)$$

Where $\sigma = \pm 1$ or $\uparrow\downarrow$

The t-J model as we have seen arises from the general Hubbard Hamiltonian (1.1) in the limit $U \gg t$, as two electrons per site is excluded in the order of perturbation theory. Let us now write the t-J model (1.12) in terms of the projected creation and annihilation operators:

$$H_{t-J} = -t \sum_{ij} \tilde{c}_{i\sigma}^+ \tilde{c}_{j\sigma} + J \sum_{ij} \left(S_i S_j - \frac{1}{4} n_i n_j \right) \dots \dots \dots (2.4)$$

where the projection operators are

$$\tilde{c}_{i\sigma}^+ = (1 - n_{i-\sigma}) c_{i\sigma}^+ \dots \dots \dots (2.5)$$

$$\tilde{c}_{j\sigma} = c_{j\sigma} (1 - n_{j-\sigma}) \dots \dots \dots (2.6)$$

The X- operators obey the completeness relation

$$X_i^{00} + \sum_{\sigma} X_i^{\sigma\sigma} = 1 \dots \dots \dots (2.7)$$

which ensures that the constraint of no double occupancy is satisfied.

Let us express the spin and number density operators in terms of X-operators as follows:

$$S_i = c_i^+ \frac{\sigma}{2} c_i = \frac{1}{2} X_i^{\sigma\bar{\sigma}} \dots \dots \dots (2.8)$$

$$S_i S_j = X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} \dots \dots \dots (2.9)$$

$$n_i n_j = n_{i\uparrow} n_{j\downarrow} = X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \dots \dots \dots (2.10)$$

We may now add the chemical potential μ to (2.4) to obtain

$$H_{t-J} = -t \sum_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \mu \sum_{i\sigma} X_i^{\sigma\sigma} + \frac{1}{4} \sum_{i \neq j, \sigma} J_{ij} (X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}}) \dots \dots \dots (2.11)$$

The hopping energy t_{ij} of (1.1) has been replaced here by t for nearest neighbours and the exchange interaction J_{ij} by J on the 2D square lattice .

SUPERCONDUCTIVE PAIRING

An approach to the electron or hole d-wave pairing mechanism can be made by introducing the two components Nambu operators

$$X_i^\sigma = \begin{pmatrix} X_i^{0\sigma} \\ X_i^{\bar{\sigma}0} \end{pmatrix}, X_i^{\sigma+} = (X_i^{\sigma 0}, X_i^{0\bar{\sigma}}) \dots \dots \dots (3.1)$$

The two time anticommutator matrix Green function in the above representation is written as

$$G_{ij}^\sigma(t-t') = \langle\langle X_i^\sigma(t) X_j^{\sigma+} \rangle\rangle = \left(\begin{array}{cc} \langle\langle X_i^{0\sigma}(t) X_i^{\sigma 0}(t') \rangle\rangle & \langle\langle X_i^{0\sigma}(t) X_j^{0\bar{\sigma}}(t') \rangle\rangle \\ \langle\langle X_i^{(\bar{\sigma})0}(t) X_j^{\sigma 0}(t') \rangle\rangle & \langle\langle X_i^{(\bar{\sigma})0}(t) X_j^{0\bar{\sigma}}(t') \rangle\rangle \end{array} \right) \dots\dots\dots(3.2)$$

The diagonal matrix elements are the normal Green functions while the non –diagonal elements represents the anomalous Green functions.The Fourier transform of the Green function is

$$G_{ij}^\sigma(t-t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} G_{ij}^\sigma(\omega) e^{-i\omega(t-t')} d\omega \dots\dots\dots(3.3)$$

To obtain the quasiparticle spectrum of the system one can use the method of the irreducible. Green functions .In this method (Plakida N.M. et al., 1989;Kuzemsky A.L,2002),the equation of motion for the Green function is first obtained as

$$i \frac{d}{dt} \langle\langle X_i^\sigma(t) X_j^{\sigma+}(t') \rangle\rangle = \delta(t-t') \langle[X_i^\sigma(t), X_j^{\sigma+}(t')]\rangle + \langle\langle [X_i^\sigma(t), H] X_j^{\sigma+}(t') \rangle\rangle \dots\dots\dots(3.4)$$

The quantity $\langle[X_i^\sigma(t), H]\rangle$ in (3.4) is found by expressing the equation of motion for a dynamical variable $X_i^\sigma(t)$ in the form

$$i \frac{d}{dt} X_i^\sigma(t) = [X_i^\sigma, H] = \sum_l A_{il}^\sigma X_l^\sigma(t) + L_i^\sigma(t') \dots\dots\dots(3.5)$$

In the last expression $L_i^\sigma(t')$ is the irreducible part of the operator $X_i^\sigma(t)$.The quantity $L_i^\sigma(t')$ is defined as an operator orthogonal to the linear term $\sum_l A_{il}^\sigma X_l^\sigma$ by the form

$$\langle[L_i^\sigma, X_l^{\sigma+}] \rangle = 0 \dots\dots\dots(3.6)$$

Now substituting eqn.(3.5)in (3.6), we have

$$\sum_l A_{il}^\sigma \langle[X_l^\beta, X_j^{\sigma+}] \rangle = \langle[[X_i^\sigma, H], X_j^{\sigma+}] \rangle \dots\dots\dots(3.7)$$

In this way the coefficients $(A_{ij}^\sigma)_{\alpha\beta}$ are defined ,and they reflect the irreducible part of the Green function .The normal components of the $(A_{ij}^\sigma)_{\alpha\beta}$ matrix are $(A_{ii}^\sigma)_{11}, (A_{ii}^\sigma)_{22}$,

the anomalous ones are $(A_{ii}^\sigma)_{12}, (A_{ii}^\sigma)_{21}$. The Fourier transform of the components are $\Omega_q^\sigma = (A_{ii}^\sigma)_{11} + \sum_{i \neq l} (A_{il}^\sigma)_{11} e^{-iq(\vec{i}-\vec{l})} \dots\dots\dots(3.8)$

$$\Delta_q^\sigma = (A_{il}^\sigma)_{12} + \sum_{i \neq l} (A_{i,l}^\sigma)_{12} e^{-iq(\vec{i}-\vec{l})} \dots\dots\dots(3.9)$$

In view of eqn. (3.5) ,(3.4) becomes

$$i \frac{d}{dt} \langle\langle X_i^\sigma(t) X_j^{\sigma+} \rangle\rangle = \langle[X_i^\sigma, X_j^{\sigma+}] \rangle + \left\langle \left\langle \sum_l A_{il}^\sigma X_l^\sigma(t) + L_i^\sigma(t') X_j^\sigma \right\rangle \right\rangle = \langle[X_i^\sigma, X_j^{\sigma+}] \rangle + \sum_l A_{il}^\sigma \langle\langle X_i^\sigma(t) X_j^\sigma(t') \rangle\rangle + \langle\langle L_i^\sigma(t') X_j^\sigma(t) \rangle\rangle \dots\dots\dots(3.10)$$

The last term represents the irreducible Green function,on one hand it is proportional to the scattering matrix $\langle\langle L_i^\sigma | L_i^{\sigma+} \rangle\rangle$.All inelastic processes are described by this matrix and it is proportional to higher order of t and J; on the

other hand it can be approximated to the chemical potential μ . We shall use the latter consideration to write (3.10) as follows

$$i \frac{d}{dt} G_{ij}(t-t') = \langle [X_i^\sigma, X_j^{\sigma+}] \rangle + \sum_{l=i} A_{il}^\sigma G_{lj}(t-t') - \sum_{l=i} \mu_{il} G_{ij} \dots (3.11)$$

$$\text{Hence } \left(i \frac{d}{dt} - (A_{ij}^\sigma)_{\alpha\beta} + \mu_{ii} \right) G_{ij}(t) = \langle [X^\sigma, X^{\sigma+}] \rangle \dots (3.12)$$

Taking the Fourier transform of the last expression, we can represent the result in a matrix form

$$\begin{pmatrix} \omega - \Omega_q^\sigma + \mu & \Delta_q^\sigma \\ (\Delta_q^\sigma)^* & \omega + \Omega_q^\sigma - \mu \end{pmatrix} \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} = \begin{pmatrix} \langle Q_i^\sigma \rangle & o \\ o & \langle Q_i^{\bar{\sigma}} \rangle \end{pmatrix} \dots (3.13)$$

$$\text{where } \mu_{11} = -\mu_{22}, \Delta_{12}^\sigma = (\Delta_{21}^\sigma)^*, (\Omega_{ij}^\sigma)_{11} = (\Omega_{ij}^\sigma)_{22}$$

In the diagram technique developed by (Izuykov et al., 1990) the quantity $\langle Q_i^\sigma \rangle$ is equivalent to the end point $\langle F^{\sigma 0} \rangle = 1 - n_\sigma$. When we replace G_{ij} of (3.13) with the definition (3.2) we obtain the normal and anomalous Green functions respectively as

$$\langle \langle X^{0\sigma} | X^{\sigma 0} \rangle \rangle_{w,q} = \langle Q_i^\sigma \rangle \frac{\omega + \Omega_q^\sigma - \mu}{\omega^2 - (\Omega_q^\sigma - \mu)^2 - |\Delta|^2} \dots (3.14)$$

$$\langle \langle X^{\bar{\sigma} 0} | X^{\sigma 0} \rangle \rangle_{w,q} = -\langle Q_i^\sigma \rangle \frac{(\Delta_q^\sigma)^*}{\omega^2 - (\Omega_q^\sigma - \mu)^2 - |\Delta|^2} \dots (3.15)$$

The quasiparticle energy spectrum is

$$(E_q^\sigma)^2 = (\Omega_q^\sigma - \mu)^2 - |\Delta|^2 \dots (3.16)$$

Since the Green function $G_{ij}(t-t')$ is a linear combination of correlation functions, then it is clear that (3.14) and (3.15) may be written in terms of the correlation functions

$$\langle X^{0\sigma} X^{\sigma 0} \rangle = \left(1 - \frac{n}{2} \right) \frac{\omega + \Omega_q^\sigma - \mu}{\omega^2 - (E_q^\sigma)^2} \dots (3.17)$$

$$\langle X^{\bar{\sigma} 0} X^{\sigma 0} \rangle = -\left(1 - \frac{n}{2} \right) \frac{(\Delta_q^\sigma)^*}{\omega^2 - (E_q^\sigma)^2} \dots (3.18)$$

The energy gap in the quasiparticle spectrum is determined by the anomalous correlation function (3.18). The anomalous Green function (3.15) can be calculated to give

$$\langle \langle X^{\bar{\sigma} 0} | X^{\sigma 0} \rangle \rangle_{q,w} = -\langle Q_i^\sigma \rangle \frac{(\Delta_q^\sigma)^*}{2E_q^\sigma} \tanh \frac{E_q^\sigma}{2T} \dots (3.19)$$

Finding the complex value of the last equation one obtains

$$\langle \langle X^{0\bar{\sigma}} | X^{0\sigma} \rangle \rangle_{q,w} = -\left(1 - \frac{n}{2} \right) \frac{\Delta_q^\sigma}{2E_q^\sigma} \tanh \frac{E_q^\sigma}{2T} \dots (3.20)$$

and the correlation function is now

$$\langle X_{-q}^{\bar{\sigma} 0} X_q^{\sigma 0} \rangle = \left(1 - \frac{n}{2} \right) \frac{\Delta_q^\sigma}{2E_q^\sigma} \tanh \frac{E_q^\sigma}{2T} \dots (3.21)$$

Equation (3.7) can now be solved to yield the coefficients (3.9) in the form

$$\Delta_q^\sigma = -\frac{2}{\langle Q^\sigma \rangle} \sum_q \{t(q) - J(k-q)\} \langle X_{-q}^{\bar{\sigma}0} X_q^{\sigma 0} \rangle \dots (3.22)$$

Combining the last two expressions, a self consistent equation for the superconducting gap is obtained

$$\Delta_k^\sigma = \frac{2}{N \langle Q_i^\sigma \rangle} \sum_q \{t(q) - J(k-q)\} \frac{\Delta_q^\sigma}{2E_q^\sigma} \tanh \frac{E_q^\sigma}{2T} \dots (3.23)$$

There are two contributions to the gap equation :the k –independent kinematic interaction (t) and the k-dependent exchange interaction J(k-q).The kinematic term does not contribute to the d-wave pairing (Plakida N.M,1996),as a result that term vanishes in (3.23).For the singlet pairing in the d-wave symmetry the gap function is

$$\Delta_d(k) = \Delta_d(\cos k_x a - \cos k_y a) \dots (3.24)$$

This gap function must be subjected to the restriction of no double occupation of the same site through the anomalous correlation function

$$\langle X_{-q}^{\bar{\sigma}0} X_q^{\sigma 0} \rangle = \frac{\langle Q^\sigma \rangle}{N} \sum_q \frac{\Delta_q^\sigma}{2E_q^\sigma} \tanh \frac{E_q^\sigma}{2T} = 0 \dots (3.25)$$

Obviously this equation is satisfied only by the d-wave pairing gap. Thus the d-wave solution to (3.23) is

$$\Delta_d(k) = \frac{J}{N} \sum_q \frac{\Delta_d(q)}{E_q^\sigma} \tanh \frac{E_q^\sigma}{2T} \dots (3.26)$$

This is a BCS-type equation (see e.g ,Schrieffer J.R 1964) and its solution gives the critical temperature T_c .

DISCUSSION

Based on the Hubbard operators the strong correlation of electrons or holes in the CuO_2 plane of the cuprate ($\text{La}_{1-x}\text{Sr}_x\text{CuO}_4$) has been studied and found to yield a BCS –type spectrum in the mean field approximation. The irreducible Green function method is an approach based on the equation of motion for the two-time Green function. It naturally precipitates the last term in (3.10) that indicates inelastic scattering in the system.

The Hubbard operators are particularly useful for studying inelastic scattering since they describe the altered final and initial states of the system very adequately.

The greatest problem in high temperature superconductivity theory is the justification of pairing of two holes or electrons with a large Coulomb repulsion between them .This problem can be examined by using Hirsch's (Hirsch J.E ,2009) suggestions of dressing and undressing of holes.

This, however shall receive attention in another paper.

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