The Driving Force of Superconducting Transition in High Temperature Superconductors

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Abstract

We show that both the kinetic energy and the exchange energy of the t-J model can be read off from the optical data. We show that the optical data indicates that the superconducting transition in high temperature superconductors is kinetic energy driven and the exchange energy resist the transition. We also show that kinetic energy may also be the driving force of the pseudogap phenomenon.
The question of the driving force of the superconducting transition in high temperature superconductors is hotly debated upon in recent years. Two school of thoughts compete. In terms of the t-J model, they are called kinetic energy driving mechanism and exchange energy driving mechanism. Since the competition of the kinetic energy and the exchange energy is the key to understanding the high-Tc physics in the t-J model perspective, an unambiguous answer to the driving force question is important.

In conventional BCS superconductors, the superconducting transition is driven by some attractive pairing potential between electrons and the kinetic energy is frustrated in the paired superconducting state. In the high temperature superconductors, the kinetic energy is frustrated in the half-filled parent compounds which are Mott insulators. Carrier doping releases the frustrated kinetic energy and lead to high temperature superconductivity for sufficiently large doping concentration. Hence a kinetic energy driving mechanism seems quite reasonable at least on the underdoped side of the phase diagram. However, arguments for exchange energy driving mechanism can also be made since it is the antiferromagnetic exchange that pair the electrons into local spin singlet. Especially, the SO(5) theory claims that the superconducting transition in the high Tc superconductors is driven by the exchange energy saving as the so called π - resonance open a new channel for antiferromagnetic spin fluctuation in the superconducting state.

Experimentally, the kinetic energy can be measured with the help of the optical sum rule. According to this rule, the absolute value of the kinetic energy of a single band model is equal to the total intraband optical transition rate, i.e.

$$\langle -K \rangle = \int_0^\Omega \sigma_1(\omega)\,d\omega$$

here $K$ is the kinetic energy of the model, $\sigma_1(\omega)$ is the real part of the optical conductivity, $\Omega$ is the energy cutoff for intraband transition. In the case of the t-J model, an intraband transition is a transition within the subspace of no double occupancy. The corresponding cutoff energy $\Omega$ is set by the gap between this subspace and the subspace with doubly occupied sites, i.e. the Hubbard gap. Recently, optical measurement on $BSCCO_{2212}$ find a spectral weight transfer from the high energy part of the spectrum($10^4 cm^{-1}$ to $2 \times 10^4 cm^{-1}$) to the low energy part of the spectrum(below $10^4 cm^{-1}$ ) with decreasing temperature in both optimally doped and underdoped samples. If we take $10^4 cm^{-1}$ as the energy cutoff of the intraband transition in the t-J model, then the experimental result indicates that the
kinetic energy is lowered with decreasing temperature. This result is taken as evidence in support of the kinetic energy driving mechanism. The decrease of the kinetic energy in the superconducting state estimated from the optical data is about $1\,\text{meV}$ per cooper atom, an order of magnitude larger than the superconducting condensation energy estimated from thermodynamical measurements.[8]

However, the neutron scattering experiments tell a quite different story[7]. The neutron scattering experiments measure the spin fluctuation spectrum of the system. By integrating the spectrum with suitable weighting factor, the exchange energy can be deduced[5]. This is expressed as the following sum rule

$$\langle S_i \cdot S_j \rangle = 3 \int \frac{dq^2}{(2\pi)^2} \int_{0}^{\infty} \frac{d\omega}{\pi} \text{Im} \chi(q, \omega) \cos[q \cdot (i - j)]$$

where $\text{Im} \chi(q, \omega)$ is the spin fluctuation spectrum of the system. In high temperature superconductors, the spin fluctuation spectrum develops a resonant mode around $(\pi, \pi)$ in the superconducting state[9]. This mode give a negative contribution to the exchange energy which is argued by some author to be the source of the superconducting condensation energy[6, 7]. The superconducting condensation energy estimated in this way is also an order of magnitude larger than that estimated from thermodynamical measurements. Obviously, the conclusions reached by optical measurements and the neutron measurements can not be both correct. Since optical data has higher resolution and covers larger energy range as compared with the neutron data, we expect the optical conclusion to have a better chance to survive.

The key observation made in this paper is that both the kinetic energy and the exchange energy in the t-J model are kinetic energy in nature and can both be measured with optics. This is almost obvious if we realize that the t-J model is in fact a low energy effective theory of an underlying Hubbard-type model. The kinetic energy term in the t-J model corresponds to the real kinetic process within the subspace of no double occupancy while the exchange energy term corresponds to the virtual kinetic process which involve doubly occupied sites in intermediate step. Here we take the standard Hubbard model to demonstrate the idea

$$H = H_t + H_U = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

In the large $U$ limit, the Hubbard model reduce to the t-J model in the low energy subspace
of no double occupancy. This is usually done by dividing the Hilbert space into the low energy subspace of no double occupancy and the high energy subspace with nonzero doubly occupied sites. In the large $U$ limit, the two subspaces are separated by a gap of order $U$. Correspondingly, the Hamiltonian can be divided into intra-subspace pieces and inter-subspace pieces. Introducing the projection operator $P_L$ and $P_H$ for the low energy subspace and the high energy subspace, the Hubbard Hamiltonian can be written as

$$H = H_L + H_H + H_{\text{mix}}$$

in which

$$H_L = P_L H t P_L$$
$$H_H = P_H H t P_H + H_U$$
$$H_{\text{mix}} = P_L H t P_H + P_H H t P_L$$

are the Hamiltonian in the low energy subspace, Hamiltonian in the high energy subspace and the subspace-mixing term. The subspace-mixing term can be removed by a canonical transformation $e^{iS}$. To first order of $\frac{t}{U}$, the transformed Hamiltonian in the low energy subspace is the standard t-J model

$$e^{iS} H e^{-iS} = H_{t-j} = P_L H t P_L + \frac{i}{2} [S, H_{\text{mix}}]$$

$$= -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c.) + J \sum_{\langle i,j \rangle} (S_i \cdot S_j - \frac{1}{4} n_i n_j)$$

where $\hat{c}_{i,\sigma} = (1 - n_{i,\sigma}) c_{i,\sigma}$, $\vec{S}_i = \frac{1}{2} c_{i,\alpha}^\dagger \vec{\sigma} c_{i,\beta}$, $J = \frac{4t^2}{U}$. Under the canonical transformation, the kinetic energy of the Hubbard model transforms into

$$e^{iS} H t e^{-iS} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c.) + 2J \sum_{\langle i,j \rangle} (S_i \cdot S_j - \frac{1}{4} n_i n_j)$$

in the low energy subspace to first order of $\frac{t}{U}$. The potential energy of the Hubbard model transforms into
\[e^{iS} H_U e^{-iS} = -J \sum_{\langle i,j \rangle} \left( S_i \cdot S_j - \frac{1}{4} n_i n_j \right)\]

in the low energy subspace to the same order. Note the transformed form of \( H_U \) is still positive definite. From these formulas, we see explicitly the relation between the charge response in the t-J model and that of the underlying Hubbard model. Especially, we see how the exchange term of the t-J model (which is charge neutral in the subspace of no double occupancy) contribute to the charge response of the underlying Hubbard model. According to the optical sum rule, the kinetic energy of the Hubbard model is related to its total optical response in the following way

\[
\langle -e^{iS} H_t e^{-iS} \rangle = \int_0^\Lambda \sigma_1 (\omega) d\omega
\]

where \( \Lambda \) is the energy cutoff for the Hubbard model. Here we assume that other bands of the system are far away from the Fermi surface and the optical weight measured in experiment is due to a single band. The total optical weight of the Hubbard model is composed of two contributions, namely the optical response within the subspace of no double occupancy and the optical response involving doubly occupied sites. The first contribution is just the optical response of the t-J model. According to the optical sum rule, this contribution is related to kinetic energy of the t-J model in the following way

\[
\left\langle t \sum_{(i,j),\sigma} (\hat{c}_i^\dagger \sigma \hat{c}_j^\sigma + h.c.) \right\rangle = \int_0^\Omega \sigma_1 (\omega) d\omega
\]

Hence the high energy optical weight, i.e. the optical weight between \( \Omega \) and \( \Lambda \) is related to the exchange energy of the t-J model in the following way

\[
\left\langle -2J \sum_{\langle i,j \rangle} \left( S_i \cdot S_j - \frac{1}{4} n_i n_j \right) \right\rangle = \int_\Omega^\Lambda \sigma_1 (\omega) d\omega
\]

Thus, if we can determine the energy cutoff \( \Lambda \) and \( \Omega \), we can read off both the kinetic energy and the exchange energy of the t-J model from the optical data.

The energy cutoff \( \Omega \) of the t-J model for cuprates is about \( 10^4 cm^{-1} \) where a conductivity minimum separate the intraband transition and the interband transition\[4\]. The value of the energy cutoff \( \Lambda \) of the Hubbard model is subjected to some uncertainty. Here we adopt the value \( 2 \times 10^4 cm^{-1} \) below which reliable optical data is available\[4\]. Experimentally, the
spectral weight between $10^4 cm^{-1}$ to $2 \times 10^4 cm^{-1}$ transfers steadily to below $10^4 cm^{-1}$ with decreasing temperature with the total spectral weight approximately conserved [4]. According to our analysis in the last paragraph, this indicates that the kinetic energy of the t-J model decreases steadily with decreasing temperature while the exchange energy increases steadily with decreasing temperature. Closer examination on the data shows that both energies change more rapidly upon entering the superconducting state. This shows convincingly that the superconducting transition is kinetic energy driven while the exchange energy resist the transition. Also, we note since the kinetic energy and the exchange energy evolve in opposite direction with temperature, the true superconducting condensation energy should be smaller than that estimated from the kinetic energy alone.

Finally, we note the optical measurement can also serve as a probe of driving force for other phenomena in high temperature superconductors such as pseudogap, stripes and et al. For example, the steady increase of the exchange energy with decreasing temperature seems at odd with the conventional understanding of the pseudogap as some kind of spin pairing gap driven the exchange energy of the t-J model [10]. This indicates that the kinetic energy of the t-J model plays an important role in the formation of the pseudogap [11, 12]. In this respect it is interesting to do optical measurement on overdoped samples where the spin gap and the superconducting transition are believed to be exchange energy driven.

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