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Current flow around small polarons embedded in a Mott insulator

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Abstract

A doped hole in the parent compound of the superconducting cuprate is believed to form so-called, ''Zhang–Rice Singlet'' (ZRS). Recent theoretical calculations indicate that the ZRS causes local lattice deformation and the doped hole becomes a small polaron (pseudo Jahn–Teller polaron) that moves with large effective mass. The formation of pseudo Jahn–Teller polarons with large effective mass seems to contradict the observed small effective mass of the charge carrier ($m^*/m \approx 3$); however, we argue that this contradiction is removed if the small polaron becomes a core of a meron (a vortex in spin configuration with winding number +1) or an antimeron (a vortex in spin configuration with winding number −1). We show that if polaronic cores of merons and antimerons are formed, electrons surrounding the cores become itinerant.

Keywords: Theoretical calculations; Mott Insulator; Cuprate superconductivity

1. Introduction

It has been already 20 years since the high temperature superconductivity was discovered in cuprates [1]. In spite of very intensive and extensive researches, the mechanism for it is still not elucidated.

The parent (undoped) cuprate is believed to be a Mott insulator which is well described by the Hubbard model; however, for the electronic state when holes are doped in the parent compound, no clear picture has been obtained, yet. According to photoemission measurements, doped holes are mainly in oxygen p-orbitals that surround a copper in the CuO_2 plane [2]; the hole in the oxygen p-orbitals and that in the copper $d_{x^2-y^2}$ orbital form a spin singlet pair called the ''Zhang–Rice singlet'' (ZRS) [3]. It is now widely believed that metallic conductivity is due to the hopping of the ZRS; and effective Hamiltonian that describes correlated hopping of ZRS's are enough to understand the cuprate superconductivity. However, this view should be more critically examined since strong electron–lattice interaction exists in this system.

The relevance of the electron–lattice interaction to the cuprate superconductivity has been a controversial issue. The motivation behind the discovery of the high T_c cuprates by Bednorz and Müller is the expected strong vibronic interaction within the building block CuO_6 complex [4]. But it has been argued that the only on-site Coulomb repulsion is relevant; the observation of a Drude like peak in the optical conductivity measurement [5] and Fermi arc [6] in relatively low doping samples indicate small effective mass ($m^*/m \approx 3$) for the charge carrier; which is interpreted to indicate that the small polaron formation by the strong electron–lattice interaction is irrelevant. On the other hand, recent molecular orbital cluster calculations by Hozoi et al. [7] and Miyaki et al. [8] clearly show that the vibronic interaction is very strong; the Zhan–Rice singlet has a character of pseudo Jahn–Teller polaron [9]. This suggests that in the low hole doping region where small polarons are intact, the hopping of ZRS's may not be the dominant current generation process.

In the present work, we give theoretical result that suggests the small effective mass of charge carrier observed in underdoped cuprates may be attributed to itineracy of the background electrons that surround the holes. We show that the itinerancy of the electrons is retrieved and current

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flow regions appear around the holes when the holes become cores of merons (vortices in spin configuration with winding number +1) or antimerons (vortices in spin configuration with winding number −1) [10].

2. Current flow region in Mott insulator

We use the Hubbard model given by

$$H = -t\sum_{\langle i,j\rangle,\sigma}(c^{\dagger}_{j\sigma}c_{i\sigma} + \text{h.c.}) + U\sum_{j} c^{\dagger}_{j\uparrow}c_{j\uparrow}c^{\dagger}_{j\downarrow}c_{j\downarrow}, \tag{1}$$

in a two-dimensional square lattice; the first term is the kinetic energy term where the sum is taken over nearest neighbor pairs of sites, and the second term describes the on-site Coulomb interaction. It is known that parent (undoped) compounds of superconducting cuprates are well described by this model.

For a Mott insulator, the Coulomb interaction parameter U is much larger than the transfer integral t; thus, the Coulomb interaction term is the dominant one. In this situation, the representation that diagonalizes the Coulomb term is useful. We use creation and annihilation operators that diagonalize the following mean field version of the Coulomb term

$$-U\left(\Delta^{*}_{j}c^{\dagger}_{j\uparrow}c_{j\downarrow} + \Delta_{j}c^{\dagger}_{j\downarrow}c_{j\uparrow}\right) = -U|\Delta_{j}|\left(a^{\dagger}_{j}a_{j} - b^{\dagger}_{j}b_{j}\right), \tag{2}$$

where the mean field at site j is defined as $\Delta_j = |\,\Delta_j\,|\,e^{i\xi_j} = \langle c^{\dagger}_{j\uparrow}c_{j\downarrow}\rangle$, and the new annihilation operators a_j and b_j are defined in relation to the original as

$$\begin{pmatrix} b_j \\ a_j \end{pmatrix} = \frac{e^{i\frac{\chi_j}{2}}}{\sqrt{2}}\begin{pmatrix} e^{i\frac{\xi_j}{2}} & -e^{-i\frac{\xi_j}{2}} \\ e^{i\frac{\xi_j}{2}} & e^{-i\frac{\xi_j}{2}} \end{pmatrix}\begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow} \end{pmatrix}. \tag{3}$$

The phase factor $e^{i\frac{\chi_j}{2}}$ is added in Eq. (3) so that the transformation matrix is single-valued. When ξ is changed by 2π, $e^{\pm i\frac{\xi}{2}}$ changes sign, $e^{\pm i\frac{\xi_j+2\pi}{2}} = -e^{\pm i\frac{\xi_j}{2}}$, although ξ and $\xi+2\pi$ are physically the same. The added phase factor compensates this sign change by the sign change $e^{i\frac{\chi_j+2\pi}{2}} = -e^{i\frac{\chi_j}{2}}$. We may choose $\chi = \xi$ for this purpose; however, it is not necessary to specify it in the following discussion.

The expectation values of the x and y components of the spin operator are given by

$$\langle S_x(j)\rangle = \frac{1}{2}\langle c^{\dagger}_{j\uparrow}c_{j\downarrow} + c^{\dagger}_{j\downarrow}c_{j\uparrow}\rangle = |\,\Delta_j\,|\cos\xi_j$$

$$\langle S_y(j)\rangle = \frac{i}{2}\langle -c^{\dagger}_{j\uparrow}c_{j\downarrow} + c^{\dagger}_{j\downarrow}c_{j\uparrow}\rangle = |\,\Delta_j\,|\sin\xi_j,$$

thus, the phase ξ_j has the meaning of the spin polarization direction in the x–y plane.

Using the new creation and annihilation operators, the kinetic energy term in Eq. (1) becomes

$$K = -\sum_{\langle k,j\rangle}\left[te^{\frac{i}{2}(\chi_j-\chi_k)}\cos\frac{\xi_j-\xi_k}{2}\left(a^{\dagger}_{j}a_{k} + b^{\dagger}_{j}b_{k}\right) + ite^{\frac{i}{2}(\chi_j-\chi_k)}\sin\frac{\xi_j-\xi_k}{2}\left(a^{\dagger}_{j}b_{k} + b^{\dagger}_{j}a_{k}\right) + \text{h.c.}\right], \tag{4}$$

and the Coulomb energy term in Eq. (1) becomes

$$H_U = U\sum_{j} a^{\dagger}_{j}a_{j}b^{\dagger}_{j}b_{j}. \tag{5}$$

Let us split the Hamiltonian as $H = H_0 + H_1$, where H_1 is a perturbation given by

$$H_1 = -\sum_{\langle k,j\rangle}\left[ite^{\frac{i}{2}(\chi_j-\chi_k)}\sin\frac{\xi_j-\xi_k}{2}\left(a^{\dagger}_{j}b_{k} + b^{\dagger}_{j}a_{k}\right) + \text{h.c.}\right] \tag{6}$$

and $H_0 = K + H_U - H_1$.

The Eq. (2) indicates that the energy for the state vector $a^{\dagger}_{j}\,|\,\text{vac}\rangle$ ($|\text{vac}\rangle$ is the vacuum) is lower than that for $b^{\dagger}_{j}\,|\,\text{vac}\rangle$. Then, in the large U limit with half-filling, the ground state vector for H_0 is given by

$$|\,0\rangle = \prod_{j} a^{\dagger}_{j}\,|\,\text{vac}\rangle, \tag{7}$$

where j runs through all the sites. The total energy for this state is zero.

Now we take into account the perturbation H_1. We denote excited states as

$$|i,\alpha\rangle = \tilde{b}^{\dagger}_{\alpha}a_{i}|0\rangle, \tag{8}$$

where the creation operators $\tilde{b}^{\dagger}_{\alpha}$ are related to $b^{\dagger}_{j}$ as

$$\tilde{b}_{\alpha} = \sum_{j} e^{-\frac{i}{2}\chi_j}U_{\alpha j}b_{j}. \tag{9}$$

The matrix $\{U_{\alpha j}\}$ is an orthogonal matrix, with which the kinetic energy term for the upper band is diagonalized as

$$-t\sum_{\langle k,j\rangle} e^{\frac{i}{2}(\chi_j-\chi_k)}\cos\frac{\xi_j-\xi_k}{2}\left(b^{\dagger}_{j}b_{k} + b^{\dagger}_{j}b_{k}\right) = \sum_{\alpha}\varepsilon_{\alpha}\tilde{b}^{\dagger}_{\alpha}\tilde{b}_{\alpha}. \tag{10}$$

Within the first order perturbation in H_1, the ground state vector $|0'\rangle$ is given as $|0'\rangle = |0\rangle + |1\rangle$, where

$$|1\rangle = \sum_{m,j,\alpha}\frac{it_{mj}|j,\alpha\rangle}{U+\epsilon_{\alpha}}e^{-\frac{i}{2}\chi_m}e^{\frac{i}{2}(\chi_m-\chi_j)}\sin\frac{\xi_m-\xi_j}{2}U_{\alpha m}, \tag{11}$$

t_{mj} are parameters equal to t if m and j are the nearest neighbor sites, and to zero otherwise.

Let us calculate current density for $|0'\rangle$. The operator for the x-component of current density with spin σ is given by

$$\hat{j}_{x\sigma}(l) = it\left(c^{\dagger}_{l+x\sigma}c_{l\sigma} - c^{\dagger}_{l\sigma}c_{l+x\sigma}\right) \tag{12}$$

where $l+x$ denotes the nearest neighbor site of l in the x direction (electric current density is $-e\hat{j}_{x\sigma}(l)$, where $-e$ is electron charge).

Using Eqs. (7), (11) and (12), the expectation value for the up-spin current density is obtained as