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Effect of the Fermi surface reconstruction on the self-energy of the copper-oxide superconductors

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ABSTRACT

We calculated the self-energy corrections beyond the mean-field solution of the rotating antiferromagnetism theory using the functional integral approach. The frequency dependence of the scattering rate $1/\tau$ is evaluated for different temperatures and doping levels, and is compared with other approaches. The general trends we found are fairly consistent with the nearly antiferromagnetic Fermi liquid as far as the **k**-anisotropy and some aspects of the marginal-Fermi liquid behavior are concerned. The present approach provides the justification from the microscopic point of view for the phenomenology of the marginal Fermi liquid ansatz, which was used in the calculation of several physical properties of the high-T_C cuprates within the rotating antiferromagnetism theory. In addition, the expression of self-energy we calculated takes into account the two currently hot issues of the high-T_C cuprate superconductors, namely the Fermi surface reconstruction and the hidden symmetry, which are closely related to the pseudogap.

1. Introduction

The origin of the pseudogap (PG) [1] behavior of the high-T_C cuprate superconductors (HTSC) remains an issue despite more than one quarter of a century has passed after the discovery of superconductivity in these materials [2]. The PG phase turned out to be more challenging and subtle than the superconducting phase itself. Indeed, the PG has been measured as a depression in the density of states at the Fermi energy below the doping dependent PG temperature T^*, but no broken symmetry has so far been observed beyond any doubt [3]. A number of theoretical models have been proposed in order to explain this PG phenomenon, with some based on the preformed-pairs scenario and others based on competing orders [4]. The rotating antiferromagnetism theory (RAFT), which belongs in the latter, is characterized by two competing orders; namely the *d*-wave superconductivity and the rotating antiferromagnetic (RAF) order. The RAF order parameter has a finite magnitude below a temperature, which was identified with T^*, and a phase that varies with time [5–10]. RAFT yield results in good agreement with several experimental data of the HTSCs. Resistivity [11], optical conductivity [12], Raman [13], and ARPES [14,9] have been analyzed within RAFT assuming the phenomenological marginal-Fermi liquid (MFL) self-energy [15]. Until before the completion of this work, the justification for using this assumption was missing. The present work shows that a self energy that is consistent with a MFL is derived beyond the mean-field point of RAFT. This self-energy is due only to the longitudinal fluctuations of the order parameter.

In the limit of the tight-binding bare electrons our self-energy satisfies the same equation as in the second-order Born approximation, which was used in the nearly antiferromagnetic Fermi liquid (NAFL) theory [16,17]. Moreover, we generalize this approximation into a gapped second-order Born approximation that takes into consideration the PG explicitly. Interestingly, we can qualify the RAF state as a state that is nearly antiferromagnetic because the RAF state has the same (free) energy as that of a true ordered antiferromagnetic state but is a disordered state because of the time dependence of the phase of the RAF order parameter. The self-energy calculation results from only the longitudinal fluctuations of the RAF order parameter, in agreement with the assumption made in NAFL. RAFT is also consistent with the assumption made in NAFL concerning the existence of a gap-like behavior without a condensate. In RAFT, a gap exists in the electronic energy spectrum but long-range order does not occur.

Below the PG temperature in the underdoped regime, we find that the relaxation rate displays a linear behavior at large frequencies consistent with a MFL, but it displays strong deviation from linearity at low frequencies, which is characterized by a hump

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due to the PG. In the overdoped regime at any temperature or above the PG temperature in the underdoped regime, the relaxation rate shows a mixture of Fermi liquid (FL) and MFL behaviors. We argue that this evolution with doping is related to the Fermi surface (FS) reconstruction [9].

This work is organized as follows. In Section 2 we calculate the Gaussian corrections to the mean-field solution of RAFT using a Hubbard–Stratanovich identity that decouples the quartic term of the Hubbard model in the channel of RAF order. This yields the propagator of the Gaussian fluctuations. Self-energy is calculated in Section 3 using this propagator, and a gapped second-order Born approximation is derived for self-energy in the presence of the PG. Some numerical results are presented in Section 4, and conclusions are drawn in Section 5.

2. Method

RAFT has been developed using the extended Hubbard model, with a repulsive on-site Coulomb interaction and a nearest-neighbor attractive interaction that simulates d-wave pairing. Here, we focus on the normal (non superconducting) state, where the Hamiltonian on a two-dimensional lattice reads as

$$\begin{aligned} H &= H_0 + H_I \\ &= -t\sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\sigma}c_{j,\sigma} - t'\sum_{\langle\langle i,j\rangle\rangle,\sigma} c^\dagger_{i,\sigma}c_{j,\sigma} - \mu\sum_{i,\sigma} c^\dagger_{i,\sigma}c_{j,\sigma} + U\sum_i n_{i,\uparrow}n_{i,\downarrow}. \end{aligned} \tag{1}$$

In (1), H_0 stands for the kinetic and chemical potential energies, and $H_I = U\sum_i n_{i\uparrow}n_{i\downarrow}$ is the sum of all on-site Coulomb energies. t and t' designate the electron's hopping energies between the nearest-neighbor ($\langle i,j\rangle$) and next-nearest-neighbor ($\langle\langle i,j\rangle\rangle$) sites respectively, μ is the chemical potential, $c^\dagger_{i,\sigma}$ ($c_{j,\sigma}$) creates (annihilates) an electron with spin σ at site i, and $n_{i,\sigma} = c^\dagger_{i,\sigma}c_{i,\sigma}$ is the number operator.

The partition function can be written as [18]

$$Z = \int \prod_{i,\sigma} dc^*_{i,\sigma}dc_{i,\sigma}\, e^{-\int_0^\beta d\tau[\sum_{i,\sigma}c^*_{i,\sigma}\frac{\partial}{\partial\tau}c_{i,\sigma}+H_0+H_I]}, \tag{2}$$

where c and c^* are from now on anticommuting Grassmann variables. For the RAF order, we decouple the interacting U-term of (1) using a Hubbard–Stratanovich transformation by considering the RAF order parameter $Q = \langle c_{i,\sigma}c^\dagger_{i,-\sigma}\rangle$, which has been used to model the PG behavior [5,6]. This gives

$$\begin{aligned} e^{-\int d\tau H_I} = \int \prod_i db_i \\ \times \exp\left\{\int d\tau\left[-\sum_i b^*_i U^{-1} b_i + \sum_i c_{i\downarrow}c^*_{i\uparrow}b_i + \sum_i c_{i\uparrow}c^*_{i\downarrow}b^*_i\right]\right\}, \end{aligned} \tag{3}$$

where b_i is a Hubbard–Stratanovich complex field. In order to recover the RAF state at the mean-field level in the present treatment we write the field b_i as

$$b_i = |b_i|e^{i[\pi(x_i+y_i)+\phi(t)]}. \tag{4}$$

The phase term $e^{i\pi(x_i+y_i)} = (-1)^{x_i+y_i}$ guarantees that the rotating order parameter is staggered due to the antiferromagnetic correlations, and the time-dependent phase $\phi(t)$ insures that the staggered magnetization rotates [10,12,6,7]. Using the Grassmann variables and the transformation (3), the partition function takes on the form

$$Z = \int \prod_{i,\sigma} dc^*_{i,\sigma}dc_{i,\sigma}db_i \exp(-S_{eff}), \tag{5}$$

with

$$S_{eff} = \int_0^\beta d\tau\left[\sum_{i\sigma}\sum_{\alpha=A,B} c^{\alpha^*}_{i\sigma}\frac{\partial}{\partial\tau}c^\alpha_{i,\sigma} + H^\alpha_0 + \sum_{i;\alpha=A,B}(c^{\alpha^*}_{i\uparrow}c^\alpha_{i\downarrow}b_i + c^{\alpha^*}_{i\downarrow}c^\alpha_{i\uparrow}b^*_i) + \sum_i\frac{|b_i|^2}{U}\right]. \tag{6}$$

Here $\beta = \frac{1}{k_BT}$ is inverse temperature, and A and B designate the two sublattices of the bipartite lattice. The upper index α in H^α_0 means that the single particle part of the Hamiltonian has now to be written using the two sublattices, A and B. The mean-field solution, where $b_i \equiv b_0$ is time and space independent, allows us to recover the RAFT's mean field equation for the parameter $Q = \langle c_{i,\uparrow}c^\dagger_{i,\downarrow}\rangle$, Ref. [5]:

$$1 = \frac{U}{2N}\sum_{\mathbf{k}}\frac{n_F[E_-(\mathbf{k})] - n_F[E_+(\mathbf{k})]}{E_q(\mathbf{k})}, \tag{7}$$

where $n_F(E) = \frac{1}{1+e^{\beta E}}$, $E_q(\mathbf{k}) = \sqrt{\epsilon_1(\mathbf{k})^2 + b_0^2}$, and N is the total number of lattice sites. The mean field energies

$$E_\pm = -\mu'(\mathbf{k}) \pm E_q(\mathbf{k}), \tag{8}$$

become the same as those derived earlier in Ref. [5] when we let $b_0 = UQ$; Q being then the RAF order parameter satisfying Eq. (7). Here, $\epsilon_1(\mathbf{k}) = -2t(\cos k_x + \cos k_y)$ and $\mu'(\mathbf{k}) = -\mu - 4t'\cos k_x \cos k_y + Un$. $n = \langle c_{i\sigma}\rangle$ is the electron's density, which satisfies the following mean-field equation [5]

$$n = \frac{1}{2N}\sum_{\mathbf{k}} n_F[E_+(\mathbf{k})] + n_F[E_-(\mathbf{k})]. \tag{9}$$

Note that the decoupling of the quartic interacting term of the Hubbard Hamiltonian using this density order parameter led to adding Un in the expression of $\mu'(\mathbf{k})$ [5]. The fluctuations beyond the mean-field solution are considered for the RAF order only for simplicity. Also, the fluctuations considered here are in the longitudinal direction of the RAF parameter, since we argue that these are much more important than the transverse fluctuations, given that the phase of the local RAF parameter is time dependent, so already fluctuating at the mean-field level. The only possible transverse fluctuations are not local but due to the fluctuations in the phase difference between adjacent sites. These are not considered here.

Upon Fourier transforming to $\mathbf{k}$ and frequency space, the mean-field action takes on the form

$$S_0 = \sum_{\tilde{k}}\psi^*_{\tilde{k}}\mathcal{G}^{-1}\psi_{\tilde{k}} + N\frac{|b_0|^2}{U}, \tag{10}$$

where $\tilde{k} \equiv (\mathbf{k}, \omega_n)$; $\mathbf{k}$ being the wavevector and ω_n the fermionic Matsubara frequency. Here, $\psi^*_{\tilde{k}} = (c^{A^*}_{\tilde{k}\uparrow}\ c^{B^*}_{\tilde{k}\uparrow}\ c^{A^*}_{\tilde{k}\downarrow}\ c^{B^*}_{\tilde{k}\downarrow})$ is a 4-component spinor, and the mean-field Green's function is [11]

$$\mathcal{G}(\mathbf{k}, i\omega_n) = \frac{[i\omega_n + \mu'(\mathbf{k})]I + \epsilon(\mathbf{k})\mathcal{M} + b\mathcal{N}}{[i\omega_n + \mu'(\mathbf{k})]^2 - [\epsilon^2(\mathbf{k}) + b_0^2]}, \tag{11}$$

with

$$\mathcal{M} = \begin{pmatrix}\tau_1 & 0\\ 0 & \tau_1\end{pmatrix}, \quad \mathcal{N} = \begin{pmatrix}0 & \tau_3\\ \tau_3 & 0\end{pmatrix}, \tag{12}$$

where τ_1 and τ_3 are the first and third Pauli matrices.

In order to go beyond the mean-field solution, we consider the Gaussian fluctuations by writing

$$b_i = b_0 + \delta b(\mathbf{r_i}, \tau), \tag{13}$$

with $\delta b(\mathbf{r_i}, \tau)$ a small deviation around the mean-field point. Using the approach for calculating Gaussian contributions to the partition function described in Ref. [18] one finds