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Superconducting correlation function in a 2D Hubbard model: The Knight shift and (T_C, μ) transition line

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We calculate the superconducting correlation function $\pi_{SC}(\mathbf{q}, i\nu_n)$ in the frame of a 2D Hubbard model $t - t' - U$ $(U > 0)$ using the finite temperature Green's function formalism into the RPA technique, in order to obtain the temperature dependence of the Knight shift, and the (T_C, μ) transition line in the d-wave pairing scenario. Under this regime, we show that the Knight shift exhibits a strong peak at T_C associated to $\Delta_{SC}(T_C) = 0$ instability.

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INTRODUCTION

There has been a remarkable trend for using the 2D Hubbard model [1] since it describes a set of interesting properties associated to superconductivity phenomenon, such as magnetic phase stability, band-structure effects, pairing correlations and Fermi surface topology variations [2],[3],[4], [5]; additionally, INS and Raman scattering experiments have proven to be a useful tool in exploring the incommensurate magnetic response $\chi''(\mathbf{q}, i\omega_n)$ [6], and the gap anisotropy. In the frame

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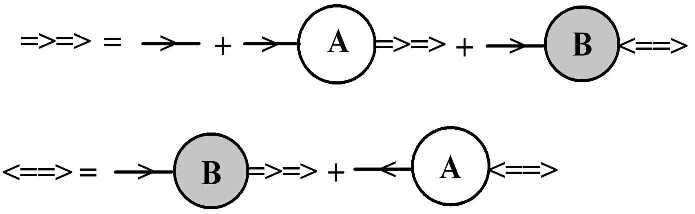
of finite temperature Green's function and RPA formalism, we calculate the second sites hopping contributions on the lowest-order polarization propagator; furthermore, we start from Vozyakov's insight [7] in order to obtain the set of self-consistent equations for the superconducting gap, particularly those attached for d-wave symmetry in the *saddle point* approximation.

FORMALISM FOR NORMAL AND ANOMALOUS GREEN FUNCTIONS

The complete and noninteracting finite temperature Green functions $(\mathcal{G}, \mathcal{G}^0)$ are related through the *Dyson-Gorkov* coupled equations, whose diagrammatic representations are given by:



where $A \equiv A(p)$ and $B \equiv B(p)$ are the associated self-energy functions into the perturbation theory approach, with $p = (\mathbf{k}, i\omega_n)$ as the momentum 4-vector, and $i\omega_n$ denoting the fermionic Matsubara frequencies. The analitycal definitive expressions for normal $(\mathcal{G})$ and anomalous $(\mathcal{G}_a)$ Green functions can be written as:

$$\mathcal{G}(p) = \frac{\mathcal{G}_0^{-1}(-p) - A(-p)}{\Big(\mathcal{G}_0^{-1}(p) - A(p)\Big)\Big(\mathcal{G}_0^{-1}(-p) - A(-p)\Big) - B(p)\,B(-p)}, \quad (1)$$

$$\mathcal{G}_a(p) = \frac{B(-p)\,\mathcal{G}(p)}{\mathcal{G}_0^{-1}(-p) - A(-p)}. \quad (2)$$

The noninteracting Green's function $\mathcal{G}^0(p)$ is defined by: $\mathcal{G}^0(p) = \Big(i\omega_n - \varepsilon_0(\mathbf{k}) + \mu\Big)^{-1}$, where μ is the chemical potential and $\varepsilon_0(\mathbf{k})$ is the dispersion relation given by the tight-binding model for a unitary square lattice, in the noninteracting limit and taking into account the next-nearest hopping contribution t':

$$\varepsilon_0(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y. \quad (3)$$

We will use the Vozyakov's approximation for the self-energies $A(p)$ and $B(p)$ according with:

$$A(p) = \lim_{\eta\to 0} \frac{U}{\beta\mathcal{N}} \sum_{p_1} e^{i\omega_1\eta} \mathcal{G}(p_1), \qquad B(p) = \frac{1}{\beta\mathcal{N}} \sum_{p1} K(p+p_1)\, \mathcal{G}_a(p_1). \tag{4}$$

The first one is associated to one-loop contribution, while the second one establishes the irreducible component of the scattering amplitude in the Bethe-Salpeter equation [8], containing the vertex and the single closed fermionic loop:

$$K \approx K_1 + K_2; \qquad K_1 \equiv U; \qquad K_2(q) \equiv -\frac{U^2}{2}\pi^0(\mathbf{q}, i\nu_n), \tag{5}$$

where $i\nu_n$ are the set of bosonic Matsubara frequencies given by: $2\pi n/\beta\hbar$. Assuming that $A(p)$ does not depend on p, we define $A = \mu - x$, that represents the hole-doping concentration level. $\xi(\mathbf{k}) = \varepsilon_0(\mathbf{k}) - \mu$, $B(p) = \Delta(p)$. $\pi^0(\mathbf{q}, i\nu_n)$ is the lowest-order in the non-interacting polarization propagator given by:

$$\pi^0(\mathbf{q}, i\nu_n) = \frac{2}{\beta} \sum_{\mathbf{p}, i\omega_n} \mathcal{G}^0(\mathbf{p}, i\omega_n)\, \mathcal{G}^0(\mathbf{p}+\mathbf{q}, i\omega_n + i\nu_n). \tag{6}$$

Therefore equations (1), (2) can be rewritten as:

$$\mathcal{G}(p) = -\frac{i\omega_n + \xi(\mathbf{k})}{\omega_n^2 + \xi^2(\mathbf{k}) + \Delta^2(p)}, \qquad \mathcal{G}_a(p) = \frac{\Delta(-p)}{\omega_n^2 + \xi^2(\mathbf{k}) + \Delta^2(p)}. \tag{7}$$

Evaluating the replacement of (5) in (4), and under the consideration that $B(p)$ and $K(p)$ do not have dependence on Matsubara frequencies, we arrive to the coupled equations for the *order parameter* $(\Delta(\mathbf{k}, T))$ and *chemical potential* (μ):

$$\Delta(\mathbf{p}) = \frac{1}{2\mathcal{N}} \sum_{\mathbf{k}} \frac{K(\mathbf{p}+\mathbf{k})\,\Delta(-\mathbf{k})}{\varepsilon_\Delta(\mathbf{k})} \tanh\frac{\beta\varepsilon_\Delta(\mathbf{k})}{2}, \tag{8}$$

$$\mu - \frac{U}{2} = x - \frac{U}{2\mathcal{N}} \sum_{\mathbf{k}} \frac{\xi(\mathbf{k})}{\varepsilon_\Delta(\mathbf{k})} \tanh\frac{\beta\varepsilon_\Delta(\mathbf{k})}{2}, \tag{9}$$

where $\varepsilon_\Delta(\mathbf{k}) = \sqrt{\varepsilon_0^2(\mathbf{k}) + \Delta^2(\mathbf{k})}$ is the excitation spectrum in the superconducting state, with the *d*-wave gap symmetry relationship

[6],[9],[10]:

$$\Delta(\mathbf{k}) = \Delta_{SC}(T)\,\Delta_0(\mathbf{k})\,; \qquad \Delta_0(\mathbf{k}) = \frac{1}{2}(\cos k_x - \cos k_y). \tag{10}$$

In the superconducting state, we calculate the correlation function $\pi_{SC}(\mathbf{q}, i\nu_n)$ defined by: (in units of $\hbar$)

$$\pi_{SC}(\mathbf{q}, i\nu_n) \equiv \frac{1}{\beta}\sum_{i\omega_n}\sum_{\mathbf{k}} \mathcal{G}(\mathbf{k}, i\omega_n)\,\mathcal{G}(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_n)\,; \tag{11}$$

where $\mathcal{G}$ takes the structure given by Eq. (7). Performing the limits for $i\nu_n \to 0$ and $\mathbf{q} \to 0$, the superconducting propagator takes the analitycal form:

$$\pi_{SC}(\mathbf{q}, i\nu_n)_{q\to 0} = -\frac{1}{4}\sum_{\mathbf{k}}\left[\frac{\varepsilon_{\mathbf{k}}^2 + \xi_{\mathbf{k}}^2}{2\varepsilon_{\mathbf{k}}^2}\frac{\beta}{\cosh^2\left(\frac{\beta}{2}\varepsilon_{\mathbf{k}}\right)} + \frac{\Delta_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}}^3}\right]. \tag{12}$$

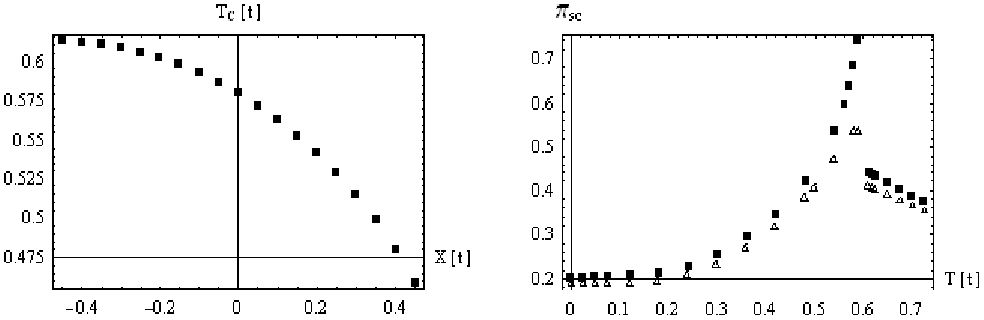


Figure 1: (Left) Critical temperature against *modified* doping parameter $X = \mu - x$, $t' = -0.16t$, $U = t$. (Right) The Knight shift (Eq. (12) in arbitrary units) vs temperature, for $t' = -0.16t$ and $X = -0.45t$ ($\square$), $X = -0.25t$ ($\triangle$). Note that the sharper peak existence is directly associated with the X raising.

The figure 1(left) exhibits the critical temperature decreasing as $X = \mu - x$ increases in the range of $\{-0.45t, 0.45t\}$ (hole-doping concentration) in agreement with several evidences [11]. The right-hand figure shows the superconducting correlation function in the $q \to 0$ limit. We note a strong peak for $T \approx 0.61t$ associated to critical temperature for $X = -0.45t$. $\pi_{SC}(\mathbf{q}, i\nu_n)_{q\to 0}$ follows a typical Yosida-type increasing for $T < T_C$. Consequently, the $T > T_C$ regime belongs to the *normal* state defined by $\Delta_{SC} = 0$, and the main feature in this phase is characterized by a marked decreasing with the temperature.

CONCLUDING REMARKS

We have obtain a set of coupled self-consistent equations for the gap-temperature dependence $\Delta_{SC}(T)$, (Eqs. (8), (9)) and the Knight shift in the superconducting state (Eq. (12)), using the finite temperature formalism for the normal and anomalous Green's functions. This approach involves two kind of contributions: the first one is attached to the Hartree-Fock term ($\sim U$); and the second one reproduces the antiferromagnetic-channel fluctuation (K_2). The numerical results provide good agreement with those obtained in several references (see text), and the running calculations are all linked into Van-Hove singularities formalism. These expressions constitute the base for a subsequent study of the gap symmetries effects introduced through $\Delta_0(\mathbf{k})$ (Eq. (10)), i.e., we must consider another type of pairing scenario such as the $s + id$ mixed state, and their properties under t' as well as X influence.

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