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Thermal and quantum fluctuations induced additional gap in single-particle spectrum of d–p model

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Abstract

The possibility of thermal and quantum fluctuations induced attractive interaction leading to a pairing gap Δ_{tq} in the single-particle spectrum of d–p model in the limit of a large N of fermion flavor is investigated analytically. This is an anomalous pairing gap in addition to the one with d-wave symmetry originating from partially screened, inter-site coulomb interaction. The motivation was to search for a hierarchy of multiple many-body interaction scales in high-T_c superconductor as suggested by recent experimental findings. The pairing gap anisotropy stems from more than one source, namely, nearest neighbor hoppings and the p–d hybridization, but not the coupling of the effective interaction. The temperature at which Δ_{tq} vanishes may be driven to zero by using a tuning parameter to have access to quantum criticality (QC) only when $N \gg 1$. For the physical case $N = 2$, the usual coherent quasi-particle feature surfaces in the spectral weight everywhere in the momentum below the pairing gap Δ_{tq}. Thus it appears that the reduction in spin degeneracy has the effect of masking quantum criticality.

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Keywords: Quantum fluctuation; Fermion flavor; Anomalous pairing; Gap anisotropy

1. Introduction

There are a number of features of high-temperature superconductors which do not completely fit within the single-band Hubbard model framework [1,2]. For example, the cuprate gap is set by the charge transfer energy separating the copper and oxygen orbitals [3,4] as opposed to a Mott gap between copper d-states split by the on-site repulsion U. Furthermore, the metal–insulator transition (MIT) and superconductivity (SC) seem [5] to be difficult to explain in this framework at any finite U in two dimensions and higher. These were the reasons for considering a three-band Hubbard model [6,7] (with spin degeneracy $N \geqslant 2$) to investigate MIT in an earlier work [8] (hereinafter referred to as I). A variant of the slave-boson (SB) mean field theoretic approach proposed by Kotliar and Ruchenstein (KR) [9] was applied in I. The advantages of the former over the latter were mentioned there. In the present work, which is a sequel to I, a novel d-fermion pairing mechanism leading to a gap Δ_{tq} in the single-particle excitation spectrum and the role played by the spin degeneracy vis-à-vis quantum criticality (QC) when this pairing instability sets in are reported. The motivation is to initiate the formulation of a multi-gap model for a high-T_c superconductor to explain the recent experimental observations [10–13], where (i) the pseudo-gap (PG) is reported to have two distinct energy scales (with a low-energy PG comparable to that of the SC gap and a larger high-energy PG) and (ii) the possibility of multiple many-body interaction scales in high-T_c superconductors is demonstrated. The p- and d-fermion nearest neighbor hoppings are introduced additionally keeping in view a previous report [14] in which it was shown that all the underlying d–p parameters have significant role. The specific aim here, of course, is to generate k-dependence of the onsite energies and to find

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their effect on nodal and anti-nodal gap contributions $\Delta_{tq}(\mathrm{N})$ and $\Delta_{tq}(\mathrm{AN})$.To capture the widely accepted d-wave gap anisotropy [2] in cuprates, the nearest-neighbor interaction counterpart in momentum space $U(\mathbf{k},\mathbf{q})$ is to be introduced [15] for transition from a momentum $\mathbf{q}$ to $\mathbf{k}$. This is taken to be separable in Ref. [15] and is expanded in terms of basis functions corresponding to mixed symmetry states involving d_{xy} and $d_{x^2-y^2}$. Once the singlet superconducting instability sets in, it will be shown that the effective gap involves the dominant one ($\Delta_{x^2-y^2}$) corresponding to pure $d_{x^2-y^2}$ wave and the sub-dominant Δ_{tq}. The gaps (Δ_{xy}, Δ_{tq}) will be shown to be relevant for the normal phase.

As the first step to achieve the goals set above, the bose field fluctuations are integrated out completely taking partial trace in the grand partition function of the system for the metallic phase close to MIT to obtain an effective fermion Hamiltonian H_{eff} in the momentum space. Due to weak attraction induced by thermal and λ-field fluctuations (the field λ is responsible for enforcing the anti-commutativity of pseudo-fermion operators in the SB method in I and therefore the corresponding fluctuations are quantum-mechanical), it has been possible to show that the anomalous pairing of d-fermion field is nonzero. The corresponding gap (Δ_{tq}) anisotropy in the single-particle excitation spectrum stems from more than one source, namely, p- and d-fermion nearest neighbor hoppings (t_{pp}, t_{dd}) and the p–d hybridization, but not the coupling of the effective interaction. Since the coupling involves both thermal and quantum fluctuations, the transition temperature may be driven to zero by tuning, say, the parameter 'u' in I to have access to QC only when the spin degeneracy $N \gg 1$ and the other gaps are zero. For $N=2$, the access to QC is denied as then the attractive interaction would diverge. The usual coherent quasi-particle feature appearing in the spectral weight everywhere in the momentum space, for $N=2$, below the pairing gap is a confirmation of this fact. In the paired state the anti-nodal gap contribution $\Delta_{tq}(\mathrm{AN})$ monotonically increases with decreasing hole doping. The nodal gap contribution $\Delta_{tq}(\mathrm{N})$, expressible in the form $\Delta_{tq}^2(\mathrm{N}) = \Delta_{tq}^2(\mathrm{AN}) - 4(\sqrt{2}t_{\mathrm{dd}} + t_{\mathrm{pp}})^2$, also shows the same behavior. It is found that $T_{\mathrm{AN}} > T_{\mathrm{N}}$, where T_{AN} and T_{N}, respectively, are the temperatures at which $\Delta_{tq}(\mathrm{AN})$ and $\Delta_{tq}(\mathrm{N})$ vanish. Furthermore, the characteristic energy of Δ_{tq} is found to be much greater than the SC gap energy.

The paper is organized as follows: In Section 2, starting with the momentum space three-band Hubbard Hamiltonian (or d–p Hamiltonian) involving nearest-neighbor (NN) hoppings and the bose field fluctuations, an effective fermionic Hamiltonian is obtained taking partial trace of the grand partition function. The Hamiltonian involves an attractive interaction, which has its origin in the fluctuations of the field λ. In Section 3 it is shown that this interaction leads to a novel pairing gap Δ_{tq} in the single-particle spectrum of the model under consideration in the limit of a large N of fermion flavor. The paper ends in Section 4 with the reporting of a possible energy scale, corresponding to the gap Δ_{tq}, about six times greater than the SC gap energy.

2. Effective fermion hamiltonian

We start with the d–p model Hamiltonian in I involving boson fields (φ,ψ) and the field (λ) enforcing the usual constraint of SB method. In momentum space the model Hamiltonian, involving bose mean-field values (e_0,D_0) (of φ and ψ) and the corresponding fluctuations (e_q, D_q), can be written as (cf. Eqs. (6) and (7) in I)

$$H' = C_1 + H_{\mathrm{mean}} + H_{\mathrm{b}}^{(0)} + H_{\mathrm{b,f}} \tag{1}$$

$$C_1 = N_{\mathrm{s}} N \lambda (e_0^2 + D_0^2 - q_0) + N_{\mathrm{s}} N U'_{\mathrm{d}} D_0^2 \tag{2}$$

$$H_{\mathrm{b}}^{(0)} = \lambda \sum\nolimits_q e_q^\dagger e_q + (\lambda + U'_{\mathrm{d}}) \sum\nolimits_q D_q^\dagger D_q \tag{3}$$

$$\begin{aligned} H_{\mathrm{mean}} = {} & \sum\nolimits_{k\sigma} (\varepsilon_{\mathrm{d}}^{\mathrm{o}} + \lambda - \mu) d_{k\sigma}^\dagger d_{k\sigma} + \sum\nolimits_{k\alpha\sigma} (\varepsilon_{\mathrm{p}}^{\mathrm{o}} - \mu) p_{k\alpha\sigma}^\dagger p_{k\alpha\sigma} \\ & - \sum\nolimits_{k\eta\sigma} (2it \sin(k_\eta a/2)) \{ p_{k\eta\sigma}^\dagger (e_0 d_{k\sigma} + D_0 \mathrm{sgn}(\sigma) d_{-k,-\sigma}^\dagger) \\ & - (e_0 d_{k\sigma}^\dagger + D_0 \mathrm{sgn}(\sigma) d_{-k,-\sigma}) p_{k\eta\sigma} \} \end{aligned} \tag{4}$$

$$\begin{aligned} H_{\mathrm{b,f}} = {} & \sum\nolimits_q' \lambda_q \{ e_0 (e_{-q} + e_q^\dagger) + D_0 (D_{-q} + D_q^\dagger) \} \\ & + \sum\nolimits_q' \lambda_{-q} \{ e_0 (e_q + e_{-q}^\dagger) + D_0 (D_q + D_{-q}^\dagger) \} \\ & + \sum\nolimits_{k\sigma q\eta}' (1/\sqrt{N}) (2it \sin(q_\eta a/2)) \{ (d_{\pm q,\sigma}^\dagger e_{\pm q-k} \\ & + \mathrm{sgn}(\sigma) D_{\pm q+k}^\dagger d_{\pm q,-\sigma}) p_{k\eta,\sigma} \\ & - p_{k\eta,\sigma}^\dagger (e_{\pm q-k}^\dagger d_{\pm q,-\sigma} + \mathrm{sgn}(\sigma) d_{\pm q,-\sigma}^\dagger D_{\pm q+k}^\dagger) \} \\ & + \sum\nolimits_{q,k}' (1/\sqrt{N}) \lambda_q (e_{q+k}^\dagger e_k \\ & + D_{q+k}^\dagger D_k) + \sum\nolimits_{q,k}' (1/\sqrt{N}) \lambda_q (d_{k+q,\sigma}^\dagger d_{k+q,\sigma}) \end{aligned} \tag{5}$$

The $\varepsilon_{\mathrm{d}}^{\mathrm{o}}$ and $\varepsilon_{\mathrm{p}}^{\mathrm{o}}$, respectively, are the d- and p-fermion onsite energies plus the corresponding nearest-neighbor hopping terms; μ is the chemical potential for fermion number. The hopping terms are given by [$-2t_{\mathrm{dd}}$ $(\cos k_x a + \cos k_y a)$] and [$-4t_{\mathrm{pp}} \sin(k_x a/2) \sin(k_y a/2)$]. The quantities ($e_0$,$D_0$,$\lambda$,$\mu$) can be determined from the mean field equations (Eqs. (8)–(11) in I). Here the primed summations correspond to $q \neq 0$. In what follows it will be shown that the last term in Eq. (5) yields the required attractive interaction. The Bose and Fermi parts are separated as far as possible in Eqs. (1)–(5). One may consider the grand partition function (GPF) $Z = \mathrm{Tr} \exp(-\beta H')$. In order to integrate out boson degrees of freedom the Hilbert space of the system may be factorized as $B \otimes F$ where B is the subspace on which boson operators act and F is the one on which fermion operators act. One can thus write $Z = Z_0 Z_{\mathrm{f}} Z_{\mathrm{b-f}}$ where $Z_0 = \mathrm{Tr} \exp(-\beta\ (C_1 + H_{\mathrm{b}}^{(0)}))$, $Z_{\mathrm{f}} = \mathrm{Tr} \exp(-\beta\ H_{\mathrm{mean}})$ and $Z_{\mathrm{b,f}} = \mathrm{Tr} \exp(-\beta\ H_{\mathrm{b,f}})$. The assumptions of large spin degeneracy and proximity to MIT (where e_0^2 and $D_0^2 \to 0^+$) provide a $(1/N)$-expansion for GPF ($(1/N)$ is used as an expansion parameter to extrapolate to the physical