Upward curvature of the upper critical field in the Boson–Fermion model

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We report on a non–conventional temperature behavior of the upper critical field ($H_{c2}(T)$) which is found for the Boson–Fermion (BF) model. We show that the BF model properly reproduces two crucial features of the experimental data obtained for high-$T_c$ superconductors: $H_{c2}(T)$ does not saturate at low temperatures and has an upward curvature. Moreover, the calculated upper critical field fits very well the experimental results. This agreement holds also for overdoped compounds, where a purely bosonic approach is not applicable.

Some of the unusual properties observed experimentally in the high temperature superconductors (HTSC) can be explained in terms of the effective two component models, which involve boson and fermion degrees of freedom. There are numerous examples of such theoretical scenarios, for instance: electron fields coupled to gauge fluctuations, the RVB spinon-holon theory, the coupled electron-phonon systems, etc. In this paper we consider one of these models, where the conduction band particles (fermions) coexist and interact with the localized electron pairs (hard-core bosons). This, so called Boson Fermion (BF) model, had initially been introduced [12] a couple of years before the discovery of HTSC materials. The authors have conjectured that it might describe an emerging physics of the electron-phonon systems for the intermediate coupling strength.

From a formal point of view, the Hamiltonian of this BF model can be considered as an effective one for several models, which are often used in the solid state physics. It has been derived so far: (1) from the generalized periodic Anderson model with the large on-site attraction by eliminating the hybridization between the wide and narrow band electrons via canonical transformation [2], (2) from a purely fermionic single band system described by the extended Hubbard model using the concept of bosonization for lattice fermions [3], (3) from the Hubbard model on the two dimensional plaquetized lattice in the strong interaction limit using the contractor method [4], and (4) from the resonating valence bond state of the $t$–$J$ model in the path integral technique [5].

The same BF model has been considered also by many other authors who postulated it in a more ad hoc way. For example in the Ref. [6] author has proposed the BF type charge transfer Hamiltonian basing his arguments on interpretation of the optical experiments. Other ideas could be found in the Ref. [7]. Authors have represented the patches of the 2D Brillouin zone near the so called hot spots via dispersionless bosons, which are coupled to fermions of a remaining part of the Brillouin zone.

The BF model is not only considered in a context of HTSC. There are recent attempts to apply the same type of picture for a description of the magnetically trapped atoms of alkali metals [8].

Unconventional mechanism of superconductivity within the BF model has been studied in a number of papers [1, 2, 7, 10, 11, 12, 13, 14]. Fermions acquire superconducting coherence via exchange of the hard-core bosons. The same processes lead also to the effective mobility of bosons. Fermions/bosons can undergo a phase transition into the superconducting/superfluid phase at identical the same critical temperature $T_c = T_{sc} = T_{BE}$. It is worth to point out some of the unusual properties obtained for the BF model which are known in the most of the HTSC materials: (i) a non-BCS ratio $\Delta_s(T = 0)/kT_c > 4$ (except for the far under- and over-doping regimes) [12, 13]; (ii) linear in $T$ resistivity of a normal phase up to very high temperatures [1]; (iii) change of sign of the Hall constant above $T_c$ and the anomalous Seebeck coefficient [7]; (iv) appearance of the pseudogap in a normal phase for temperatures $T^* > T > T_c$ [10, 14]; (v) a particle-hole asymmetry of the single particle excitation spectrum in the normal phase [1].

Some of unusual properties of HTSC are related to the upper critical field. $H_{c2}$ can achieve values of a few hundred Tesla. Moreover, the resistivity measurements for HTSC clearly show an upward curvature of $H_{c2}(T)$, with no evidence of saturation even at low temperatures [6, 7]. From the theoretical point of view the upward curvature of the critical field occurs for instance in: Bose-Einstein condensation of charged bosons [2], Josephson tunneling between superconducting clusters [3], and in mean-field–type theory of $H_{c2}$ with a strong spin–flip scattering [4]. However, this feature cannot be explained within a conventional theory of $H_{c2}$ [5]. Therefore, it is a natural test for theoretical approaches to HTSC.

In the present study we show that the upward curva-
ture of $H_{c2}(T)$ is an intimate feature of the BF model. This result strongly supports the BF Hamiltonian as a model of HTSC.

We consider the Hamiltonian of the two-dimensional BF system, immersed in a perpendicular, uniform magnetic field

$$H^{BF} = \sum_{i,j,\sigma} (t_{ij}(A) - \delta_{ij} \mu) c_{i\sigma}^\dagger c_{j\sigma} + \sum_i (\Delta_B - 2\mu) b_i^\dagger b_i + v \sum_i (b_i^\dagger c_{i\uparrow} + \text{h.c.})$$

We use the standard notation for annihilation (creation) operators of fermion $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) with spin $\sigma$ and of the hard core boson $b_i$ ($b_i^\dagger$) at site $i$. Fermions interact with bosons via the charge exchange interaction $v$. $\mu$ is the chemical potential and $t_{ij}(A)$ is the hopping integral that depends on the magnetic field through the vector potential $A$:

$$t_{ij}(A) = t_{ij}(0) \exp \left( \frac{ie}{\hbar c} \oint_{R_i} A \cdot dl \right) .$$

To proceed, we apply the mean field decoupling for the boson–fermion interaction

$$b_i^\dagger c_{i\downarrow} c_{i\uparrow} \simeq \langle b_i \rangle^* c_{i\downarrow} c_{i\uparrow} + b_i^\dagger \langle c_{i\downarrow} c_{i\uparrow} \rangle,$$

which is justified when $v$ is small enough in comparison to the kinetic energy of fermions. After the decoupling we deal with the effective Hamiltonian composed of the fermion and boson contributions $H \simeq H^F + H^B$, coupled through the self-consistently determined expectation values $\langle c_{i\downarrow} c_{i\uparrow} \rangle$ and $\langle b_i \rangle$.

$$H^F = \sum_{i,j,\sigma} [t_{ij}(A) - \delta_{ij} \mu] c_{i\sigma}^\dagger c_{j\sigma} + \sum_i (\rho_i^2 c_{i\downarrow} c_{i\uparrow}^\dagger + \text{h.c.}),$$

$$H^B = \sum_i \left[ (\Delta_B - 2\mu) b_i^\dagger b_i + \Delta_i b_i^\dagger + \Delta_i^* b_i \right],$$

where $\Delta_i = v \langle c_{i\downarrow} c_{i\uparrow} \rangle$ and $\rho_i = v \langle b_i \rangle$.

One can exactly diagonalize the bosonic subsystem using a suitable unitary transformation. Statistical expectation values of the number operator $b_i^\dagger b_i$ and the parameter $\rho_i$ are given by:

$$\langle b_i^\dagger b_i \rangle = \frac{1}{2} - \frac{\Delta_B - 2\mu}{4\gamma_i} \tanh \left( \frac{\gamma_i}{kT} \right),$$

$$\rho_i = \frac{v \Delta_i}{2\gamma_i} \tanh \left( \frac{\gamma_i}{kT} \right),$$

where $\gamma_i = \frac{1}{2}(\Delta_B - 2\mu)^2 + 4\Delta_i^2$ and $k$ is the Boltzmann constant. At the phase transition the superconducting order parameter is infinitesimally small and one can expand $\rho_i$ in powers of $\langle c_{i\downarrow} c_{i\uparrow} \rangle$ up to the leading order. Then, the fermionic subsystem is described by

$$H^F = \sum_{i,j,\sigma} [t_{ij}(A) - \delta_{ij} \mu] c_{i\sigma}^\dagger c_{j\sigma} - V(T) \sum_i \left( \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle c_{i\downarrow} c_{i\uparrow} + \text{h.c.} \right),$$

where

$$V(T) = \frac{v^2}{2} \frac{\Delta_B - 2\mu}{\Delta_B - 2\mu} \tanh \left( \frac{\Delta_B - 2\mu}{2kT} \right).$$

The effective Hamiltonian (8) represents a BCS–type model with isotropic on–site pairing. The boson–fermion coupling enters $H^F$ through the pairing interaction and the chemical potential. The latter quantity should be evaluated from the conservation of the total charge $n_{\text{tot}} = 2n_B + n_F = 2/N \sum_i \langle b_i^\dagger b_i \rangle + 1/N \sum_{i,\sigma} \langle c_{i\sigma} c_{i\sigma} \rangle$. We restrict further investigation only the nearest–neighbor hoping, when the fermionic energy spectrum is known as the Hofstadter butterfly.

First, we assume that the bosonic level is in the middle of the fermionic band ($\Delta_B = 0$) and $n_{\text{tot}} = 2$. It is the simplest case, when the parameters of the Hamiltonian can be evaluated without a numerical investigation of the Hofstadter butterfly. Namely, since the Hofstadter energy spectrum is symmetric, for $\mu = 0$ one gets $n_F = 1$, $n_B = 1/2$, $n_{\text{tot}} = 2$ and $V(T) = v^2/(2kT)$. In order to calculate $H_{c2}$ one can apply a two–dimensional version of the Helfand-Werthamer (HW) theory, where the coupling constant, $\lambda$, depends on temperature. Since, $\lambda = V \rho_{\text{FS}}$, where $\rho_{\text{FS}}$ is the density of states at the Fermi level, one gets

$$\lambda(T) = \lambda(T_c) \frac{T_c}{T}.$$

The HW theory was derived for a free–electron gas and neglects the Landau level structure (so called quasiclassical limit). However, for a weak magnetic field these effects do not lead to an essential modification of $H_{c2}(T)$. Figure 1 shows $H_{c2}(T)$ calculated within the HW approach with the coupling constant determined by Eq. (10). In order to predict the qualitative temperature dependence of the critical field it is sufficient to recall the following facts: (i) when $\lambda(T) = \text{const}$ (standard HW theory), $H_{c2}(T)$ is linear for a weak magnetic field; (ii) in the BF model $\lambda$ increases with the decrease of temperature and diverges when $T \to 0$ (Eq. (10)). Then, it becomes obvious that BF model properly reproduces two crucial features of the experimental data: $H_{c2}(T)$ does not saturate at low temperatures and has an upward curvature, at least for a weak magnetic field. Numerical results (see Fig. 1) show that the latter property holds in the whole range of temperature.

Next, we show that the BF model properly describes $H_{c2}(T)$ for a wide range of model parameters, when the
FIG. 1: Temperature dependence of the upper critical field, obtained from the HW approach with the coupling constant given by Eq. (9). We have assumed $kT_c(H = 0) = 0.02t$.

problem cannot be reduced to the effective HW theory. In this case we apply a lattice version of the Gor’kov equations [27]

$$
\Delta_i = \frac{V(T)}{\beta} \sum_{j,\omega_n} \Delta_j G(i, j, \omega_n) G(i, j, -\omega_n).
$$

(10)

Here, $G(i, j, \omega_n)$ is the one–electron Green’s function in the presence of a uniform and static magnetic field and $\omega_n$ is the fermionic Matsubara frequency. With the help of the Hofstadter approach [26], equation (10) can exactly be solved for clusters of the order of $10^4$ lattice sites. For the details we refer to Ref. [27]. In contradistinction to the quasiclassical approaches (e.g., HW or Ginsburg–Landau theory) we explicitly account for the actual structure of Landau levels.

Figure 2 shows the upper critical field obtained for $n_{tot} = 1$ and different positions of the bosonic level. We consider two cases: (i) when this level is below the Fermi energy ($\Delta_B < 0$) there is a finite number of bosons also at $T \rightarrow 0$, (ii) for $\Delta_B > 0$ bosonic states are occupied only virtually. The upward curvature of $H_{c2}(T)$ appears predominantly in the first case (solid line in Fig. 2). When $\Delta_B$ is shifted above the Fermi energy, the curvature is gradually reduced. Finally, when $\Delta_B \gg kT$ the curvature changes from positive to negative (dashed line in Fig. 2) and one reproduces standard results for a purely fermionic system [27]. In Fig. 2 we have not presented results in the low temperature regime. Although, we have carried out numerical calculations for large clusters, this approach is not applicable at genuinely low temperatures. In this case the Cooper pair susceptibility accounts only for very few fermionic states (with energy close to the Fermi level) instead of a continuous density of states. However, one can prove that BF model qualitatively reproduces $H_{c2}(T)$ also for $T \rightarrow 0$. Combining Eqs. (8) and (9) one can express the effective pairing potential in terms of the bosonic occupation number

$$
V(T) = \frac{2v^2}{\Delta_B - 2\mu} \left( \frac{1}{2} - \left\langle b_i^\dagger b_i \right\rangle \right).
$$

(11)

It is straightforward to note that for $\left\langle b_i^\dagger b_i \right\rangle = 1/2$ one gets $\Delta_B = 2\mu$ and Eq. (8) is reduced to $V(T) = v^2/2kT$. On the other hand, when $\left\langle b_i^\dagger b_i \right\rangle \neq 1/2$ but $0 < n_B < 1$ the denominator in Eq. (11) vanishes for $T \rightarrow 0$. Therefore, $V(T)$ diverges for $T \rightarrow 0$ provided that $0 < n_B < 1$. It means that a requirement of partial occupation of bosonic states is sufficient to reproduce the experimental low temperature behavior of $H_{c2}$.

To complete the discussion, we show that BF model accurately reproduces the experimental data (see Fig. 3). We have chosen an appropriate set of model parameters, for which $H_{c2}(T)$ fits very well the results pre-
sented in Refs. [20, 21]. The theoretical curve was calculated for bosonic level that is situated slightly above the Fermi energy (n_{tot} = 1 and \Delta_B = 0). In this case n_F \gg n_B and the BF system is mainly of fermionic character. The experimental data were obtained for overdoped compounds, when HTSC exhibits a Fermi liquid character [28]. Therefore, BF model is fully consistent with fermionic–type behavior of the overdoped HTSC, whereas the purely Bosonic approach [22] is not applicable in this regime.

To conclude, we have shown that the BF model accurately describes the upper critical field observed in HTSC. It is known that the BF model correctly describes the pseudogap phenomenon and some other unconventional normal–state properties of HTSC. In this letter we have shown that this model reproduces also other unusual feature of HTSC, which cannot be explained within a standard BCS–type approach. Moreover, our results remain in agreement with the Fermi liquid behavior of the overdoped compounds. Therefore, it is an important support for the BF Hamiltonian as a model of HTSC.

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