Upward curvature of the upper critical field in the boson-fermion model

Tadeusz Domański
Centre de Recherches sur les Très Basses Temperatures CNRS, 38042 Grenoble, France and Institute of Physics, M. Curie Skłodowska University, 20-031 Lublin, Poland

Maciej M. Maśka and Marcin Mierzejewski
Institute of Physics, University of Silesia, 40-007 Katowice, Poland

(Received 27 November 2002; published 4 April 2003)

We report on a nonconventional 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 the experimental results very well. This agreement also holds for overdoped compounds, where a purely bosonic approach is not applicable.

DOI: 10.1103/PhysRevB.67.134507 PACS number(s): 74.20.Mn, 71.10.−w, 74.25.Bt

I. INTRODUCTION

Some of the unusual properties observed in high temperature superconductors (HTSCs) can be explained in terms of 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 resonating valence bond (RVB) spinon-holon theory, coupled electron-phonon systems, etc. In this paper we consider one such model, where the conduction band particles (fermions) coexist and interact with the localized electron pairs (hard-core bosons). This so-called *boson fermion* (BF) model was introduced[1] a couple of years before the discovery of HTSC materials. Initially it was proposed to describe the electron-phonon system in a crossover regime between the adiabatic and antiadiabatic limits.

It has been shown that the BF model describes the emerging physics of several theoretical models often used in studies of strongly correlated systems. It has been derived so far from (a) the periodic Anderson model with large on-site attraction by eliminating the hybridization between the wide and narrow band electrons,[2] (b) the extended Hubbard model using the concept of bosonization for fermions on a lattice,[3] (c) the Hubbard model on the plaquettized two-dimensional lattice in the strong interaction limit using the contractor method,[4] and (d) the resonating valence bond state of the *t-J* model in the path integral technique.[5]

Some authors postulated the BF model in an *ad hoc* way. For example Enz[6] proposed a BF–type model basing his arguments on an interpretation of the optical experiments on HTSC materials. Other ideas were explored by Geshkenbein *et al.*,[7] who represented patches of the two-dimensional Brillouin zone near so called *hot spots* via dispersionless bosons which could dissociate into the fermion pairs from a remaining part of the Brillouin zone. The same model is used not only in a context of HTSCs. There are recent attempts to apply a similar approach for a description of the magnetically trapped atoms of alkali metals.[8]

As far as superconductivity is concerned its mechanism is unconventional within the BF model. This issue was thoroughly investigated in a number of papers.[1,2,7,9–13] Fermions acquire the superconducting correlations due to the coupling with bosons. This coupling gives rise to the finite boson mobility ($m_B<\infty$). Under proper conditions bosons/and fermions undergo a phase transition into a superfluid/superconducting phase at a common critical temperature $T_c=T_{sc}^F=T_{BE}^B$.[14] It is worth pointing out some unusual properties obtained within the BF model which were observed in most of the HTSC materials: (i) a non-BCS ratio $\Delta_{sc}(0)/k_BT_c>4$ (except for the far under-doping and overdoping regimes);[11,12] (ii) a linear in T resistivity in a normal phase up to very high temperatures;[15] (iii) change of sign of the Hall constant above T_c and the anomalous Seebeck coefficient;[7] (iv) the appearance of the pseudogap in a normal phase for temperatures $T^*>T>T_c$;[16–19] and (v) a particle-hole asymmetry of the single particle excitation spectrum in the normal phase.[4,7,20]

In this paper we address a problem of the unusual behavior of the upper critical field observed in the HTSC materials. H_{c2} can achieve values of a few hundred Tesla. Moreover, the resistivity measurements clearly show an upward curvature of $H_{c2}(T)$, with no evidence of saturation even at low temperatures.[21,22] The positive curvature of the upper critical field $H_{c2}(T)$ was earlier known for layered superconductors,[23] and then the effect was assigned to the dimensional crossover. A similar behavior was also observed in electron-doped high-T_c copper oxides.[24] Acsusceptibility measurements showed a slight upward curvature of $H_{c2}(T)$ in $K_xBa_{1-x}BiO_3$ single crystals[25] as well. Authors attributed this to the presence of the Landau quantization that becomes important in the strong magnetic field.[26]

From a theoretical point of view the upward curvature of $H_{c2}(T)$ can occur, for instance, in systems with a strong disorder sufficiently close to the metal–insulator transition,[27] is disordered superconductors due to mesoscopic fluctuation,[28] during Josephson tunneling between superconducting clusters,[29] in a mean–field–type theory of H_{c2} with a strong spin-flip scattering,[30] and due to a reduction of the diamagnetic pair–breaking in the stripe phase.[31] These approaches require the system to be inhomogeneous, whereas the positive curvature has also been observed in a clean state.[22] Other theoretical approaches to this problem include, e.g., the superconductivity with a mixed symmetry $(s+d)$ order parameter[32] and a Bose-Einstein condensation of charged bosons.[33] However, the latter scenario cannot be applied to overdoped compounds, which exhibit a Fermi–liquid–type behavior.[34]

As this feature cannot be explained within a conventional theory of H_{c2},[35] it is a natural test for various models proposed for HTSCs. In the present study we show that the peculiarities of $H_{c2}(T)$ are immanent features of the BF model. We obtain our results both on the level of semiclassical Helfand–Werthammer (HW) theory[36] and in the Hofstadter approach taking into account the actual Landau level quantization.[37] Our findings strongly support the BF scenario as a relevant model for description of the HTSC materials.

II. MODEL

We consider the BF Hamiltonian of the 2D system immersed in a perpendicular, uniform magnetic field:

$$H^{BF}=\sum_{i,j,\sigma}(t_{ij}(\mathbf{A})-\delta_{ij}\mu)c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{i}(\Delta_B-2\mu)b_i^{\dagger}b_i+v\sum_{i}(b_i^{\dagger}c_{i\downarrow}c_{i\uparrow}+\text{H.c.}). \tag{1}$$

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

$$t_{ij}(\mathbf{A})=t_{ij}(0)\exp\left(\frac{ie}{\hbar c}\int_{\mathbf{R}_j}^{\mathbf{R}_i}\mathbf{A}\cdot d\mathbf{l}\right).$$

To proceed, we first apply a mean–field decoupling for the boson fermion interactions,

$$b_i^{\dagger}c_{i\downarrow}c_{i\uparrow}\simeq\langle b_i\rangle^{*}c_{i\downarrow}c_{i\uparrow}+b_i^{\dagger}\langle c_{i\downarrow}c_{i\uparrow}\rangle, \tag{2}$$

which is justified only when v is small enough. Indeed, it is the case here because it was shown[12] that the realistic values $T_c\sim 100$K can be obtained using a small interaction strength $v\simeq 0.1D$, where $D=0.5$eV is a typical fermion bandwith. By applying the mean-field approximation [Eq. (2)] we neglect fluctuations of the order parameter which may partly suppress the superconducting correlations.[38] However, in this paper we show that even without taking into account the fluctuations we reproduce the anomalies of the upper critical field.

Using the decoupling [Eq (2)] we deal with the effective Hamiltonian composed of the separated fermion and boson parts $H^{BF}\simeq H^F+H^B$:

$$H^F=\sum_{i,j,\sigma}[t_{ij}(\mathbf{A})-\delta_{ij}\mu]c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{i}(\rho_i^{*}c_{i\downarrow}c_{i\uparrow}+\text{H.c.}), \tag{3}$$

$$H^B=\sum_{i}[(\Delta_B-2\mu)b_i^{\dagger}b_i+\Delta_i b_i^{\dagger}+\Delta_i^{*}b_i]. \tag{4}$$

They are coupled through the order parameters $\Delta_i=v\langle c_{i\downarrow}c_{i\uparrow}\rangle$ and $\rho_i=v\langle b_i\rangle$, which have to be determined self-consistently.[2,12] One can diagonalize the boson subsystem using a suitable unitary transformation. Statistical expectation values of the number operator $b_i^{\dagger}b_i$ and the parameter ρ_i are given by[2,12]

$$\langle b_i^{\dagger}b_i\rangle=\frac{1}{2}-\frac{\Delta_B-2\mu}{4\gamma_i}\tanh\left(\frac{\gamma_i}{k_BT}\right), \tag{5}$$

$$\rho_i=-\frac{v\Delta_i}{2\gamma_i}\tanh\left(\frac{\gamma_i}{k_BT}\right), \tag{6}$$

where $\gamma_i=\frac{1}{2}\sqrt{(\Delta_B-2\mu)^2+4|\Delta_i|^2}$, and k_B is the Boltzmann constant. Near the superconducting phase transition the order parameters are infinitesimally small, and one can expand ρ_i in powers of $\langle c_{i\downarrow}c_{i\uparrow}\rangle$ up to the leading order. The fermionic subsystem is then described by

$$H^F=\sum_{i,j,\sigma}[t_{ij}(\mathbf{A})-\delta_{ij}\mu]c_{i\sigma}^{\dagger}c_{j\sigma}-V(T,\mu)\sum_{i}[\langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}\rangle c_{i\downarrow}c_{i\uparrow}+\text{H.c.}], \tag{7}$$

where

$$V(T,\mu)=\frac{v^2}{\Delta_B-2\mu}\tanh\left(\frac{\Delta_B-2\mu}{2k_BT}\right). \tag{8}$$

Hamiltonian H^F [Eq. (7)] has a BCS–type structure where the boson–fermion coupling enters through the effective pairing potential $V(T,\mu)$. Chemical potential μ should be evaluated from the conservation of the total charge $n_{\text{tot}}\equiv 2n_B+n_F=2/N\Sigma_i\langle b_i^{\dagger}b_i\rangle+1/N\Sigma_{i\sigma}\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle$. We restrict further investigation only to a case of the nearest neighbor hopping, when the fermionic energy spectrum is known as the Hofstadter butterfly.[37]

III. RESULTS AND DISCUSSION

First we consider a situation when the boson level is located in the middle of the fermionic band ($\Delta_B=0$) and $n_{\text{tot}}=2$. In this *symmetric case* both fermion and boson subsystems are half–filled, $n_B=1/2$, $n_F=1$, and $V(T,\mu)=v^2/2k_BT$, because $\mu=0$. In order to calculate H_{c2} one can apply a two-dimensional version of the Helfand-Werthamer theory,[30] where the coupling constant λ, depends on the temperature. Since $\lambda=V\rho_{\text{FS}}$, where ρ_{FS} is the density of states at the Fermi level, one obtains

$$\lambda(T)=\lambda(T_c)\frac{T_c}{T}. \tag{9}$$

The HW theory was derived for a free-electron gas and neglects the Landau level structure (the so called quasiclassical limit). However, for a weak magnetic field the Landau level

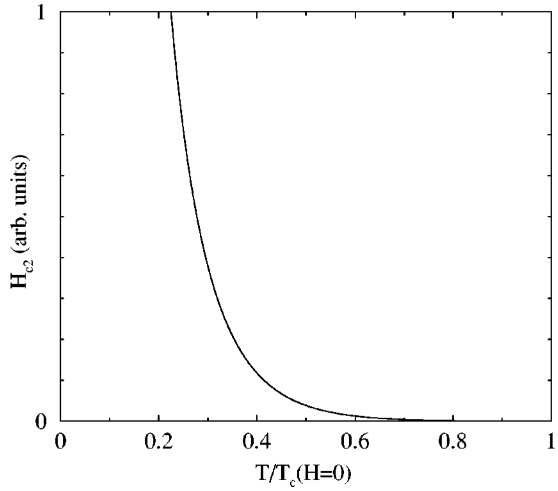

FIG. 1. Temperature dependence of the upper critical field, obtained from the HW approach with the temperature dependent coupling constant given by Eq. (9). We have assumed $k_B T_c(H=0) = 0.02t$.

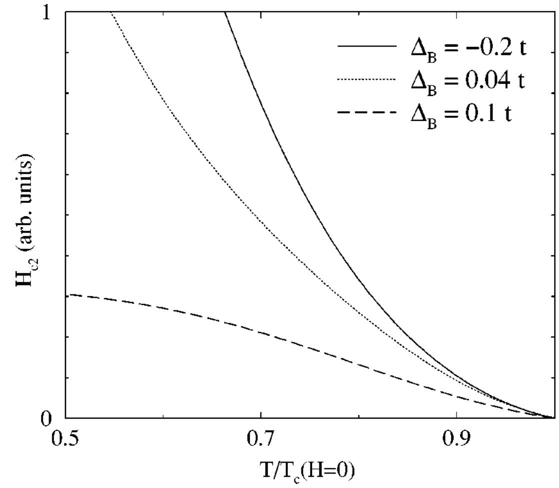

FIG. 2. $H_{c2}(T)$ obtained from Eq. (10) for $n_{tot}=1$ and different bosonic levels. The fermion-boson coupling was adjusted to obtain the same critical temperature in the absence of a magnetic field.

quantization does not lead to an essential modification of $H_{c2}(T)$.[39] Figure 1 shows $H_{c2}(T)$ calculated within the HW approach with the coupling constant determined by Eq. (9). In order to explain the temperature dependence of the critical field qualitatively let us recall the following facts: (i)when $\lambda(T)=\text{const}$ (standard HW theory), $H_{c2}(T)$ is almost linear for a weak magnetic field; (ii) in the BF model λ increases with the decrease of temperature and diverges when $T\to 0$ [Eq. 9]. Thus the BF model properly reproduces two 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 confirm (see Fig. 1) that the upward curvature is preserved in the whole range of temperature. This result is opposite to the standard HW approach, where $H_{c2}(T)$ has a negative curvature.

Next, we show that the BF model properly describes $H_{c2}(T)$ for a wide range of model parameters, when the problem cannot be reduced to the effective HW theory. In this case we apply a lattice version of the Gor'kov equations[39]

$$\Delta_i = \frac{V(T)}{\beta} \sum_{j,\omega_n} \Delta_j G(i,j,\omega_n) G(i,j,-\omega_n). \qquad (10)$$

Here, $G(i,j,\omega_n)$ is the one-electron Green's function in the presence of a uniform and static magnetic field, and ω_n is the fermionic Matsubara frequency. With the help of the Hofstadter approach,[37] Eq. (10) can exactly be solved for clusters of the order of 10^4 lattice sites. For details we refer to Ref. 39. 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 various 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 $T\to 0$; and (ii) for $\Delta_B>0$, bosonic states are occupied only virtually. The concentration of bosons as a function of Δ_B is presented in Fig. 3. The upward curvature of $H_{c2}(T)$ appears predominantly in the first case (solid line in Fig. 2). When Δ_B is shifted above the Fermi energy, the curvature is gradually reduced. Finally, when $\Delta_B \gg k_B T$ the curvature changes from positive to negative (dashed line in Fig. 2) and one reproduces standard results for a purely fermionic system[39]. In Fig. 2 we have not presented results in the low temperature regime. However, one can prove that the BF model qualitatively reproduces $H_{c2}(T)$ also for $T\to 0$. Combining Eqs. (5) and (8), one can express the effective pairing potential in terms of the bosonic occupation number:

$$V(T,\mu) = \frac{2v^2}{\Delta_B - 2\mu}\left(\frac{1}{2} - \langle b_i^\dagger b_i \rangle\right). \qquad (11)$$

It is straightforward to note that for $\langle b_i^\dagger b_i\rangle = 1/2$ one obtains $\Delta_B = 2\mu$ and Eq. (8) is reduced to $V(T)=v^2/2k_BT$. On the other hand, when $\langle b_i^\dagger b_i\rangle \neq 1/2$, but $0<n_B<1$, the denomina-

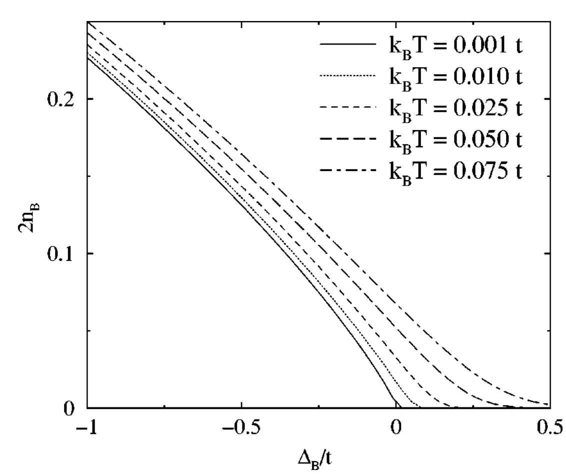

FIG. 3. The boson concentration n_B as a function of Δ_B calculated for $n_{tot}=1$. Temperature dependence of n_B is rather negligible.

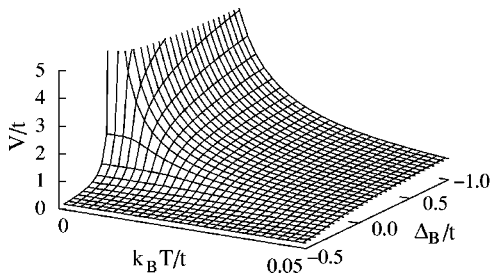

FIG. 4. The effective pairing potential between fermions as a function of temperature T and the boson energy level Δ_B for $v=0.1t$ and $n_{\rm tot}=1$.

tor in Eq. (11) vanishes for $T\rightarrow 0$. Therefore, $V(T,\mu)$ diverges for $T\rightarrow 0$ provided that $0<n_b<1$. Figure 4 illustrates the effective pairing potential $V(T,\mu)$ calculated self-consistently for $n_{\rm tot}=1$ and $v=0.1t$. Note a strong temperature dependence of $V(T,\mu)$ for such values of Δ_B when the boson concentration is non-negligible. This means that a requirement for a partial occupation of bosonic states is sufficient to reproduce the experimental low temperature behavior of H_{c2}.

To complete the discussion, we show that the BF model accurately reproduces the experimental data (see Fig. 5). We have chosen an appropriate set of model parameters, for which $H_{c2}(T)$ fits the results presented in Refs. 21 and 22 very well. The theoretical curve was calculated for a bosonic level that is situated slightly above the Fermi energy, i.e., $n_{\rm tot}=1$, $\Delta_B=0$, and $v=0.5t$. In this case $\mu<0$, $n_F\gg n_B$ and the BF system is mainly of fermionic character. The experimental data were obtained for overdoped compounds, when HTSCs exhibit a Fermi liquid character.[34] Therefore, the BF model is fully consistent with the fermionic–type behavior of the overdoped HTSC, whereas the purely bosonic approach[33] is not applicable in this regime. The most unusual properties of HTSCs occur in underdoped systems. In order to restore these properties one should appropriately adjust the BF model parameters. In the underdoped case, the bosonic occupation number is generally much larger than n_B obtained for parameters, which we have used for overdoped HTSC (Fig. 5). This is due to the fact that the boson concentration controls the width of the pseudogap. In particular, investigations of the pseudogap in Ref. 17 have been carried out for $n_{\rm tot}=1.25$, $n_F\leqslant 1$, and $v=0.1$.

Figures 2 and 5 show $H_{c2}(T)$ obtained numerically for $T>0.4T_c$. 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 sus-

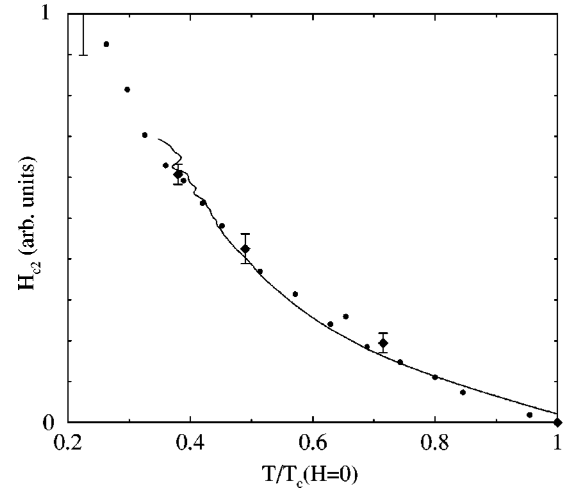

FIG. 5. Fit to experimental results (continuous curve) obtained for $n_{\rm tot}=1$, $\Delta_B=0$ and $v=0.5t$. The experimental data (points) were taken for $Tl_2Ba_2CuO_6$ from Ref. 22, and for $Bi_2Sr_2CuO_y$ from Ref. 21.

ceptibility accounts only for very few fermionic states (with energy close to the Fermi level) instead of a continuous density of states. For a sufficiently strong magnetic field the Landau level quantization becomes important, and $H_{c2}(T)$ may be a nonmonotonic function .[26,40] This feature is visible in the low temperature region in Fig. 5. These oscillations may be smeared out by fluctuations which, however, are neglected within a mean–field approach. In real materials the disorder–induced broadening of Landau levels also smooths out the density of states, and these irregularities do not appear.

To conclude, we have shown that the BF model properly reproduces the anomalous features of the upper critical field observed in HTSC materials. Such an unusual behavior cannot be explained within a standard BCS-type approach. Moreover, our results are correct not only in the underdoped region but also for the overdoped compounds, where a Fermi liquid behavior is observed. Together with other unconventional properties such as the pseudogap, our results strongly support the BF model as a relevant scenario for high-T_c superconductivity.

ACKNOWLEDGMENTS

T.D. kindly acknowledges financial support from the Joseph Fourier University and the hospitality of the Centre de Recherches sur les Trѐs Basses Temperatures in Grenoble.

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