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BCS–BEC and observed sharp vs. BCS exponential rise in T_c

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ABSTRACT

We show how a recent generalized Bose–Einstein condensation (GBEC) formalism predicts a *sharp* rise in T_c with charge-carrier density as observed in variably-doped cuprates, in contrast with the *exponential* rise predicted by BCS theory.

1. Introduction

Boson–fermion (BF) models of superconductivity were apparently introduced as early as 1985 [1]. Soon, a Bose–Einstein condensation (BEC) BF field theory by Friedberg and Lee appeared [2]. Both these efforts, however, were *binary* BF models as they neglected the possibility of two-*hole* Cooper-pair (CP) bosons. Inclusion of 2 h-CPs lead to a generalized BEC (GBEC) formalism [3] describing a *ternary* BF model. This contained the 2e-/2 h-CP energies $E_{\pm}(K)$ *phenomenologically*, where K is the CP center-of-mass momentum (CMM) wavenumber. A BEC (or macroscopic occupation of a given state that appears below a certain fixed $T = T_c$) was found [3] numerically *a posteriori* in the GBEC theory.

2. GBEC formalism

Two *new* phenomenological dynamical energy parameters $E_f \equiv \frac{1}{4}[E_+(0) + E_-(0)]$ and $\delta\varepsilon \equiv \frac{1}{2}[E_+(0) - E_-(0)] \geqslant 0$ can then be defined, where $E_{\pm}(0)$ are the (empirically *un*known) zero-CMM energies of the 2e- and 2 h-CPs, respectively.

One can refer to E_f as a "pseudoFermi" energy. It serves as a convenient energy scale and is not to be confused with the usual Fermi energy $E_F = \frac{1}{2}mv_F^2 \equiv k_B T_F$ where T_F is the Fermi temperature. If n is the total number-density of charge-carrier electrons of effective mass m, the Fermi energy $E_F = (\hbar^2/2m)(3\pi^2 n)^{2/3}$ in 3D, while E_f is similarly related to another density n_f which serves to scale the ordinary density n. The two quantities E_f and E_F, and consequently also n and n_f, coincide *only* when perfect 2e/2 h-CP symmetry holds as in the BCS instance.

With the GBEC Hamiltonian explicitly diagonalized, one can straightforwardly construct the thermodynamic potential $\Omega \equiv -PL^d$, with L^d the system "volume" and P its pressure, defined as $\Omega(T, L^d, \mu, N_0, M_0) = -k_B T \ln \times [Tr \exp\{-\beta(H - \mu\widehat{N})\}]$ where "Tr" stands for "trace", and N_0 and M_0 are the number of zero-CMM 2e- and 2 h-CPs, respectively. After some algebra an explicit expression for Ω follows.

3. Helmholtz free energy

The Helmholtz free energy is then, by definition,

$$F(T, L^d, \mu, N_0, M_0) \equiv \Omega(T, L^d, \mu, N_0, M_0) + \mu N.$$

Minimizing it with respect to N_0 and M_0, and simultaneously fixing the total number N of electrons by introducing the electron chemical potential μvia the usual way, specifies an *equilibrium state* of the system at fixed volume L^d and temperature T. The necessary conditions for an equilibrium thermodynamic state are $\partial F/\partial N_0 = 0$, $\partial F/\partial M_0 = 0$, and $\partial\Omega/\partial\mu = -N$, where N evidently includes both paired and unpaired fermions. Second partial derivatives of F have also been examined [4]. After some algebra these conditions lead to the three coupled transcendental found in Ref.[3]. These can be rewritten somewhat more transparently as: (a) two *"gap-like equations"*

$$[2E_f + \delta\varepsilon - 2\mu(T)] = \frac{1}{2}f^2 \int_{E_f}^{E_f+\delta\varepsilon} d\epsilon N(\epsilon) \times \frac{\tanh\frac{1}{2}\beta\sqrt{[\epsilon - \mu(T)]^2 + f^2 n_0(T)}}{\sqrt{[\epsilon - \mu(T)]^2 + f^2 n_0(T)}} \quad (1)$$

and

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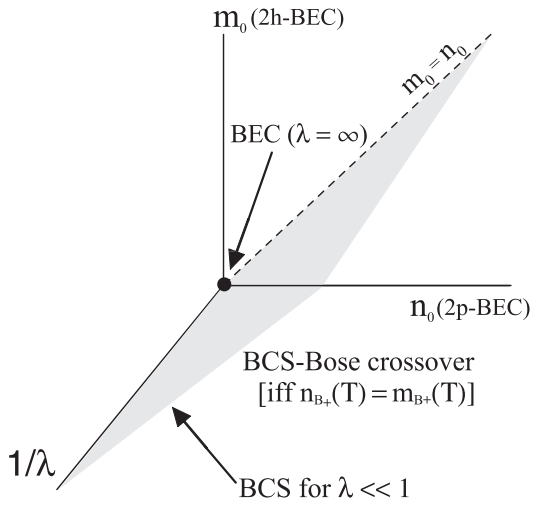

Fig. 1. Parameter octant defined by the two condensate densities $n_0(T) \geqslant 0$ and $m_0(T) \geqslant 0$ as well as the (also nonnegative) *inverse* $1/\lambda \geqslant 0$ of the interelectronic BCS dimensionless coupling $\lambda \geqslant 0$, and applicable in principle at all temperatures T. The GBEC describes a ternary gas and applies in the *entire* octant. The BCS–Bose crossover theory applies *only* on the shaded plane defined by $n_0(T) \equiv m_0(T)$ provided the additional restriction $n_{B+}(T) = m_{B+}(T)$ is imposed whereby the total number of 2p (two-electron) *non* condensate CPs equals that of 2 h (two-hole) CPs. BCS theory is valid along the *forefront* of the shaded plane where $\lambda \ll 1$ of the shaded BCS–Bose crossover plane. For quadratically-dispersive bosons the usual BEC theory ensues at the origin of the octant where $m_0(T) = 0$ for all T and $n_0(T_c) = 0$, giving there the *implicit* expression $T_c \simeq 3.31\hbar^2 n_B(T_c)^{2/3}/2mk_B$. This has the same *form* as the standard *explicit* BEC T_c-formula for mass $2m$ bosons and where the boson number density n_B is, of course, independent of T_c.

$$[2\mu(T) - 2E_f + \delta\varepsilon] = \frac{1}{2}f^2 \int_{E_f - \delta\varepsilon}^{E_f} d\epsilon N(\epsilon) \times \frac{\tanh\frac{1}{2}\beta\sqrt{[\epsilon - \mu(T)]^2 + f^2 m_0(T)}}{\sqrt{[\epsilon - \mu(T)]^2 + f^2 m_0(T)}} \quad (2)$$

with $\beta \equiv 1/k_B T$, as well as b) a single *"number equation"* $2n_B(T) - 2m_B(T) + n_f(T) = n$ that ensures charge conservation in the ternary mixture.

Here $n \equiv N/L^d$ is the total number density of electrons, $n_f(T)$ is the number density of *unpaired* electrons, while $n_B(T)$ and $m_B(T)$ are respectively those of 2e- and 2 h-CPs in *all* bosonic states, ground plus excited, i.e., condensed $n_0(T)$ plus noncondensed $n_{B+}(T)$. They turn out to be $n_B(T) \equiv n_0(T) + n_{B+}(T)$ and $m_B(T) \equiv m_0(T) + m_{B+}(T)$ where

$$n_{B\pm}(T) \equiv \int_{0+}^{\infty} d\varepsilon M(\varepsilon)(\exp\beta[\pm 2E_f + \delta\varepsilon \mp 2\mu + \varepsilon] - 1)^{-1}$$

clearly evidencing the bosonic nature of both kinds of CPs. Here $N(\epsilon) \equiv m^{3/2}\sqrt{\epsilon}/2^{1/2}\pi^2\hbar^3$ while $M(\varepsilon) \equiv 2m^{3/2}\sqrt{\varepsilon}/\pi^2\hbar^3$ for $d = 3$. One picks $\delta\varepsilon = \hbar\omega_D$, and if f in (1) and (2) is taken as $\sqrt{2\hbar\omega_D V}$, where V is the BCS model attractive-interaction strength, one recovers both the BCS gap equation precisely for all T and all interaction parameters as well as the $T = 0$ BCS condensation energy for all such. The number density of unpaired electrons at any T is

$$n_f(T) \equiv \int_0^{\infty} d\epsilon N(\epsilon)\left[1 - \{[\epsilon - \mu]/E(\epsilon)\}\tanh\frac{1}{2}\beta E(\epsilon)\right] \quad (3)$$

with $E(\epsilon) = \sqrt{(\epsilon - \mu)^2 + \Delta^2(\epsilon)}$. The octant defined by Fig. 1 illustrates the applicability at any temperature T and any electron

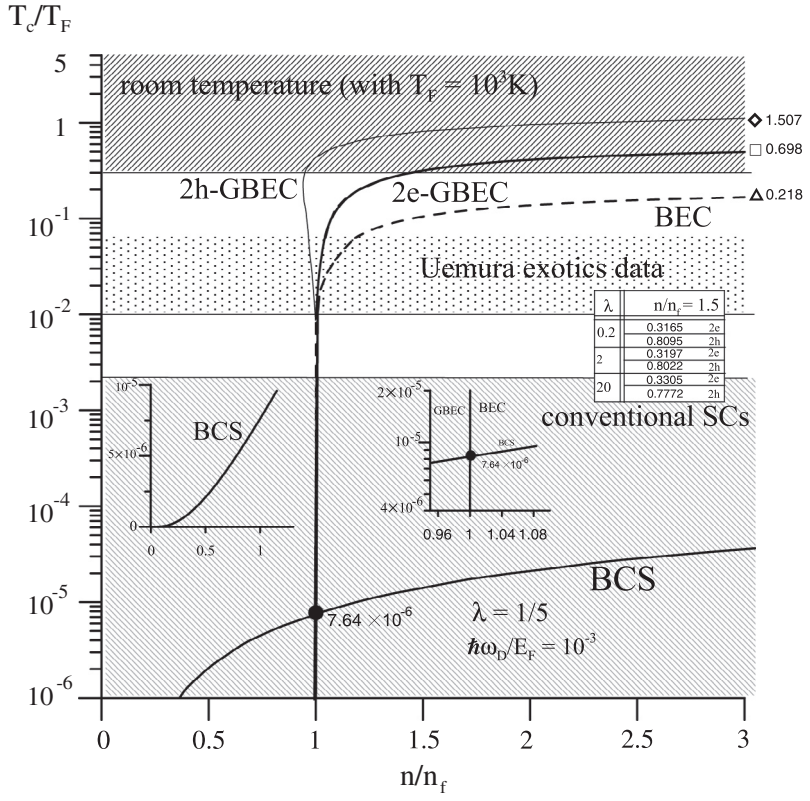

Fig. 2. Phase boundaries of pure GBEC of 2 h-CPs (thin curve) and of 2e-CPs (thick full curve) compared to the standard BEC curve (dashed) and the BCS (lower full curve), for a BCS model interaction creating the CPs, all for $\lambda = 1/5$ and $\hbar\omega_D/E_F = 10^{-3}$ vs. dimensionless charge-carrier densities n/n_f with n_f as defined in text. Exotics data are from Ref. [5]. Insets are zoom-ins except for table reporting values at $n/n_f = 1.5$ of the 2e-GBEC phase boundary for $\lambda = 0.2,2$ and 20.

concentration n of the BCS–Bose crossover picture and the BCS theory implying its dimensionless coupling $\lambda \equiv N(E_F)V$ where V is the net attractive interelectronic interaction causing the formation of CPs. The applicability of the GBEC formalism spans the entire octant with vertical and horizontal axes defined by $m_0(T,n)$ and $n_0(T,n)$, respectively.

4. Sharp vs. BCS exponential rise of T_c

Numerical elimination of $\mu(T,n)$ has shown that, in addition to a normal phase defined by $n_0(T,n) = m_0(T,n) = 0$ at high T, at lower temperatures *three* condensed phases appear: two pure phases of 2e-CP- and 2 h-CP-BE-condensed states and one mixed phase with arbitrary proportions of both kinds of BE-condensed CPs. Fig. 2 shows the phase boundaries for the specific set of BCS interaction parameters $\lambda = 1/2$ and $\hbar\omega_D = 10^{-3}E_F$. These results would seem to suggest a possible explanation, to be explored in the near future, for the intriguing experimental fact emphasized by Hirsch (Ref. [6] §6) that regardless of whether charge carriers *above* T_c are holes or electrons, they are always electrons *below* T_c.

5. Conclusions

The GBEC formalism predicts the observed *linear*rise of T_c with charge-carrier density (i.e., doping) in contrast with the *exponential* rise of BCS theory. The hopefully practical outcome of the BCS–BEC unification via the GBEC formalism is *enhancement* in T_c by up to *four* orders-of-magnitude in 3D. These enhancements fall within empirical ranges for 2D and 3D "exotic" SCs, whereas BCS T_c values remain much lower—being within the empirical ranges for conventional, elemental SCs using standard interaction-parameter values. Lastly, room temperature superconductivity is possible for a material with a Fermi temperature $T_F \leqslant 10^3 K$, with the *same* interaction parameters used in BCS theory for conventional SCs.

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