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COOPER PAIRING AND LADDER CORRELATIONS IN A BCS GROUND STATE

V. C. AGUILERA-NAVARRO

Depto. de Física, UNICENTRO, 85015, Guarapuava, PR, Brazil

M. FORTES

Instituto de Física, Universidad Nacional Autónoma, de México
Apdo. Postal 20-364, 01000, México D.F. México

M. DE LLANO

Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México
Apdo. Postal 70-360, 04510 México DF, México

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A Bethe–Salpeter treatment of Cooper pairs (CPs) based on an ideal Fermi gas (IFG) "sea" produces unstable CPs if holes are not ignored. Stable CPs with damping emerge when the BCS ground state replaces the IFG, and are positive-energy, finite-lifetime resonances for nonzero center-of-mass momentum with a *linear* dispersion leading term. Bose–Einstein condensation of such pairs may thus occur in exactly two dimensions as it cannot with quadratic dispersion.

Keywords: Cooper-pairs; Bethe–Salpeter.

Shortly after the appearance of the BCS theory of superconductivity, charged Cooper pairs[1] (CPs) observed in magnetic flux quantization experiments with 3D conventional, and much later with quasi-2D cuprates, superconductors, suggested CPs as a fundamental ingredient of this phase. Although BCS theory only considers the presence of Cooper "correlations," several boson-fermion (BF) models with real, bosonic CPs have been introduced after the pioneering work of Schafroth;[2] for a superb review see Ref. 3. However, with one exception,[4–6] all such models neglect the effect of two-hole (2h) CPs taken on an equal footing with two-particle (2p) CPs — as Green's functions can naturally guarantee. Strong physical motivation for this paper comes from the unique but unexplained role played by *holes* in the normal state of superconductors in general. Additional motivation stems from the fact that the "complete (in that both 2h- and 2p-CPs are allowed) BF model" of Refs. 4–6 is able to "unify" both BCS and Bose–Einstein condensation (BEC) theories as special cases, and predict substantially higher T_c's than BCS theory without abandoning electron-phonon dynamics. Compelling evidence for a significant presence of the latter in high-T_c cuprate superconductors from angle-resolved photoemission spectroscopy data has recently been reported.[7]

Here, the Bethe–Salpeter (BS) many-body equation (in the ladder approximation) treating both particles and holes on an equal footing is used to recall that:

(i) The CP problem [based on an ideal Fermi gas (IFG) ground state (the usual "Fermi sea")] does *not* possess stable energy solutions, i.e. with nonzero real energies.
(ii) CPs based not on the IFG-sea but on the BCS ground state survive as *positive* energy resonances.
(iii) Their dispersion relation in the total (or center-of-mass) momentum (CMM) $\hbar\mathbf{K} \equiv \hbar(\mathbf{k}_1 + \mathbf{k}_2)$ in leading order is *linear* rather than the quadratic $\hbar^2K^2/4m$ of a composite boson (e.g., a deuteron) of mass $2m$ moving not in the Fermi sea but in vacuum.
(iv) This latter "moving CP" solution, though often confused with it, is physically *distinct* from another more common solution sometimes called the Anderson–Bogoliubov–Higgs (ABH),[8] (Ref. 9, p. 44) collective excitation.

The ABH sound mode is also linear in leading order and goes over into the IFG ordinary sound mode in zero coupling. Though most of our results hold in 3D,[10] they are here detailed in 2D because of its interest for quasi-2D cuprate superconductors, and will be seen to be crucial in Bose–Einstein condensation (BEC) scenarios with BF models of superconductivity, as well as for neutral-atom superfluidity, *in exactly 2D.* In general, for free bosons with energy $\varepsilon_K = C_s K^s + o(K^s)$ (for small enough CMM K, with C_s a constant) BEC occurs in a box if and only if $d > s$, since $T_c \equiv 0$ for all $d \leq s$ as it is then given by an expression with an integral in the denominator which diverges in its *lower* limit. We distinguish between CPs and BCS pairs since the former satisfy BE statistics while the latter do not obey BE commutation relations.

In dealing with the many-electron system we assume an s-wave BCS-like electron-phonon model interelectron interaction, whose double Fourier transform $\nu(|\mathbf{k}_1 - \mathbf{k}_1'|)$ is just

$$\nu(k_1, k_1') = -(k_F/k_1')V \tag{1}$$

if $k_F - k_D < k_1 < k_F + k_D$, and $= 0$ otherwise, where $V > 0$, $\hbar k_F \equiv m v_F$ the Fermi momentum, m the effective electron mass, v_F the Fermi velocity, and $k_D \equiv \omega_D/v_F$ with ω_D the Debye frequency. The usual condition $\hbar\omega_D \ll E_F$ then implies that $\hbar\omega_D/2E_F \equiv k_D/k_F \ll 1$. The BS wavefunction equation[10] in the ladder approximation for the IFG-based CP problem using (1), with both particles and holes, leads to an equation for the wavefunction $\psi_{\mathbf{k}}$ in momentum space for *zero* CMM CPs, with $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ the relative wavevector of the pair, namely

$$(2\xi_k - \mathcal{E}_0)\psi_{\mathbf{k}} = V{\sum_{\mathbf{k}'}}'\psi_{\mathbf{k}'} - V{\sum_{\mathbf{k}'}}''\psi_{\mathbf{k}'}\,. \tag{2}$$

Here $\xi_k \equiv \hbar^2 k^2/2m - E_F$ and $\mathcal{E}_0$ is the eigenvalue energy. The single prime over the first (2p-CP) summation term denotes the restriction $0 < \xi_{k'} < \hbar\omega_D$ while the double prime in the last (2h-CP) term signifies $-\hbar\omega_D < \xi_{k'} < 0$. Without this latter term we have the Cooper Schrödinger-like equation[1] for 2p-CPs whose implicit solution is clearly

$$\psi_{\mathbf{k}} = (2\xi_k - \mathcal{E}_0)^{-1} V \sum_{\mathbf{k}'}{}' \psi_{\mathbf{k}'} \, .$$

Since the summation term is constant, performing that summation on both sides allows canceling the $\psi_{\mathbf{k}}$-dependent terms, leaving the eigenvalue equation

$$\sum_{\mathbf{k}'}{}' (2\xi_k - \mathcal{E}_0)^{-1} = 1/V$$

with the familiar solution (exact in 2D and to a very good approximation otherwise if $\hbar\omega_D \ll E_F$):

$$\mathcal{E}_0 = -2\hbar\omega_D/(e^{2/\lambda} - 1) \, ,$$

where $\lambda \equiv VN(E_F)$ with $N(E_F)$ the electronic density of states (DOS) for one spin. This corresponds to a negative-energy bound pair. Without the first summation in (2) the same result for $\mathcal{E}_0$ (apart from a sign change) follows for 2h-CPs. However, solving by similar techniques the *full* equation (2) — which *cannot* be derived from an ordinary (non-BS) Schrödinger-like equation in spite of its simple appearance — gives the purely-imaginary $\mathcal{E}_0 = \pm i2\hbar\omega_D/\sqrt{e^{2/\lambda} - 1}$, thus implying an obvious instability. This was reported in Refs. 9 (p. 44) and 11, Sec. 33 — without mentioning the pure 2p and 2h cases just discussed. *The CP problem is thus unstable and hence meaningless if particles and holes are treated on an equal footing.*

However, a BS treatment not about the IFG sea but about the BCS ground state *vindicates the CP problem*, and adds something new. In either 3D or 2D it yields two *distinct* solutions, the usual ABH sound solution and a highly nontrivial "moving-CP" solution. These wavefunction equations are too lengthy, and will be derived in detail elsewhere. The *ABH collective excitation mode* energy $\mathcal{E}_K$ is found to give for small λ:

$$\pm\mathcal{E}_K \simeq \frac{\hbar v_F}{\sqrt{2}} K + O(K^2) \, . \tag{3}$$

Note that the leading term is just the IFG ordinary sound mode whose sound speed $c = v_F/\sqrt{d}$ in d dimensions follows trivially from the zero-temperature IFG pressure $P = n^2[d(E/N)/dn] = 2nE_F/(d+2)$ on applying the familiar thermodynamic relation $dP/dn = mc^2$. Here E is the ground-state energy and $n \equiv N/L^d = k_F^d/d2^{d-2}\pi^{d/2}\Gamma(d/2)$ the fermion-number density.

The second *moving-CP* solution in the BCS-ground-state-based BS treatment has a pair energy $\mathcal{E}_K$ which in 2D is contained in

$$\frac{1}{2\pi}\,\lambda\hbar v_F\int_{k_F-k_D}^{k_F+k_D}dk\int_0^{2\pi}d\varphi u_{\mathbf{K}/2+\mathbf{k}}v_{\mathbf{K}/2-\mathbf{k}}\{u_{\mathbf{K}/2-\mathbf{k}}v_{\mathbf{K}/2+\mathbf{k}}-u_{\mathbf{K}/2+\mathbf{k}}v_{\mathbf{K}/2-\mathbf{k}}\}$$
$$\times\,\frac{E_{\mathbf{K}/2+\mathbf{k}}+E_{\mathbf{K}/2-\mathbf{k}}}{-\mathcal{E}_K^2+(E_{\mathbf{K}/2+\mathbf{k}}+E_{\mathbf{K}/2-\mathbf{k}})^2}=1\,, \tag{4}$$

where φ is the angle between $\mathbf{K}$ and $\mathbf{k}$; $\lambda \equiv VN(E_F)$ as before with $N(E_F) \equiv m/2\pi\hbar^2$ the constant 2D DOS; $E_{\mathbf{k}} \equiv \sqrt{\xi_k^2+\Delta^2}$ with Δ the familiar BCS $T=0$ gap which for interaction (1) is $\Delta = \hbar\omega_D/\sinh(1/\lambda)$; while $u_k^2 \equiv \frac{1}{2}(1+\xi_k/E_{\mathbf{k}})$ and $v_k^2 \equiv 1-u_k^2$ are the Bogoliubov functions. In addition to the pp and hh wavefunctions (depicted diagrammatically in Ref. 10, Fig. 2), diagrams associated with the ph channel give zero contribution at $T=0$. A third equation for the ph wavefunction describes the ph bound state but turns out to depend only on the pp and hh wavefunctions. Using a Taylor expansion of $\mathcal{E}_K$ in powers of K around $K=0$ in (4) and on introducing a damping factor by adding an imaginary term $-i\Gamma_K$ in the denominator, a direct integration yields, to order K^2 and for small λ

$$\pm\mathcal{E}_K \simeq 2\Delta+\frac{\lambda}{2\pi}\,\hbar v_F K+\frac{1}{9}\frac{\hbar v_F}{k_D}\,e^{1/\lambda}K^2$$
$$-\,i\left[\frac{\lambda}{\pi}\hbar v_F K+\frac{1}{12}\frac{\hbar v_F}{k_D}e^{1/\lambda}K^2\right]+O(K^3)\,, \tag{5}$$

where the upper and lower sign refers to 2p- and 2h-CPs, respectively. A linear dispersion in leading order again appears which, unlike the sound mode in (3), now vanishes in zero coupling as expected. The *positive*-energy 2p-CP resonance

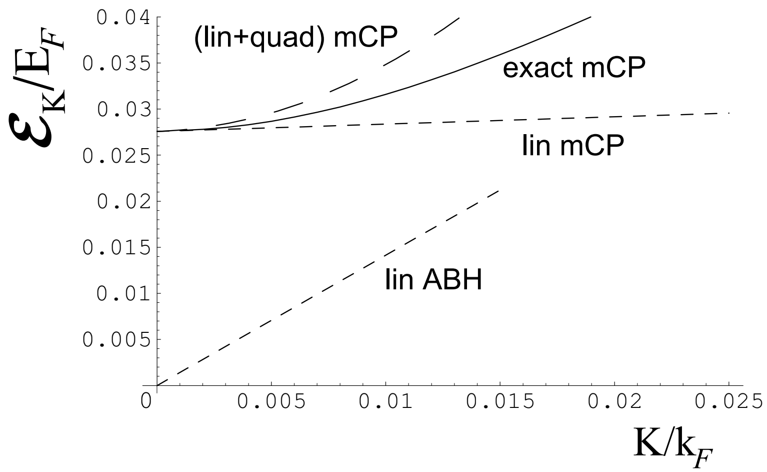

Fig. 1. Exact "moving Cooper pair" energy $\mathcal{E}_K$ (in units of E_F) (full curve) extracted from (44), compared with its linear leading term (upper short-dashed line) and its linear plus quadratic expansion (long-dashed curve) from (5), *vs* CMM wavenumber K (in units of k_F), for BCS model interfermion interaction with parameters $\lambda=\frac{1}{2}$ and $\hbar\omega_D/E_F=0.05$. For reference, the leading linear term (3) of the ABH sound mode is also plotted (lower short-dashed line).

has a lifetime $\tau_K \equiv \hbar/2\Gamma_K = \hbar/2[(\lambda/\pi)\hbar v_F K + (\hbar v_F/12k_D)e^{1/\lambda}K^2]$ diverging only at $K = 0$, and falling to zero as K increases. Figure 1 graphs the exact moving CP (mCP) solution, along with its leading linear-dispersion term, and this plus the next, quadratic, term. The interaction parameter values used in (4) were $\hbar\omega_D/E_F = 0.05$ (a typical value for cuprates) and $\lambda = \frac{1}{2}$, which give $2\Delta/E_F = 2\hbar\omega_D/E_F \sinh(1/\lambda) \simeq 0.028$. For reference we also plot the linear term $\hbar v_F K/\sqrt{2}$ of the ABH sound solution (3).

To conclude, we see that holes treated on a par with electrons play a vital role in determining the precise nature of CPs even at zero temperature, but only when based not on the usual ideal-Fermi-gas (IFG) "sea" but on the BCS ground state. Their treatment with a BS equation gives purely-imaginary energies based on the IFG and positive-energy resonant-state CPs with a finite lifetime for nonzero CMM when based on the BCS ground state, instead of the more familiar negative-energy stationary states emerging from the original IFG-based CP problem that neglects holes, as sketched just below (2). The BS moving-CP dispersion relation is gapped by twice the BCS gap energy, followed by a *linear* leading term in the CMM expansion. This linearity is *distinct* from the better-known one associated with the sound or ABH collective excitation mode whose energy vanishes with zero total pair momentum. Thus, BF models accounting for this CP linearity in the boson component can give rise to BEC in $d > 1$, including exactly 2D, and thus in principle addressing not only quasi-2D cuprate but also quasi-1D organo-metallic superconductors.

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References

1. L. N. Cooper, *Phys. Rev.* **104**, 1189 (1956).
2. M. R. Schafroth, *Phys. Rev.* **96**, 1442 (1954).
3. J. M. Blatt, *Theory of Superconductivity* (Academic, New York, 1964).
4. V. V. Tolmachev, *Phys. Lett.* **A266**, 400 (2000).
5. M. de Llano and V. V. Tolmachev, *Physica* **A317**, 546 (2003).
6. J. Batle, M. Casas, M. Fortes, M. de Llano, M. A. Solís and V. V. Tolmachev, *Cond. Matter Theories* **18**, (in press) (2003); cond-mat/0211456.
7. A. Lanzara, P. V. Bogdanov, X. J. Zhou, S. A. Kellar, D. L. Feng, E. D. Lu, T. Yoshida, H. Eisaki, A. Fujimori, K. Kishio, J.-I. Shimoyama, T. Noda, S. Uchida, Z. Hussain and Z.-X. Shen, *Nature* **412**, 510 (2001).
8. P. W. Anderson, *Phys. Rev.* **112**, 1900 (1958).
9. N. N. Bogoliubov, V. V. Tolmachev and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (Consultants Bureau, New York, 1959).

10. M. Fortes, M. A. Solís, M. de Llano and V. V. Tolmachev, *Physica* **C364–365**, 95 (2001).
11. A. A. Abrikosov, L. P. Gorkov and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975).