RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 36, NUMBER 4 1 AUGUST 1987

Tensor-boson condensation in superconductivity of heavy-fermion systems

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(Received 17 November 1986)

A theory of heavy-fermion superconductivity is proposed based on a tensor-boson condensation within an SU(N) Anderson-lattice model in which f^0, f^1, and f^2 states are allowed. The order parameter is a multiplet for $N>2$. In an s-wave model, a Kondo-like expression for the gap is obtained, and T_c and H_c are calculated. Estimates for $CeCu_2Si_2$ give T_c of the correct order of magnitude.

The superconductivity of heavy-fermion systems such as $CeCu_2Si_2$ and UBe_{13} is known to involve the heavy-fermion bands[1] and is thought to be an intrinsic property of the heavy-fermion fluid. It is widely believed that superconductivity has the same origin in the strong, short-range repulsion between f electrons as the heavy-fermion behavior itself.[2-4] But at this time we do not know specifically the nature of the pairing mechanism.

Lavagna, Millis, and Lee[5] consider an Anderson lattice with an infinitely repulsive local interaction between f electrons, constraining the f sites to f^0 and f^1 configurations. This constraint leads to a repulsion between quasiparticles in the $l=0$ channel, so pairing must be in a higher-l channel. With the use of an s-wave SU(N) model, a weak attractive interaction is found in the $l=2$ channel, leading to $l=2$ pairing. However, Zhang and Lee point out[6] that outside the highly idealized SU(N) model, the $l=2$ channel may no longer be attractive.

Experimental evidence from tunneling[7] is compatible with higher-l pairing for UBe_{13}, and specific-heat data[4] suggest a vanishing gap at spots or lines on the Fermi surface. This can arise in an $l\neq 0$ pairing theory, as it does in ^{3}He-A but not in ^{3}He-B. Other characteristic features of heavy-fermion superconductivity, e.g., high critical field, arise essentially from the high fermion mass[8] and are not diagnostic of the pairing mechanism.

In this paper I show, and justify quantitatively, for the first time that when we introduce an additional f^2 occupation into the f^0-f^1 model, an attractive interaction is generated leading to superconductivity, which formally appears as a kind of superfluidity. A conceptual argument is to imagine f^2 as the lowest state (i.e., an attractive electron-electron interaction U) and choose the chemical potential so as to keep the f^2 concentration low. Then the f^2 sites form a dilute Bose gas which is superfluid at low temperatures. In this paper, I first consider an s-wave SU(N) model and, assuming that f^2 is the *highest* state, show that condensation to a superconducting state, which maps onto the U-negative superfluid state, occurs. Pairing is a $l=0$ multiplet and the gap is isotropic. But in a realistic model, pairing is $l>0$ and the gap vanishes at points on the Fermi surface, as indicated by the data.[4,7]

For specificity, consider a Ce-type system close to the $4f^1$ state, when the system is a "Kondo lattice" with very large fermion mass.[9-11] Fluctuations to the $4f^0$ states are usually considered dominant,[8-16] but when the system is close to f^1 it is essential to allow for fluctuations to the f^2 state as well, since it is not so high up relative to the f^0 state, as discussed quantitatively below. Fluctuations to f^2 are treated here as relatively weak. The theoretical approach we use is a large-N one, where N is the f^1 degeneracy. The large-N technique is one of the few approaches enabling reliable calculations to be performed in these systems.[10-17] This technique demands that some oversimplification of the couplings in the lattice be made by adopting a model with SU(N) symmetry,[10-17] an extension of ordinary spin symmetry from twofold to N-fold degeneracy. Thus some subtleties arising from coupling of the gap vector to the lattice will be missed. Finally, I adopt the slave-boson formulation of large-N theory,[10,11,14-17] which is well adapted to treating the lattice[10,11,14-17] and works well below the lattice Kondo temperature T_K.

We introduce the Hamiltonian

$$H=H_d+H_f+H_{fd}+\lambda Q \ , \tag{1}$$

where

$$H_d=\sum_{k,m}\varepsilon_k c_{km}^{\dagger}c_{km} \ , \tag{2a}$$

$$H_f=E_0\sum_k b_k^{\dagger}b_k+E_1\sum_{k,m}f_{km}^{\dagger}f_{km}+E_2\sum_{\substack{k,m,n\\(m>n)}}a_{mn}^{\dagger}(k)a_{mn}(k) \ , \tag{2b}$$

and

$$H_{fd}=\sum_{k,q,m}U_k[b(k-q)f_{qm}^{\dagger}c_{km}+\text{H.c.}]+\sum_{k,q,m,n}V_k[a_{mn}(k+q)f_{qm}^{\dagger}c_{kn}^{\dagger}+\text{H.c.}] \ . \tag{2c}$$

In (1) and (2), H_d is the Hamiltonian of the conduction electrons of wave vector k and z component of angular momentum $m_z=m$, and energy eigenvalue ε_k. Suffix m runs over N values. H_f is the Hamiltonian of the $4f$ electrons, with E_n the energy of the configuration f^n. Configuration f^1, with odd spin, is described by fermion operators f_{km} which are Bloch sums over lattice site states f_{im} on site i. Configurations f^0 and f^2, with even spin, are described, respectively, by scalar bosons b and tensor bo-

sons a_{mn}; a_{mn} is antisymmetric, and thus contains $N(N-1)/2$ independent elements, the number of ways two electrons can be put into f^2. H_{fd} describes fd mixing, f^0-f^1 with amplitude U, and f^1-f^2 with amplitude V. The presence of boson operators in H_{fd} ensures staying in the f^0, f^1, f^2 subspace provided that a local constraint is satisfied:[10,11,14-17]

$$Q_q=\sum_k\left\{\sum_m f^\dagger_{km}f_{k+q\,m}+\sum_{\substack{m,n\\(m>n)}}a^\dagger_{mn}(k)a_{mn}(k+q)+b^\dagger_k b_{k+q}\right\}=1\ . \quad (3)$$

At low temperatures it is sufficient to ensure that the mean value of (3) is satisfied,[10,11,14-17] whence a Lagrange-multiplier term λQ_0 is added to (1). Equations (1)-(3) constitute a generalization of the usual f^0-f^1 boson scheme. A superficially related but different scheme has recently been used by Kotliar and Ruckenstein[18] for the $N=2$ Hubbard model. The key element of the present scheme is that it is defined for arbitrary N and is valid in the large-N limit: specializing (1)-(3) to the single impurity case, I have verified[17] that the correct results in the large-N limit for the model are retrieved.[13,19,20]

In the theory of the f^0-f^1 model the leading-N behavior is found by taking the expectation value $\langle b(0)\rangle=\langle b^\dagger(0)\rangle$ of the $k=0$ b boson, and determining it variationally.[10,11,14-17] If this is done, and then the a-boson self-energy is calculated to formal leading order[21] in $1/N$ (see Fig. 1), a Cooper-like divergence is found in the a propagator at $k=0$. Following BCS it is natural to regulate this by the introduction of anomalous expectation values

$$\langle a^\dagger_{mn}(0)\rangle=\langle a_{mn}(0)\rangle=-\langle a_{nm}(0)\rangle\ .$$

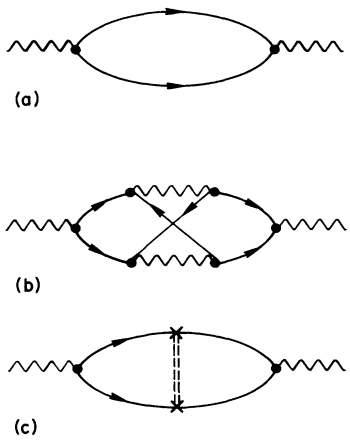

FIG. 1. Diagrams for the a-boson self-energy. Wavy line is an a boson, double broken line a complete b boson. (b) and (c) are formally down by a factor $1/N$ relative to (a).

We then have the mean-field Hamiltonian

$$H=\sum_k\left[\tfrac{1}{2}(\lambda+E_2)\sum_{m,n}\langle a_{mn}(0)\rangle^2+(\lambda+E_0)\langle b\rangle^2-\lambda\right]+\sum_{k,m}\varepsilon_k c^\dagger_{km}c_{km}+\varepsilon_f\sum_{k,m}f^\dagger_{km}f_{km}$$
$$+\sum_{k,m}u_k(f^\dagger_{km}c_{km}+\text{H.c.})+\sum_{k,m,n}V_k[\langle a_{mn}(0)\rangle f^\dagger_{-km}c^\dagger_{kn}+\text{H.c.}]\ . \quad (4)$$

Here $\varepsilon_f=E_1+\lambda$ defines a renormalized f level and $u_k=\langle b(0)\rangle U_k$; ε_f is equal to T_K, the characteristic energy scale of the Kondo lattice.[10,11,14-17]

First diagonalizing Eq. (4) in all except the last term, (4) is expressed in terms of new fermion operators $C_{km\pm}$ representing two hybrid heavy-fermion bands [they are heavy because of the smallness of $\langle b(0)\rangle\approx(1-\langle n_f\rangle)^{1/2}$, making the f-k mixing matrix element u_k small]. In this representation (4) may be written

$$H=\sum_{i(>0)}\left[(E_2+\lambda)d_i^2+\sum_k(-E_kB_{ki}B^\dagger_{ki}+E_{-k}B^\dagger_{-k\,-i}B_{-k\,-i}+E_k)+\sum_k v_k(-iB^\dagger_{-k\,-i}d_iB^\dagger_{ki}+\text{H.c.})\right]+\text{const}\ . \quad (5)$$

Equation (5) is a simplified version appropriate for weak mixing of f^2 ("weak coupling"), which includes only the lower heavy-fermion band

$$E_k=\tfrac{1}{2}(\varepsilon_f+\varepsilon_k)-\tfrac{1}{2}[(\varepsilon_k-\varepsilon_f)^2+4u_k^2]^{1/2}\ .$$

The Fermi level is assumed to lie in the E_k band. v_k is defined as

$$v_k=2u_kV_k/[(\varepsilon_k-\varepsilon_f)^2+4u_k^2]^{1/2}\ .$$

In (5) a rotation in SU(N) space has diagonalized $A\equiv\langle a_{mn}(0)\rangle$, so that $U^\dagger AU=D$, $D_{ij}=d_i\delta_{ij}$. Also the rotation brings in new fermion operators

$$B_{ki}=\sum_m U_{mi}C_{km-},\quad B_{k\,-i}=\sum_m U^\dagger_{im}C_{km-}$$

for the lower heavy-fermion band.

Equation (5) is just a sum of $N/2$ BCS Hamiltonians. Their now standard solution is exact in the limit of a large number of particles. Minimizing the ground-state energy with respect to d_i gives the $T=0$ gap equation (assuming $T_K\ll E_2-E_1$)

$$(E_2-E_1)=\tfrac{1}{2}\sum_k v_k^2/(E_k^2+\Delta_k^2)^{1/2}\ . \quad (6)$$

In (6) the half-gap $\Delta_k=d_iv_k$ is the same for all i.

In the usual s-wave SU(N) lattice model the u_k and v_k matrix elements are isotropic, leading to an analytic solution to (6),

$$\Delta_{kF}\approx 2(\varepsilon_f u_{kF})^{1/2}\exp\left[\frac{E_1-E_2}{4\rho_0V_{kF}^2}\right]\ , \quad (7)$$

where ρ_0 is the density of states of d electrons at ε_F. We thus get a Kondo-like expression for the gap Δ, which is small if the f^2 level lies far above f^1. The gap is isotropic in k space, $\Delta_{kF}=\Delta$. For the transition temperature T_c, and critical field at $T=0$ $H_c(0)$, we find the BCS-like results $T_c=(1.14/2)\Delta$, $H_c(0)=(2\pi N\rho)^{1/2}\Delta$, where ρ is the heavy-fermion density of states at ε_f. This solution is BCS-like except that, within a rotation in SU(N) space, the order parameter contains $N/2$ independent phases and one amplitude.

To estimate T_c, it is convenient to rewrite (7) in the form

$$T_c/T_K=1.14(T_K/D)^{(a-1)/4}\ , \tag{8}$$

where $a=N(E_2-E_1)/(E_0-E_1)$, $2D$ is the bandwidth of the k states, ρ_0 is assumed to be $1/2D$, and $T_K=\exp[(E_0-E_1)/NU_{k_F}^2\rho_0]$. We assume that $V_k=U_k$. Since T_K/D is small, it is evident from Eq. (8) that T_c/T_K is itself small if N is large and/or if the f^1-f^2 excitation energy is much larger than the f^1-f^0 excitation energy. But in the heavy-fermion materials, N is essentially 2 and, at least for $CeCu_2Si_2$, the two excitation energies are comparable, suggesting that superconductivity is possible by this mechanism.

To see how this works out quantitatively, we shall make estimates for $CeCu_2Si_2$ for which the relationship between atomic spectroscopy and the heavy-fermion behavior is much better understood than in the U materials. Directly from spectroscopic data, we find[22,23] $E_0-E_1=4$ eV, $E_2-E_1=5.4$ eV. We take[1] $N=2$. T_K may be defined as in Ref. 15, when within mean-field theory we derive from the observed $\gamma=1100$ mJ K^{-2}, $T_K=25$ K. Inserting into (8) gives $T_c=2$ K; the experimental value is approximately 0.6 K. Taking into account the simplest many-body effect, the blocking of the charge-fluctuation channel,[10] would give $T_c=0.8$ K, in better agreement with experiment. Note that we have neglected the effect of f^1-f^2 fluctuations on T_c (Refs. 19 and 20) which for different reasons is small both for $N=2$ and for N large. Hence, within the uncertainties, we are for the first time able to explain the order of magnitude of T_c in heavy-fermion superconductivity.

Pressure is expected to affect T_K and T_c primarily through the pressure coefficients a and b of E_1-E_0 and E_2-E_1. Assume for simplicity that $a=b$; both should be positive. Then $T_K/T_K^0=\exp(ap/N\rho_0V^2)$, $T_c/T_c^0=\exp[a(3-N)/4N\rho_0V^2]$ (putting $U=V$). $CeCu_2Si_2$ presumably has at low p $N=2<3$, giving a positive pressure coefficient of T_c. However, as p increases so does T_K, until T_K becomes comparable with crystal-field splitting. The effective N thus increases until N exceeds 3, changing the T_c coefficient to negative as observed.[24] UBe_{13} has a pressure coefficient of T_K opposite to T_c,[25] suggesting $N>3$.

In an attempt to formulate a more realistic model in which the crucial f and k degeneracies have physical origin, I considered a rocksalt structure with d_{xy}, d_{yx}, and d_{zx} orbitals on each Na site and $f_{x(y^2-z^2)}$, $f_{y(z^2-x^2)}$, and $f_{z(x^2-y^2)}$ orbitals on each Cl site. Nearest-neighbor dd's and df's are linked by tight-binding matrix elements. The model is constrained to f^0, f^1, and f^2. A simple case is where f^2 is the singlet state having both electrons in the same orbital, when the order parameter is a singlet and for some parameters the gap vanishes when $k_x=k_y=0$, $k_y=k_z=0$, $k_z=k_x=0$. Consideration of f^2 states with electrons in different f orbitals leads to nonuniversal results apparently including the possibility of lines of vanishing gap on the Fermi surface.

The effect of the local gauge symmetry (3) is to make only $|\langle a\rangle|$ and $|\langle b\rangle|$ nonzero—they cannot[10,11] independently have a phase; only their phase difference is nonzero. The combination $\sum_k\langle a^\dagger(k)b_k\rangle$ is gauge invariant and may be identified with the true order parameter. In the future we shall include the effects of the formally nonleading diagrams in Fig. 1.

Finally, I mention that my theory seems to have much in common (though an Anderson lattice is treated) with Anderson's mechanism for superconductivity in the Hubbard model applied to oxide superconductors.[26]

I am grateful to D. H. Lee, M. Rasolt, N. Read, and Z. Tesanovic for comments and criticism, and to J. W. Allen for use of unpublished data.

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