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Three-body bound states and the development of odd-frequency pairing

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Abstract

We link the formation of an odd-frequency paired state to the development of an anomalous three-body scattering amplitude. We show how a simple ansatz leads to a simple realization of odd-frequency superconductivity in a mean-field model of the Kondo lattice. The gapless quasiparticles of this state are equal mixtures of particle and hole at zero frequency and their spin and charge coherence factors vanish, unlike conventional even-paired BCS quasiparticles. We discuss the difficulties this and other models face in attempting to explain experiments in heavy-fermion superconductors.

The nature of superconductivity in heavy fermion materials is still rather controversial. The presence of gapless excitations led to the suggestion that the superconducting state is unconventional as compared to the classic paradigm of phonon mediated BCS-Eliashberg superconductivity. The strong electronic correlations in the active f-shells of its constituent rare-earth and actinide atoms suggested, from the outset, that an analogy with superfluid ^{3}He might be fruitful [1]. Indeed, the strong interactions in the latter material are known to lead to an instability towards a p-wave paired superfluid with gapless fermionic excitations [2]. This early suggestion is at the heart of many of the later attempts to understand the nature of heavy-fermion superconductivity [3] in a p-wave or d-wave scenario. Yet, unlike the case of ^{3}He, after more than a decade of scrutiny, an undisputed theory for these fascinating materials does not exist.

The distinctive feature of heavy-fermion materials is the crucial role played by the local moments in the formation of the normal *and* the superconducting state. It is only by the release of the large spin entropy into the fermionic carriers that the latter can acquire their enormous masses. In addition, the large jumps in the specific heat at the superconducting transition point to the active participation of the spin degrees of freedom in the condensation process. In the case of UBe_{13}, to take an extreme example, the condensation entropy is about $0.2R \ln 2$. It is in this sense that heavy-fermion superconductivity should be understood as a *spin ordering* process. More importantly, the puzzling case of UBe_{13}, which becomes a superconductor even before a Fermi liquid is formed, suggests that the naive approach of a heuristic separation of the formation of the heavy Fermi liquid state from the subsequent superconducting instability should be taken with caution. Finally, the 'pacific' coexistence with static antiferromagnetic order in UPt_3, URu_2Si_2, UPd_2Al_3 and UNi_2Al_3 shows the intimate connection between the two types of order.

It is noteworthy that the gapless excitations in these materials lead to ubiquitous T^3 NMR and NQR relaxation rates $1/T_1$. In the case of UPd_2Al_3 this power law has been found to be obeyed over three to four orders of magnitude of the relaxation rate [4]. This is consistent with a line of nodes in the gap, which occurs in d-wave pairing models. However, such universality is not to be found in other properties, particularly the specific heat. In superconducting UPt_3 for example, $C_v = \gamma_s T + BT^2$ [5], in UPd_2Al_3, $C_v = \gamma_s T + AT^3$ [6], and in UBe_{13}, $C_v = \gamma_s T + AT^3$ [7]. Though the presence of the

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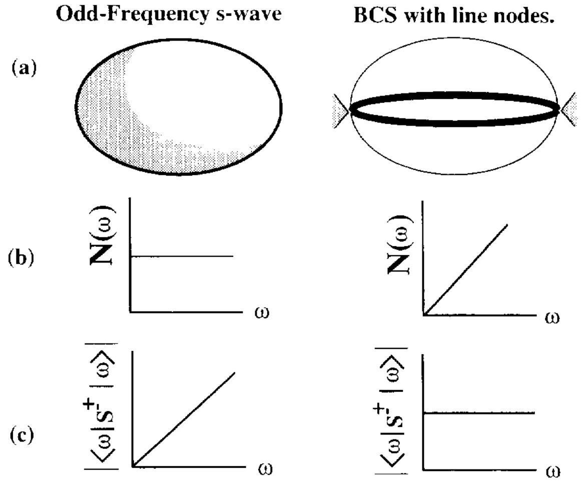

Fig. 1. (a) Contrasting gapless Fermi surface of an odd-frequency paired s-wave state, with gapless line-nodes in a BCS superconductor. Shown beneath, corresponding (b) quasiparticle density of states $N(\omega)$ and (c) spin coherence factors.

linear term in the case of UPt_3 has been attributed to disorder [8], UPd_2Al_3 seems to show an intrinsic linear term.

While it would be too unwise to rule out the p-wave or d-wave pairing hypotheses, in view of the experimental difficulties in determining the intrinsic low temperature behavior, this apparent contradiction between the two sets of experiments has led us to explore a different scenario. Since the NMR relaxation rate is always T^3, we conjecture that it is a consequence of the spin coherence factors rather than a density of states effect. In a qualitative way, the NMR relaxation rate at temperature T is

$$(T_1)^{-1} \sim T[N(\omega)|\langle\omega|S_+|\omega\rangle|]^2_{\omega\sim k_B T}, \tag{1}$$

where

$$|\langle\omega|S_\pm|\omega\rangle|^2 = \overline{|\langle \boldsymbol{k}|S_\pm|\boldsymbol{k}'\rangle|^2\delta(\omega - E_k)\delta(\omega - E_{k'})} \tag{2}$$

is a momentum average of the quasiparticle spin matrix elements and $N(\omega)$ is the density of states at energy ω. In the presence of a line of nodes, a T^3 law is accomplished by a constant spin matrix element and a linear density of states $N(\omega) \sim \omega$. An alternative way of getting the same law would be through a constant density of states $N(\omega)$ and a *linear* spin matrix element (Fig. 1)

$$|\langle\omega|S_\pm|\omega\rangle| \sim \omega. \tag{3}$$

In conventional BCS theory, the vanishing of the charge coherence factors occurs when the quasiparticle is an equal mixture of particle and holes ($u_k = v_k$). In general, $a_k = u_k c_k + v_k c^\dagger_{-k}$, where

$$\begin{pmatrix}|u_k|^2\\ |v_k|^2\end{pmatrix} = \frac{1}{2}\left[1 \pm \frac{1}{\sqrt{1+(\Delta_k/\varepsilon_k)^2}}\right]. \tag{4}$$

At a gap node $\Delta_k/\varepsilon_k = 0$ and u_k and v_k are either zero or 1, quasiparticles are unpaired and the coherent factors are unity. We consider here the possibility of *strongly paired* low-energy quasiparticles such that $\Delta_k/\varepsilon_k \to \infty$. This is achieved by an anomalous pole in the three-particle channel that leads to an odd-frequency gap function [9] that diverges at zero frequency, $\Delta_k(\omega) \propto 1/\omega$.

To illustrate this idea, consider a Kondo lattice Hamiltonian,

$$H = \sum_k \varepsilon_k \psi^\dagger_k \psi_k + \sum_j H_{\rm int}[j], \tag{5}$$

where $\psi^\dagger_k$ is a conduction electron spinor, coupled to an array of $S = \frac{1}{2}$ local f-moments $\boldsymbol{S}_j = \frac{1}{2} f^\dagger_j \boldsymbol{\sigma} f_j$ via an antiferromagnetic exchange interaction

$$H_{\rm int}[j] = J(\psi^\dagger_j \boldsymbol{\sigma} \psi_j)\cdot \boldsymbol{S}_j. \tag{6}$$

Here ψ_j denotes the conduction electron in a tight-binding representation. This Hamiltonian is the simplest toy model for a heavy fermion metal. Consider now the fundamental three-body spinor $\xi_{j\alpha} = (\boldsymbol{S}_j \cdot \boldsymbol{\sigma}_{\alpha\beta})\psi_{j\beta}$. In the normal state, strong Kondo scattering of the conduction electrons off the local moments leads to the enhancement of the mass of the carriers. This three-body operator thus behaves as a charged fermion field. We will look for a correlated state where this quantity acquires an anomalous pole. Since it has fermionic character it cannot condense [10]. However, generalizing the concept of three-body fermionic bound states, we envisage the possibility of symmetry-breaking three-body amplitudes that act as collective order parameters. For that, we write

$$-J\xi_j(t) = 2V_j\hat{\phi}_j(t) - J\delta\xi_j(t). \tag{7}$$

Here V_j is a two component complex spinor representing the anamalous three-body amplitude and carrying the charge and spin of the three-body composite, ϕ_j is a real fermionic field (a Majorana fermion, $\phi^\dagger_j = \phi_j$) that embodies the fermionic nature of ξ_j, and $\delta\xi_j$ represents fluctuations that are neglected in the mean-field theory. Eq. (6) can be rewritten as

$$H_{\rm int}[j] = -J(\xi^\dagger_j \xi_j), \tag{8}$$

by means of the identity $(\boldsymbol{S}\cdot\boldsymbol{\sigma})^2 = \frac{3}{4} - \boldsymbol{S}\cdot\boldsymbol{\sigma}$. Substitution of the ansatz Eq. (7) into Eq. (8) then leads to

$$H_{\rm MF} = \sum_j 2\left[\{\psi^\dagger_j(\boldsymbol{\sigma}\cdot\boldsymbol{S}_j)\hat{\phi}_j V_j + ({\rm H.C.})\} + \frac{V^\dagger_j V_j}{J}\right]. \tag{9}$$

This mean field theory can be solved by noting that the combination

$$\eta_j = 2\boldsymbol{S}_j\phi_j \tag{10}$$

in such that $\boldsymbol{\eta}_j = \boldsymbol{\eta}_j^\dagger$ and its components satisfy a canonical anticommutation algebra, $\{\eta_j^a, \eta_k^b\} = \delta^{ab}\delta_{jk}$. We thus end up with

$$\tilde{H} = \sum_j [\psi_j^\dagger(\boldsymbol{\sigma}\cdot\boldsymbol{\eta}_j)V_j + (\text{H.C.})] + \frac{2V_j^\dagger V_j}{J}. \tag{11}$$

This type of Hamiltonian was previously obtained via a Majorana fermion representation of spins in Ref. [11], where many details of its properties can be found. In particular, it was found that for most lattices, the free energy is minimized by a staggered configuration of the V_j spinor $V_j = \mathrm{e}^{i\boldsymbol{Q}\cdot\boldsymbol{R}_j/2}V$, $\boldsymbol{Q} = (\pi, \pi, \pi)$ [11]. The mean field Hamiltonian will then be, after gauging the staggered phase into a redefinition of the conduction electron field operators

$$H_{\text{mft}} = \sum_k \tilde{\varepsilon}_k \psi_k^\dagger \psi_k + \sum_k [\psi_k^\dagger(\boldsymbol{\sigma}\cdot\boldsymbol{\eta}_k)V + (\text{H.C.})], \tag{12}$$

where $\tilde{\varepsilon}_k = \varepsilon_{k-Q/2}$ and we dropped the constant term.

The Hermitian nature of the Majorana fields will lead to a mixing of the particle and hole components of the conduction electrons through anomalous resonant scattering off the local three-body composites. If we take a particular choice for the V spinor

$$V = V_0\begin{pmatrix}1\\0\end{pmatrix}, \tag{13}$$

the main effect of these resonant pairing processes is to generate a singular pairing self-energy for the up spin conduction electrons

$$\Delta_\uparrow(\omega) = \frac{V_0^2}{2\omega}(1 - \tau_1), \tag{14}$$

where τ_1 is a Nambu matrix. It is precisely this singular behavior that leads to the unconventional coherence factors mentioned before. Due to the odd-frequency nature of the gap function, the system exhibits surfaces of gapless excitations. We can decompose the gapless quasiparticles as

$$a_k = \sqrt{Z_k}[u_k\psi_{k\uparrow} + v_k\psi_{k'}^\dagger] + \sqrt{1 - Z_k}\eta_k^3, \tag{15}$$

where

$$\begin{pmatrix}u_k^2\\v_k^2\end{pmatrix} = \frac{1}{2}\left[1 \pm \frac{1}{\sqrt{1 + (\Delta(\omega)/\mu_k)^2}}\right]_{\omega = E_k}, \tag{16}$$

μ_k is the symmetric part of $\tilde{\varepsilon}_k$, $Z_k = [1 + \mu_k^2/V^2]^{-1}$ and E_k is the quasiparticle energy. At zero frequency, $u_k^2 = v_k^2 = \frac{1}{2}$. Quasiparticles at the Fermi surface are strongly paired and their charge and spin coherence factors vanish linearly with frequency

$$\langle\omega|S_\pm|\omega\rangle \sim u^2(\omega) - v^2(\omega) \sim \Delta(\omega)^{-1} \sim \omega. \tag{17}$$

Whilst the approach developed here clearly does *not* provide a theory of heavy fermion superconductivity, it furnishes a tentative illustration of how strongly correlated spin systems such as UBe_{13} may undergo a condensation process in which the local moments play an active role. Recently, some independent support for odd-frequency pairing in Kondo lattice systems has been obtained by Zachar, Kivelson and Emery [12]; at a special solvable Toulouse point of the one-dimensional Kondo lattice model, these authors show the presence of an incipient odd-frequency pairing instability. Various inadequacies of our approach in its current form are quite clear: this simplistic model is unable to account for the condensate anisotropy clearly seen in the thermal conductivity and ultrasonic attenuation measured for UPt_3 [13, 14]; moreover, the apparent lack of any residual linear term in the specific heat in this compound does not appear to be consistent with a Fermi surface of gapless Majorana excitations. We hope, however, that our speculations and the questions they raise will inspire others to go beyond phenomenology and consider the vital question of how the local moments of heavy fermion compounds participate in heavy fermion superconductivity.

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