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

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Abstract

We propose that the development of odd-frequency superconductivity is driven by the formation of neutral three body bound-states. Using a three-body bound-state ansatz we develop a mean-field theory for odd-frequency pairing within the Kondo Lattice model. Three body bound-state formation leads to the formation of a gapless band of fermions with a neutral, spinless Fermi surface. We discuss the low energy excitations of these modes, suggesting them as a possible explanation for the absence of anisotropy in the thermal conductivity of heavy fermion superconductors.

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Although three body fermion states are ubiquitous in many branches of particle, nuclear and atomic physics, there has been very little study of their impact on collective condensed matter behavior. In this paper, we propose that three body bound-state instabilities can precipitate a phase transition, and we identify the broken symmetry state that forms as an odd-frequency superconductor. Berezinskii originally proposed that superconductivity could occur through the development of a state with an odd frequency gap function

\[ \Delta(\omega, k) = -\Delta(-\omega, k) \]  

(1)

Unlike conventional superconductivity, there is no weak-coupling Cooper instability associated with this type of state. Indeed the proper identification of an appropriate class of many body instability for odd-frequency pairing has proved a major obstacle to concrete theoretical realization of Berezinskii’s proposal.

Our particular interest in odd-frequency pairing is motivated by heavy fermion superconductors, where superconductivity appears to involve the active participation of local moments in the condensation process. Vanishing coherence factors particular to odd frequency pairing may offer a means to reconcile the large linear specific heat and isotropic thermal conductivity observed in these superconductors with the absence of a linear Korringa relaxation in the NMR data. In this paper we show how the development of such hypothetical states can be directly associated with the formation of three-body bound-states between electrons and local moments.

A three-fermion bound-state is a composite fermion where selection rules stabilize it against decay into its constituents. A good example is the He-3 atom: a neutral bound-state formed from a $S = 1/2$ nucleus and two electrons. Since the low-energy dynamics of the atom involve rigid center-of-mass motion, correlation functions of the bound fermions are determined by their factorization into triplet contractions

\[ \psi_1(1)\psi_2(2)N_\sigma(3) = \int \Lambda(1, 2, 3; x)\Phi_\sigma(x)dx \]  

(2)

where $\Phi^\dagger(x)$ creates the He-3 fermion, $\psi$ represents the electron fields, $N$ the nucleus, and
\( \Lambda \) is the atomic wave function of the He-3 atom. It is this factorization into “three body contractions” which enables us to replace the composite operators by a single fermion \( \Phi(x) \) in the low energy physics of He-3.

Can such bound-states form \textit{collectively} in an electronic system? A well-known theorem of Yang\cite{footnote} precludes the development of any literal off-diagonal long-range order of a three-body fermion. Here we propose an alternative possibility, where two electrons and a hole bind to form a neutral fermion through the collective formation of a three-body condensate\cite{footnote}

\[
\psi_\alpha^\dagger(1)\psi_\beta(2)\psi_\gamma(3) = \int \Lambda_{\alpha\beta\gamma}(1, 2, 3; x) \hat{\phi}(x) dx
\]

Here \( \phi(x) = \phi^\dagger(x) \) represents the neutral bound-state fermion. \( \Lambda_{\alpha\beta\gamma} \) is a \textit{complex} wave function which carries the phase information associated with the charge of the bound electrons, playing the role of a collective variable. We shall argue that if the phase of the three-body wave function develops a rigidity, an odd frequency superconductor is formed. For simplicity we consider a wave function that is symmetric in electron co-ordinates 2 and 3, and hence antisymmetric in the corresponding spin variables

\[
\Lambda_{\alpha\beta\gamma}(1, 2, 3; x) = \sigma^2_{\beta\gamma}\sigma^2_{\alpha\eta}A_\eta(1, 2, 3; x)
\]

where \( \sigma^2 \) is a Pauli matrix. The coarse-grained average \( A(x) \equiv \int_{1,2,3} A(1, 2, 3; x) \) plays the role of a spinorial order parameter\cite{footnote}. By contracting the spin-indices, we see that \( A \) describes the binding between spins and electrons,

\[
\left[ \vec{S}(1) \cdot \vec{\sigma}_{\alpha\beta} \right] \psi_\beta(2) = \int dx A_\alpha(1, 1, 2; x) \hat{\phi}(x)
\]

where \( \vec{S} = \frac{1}{2}\psi^\dagger \vec{\sigma} \psi \) is the spin density.

A specific model for this type of bound-state instability is provided the “Kondo lattice” Hamiltonian

\[
H = \sum_k \epsilon_k \psi_k^\dagger \psi_k + \sum_j H_{int}[j]
\]
where \( \psi^\dagger_k \) is a conduction electron spinor, coupled to an array of \( S = 1/2 \) local moments \( \vec{S}_j \) via an antiferromagnetic exchange interaction

\[
H_{\text{int}}[j] = J (\psi^\dagger_j \vec{\sigma} \psi_j) \cdot \vec{S}_j.
\]

(7)

where \( \psi_j \) denotes the conduction electron in a tight binding representation. This Hamiltonian is of particular interest as a toy model for heavy fermion metals. An electron scattering off a magnetic ion at site \( j \) couples directly to the three-body spinor

\[
\xi_{j\alpha} = (\vec{S}_j \cdot \vec{\sigma}_{\alpha\beta}) \psi_{j\beta}
\]

(8)

Irreducible Green functions of \( \xi \) determine the self-energies of the conduction electrons. In a superconducting state, the normal and anomalous components of the electron self-energies are given by

\[
\Sigma(\kappa) = J^2 \langle \langle \xi(\kappa) \xi^\dagger(\kappa) \rangle \rangle
\]

\[
\Sigma_A(\kappa) = J^2 \langle \langle \xi(\kappa) \xi(-\kappa) \rangle \rangle
\]

(9)

where double brackets denote one-particle irreducibility with respect to conduction electrons and \( \kappa \equiv (\omega, \vec{k}) \). The development of bound-state resonances associated with \( \xi \) can thus severely modify the electronic properties of the lattice.

To provide a controlled treatment of fermionic bound-states in the Kondo lattice model, we develop a \( 1/N \) expansion within a class of “\( O(N) \) Kondo models”. In this generalization, the local anticommuting algebra of the original spin-1/2 operators is preserved

\[
\{\sigma^\mu, \sigma^\nu\} = 2\delta^\mu^\nu
\]

\[
\{S^\mu_j, S^\nu_j\} = \frac{1}{2} \delta^\mu^\nu
\]

(10)

but the number of components of each operator is generalized from three in the model of interest, to an arbitrary odd number \( N \). This is the algebra of \( N \) component gamma matrices. For general \( N \), the conduction electron spinors have dimension \( 2^{[N/2]} \), where \([ \ ]\) denotes the integer part. For all \( N \), the Kondo interaction Hamiltonian can be written

\[
H_{\text{int}}[j] = -\frac{\vec{j}}{N} (\xi^\dagger \vec{\sigma} \xi_j)
\]

(11)
where we replace \( J = \tilde{J}/N \).

We now calculate the correlation function of \( \xi \) in the normal state, in a scheme that is exact to order \( O(1/N) \). Since \( \xi \) is a fermion, a fluctuating component of the operator must survive development of bound-state singularities in its correlation functions. To describe these intrinsic fluctuations we introduce the device of a “spectator fermion” \( \phi_j \): a neutral fermion \( \phi_j = \phi_j^\dagger \), defined at each site which which satisfies canonical anticommutation rules, \( \{ \phi_j, \phi_k \} = \delta_{jk} \), commuting with the spin operators and anticommuting with all other fermions. \( \phi_j \), so defined, commutes with the Hamiltonian and decouples from the dynamics; its correlation functions display intrinsic fluctuations

\[
\langle T\phi_j(1)\phi_k(2) \rangle = \frac{\delta_{jk}}{2} \text{sgn}(\tau_1 - \tau_2)
\]  

We construct a “bosonic partner” to the three-body operator \( \xi \) as follows

\[
\hat{A}_j = 2\phi_j\xi_j.
\]  

Since \( \phi_j^2 = \frac{1}{2} \), we may invert this relation to obtain \( \xi_j = \phi_j\hat{A}_j \). The spectator fermion factors out of the dynamics, so we may relate the correlation functions of \( \hat{A}_j \) and \( \hat{\xi}_j \),

\[
\langle \hat{A}_j(\tau)\hat{A}_k^\dagger(0) \rangle = 2\text{sgn}(\tau)\delta_{jk}\langle \langle \xi_j(\tau)\xi_j^\dagger(0) \rangle \rangle
\]  

We can also reversibly transform the spin operators into fermionic counterparts

\[
\bar{\eta}_j = 2\phi_j\bar{S}_j
\]  

which satisfy \( \{ \eta^a[j], \eta^b[k] \} = \delta^{ab}\delta_{jk} \) and are real \( \eta^a[j] = \eta^{a\dagger}[j] \). The canonical commutation properties of these “Majorana” spin fermions permits us to use diagrammatic methods without invoking a Gutzwiller projection.\(^{14}\) Since \( \hat{A}_j = [\bar{\eta}_j \cdot \vec{\sigma}]\psi_j \), the original interaction can be written

\[
H_{\text{int}}[j] = -\frac{\tilde{J}}{2N} \hat{A}_j^\dagger\hat{A}_j
\]  

Consider the diagrammatic expansion for the local susceptibility
\[ \langle A_i(\tau)A_j^\dagger(0) \rangle = \delta_{ij}\chi(\tau) \] (17)

in powers of \( \bar{J}/N \). (Fig. 1.) The non-interacting value is \( \chi^0(\tau) = \frac{N}{2} \text{sgn}(\tau) G(\tau) \) where \( G(\tau) = \langle \psi_i(\tau)\psi_i^\dagger(0) \rangle \) is the local electron propagator. In the frequency domain

\[
\chi^0(i\nu_n) = \frac{N}{2} \sum_{\vec{k}} \frac{\tanh(\beta \epsilon_{\vec{k}}/2)}{\epsilon_{\vec{k}} - i\nu_n} \quad (\nu_n = 2\pi T n)
\] (18)

is logarithmically divergent at low energies \( \chi^0(0) \sim N \rho \ln[D/T] \), where \( \rho \) is the conduction electron density of states and \( D \) the bandwidth. Each fermion loop contributes a factor \( N \) and each interaction line contributes a factor \( 1/N \), thus the leading order \( O(N) \) contribution to \( \chi \) is given by the RPA sum

\[
\chi_{\text{RPA}}(i\nu_n) = N \frac{\chi^0(i\nu_n)}{1 - \frac{\bar{J}^2}{2}\chi^0(i\nu_n)}
\] (19)

\[ \{ \]

\[ \text{O(N)} \]

\[ \chi^0 \]

\[ + \]

\[ \frac{N}{1/N} \]

\[ \text{O(1)} \]

\[ 1 \]

\[ + \]

\[ \frac{1/\bar{J}}{1/N} \]

\[ \frac{1}{N} \]

Fig. 1. Diagrammatic expansion of \( \chi(i\nu_n) \) in a \( 1/N \) expansion for the \( O(N) \) Kondo model: solid lines refer to conduction electron propagators, dashed lines to spin fermions, and a wavy line denotes the interaction vertex.
where $N\tilde{\chi}^0 = \chi^0$. If we now transform back to the corresponding fermionic response function of $\xi$, we find

$$\langle \xi_i(\tau)\xi_i^\dagger(0) \rangle = \frac{1}{2} \operatorname{sgn}(\tau) \chi_{RPA}(\tau)$$

(20)

Since $\chi^0(0)$ is logarithmically divergent, this function develops a singularity at a finite temperature $T_c \sim D e^{-2/\rho J}$, where $1 = \frac{i}{2} \tilde{\chi}^0(0)$. This singularity signals the formation of a three body bound-state.

We now apply our bound-state ansatz to the three body spinor $\xi_j$, writing

$$\xi_j(t) = \langle A_j \rangle \hat{\phi}_j(t) + \delta \xi_j(t)$$

(21)

where the first term is the three body contraction of the operator. This ansatz implies long-time correlations of the three body operator

$$\langle \langle \hat{\xi}_j(\tau)\hat{\xi}_k(0) \rangle \rangle \xrightarrow{|\tau|\to\infty} \delta \frac{\delta_{jk}}{2} \operatorname{sgn}(\tau) A_j \otimes A_j^\dagger$$

$$\langle \langle \hat{\xi}_j(\tau)\hat{\xi}_k(0) \rangle \rangle \xrightarrow{|\tau|\to\infty} \delta \frac{\delta_{jk}}{2} \operatorname{sgn}(\tau) A_j \otimes A_j^T$$

(22)

For $N = 3$, The Fourier transform of (22), inserted into (9) then gives

$$\Sigma^A(\kappa) = [V \otimes V^T] \langle \phi(\kappa) \phi(-\kappa) \rangle = \frac{4[V \otimes V^T]}{\omega}.$$  

(23)

where $V_j = \frac{i}{2N} \langle A_j \rangle$. This establishes the direct link between three body bound-state formation and an odd frequency pairing amplitude that scales as $1/\omega$.

To develop the mean-field theory for the condensed phase, we substitute the bound-state ansatz into the Kondo exchange interaction, so that $H_{\text{int}}[j] \rightarrow H_{\text{int}}[V_j]$, where

$$H_{\text{int}}[V_j] = 2 \left[ (\xi_j^\dagger \phi_j^\dagger V_j + \text{(H.C.)}) + \frac{V_j^\dagger V_j}{J} \right] + O(\delta \xi^\dagger \delta \xi)$$

Using (15), $2\xi^\dagger \phi \equiv \psi^\dagger (\vec{\sigma} \cdot \vec{\eta})$, thus

$$H_{\text{int}}[V_j] = \left[ \psi^\dagger j (\vec{\sigma} \cdot \vec{\eta}_j) V_j + \text{(H.C.)} \right] + \frac{V_j^\dagger V_j}{J}$$

(24)

Remarkably, the fusion of the neutral bound-states with the the spin variables transforms them into propagating spin fermions. This form of mean-field theory was previously derived using an abstract Majorana spin-representation of spin-1/2 operators.
Formation of a gapless band of neutral fermions follows naturally from our original ansatz. If we write \( V_j = \frac{V}{\sqrt{2}} z_j \), where \( z_j \) is a unit spinor, and decompose \( \psi_j \) into four Majorana components \( \psi_j = \frac{1}{\sqrt{2}} [\psi_j^0 + i \vec{\psi}_j \cdot \vec{\sigma}] z_j \). then the scalar component \( \psi_o \) decouples from the the hybridization term \( H_{\text{int}}[V_j] = -i V \vec{\psi}_j \cdot \vec{\eta}_j \). The vector components of the conduction sea hybridize with the spin fermions to form a gap \( \Delta_g \sim V^2/D \). Residual “scalar” components of the conduction sea thus split off below the quasiparticle continuum to produce a gapless band. (Fig. 2.) Spin and charge operators are off-diagonal bilinears in this Majorana basis, which ensures the neutrality of the gapless Fermi surface and leads to coherence factors that vanish linearly with energy.

Fig. 2. Schematic illustration of the excitation spectrum predicted by the mean-field theory. Formation of the three body bound-state splits a gapless band of neutral fermions off from the charged quasiparticle continuum.

The use of spectator fields differs fundamentally from the more familiar use of “slave” fields, since the combined Hilbert space of particles and spectators replicates the physical Hilbert space. There is no unwanted subspace with unphysical matrix elements to be projected out. In a path integral language the decoupling of the spectator fields is associated with a unique fermionic gauge invariance. The appropriate Lagrangian is

\[
\mathcal{L} = \sum_j \{ \psi_j \dagger \partial_\tau \psi_j + \frac{1}{2} \vec{\eta}_j \partial_\tau \vec{\eta}_j + H_{\text{int}}[V_j] \} + H_c \tag{25}
\]
where $V_j$ is now a fluctuating bosonic spinor field. This Lagrangian is derived from the observation that the combined Hilbert space of spectator fermions and spins is equivalent to the Hilbert space of the Majorana spins: $\text{Tr}\tilde{\eta} \equiv \text{Tr}\tilde{S}_\phi$. The saddle point approximation to the path integral of this Lagrangian corresponds to the mean-field theory described above.

Suppose we couple a Grassmann source term $\alpha_j$ to the $\phi$ field

$$L \to L + \sum_j \dot{\alpha}_j \phi_j, \quad (\dot{\alpha}_j \equiv \partial_\tau \alpha_j).$$

For $N = 3$, $\phi_j \equiv -2i\eta_j^x \eta_j^y \eta_j^z$.[14] We can always gauge away such a term by a transformation

$$\phi_j \to \phi_j + \alpha_j, \quad \eta_j \to \tilde{\eta}_j + 2\alpha_j \tilde{S}_j, \quad V_j \to V_j + 2\alpha_j \phi_j V_j$$

under which the spins $\tilde{S}_j$ and the Hamiltonian $H = \sum_j H_{\text{int}}[j]$ are invariant. This is a “supersymmetric” transformation, generated by the $\phi_j$ fields in the unitary transformation $U = \prod_j (1 + \alpha_j \hat{\phi}_j)$. Splitting the Berry phase term into separate contributions from the spin ($L_B[\tilde{S}]$) and $\phi$ field,

$$\frac{1}{2} \tilde{\eta}_j \partial_\tau \tilde{\eta}_j \equiv L_B[\tilde{S}] + \frac{1}{2} \phi \partial_\tau \phi$$

$$\to L_B[\tilde{S}] + \frac{1}{2} (\phi + \alpha) \partial_\tau (\phi + \alpha)$$

we find that this term transforms as

$$\int d\tau [\frac{1}{2} \tilde{\eta}_j \partial_\tau \tilde{\eta}_j + \dot{\alpha}_j \phi_j] \to \int d\tau [\frac{1}{2} \tilde{\eta}_j \partial_\tau \tilde{\eta}_j - \frac{1}{2} \dot{\alpha}_j \partial_\tau \dot{\alpha}_j]$$

By differentiating with respect to the source fields, we confirm that the $\phi$ field is decoupled, with a free propagator $\langle \phi_j(1)\phi_j(2) \rangle = \frac{1}{\partial_\tau} \equiv \frac{1}{2} \text{sgn}(\tau_1 - \tau_2)$.

These connections between three-body bound-state formation and odd-frequency pairing provide insight into its possible application to heavy fermion physics.[6] Coherence factors that are linear in excitation energy $\langle \k|\rho|\k \rangle \propto \langle \k|S_z|\k \rangle \propto \omega$ and the development of a quadratic temperature or frequency dependence in a wide variety of response functions, such as the
normalized NMR relaxation rate $\frac{1}{T^1 T}$, the transverse ultrasound attenuation $\alpha_T$, the depletion of the superfluid density $\Delta \rho_s$ and the quasiparticle conductivity $\sigma(\omega)$,

$$\left( \frac{1}{T^1 T}, \alpha_T, \Delta \rho_s(T), \sigma(\omega) \right) \propto \max(T^2, \omega^2)$$

are seen as a necessary consequence of neutral bound-states. These features are expected to co-exist with a linear specific heat and an essentially isotropic thermal conductivity. Crystalline anisotropy, not included in our discussion, may influence bound state formation, for the local bound-states should acquire a specific crystal field symmetry $\Gamma$ of the lattice. The three-body spinor will take the form $\xi_{\Gamma j} = (\vec{\sigma} \cdot \vec{S}_j) \psi_{\Gamma j}$ where $\psi_{\Gamma j} = \sum_{\vec{k}} \gamma_{\Gamma \vec{k}} e^{i \vec{k} \cdot \vec{R}_j} \psi_{\vec{k}}$ is a conduction spinor with symmetry $\Gamma$. Hybridization with conduction electrons will reflect the same symmetry $V_{\vec{k}} = V \gamma_{\Gamma \vec{k}}$. Nodes of the microscopic crystal field f-wave function of the local moment can thus lead to gap zeroes $\Delta_{\vec{k}} \propto \gamma^2_{\Gamma \vec{k}}$, suggesting an interesting possibility of a co-existence between neutral Fermi surfaces and gap lines of conventional quasiparticles.

We have attempted to elucidate the physics of odd-frequency superconductivity with the proposal that it is driven by the formation of neutral three-body bound states. This hypothesis provides a physical interpretation of the appearance of Majorana spin excitations in the Kondo lattice model, and may be useful in developing our understanding of heavy fermion superconductors.

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Elementary defects of charge $e$ spinors correspond to a phase change of $\pi$, and are associated with a flux quantum $(h/e)\pi = h/2e$.

For odd $N$, using the property $\prod_a S^a = i^{(N-1)/2}/2^N$, we may invert the transformation, $\phi_j = (-2i)^{(N-1)/2} \prod_a \eta_a[j], \vec{S}_j = \phi_j \vec{\eta}_j$. For $N = 3$ this recovers the Majorana spin representation $\vec{S}_j = -(i/2)\vec{\eta}_j \times \vec{\eta}_j$. 