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Are Kondo insulators gapless?

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We outline a novel Majorana treatment of the Kondo lattice that suggests Kondo insulators are gapless, with a band of neutral quasiparticles, an electronic thermal conductivity in the absence of a thermopower and an NMR relaxation rate that grows as T^3.

Kondo insulators are arguably the oldest known form of a heavy fermion compound. Since the original discovery of SmB_6 [1,2], several heavy fermion insulators (HFI) have come to light [3–5], each one characterized by a local moment behavior at high temperatures, and a low carrier density ground-state with activated conductivity and gaps in the range 10–1 meV [6]. These compounds are a dramatic vindication of the role of adiabaticity in determining heavy fermion ground states. Though the f-electrons manifest themselves as local moments at high temperatures, at low temperatures they behave as *valence* electrons, quenching into a ground-state that is adiabatically related to a corresponding non interacting system. In particular, as emphasized by Allen and Martin, these systems satisfy the Luttinger sum rule [7,8] and in cases where the total conduction and f-count per unit cell is an even number, this can give rise to a highly renormalized bandgap insulator.

How strong can the interactions in the HFIs be before the adiabaticity argument begins to fail, and the ground state becomes gapless? There are a number of reasons to suspect that heavy fermion insulators lie at the very edge of validity of adiabaticity, and may already possess some form of gapless excitations within a hybridization pseudogap.

- A fully gapped insulator is expected to experience a first-order Mott transition to the metal as a function of doping or magnetic field. Experimentally, even the cleanest samples show a *crossover* to the metallic state with no Mott transitions [9,10].
- In the narrowest-gap heavy fermion insulator, CeNiSn, a T^3 NMR relaxation is observed, consistent with the presence of low-lying spin excitations [11].
- The adiabatic argument presupposes that the Kondo effect can scale completely to the *strong coupling* fixed point. But if a perfect gap forms in the spin excitation spectrum, then the Kondo scaling cannot proceed to completion. These arguments suggest that strong coupling can only be realized asymptotically by the formation of a pseudogap in the excitation spectrum.

To examine these questions in more detail, we have developed an alternate approach to the Kondo lattice model that avoids certain difficulties associated with the Gutzwiller projection [12]. We use a special *anticommuting* representation of spin 1/2 operators. Recall that the Pauli matrices are anticommuting variables $\{\sigma_a, \sigma_b\} = 2\delta_{ab}$ and can consequently be treated as real ('Majorana') Fermi fields ($\boldsymbol{\sigma}^\dagger = \boldsymbol{\sigma}$). Their Fermi statistics alone guarantees that the spin operator $\mathbf{S} = -(i/4)\boldsymbol{\sigma} \times \boldsymbol{\sigma}$ satisfies *both* the SU(2) algebra $[S^a, S^b] = i\varepsilon_{abc}S^c$ and the condition $S^2 = 3/4$. This feature can be generalized to many sites, introducing three-component anticommuting real vectors $\boldsymbol{\eta}_i$ at each site i,

$$\{\eta_i^a, \eta_j^b\} = \delta_{ij}\delta^{ab}, \qquad (\eta_j^a = \eta_j^{\dagger a}), \tag{1}$$

from which the spin operator at each site is constructed

$$\mathbf{S}_j = -\frac{i}{2}\boldsymbol{\eta}_j \times \boldsymbol{\eta}_j . \tag{2}$$

There is no constraint associated with this representation: the spin algebra *and* the condition $S = 1/2$ hold at each site between all states. In $\boldsymbol{k}$-space, the Ma-

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jorana Bloch waves behave as conventional complex fermions with one half the Brillouin zone ($\eta_k^\dagger = \eta_{-k}$).

Let us sketch how this formalism applies to the Kondo lattice. The exchange interaction between conduction band and local moment at site j is written in a tight-binding representation as

$$H_{\rm int}[j] = J(\psi^\dagger_{j\alpha}\boldsymbol{\sigma}_{\alpha\beta}\psi_{j\beta})\cdot \boldsymbol{S}_j \to -\frac{J}{2}\psi_j^\dagger[\boldsymbol{\sigma}_j\cdot\boldsymbol{\eta}_j]^2\psi_j\ ,$$

using the result $\mathrm{i}\boldsymbol{\sigma}\cdot(\boldsymbol{\eta}\times\boldsymbol{\eta}) = [\boldsymbol{\eta}\cdot\boldsymbol{\sigma}]^2 - \frac{3}{2}$ to simplify the interaction. We write the partition function as a path integral

$$Z = \int_{\rm P} \mathrm{e}^{-\int_0^\beta \mathscr{L}(\tau)\,\mathrm{d}\tau}$$

where

$$\mathscr{L}(\tau) = \sum_k \psi_k^\dagger\partial_\tau\psi_k + \sum_{k\in\frac{1}{2}\rm BZ}\boldsymbol{\eta}_k^\dagger\partial_\tau\boldsymbol{\eta}_k + H_{\rm c} + \sum_j H_{\rm int}[j]\ . \qquad (3)$$

We factorize the interaction in terms of a fluctuating two-component spinor $V_j^\dagger = (V_\uparrow^*, V_\downarrow^*)$:

$$H_{\rm int}[j] = \psi_j^\dagger(\boldsymbol{\sigma}\cdot\boldsymbol{\eta}_j)V_j + V_j^\dagger(\boldsymbol{\sigma}\cdot\boldsymbol{\eta}_j)\psi_j + 2|V_j|^2/J\ . \qquad (4)$$

Mean-field solutions where $V_j = (V/\sqrt{2})z_j$ and z_j is a unit spinor have a particularly rich structure. By integrating out the localized spin degrees of freedom, in addition to the resonant conduction electron self-energy obtained in the large-N approach, the conduction self-energy acquires an anisotropic component represented by the effective action

$$S_a = -\sum_{\omega_n, j}\Big\{\psi_j^\dagger(\omega_n)[\boldsymbol{B}_j(\omega_n)\cdot\boldsymbol{\sigma}]\psi_j(\omega_n) - [\psi_j^\dagger(\omega_n)[\boldsymbol{\Delta}_j(\omega_n)\cdot\boldsymbol{\sigma}]\mathrm{i}\sigma_2\psi_j^\dagger(-\omega_n) + \text{c.c.}]\Big\} \qquad (5)$$

where $\Delta(\mathrm{i}\omega_n) = V^2/4\mathrm{i}\omega_n$ determines the strength of the resonant scattering, and the triad of orthogonal unit vectors $\hat{b} = z^\dagger\boldsymbol{\sigma}z$, $\hat{x} + \mathrm{i}\hat{y} = z^{\rm T}[\mathrm{i}\sigma_2\boldsymbol{\sigma}]z$ defines the orientation. Most notably,

$$\begin{aligned}\boldsymbol{B}_j(\omega_n) &= \Delta(\mathrm{i}\omega_n)\hat{b}_j\ ,\\ \boldsymbol{\Delta}_j(\omega_n) &= \Delta(\mathrm{i}\omega_n)(\hat{x}_j + \mathrm{i}\hat{y}_j)\end{aligned} \qquad (6)$$

are resonant Weiss and triplet pairing fields. This is a realization of odd-frequency triplet pairing first considered by Berezinskii [13,14].

A critical feature of this mean-field theory is the appearance of a gapless neutral Fermi surface. If we decompose the conduction electrons into their four real components $\chi^\mu(\boldsymbol{k})$ ($\mu = 0,1,2,3$),

$$\psi_j = \frac{1}{\sqrt{2}}\{\chi_j^0 + i\boldsymbol{\chi}_j\cdot\boldsymbol{\sigma}\}z_0\ , \qquad (7)$$

then at each site only the last three components of the field admix resonantly with the localized moment. The remaining component forms a gapless Fermi surface. For a bipartite lattice, a stable mean-field solution is obtained with a *staggered* order parameter, where for example $\hat{b} = $ const. and $\hat{x} + \mathrm{i}\hat{y} = \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_j}[\hat{x}_0 + \mathrm{i}\hat{y}_0]$ ($\boldsymbol{Q} = (\pi,\pi,\pi)$). For the case of a half-filled conduction band, the spectrum consists of six admixed Majorana branches with a hybridization gap and a gapless branch corresponding to the conduction electrons that do not mix with the local moments:

$$E_{ki} = \frac{\tilde{\varepsilon}_k}{2} \pm \sqrt{\left(\frac{\tilde{\varepsilon}_k}{2}\right)^2 + V^2} \qquad (i = 1,3)\ , \qquad (8)$$

$$E_{k0} = \tilde{\varepsilon}_k\ .$$

The Fermi surface $\tilde{\varepsilon}_k = 0$ spans precisely one half of the Brillouin zone, corresponding to one 'half' fermion state per unit cell. These results lead to a linear specific heat $\gamma = \frac{1}{4}\gamma_n(1 + \mu^2/V^2)$, where γ_n is the linear specific heat coefficient in the absence of local moments (e.g. the Lanthanum analog) (fig. 1).

The Majorana character of the Fermi surface ensures that its quasiparticles are neutral and only conduct heat. As in a superfluid, part of the charge of a quasiparticle is transferred to the condensate, leaving behind a quasiparticle component to the charge. Away from the FS, quasiparticle charge and spin matrix elements grow linearly with the energy ε:

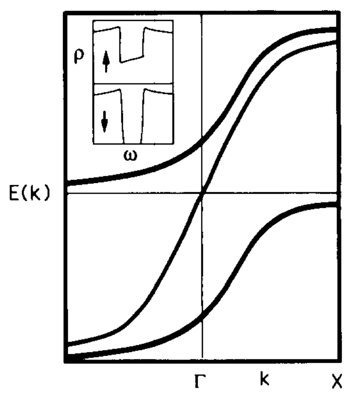

Fig. 1. Excitation spectrum of a Kondo insulator from the current approach. Insert: conduction electron density of states for up and down electrons.

$$\left.\begin{array}{l} Q(\varepsilon) = \langle n_k \rangle \\ 2S(\varepsilon) = \langle \sigma_k^z \rangle \end{array}\right\} = \langle \varepsilon | \{ i\chi_{3k}^{\dagger}\chi_{0k} + \text{c.c.} \} | \varepsilon \rangle = \varepsilon\left(\frac{\mu}{V^2}\right) . \tag{9}$$

Since paramagnetic spin and charge response functions of the quasiparticle fluid are proportional to the square of these matrix elements, the corresponding local response functions will grow quadratically with energy:

$$\chi''_{\text{sp, ch}}(\omega)/\omega \propto \left(\frac{\omega}{T_{\text{K}}}\right)^2 \left(\frac{\mu}{D}\right)^2 . \tag{10}$$

This unusual energy dependence of matrix elements thus permits this state to mimic a quasiparticle fluid with energy-independent matrix elements and a *linear* density of states. There are two key consequences of this result: (i) a T^3 NMR relaxation rate coexists with a linear specific heat and (ii) the system will display a significant thermal conductivity in the absence of a thermopower.

We have not discussed the collective properties associated with the order parameter z. For a half-filled conduction band, continuous particle–hole symmetry of the order parameter z ensures there are no topologically stable vortices, preventing the establishment of a supercurrent and stabilizing the insulator. However, this reasoning suggests that doping will stabilize vortices of the spinor field, leading to odd-frequency triplet pairing and a continuous evolution into an odd-frequency superconductor. The possibility of a link between heavy fermion superconductivity and heavy fermion insulators is rather appealing and clearly deserves further study.

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