Comment on "Low-Temperature Properties of the Two-Impurity Kondo Hamiltonian"

Recently, Jones, Varma, and Wilkins[1] found a novel type of fixed point of the two-impurity Kondo model using Wilson's numerical renormalization-group technique. The problem involves two energy scales: the single-ion Kondo temperature T_K and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction energy J. There are two stable fixed points[2]: (a) For $J/T_K > 2.2$ the ground state is the antiferromagnetic singlet (no Kondo effect) and (b) for $J/T_K < 2.2$ the impurity spins are completely quenched by the Kondo effect.[3] Separating these is a third (unstable) fixed point with highly unusual properties, namely, a diverging staggered-field response and specific heat γ, while the homogeneous-field susceptibility remains finite. At this fixed point $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle \sim -0.25$ for widely separated values of T_K.

In order to gain a phenomenological understanding of these effects we consider a simple model consisting of four spins of $\frac{1}{2}$: S_1 and S_2 representing the impurity spins and s_1 and s_2 representing the conduction-electron spin density at the impurity sites. These spins are coupled by three antiferromagnetic couplings: T_K phenomenologically describes the energy splitting between the $T=0$ Kondo ground-singlet and excited-triplet states, J is the usual RKKY coupling, and K is a cross coupling between $\mathbf{S}_1$ ($\mathbf{S}_2$) and $\mathbf{s}_2$ ($\mathbf{s}_1$),

$$H = T_K\{\mathbf{S}_1 \cdot \mathbf{s}_1 + \mathbf{S}_2 \cdot \mathbf{s}_2\} + J\mathbf{S}_1 \cdot \mathbf{S}_2 + K\{\mathbf{S}_1 \cdot \mathbf{s}_2 + \mathbf{S}_2 \cdot \mathbf{s}_1\} . \quad (1)$$

This model contains the same type of effective interactions (already representing the many-body processes) as the fixed-point Hamiltonian proposed in Ref. 2.

The sixteen eigenstates of the Hamiltonian can be classified according to the total spin S, its z component, and the parity of the wave function, and their energies are (i) ($S=2$, even) $E = T_K/2 + J/4 + K/2$, (ii) ($S=1$, even) $E = -T_K/2 + J/4 - K/2$, (iii) ($S=1$, odd) $E = -J/4 \pm 1/2[J^2 + (T_K - K)^2]^{1/2}$, and (iv) ($S=0$, even)

$$E = -T_K/2 - J/4 - K/2 \pm [T_K^2 + J^2/4 + K^2 - JK/2 - JT_K/2 - T_K K]^{1/2} . \quad (2)$$

For the parameter range of interest the ground state is a singlet, except at one point P ($J = 2K = 2T_K$) which forms the basis of our further discussion.

At this singular point P the ground state is fivefold degenerate, since the two singlets and the lower-lying odd-parity triplet all have energy $E = -1.5T_K$. The other energy levels at P are $E = -0.5T_K$ ($S=1$, even), $E = 0.5T_K$ ($S=1$, odd), and $E = 1.5T_K$ ($S=2$). The high symmetry at P is a consequence of the frustration of the spins. The singlet wave functions correspond in general to linear combinations of (a) the Kondo-compensated and (b) the antiferromagnetically correlated states, but at the singular point the mixing vanishes and the dominant character of the wave function changes abruptly between (a) and (b).

This leads to the following properties close to the singular point: (i) The degeneracy of the ground state gives rise to a specific-heat anomaly, which when coupled to the electron-gas continuum would produce a nonanalytic behavior in γ. (ii) A uniform magnetic field couples the singlets to the even-parity triplet, leading to a susceptibility $\chi \sim 1/T_K$ without irregular behavior. (iii) However, a staggered field admixes the odd-parity tripets with the singlets, giving rise to a diverging staggered susceptibility χ_s at P (Curie law). This divergence is controlled by the square root in (2) and χ_s is dramatically reduced even for small deviations away from P. (iv) $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = dE/dJ$ varies discontinuously across the singular point as a consequence of the abrupt change of dominant character of the singlet wave functions. At P, $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -\frac{11}{20}$, but the half-sum across the discontinuity is -0.25 (the average of the singlet matrix elements). The discontinuity may resemble the strong variation of $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ with J/T_K across the unstable fixed point found in Ref. 1. (v) All these properties occur for $J/T_K = 2$, as compared to 2.2 for the unstable fixed point in Ref. 1.

Thus in spite of the simplicity of our model, we recover at the singular point most of the anomalous properties of the unstable fixed point discovered in Ref. 1. Our brief calculation may suggest insights into the complicated nature of the interference between Kondo screening and intersite spin correlations.

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