NON-FERMI LIQUID versus FERMI LIQUID BEHAVIOR OF THE GENERALIZED ANDERSON IMPURITY*

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We present the Bethe ansatz solution for the generalized Anderson impurity model, in which localized electrons carrying spin and orbital degrees of freedom, interact in a shell via the Hubbard-like repulsion and Hund's rule exchange interaction. Depending on the relative position of the impurity's level with respect to the Fermi energy and strengths of Hubbard-like and Hund's couplings, a magnetic impurity can reveal either the Fermi-liquid like behavior or the non-Fermi-liquid behavior.

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The behavior of hybridization impurities has been theoretically studied in the framework of the Anderson impurity model [1]. Usually it pertains to in-shell electrons with only spin internal degrees of freedom and the Hubbard-like repulsion produces the Kondo effect. In the Kondo case the magnetic impurity hybridized with conduction electrons manifests the low energy Fermi liquid behavior, but with the large renormalized density of states, which is determined by the Kondo temperature. However there exist many materials in which the ground state of ions in the symmetric configuration has an orbital degeneracy in addition to the Kramers (spin) degeneracy. A multi-channel Kondo situation can appear, which main feature is the non-Fermi liquid behavior [2]. Here we present the Bethe ansatz solution of the generalized Anderson model, in which the Coulomb in-shell coupling reveals itself in the Hubbard-like interaction (U) and Hund's exchange (J) [3] (our results can be applied to behaviors of two-impurity Kondo problem [4],

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some rare-earth and actinide compounds [5] and a split-gate quantum dot or double-dot configurations [6]) with the Hamiltonian:

$$\mathcal{H} = -\int dx \sum_{m,\sigma} \psi^\dagger_{m,\sigma}(x)\Big(i\frac{\partial}{\partial x} + \frac{1}{\Lambda}\Big[\frac{\partial^2}{\partial x^2} - \delta(x)\frac{x}{|x|}[\delta'(x+0)$$
$$+\delta'(x-0)]\Big]\Big)\psi_{m,\sigma}(x) + \Big(\varepsilon\sum_{m,\sigma} f^\dagger_{m,\sigma} f_{m,\sigma} + \sum_{m',\sigma'\neq m,\sigma}\Big[\frac{U}{2} f^\dagger_{m,\sigma} f^\dagger_{m',\sigma'} f_{m',\sigma'} f_{m,\sigma}$$
$$-\frac{J}{2} f^\dagger_{m,\sigma} f^\dagger_{m',\sigma'} f_{m',\sigma} f_{m,\sigma'}\Big]\Big) + V\int dx\delta(x)\sum_{m,\sigma}[\psi^\dagger_{m,\sigma}(x) f_{m,\sigma} + \mathrm{H.C.}] \,, \quad (1)$$

where $\psi^\dagger_{m\sigma}(x)$ ($f^\dagger_{m,\sigma}$) creates a conduction electron at site x (in-shell) with the spin σ and orbital index $m = -l, \dots, l$, V are hybridization elements (supposed to be independent on positions, spins and orbital indices) and the Fermi velocity of conduction electrons is equated to 1. The counterterm with the parameter Λ (then $\Lambda \to \infty$, see below), which measures the curvature of the spectrum, is necessary to preserve the integrability at the position of the impurity. A crystalline electric field D (magnetic field H) can lift the degeneracy of orbitals, the latters becoming unequally populated (spin degeneracy). Bethe equations (BE) are derived on a periodic interval of the length L for quantum numbers (rapidities), which parametrize the eigenstates of the Schrödinger equation: charge rapidities $\{k_j\}_{j=1}^N$, spin $\{\lambda_\alpha\}_{\alpha=1}^M$ and orbital ones $\{\xi_q^{(r)}\}_{q=1}^{M_r}$ (with N, M, N_r being the numbers of electrons, down spins and electrons with the r-th orbital index, $N_r = M_{r-1} - M_r$, $r = 1, \dots, 2l$)

$$\mathrm{e}^{-i(k_j L + 2\hat\phi_j)} = \prod_{\gamma=1}^{M} \frac{p_j - \lambda_\gamma - i\frac{c}{2}}{p_j - \lambda_\gamma + i\frac{c}{2}} \prod_{q=1}^{M_1} \frac{p_j - \xi_q^{(1)} - i\frac{c'}{2}}{p_j - \xi_q^{(1)} + i\frac{c'}{2}} \qquad j = 1, \dots, N \,,$$
$$\prod_{q=1}^{M_{r-1}} \frac{\xi_f^{(r)} - \xi_q^{(r-1)} - i\frac{c'}{2}}{\xi_f^{(r)} - \xi_q^{(r-1)} + i\frac{c'}{2}} \prod_{q=1}^{M_{r+1}} \frac{\xi_f^{(r)} - \xi_q^{(r+1)} - i\frac{c'}{2}}{\xi_f^{(r)} - \xi_q^{(r+1)} + i\frac{c'}{2}} = -\prod_{q=1}^{M_r} \frac{\xi_f^{(r)} - \xi_q^{(r)} - ic'}{\xi_f^{(r)} - \xi_q^{(r)} + ic'} \,,$$
$$\prod_{j=1}^{N} \frac{\lambda_\alpha - p_j - i\frac{c}{2}}{\lambda_\alpha - p_j + i\frac{c}{2}} = -\prod_{\delta=1}^{M} \frac{\lambda_\alpha - \lambda_\delta - ic}{\lambda_\alpha - \lambda_\delta + ic} \,, \qquad \alpha = 1, \dots M \,, \quad (2)$$

where $f = 1, \dots, M_r$, $\xi_j^{(0)} = p_j = k_j/\Lambda$, $M_0 = N$, $M_{2l+1} = 0$, $\hat\phi_j = 2\tan^{-1}[V^2/4(k_j - \varepsilon)]$, $c = V^2(U - J)/2(2\varepsilon + U - J)$, and $c' = V^2(U + J)/2(2\varepsilon + U + J)$. The energy is equal to $E = -\sum_{j=1}^N |k_j|$. It turns out that different behaviors of scatterings in spin and orbital subspaces is not novel in the theory of exactly solvable models and is similar to the situation in the multi-channel channel-asymmetric Kondo problem [7]. The solutions to the BAE in the thermodynamic limit (with $L, N, M, M_r \to \infty$ and finite ratios N/L, M/L, M_r/L) are classified in the framework of the "string hypothesis" [1] in the following way: (a) real charge rapidities; (b) strings of complex spin rapidities (bound spin states); (c) strings of complex orbital rapidities (orbital bound states); (d) complex spin and charge rapidities (bound states of electrons with different spin components); (e) complex orbital and charge rapidities (bound states of electrons with different orbital components). Which classes are realized in the solution depends on signs and values of U, J and ε. For $c, c' \leq 0$ the repulsion exists in both spin and orbital subspaces. The solutions of the classes (a), (b) and (c) are valid. For $c \geq 0$, $c' \leq 0$ one has an effective repulsion in the spin subspace and the effective attraction in the orbital subspace, with the solutions from classes (a), (b), (c) and (e). For $c \leq 0$, $c' \geq 0$ the situation is opposite: there is an effective repulsion in the orbital subspace and an effective attraction in the spin subspace [classes (a), (b), (c) and (d)]. Finally, for $c, c' \geq 0$ all of the classes are present, because of the effective attraction in both spin and orbital subspaces. We derived integral equations for dressed energies, densities of excitations and their holes, which describe the thermodynamics of the model. The solution yields thermodynamic properties of the model as a function of U, J, ε, temperature T, chemical potential μ, H and D. It is not difficult to show that the behavior of conduction electrons of the model is the same as of a free electron gas, as it must be. For high energies ($T \gg V$) the model also describes the high-T behavior of a single noninteracting impurity shell, which properties are well-known [1, 3]. The most interesting properties are revealed by the impurity in the ground state and at low temperatures.

Consider, *e.g.*, $c' \geq 0$, $c \leq 0$ (for $|c| \geq |c'|$) for $l = \frac{1}{2}$. Here only solutions of classes (a), (c) and (d) — spin-singlet orbital-triplet Cooper-like pairs carrying charge $-2e$, spin zero and orbital moment 1, have Dirac seas for any μ, H and D. The way of solving the BE is, *e.g.*, the fusion procedure [7], which is the search of a solution to BE for charge rapidities within the class of orbital bound states. Those of them, which have maximal spin, are only important for the low-energy physics. One conduction electron, however, is bound at the impurity (*i.e.*, its charge rapidity is real, $k_j = \varepsilon$, with the fixed ratio ε/Λ). In the limit of $\Lambda \to \infty$ all real parts of those string solutions can be neglected, except of the rapidity of the conduction electron bound at the impurity. For the behavior of an impurity two low energy scales are important, one of which, T_{K}, is determined by c, and the smaller one, T_a, is determined by c' and c/c'. The solution of BE reveals that in the ground state the mixed valence of the impurity increases with growth of the band filling of conduction electrons (*i.e.*, the valence of the impurity explicitly depends on the total number of electrons in the system.) The ground state magnetization of the impurity for $H \ll T_a \ll T_{\rm K}$ is proportional to H/T_a with standard Kondo logarithmic corrections, *i.e.*, $M^z \sim H/T_a(1 + |\ln H/aT_a|^{-1} - \ldots)$ (a is some non-universal constant). It is usual for a single-channel Kondo problem [1]. However for $T_a \ll H \ll T_{\rm K}$ the magnetization of the impurity reveals the logarithmic behavior $M^z \sim (H/T_a)\ln(aT_{\rm K}/H)$, typical for the two-channel Kondo problem. For low temperatures $T \ll T_a \ll T_{\rm K}$ the Sommerfeld coefficient of the specific heat for the impurity is $\gamma \sim T_a^{-1}[1-(3T_a/\pi T_{\rm K})\ln(T_a/T_{\rm K})](1+|\ln T/T_a|^{-1} - \ldots)$ and the finite ground state susceptibility $\chi \sim T_{\rm K}^{-1}\ln(T_a/T_{\rm K})(1+|\ln T/T_{\rm K}|^{-1} - \ldots)$. This case pertains to the single-channel Kondo physics, though two different energy scales for χ and γ mean that the Wilson ratio differs from the Fermi liquid one. For $T_a \ll T \ll T_{\rm K}$ we have $\gamma \propto \chi \sim (T_{\rm K})^{-1}\ln(T_{\rm K}/T)$ and the remnant entropy of the impurity $\mathcal{S} = \ln\sqrt{2}$. For higher temperatures $T \geq T_{\rm K}$ the magnetic susceptibility of the impurity manifests the Curie-like behavior. The temperature dependence of the resistivity is determined by the scattering of conduction electrons off the spin of localized electron at low temperatures by $\Delta\rho(T) \sim A(T/T_a)^2$ for $T \ll T_a \ll T_{\rm K}$ and $\Delta\rho(T) \sim B(T/T_{\rm K})^{1/2}$ for $T_a \ll T \ll T_{\rm K}$. For $c' \leq 0$, $c \geq 0$ the situation is opposite to the above. One has the formal similarity to the previous case with the interchange $c \leftrightarrow c'$, $H/2 \leftrightarrow D$ and $L^z \leftrightarrow 2S^z$. The case $c, c' \geq 0$ pertains to all possible bound states being the solutions of the BE. This case is similar to the case of the degenerate Anderson model [1], but with different values of effective interactions for orbital and spin degrees of freedom. For $c, c' \leq 0$ only unbound electron excitations, spinons and orbitons can have their Dirac seas. In this case the situation is reminiscent of the Anderson impurity model with the in-shell attraction of electrons [1].

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