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Exactly Solvable Model for the Kondo Problem*

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A model for magnetic impurities in metals is introduced and solved exactly. It treats longitudinal impurity-electron coupling in the long-time approximation of the x-ray threshold problem and treats transverse spin-density operators in a fermion representation. For antiferromagnetic coupling, the magnetization in field H vanishes as $H^{2J_\parallel}$ and saturates when H is of order $(J_\perp^2/J_\parallel)^{1/2J_\parallel}$ ($J_\parallel$ and $J_\perp$ are longitudinal and transverse exchange constants). For ferromagnetic coupling, the free moment is only slightly renormalized.

Interest in the possibility of an exact solution of the Kondo problem has greatly increased since Anderson, Yuval, and Hamann[1] reformulated it using results from the x-ray threshold problem.[2] With their method, it is possible to treat the longitudinal exchange exactly and study the perturbation series in the transverse exchange. The result is a formal expression for the partition function, which must then be evaluated.

Subsequently, it was pointed out that the Tomonaga model of the electron gas gave the same formal expression for the partition function.[3] This model treats the *longitudinal* density operators of the unperturbed electron gas as bosons, and had previously been shown to give the weak-coupling limit of the x-ray threshold problem correctly.[4] On the other hand, as mentioned above, it is possible to diagonalize the longitudinal exchange term of the Kondo Hamiltonian and then to study the transverse spin-density operators in this new representation. We wish to point out here that there is a physically plausible model of *these* operators which makes the Hamiltonian exactly solvable.

Two separate reasons suggest the importance of this approach. The long-time approximation, as applied to the Kondo model,[1] is based on the intuitive idea that observable quantities should be governed by excitations near the Fermi level. These excitations lead to infrared singularities; and, within the framework of our model, we can study their importance and resolve whether they alone determine the observables. Alternatively, one can regard this approach as a particular partial summation of perturbation theory for the Kondo Hamiltonian, which is an exact solution of our model Hamiltonian. As discussed below, the two perturbation series have similar Kondo singularities, and in our exact solution we can study their renormalization.

The content of our model is best understood by comparison with the Kondo model. Consider the formal derivation of perturbation theory in the transverse exchange constant, using the eigenstates of the longitudinal exchange as the unperturbed basis set. The Kondo Hamiltonian is

$$\mathcal{H}_K=\sum_{\vec{k}}\epsilon_{\vec{k}}a_{\vec{k}}^{\dagger}a_{\vec{k}}+\frac{2J_\parallel}{N}\rho_z\sigma_z+2H\sigma_z+\frac{J_\perp}{N}(\rho_+\sigma_-+\rho_-\sigma_+), \tag{1}$$

where $\rho_i=\sum_{\vec{k}\vec{k}'}a_{\vec{k}'\alpha}^{\dagger}a_{\vec{k}\alpha'}s_{\alpha\alpha'i}$ is the ith component of the conduction-electron spin-density operator at the impurity site, σ_i and s_i are spin-$\frac{1}{2}$ operators, and N is the number of electrons. Taking $\sum_k 1=N$,

the operators ρ_i/N satisfy spin-operator algebra. We have omitted the coupling of the external field to the electrons since it is a negligible correction.[3] The first three terms on the right of Eq. (1) can be diagonalized by a unitary transformation $\exp(S\sigma_z)$. The transverse spin operator in this new representation, $\tilde{\rho}_\pm = \exp(S\sigma_z)\rho_\pm \exp(-S\sigma_z)$ and $\tilde{\sigma}_\pm = \exp(S\sigma_z)\sigma_\pm \exp(-S\sigma_z)$, still, of course, obey spin commutation relations. Our model replaces these operators by a fermion representation which preserves this spin algebra and the $\tilde{\rho}_\pm$ pair-correlation functions.

The model Hamiltonian is

$$\mathcal{H}_M = \sum_k E_k c_k^\dagger c_k + 2H\sigma_z + (J_\perp/N)(\rho_{M+}\sigma_- + \rho_{M-}\sigma_+), \tag{2}$$

where $\rho_{M+} = N^{1/2}\sum_k u_k c_k^\dagger d$ and $\rho_{M-} = (\rho_{M+})^\dagger$ are the transverse spin operators at the impurity site, the c and d operators describe fermions, and the functions E_k and u_k are specified below. Choosing $\sum_k u_k^2 = N$ insures that the operator ρ_{Mi}/N defined here obey spin algebra. The perturbation series for the partition function $Z_M = \mathrm{tr}\exp(-\beta\mathcal{H}_M)$ in $J_\perp$ is given by

$$\frac{Z_M}{Z_0} = \sum_{n=0}^{\infty}\left(\frac{J_\perp}{N}\right)^{2n}\int_0^\beta dt_1\cdots\int_0^{t_{2n-1}} dt_{2n}\{\langle\rho_{M+}(t_1)\rho_{M-}(t_2)\cdots\rho_{M-}(t_{2n})\rangle_0 \exp[\beta\mathcal{H} - 2H(t_1 - t_2)\cdots] + (+ - - -)\}, \tag{3}$$

where averages are taken in $\sum_k E_k c_k^\dagger c_k$, $\rho_{M\pm}(t)$ is temperature evolved with $\sum_k E_k c_k^\dagger c_k$, Z_0 is the partition function with $J_\perp = H = 0$, and the trace over the spin variable σ_z has been carried out. A very similar result obtains for the Kondo-model partition function, $Z_K = \mathrm{tr}\exp(-\beta\mathcal{H}_K)$, as a perturbation series in $J_\perp$. However, by Wick's theorem, it is seen that the averages which appear in Eq. (3) factorize into all possible contractions of the c_k operators since the trace over the d operators is trivial. As a result of this factorization, only the spin pair-correlation functions $\langle\rho_{M+}(t)\rho_{M-}\rangle_0$ and $\langle\rho_{M-}(t)\rho_{M+}\rangle_0$ occur in Eq. (3). The quantities E_k and u_k are then determined such that these pair-correlation functions are identical to the corresponding Kondo-model pair-correlation functions. This determination can best be done by comparing second-order perturbation theory in $J_\perp$, from Eq. (3), with the corresponding expression[1] for $\mathcal{H}_K$. The result is that $\langle\rho_{M+}(t)\rho_{M-}\rangle_0$ and $\langle\rho_{M-}(t)\rho_{M+}\rangle_0$ must both be equal to the square of the origin-to-origin Green's function[1] of the x-ray threshold problem.[1] This is achieved by choosing $\sum_k E_k c_k^\dagger c_k$ to describe a symmetric half-filled band of states and $\sum_k u_k^2 \times\langle c_k^\dagger c_k\rangle_0 \exp(-E_k t)$ to give the correct t dependence.

Although $\mathcal{H}_M$ should properly be viewed as a new model for the magnetic-impurity problem, it is closely related to the Kondo model. Considered as a partial summation for $\mathcal{H}_K$, it first differs from the Kondo model in order $J_\perp$.[4] It also reproduces the Toulouse limit[5] exactly, and agrees with perturbation expansions which can be derived for very large $J_\parallel$ using the spin-boson representation[3] of $\mathcal{H}_K$. Furthermore, it has the same symmetry properties as the general anisotropic $\mathcal{H}_K$.

In order to solve for the partition function Z_M we establish that it is formally identical to the partition function for a solvable single-particle problem. This problem is described by

$$\mathcal{H}_F = \sum_k E_k c_k^\dagger c_k + H(2d^\dagger d - 1) + (J_\perp/N)(cd^\dagger + dc^\dagger), \tag{4}$$

where $c = \sum_k u_k c_k$, the operators c_k and d are fermion operators as before, and u_k and E_k are the same as in Eq. (2). The perturbation series for $Z_F = \mathrm{tr}\exp(-\beta\mathcal{H}_F)$ is identical to that given by Eq. (3), with the $c(t)$ operators replacing the $\rho_M(t)$ operators. The H dependences, which were produced by the σ operators in Eq. (3), are here produced by the d operators. In both cases, the resulting averages of products of c_k operators factorize, by Wick's theorem, in exactly the same way. Thus the two partition functions Z_M and Z_F are identical.

Since $\mathcal{H}_F$ is a one-particle Hamiltonian, the single-particle Green's function $\langle\langle d; d^\dagger\rangle\rangle_\omega$ may be evaluated exactly. The correlation function $\langle d^\dagger d\rangle$ is then obtained by integration over the frequency and this gives the magnetization $M = 1 - 2\langle d^\dagger d\rangle$. In the usual way, the free energy F may be obtained by integrating the expectation value of the interaction energy with respect to the coupling constant. The result may be expressed in terms of the self-energy $\Sigma(\omega + i0) = \Sigma'(\omega) + i\Sigma''(\omega)$ for $\langle\langle d; d^\dagger\rangle\rangle_\omega$ as

$$F - F_0 = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{d\omega}{e^{\beta\omega}+1}\tan^{-1}\left(\frac{\Sigma''(\omega)}{\omega - \Sigma'(\omega) + 2H}\right), \tag{5}$$

where F_0 is the free energy when $J_\perp = 0$. Solving

the equations of motion gives

$$\Sigma(\omega)=\int_0^\infty \frac{dt}{i}e^{i\omega t}\frac{J_\perp^2}{N^2}\{[c(t),c^\dagger\}]_0$$

$$=\int_0^\infty \frac{dt}{i}e^{i\omega t}\frac{J_\perp^2}{N^2}\langle\{\rho_{M+}(t),\rho_{M-}\}\rangle_0, \qquad (6)$$

where t is real, $\{a,b\}$ denotes the anticommutator of a and b, and the second equation follows from the condition that the pair-correlation functions, which occur in the partition functions Z_K, Z_M, and Z_F, are set equal. It is thus not necessary explicitly to determine the u_k. We shall consider only zero temperature in detail. Since $\langle\rho_{M+}(t)\rho_{M-}\rangle_0$ is the square of the origin-origin Green's function, it takes the form $\langle\rho_{M+}(t)\rho_{M-}\rangle_0=(\rho_0/it)^{2-\epsilon}$, determined by Nozières and de Dominicis[2] for the x-ray threshold problem. Here ρ_0 is the Fermi-surface density of states; ϵ is related to the phase shift for scattering from the Kondo longitudinal exchange term[1] for large $J_\parallel\rho_0$, and is equal to $2J_\parallel\rho_0$ for small $J_\parallel\rho_0$. This time dependence is correct provided $t\gtrsim t_0$ is a cutoff of order a reciprocal band width. In usual metals, $t_0\approx\rho_0$, but it is important here to keep the two different to distinguish the long-time, or infrared, regime from the ultraviolet regime. An answer independent of t_0 indicates that infrared singularities do indeed dominate, and that the details of the band structure are unimportant. Thus we take

$$\frac{1}{N^2}\langle\rho_{M+}(t)\rho_{M-}\rangle_0=\left(\frac{\rho_0}{t_0+it}\right)^{2-\epsilon},$$

corresponding to a single-electron density of states $\rho(E)=\rho_0 e^{-|E|t_0}$. Substituting this into Eq. (6) gives the following result for $\omega t_0\ll 1$:

$$\Sigma(\omega+i0)=J_\perp^2\rho_0^{2-\epsilon}\Gamma^{-1}(2-\epsilon)\{-\pi i|\omega|^{1-\epsilon}-\omega|\omega|^{-\epsilon}\pi\cot(\tfrac{1}{2}\pi\epsilon)+2\omega\Gamma(1+\epsilon)t_0^{\epsilon}\cos(\tfrac{1}{2}\pi\epsilon)\epsilon^{-1}\}, \qquad (7)$$

where Γ is the gamma function. It is seen that the limit $t_0\to 0$ is meaningful only for $\epsilon>0$, corresponding to antiferromagnetic coupling. Furthermore, for $\epsilon>0$ this self-energy dominates the $\omega+2H$ terms in the argument of the inverse tangent in Eq. (5) at small ω, while for $\epsilon<0$ the corrections due to $\Sigma(\omega)$ are negligible at small ω. The thermodynamics for ferromagnetic coupling thus depends on the details of the band structure. We treat these two cases separately below.

Antiferromagnetic coupling.—The ground-state energy for $H=0$ is found by substituting Eq. (7) into Eq. (5). In $\Sigma(\omega)$, the limit $t_0\to 0$ can be taken, but the frequency integral must be cut off at t_0^{-1} in general since Eq. (7) is only valid for $\omega t_0\ll 1$. The result can be written as

$$F-F_0=-\int_0^{t_0^{-1}}\frac{d\omega}{\pi}\tan^{-1}\left\{\frac{J_\perp^2\rho_0^{2-\epsilon}\pi\omega^{-\epsilon}}{\Gamma(2-\epsilon)+J_\perp^2\rho^{2-\epsilon}\pi\omega^{-\epsilon}\cot\frac{1}{2}\pi\epsilon}\right\}. \qquad (8)$$

The upper cutoff can be extended to infinity if $\epsilon>1$, resulting in a ground-state energy which is proportional to $\rho_0^{-1}(J_\perp\rho_0)^{2/\epsilon}$ times a simple integral which depends only on ϵ. The importance of this result is the nonanalytic dependence on $J_\perp$, resulting from divergences in perturbation theory. If the inverse tangent in Eq. (8) is expanded in $J_\perp^2$, infrared divergences are encountered in nth order when $n\epsilon>1$. For small ϵ, these divergences occur first at very high orders, but they sum to produce the nonanalytic dependence of F on $J_\perp$.

The upper cutoff in Eq. (8) must be retained for $\epsilon<1$, and the ground-state energy becomes dependent on t_0. Numerically, however, perturbation theory in $J_\perp$ is adequate to compute F, because the divergences sum to produce a $(J_\perp\rho_0)^{2/\epsilon}$ contribution which is negligible compared to the second-order result of $-J_\perp^2\rho^{2-\epsilon}t_0^{\epsilon-1}$ for sufficiently small ϵ.

The magnetization is given by differentiating Eq. (5) with respect to H, then setting $t_0=0$. The result is

$$1-M=\frac{2}{\pi\epsilon}\int_0^\infty dx\left[\left(x+\frac{2H}{\omega_s}x^{1-1/\epsilon}+\cot\frac{\pi\epsilon}{2}\right)^2+1\right]^{-1}, \qquad (9)$$

where $\omega_s=\rho_0^{-1}[J_\perp^2\rho_0^2\pi/\Gamma(2-\epsilon)]^{1/\epsilon}$ and the variable $x=(\omega/\omega_s)^\epsilon$ has been introduced. With $H=0$, the result $M=0$ is readily found. It is also evident from Eq. (9) that the susceptibility $(\partial M/\partial H)_{H=0}$ is divergent when $\epsilon<\frac{1}{2}$. This divergent susceptibility results from a power-law magnetization which behaves as $M\approx\epsilon(2H/\omega_s)^\epsilon\pi/2$ for small ϵ and H. From these results, we can also deduce the characteristic saturation field $2H_s$ to be roughly $\rho_0^{-1}(J_\perp^2\rho_0^2\pi/\epsilon)^{1/\epsilon}$, which corresponds to the typical fluctuation

energy described by the self-energy in Eq. (7).

Ferromagnetic coupling.—Equation (8) can also be used for $\epsilon < 0$, provided the additional assumption $J_\perp{}^2\rho_0{}^{2-\epsilon} t_0{}^{\epsilon} \ll \epsilon$ is made. This restriction includes the physically interesting isotropic Kondo problem, and serves to simplify the results. Otherwise the computations are quite complicated, but qualitatively unchanged. Obviously Eq. (8) has only ultraviolet singularities if expanded in $J_\perp{}^2$. Since the band width $t_0{}^{-1}$ cuts them off, the perturbation series converges rapidly and, for numerical purposes, the second-order result of $-J_\perp{}^2\rho_0{}^{2-\epsilon} t_0{}^{\epsilon-1}$ suffices. Obviously this result depends on the details of the band structure, but the conclusion that the series converges does not.

An examination of $\Sigma(\omega)$ in Eq. (7) for $\epsilon < 0$ indicates that $\Sigma'(\omega)$ is negligible compared to $2H$ when inserted in Eq. (5). Consequently, the free-spin nature of the $\langle\langle d; d^\dagger\rangle\rangle_\omega$ Green's function is only slightly renormalized, and the $\omega + 2H$ behavior is dominant in Eq. (5). Differentiating Eq. (5) with respect to H gives a result for the magnetization which can be evaluated by perturbation theory to be

$$M = 1 - \frac{J_\perp{}^2\rho^{2+|\epsilon|}\pi t_0{}^{-|\epsilon|}}{|\epsilon|\Gamma(2-\epsilon)} + \cdots . \qquad (10)$$

As in F, the magnetization depends on the band structure, but we can conclude that, unlike $\epsilon > 0$, there is no problem of infrared singularities in the perturbation series for M.

The finite-temperature field dependence is qualitatively similar to that obtained for the ground state. For $k_B T \gg H_s$, the antiferromagnetic susceptibility follows a Curie law, and for $k_B T \ll H_s$ it approaches the $T = 0$ susceptibility which is nonlinear in general. The ferromagnetic case, of course, is simply a free spin with only weak temperature-dependent renormalizations.

It is interesting that this model and the Kondo Hamiltonian have the same magnetization at $H = 0$ but the susceptibilities[7] differ for $\epsilon > 0$. A more complete comparison with these results will be made in a future publication. However, it may be noted that, for the case of isotropic exchange, $J_\perp = J_\parallel = J$, both are also identical to order J^3 for the resistivity and the susceptibility. In particular the usual $J\rho_0 \ln(H\rho_0)$ singularities are found, and they are summed exactly in our model to give the results of Eqs. (9) and (10). For $J > 0$ the discussion following Eq. (9) demonstrated that the characteristic field $\rho_0{}^{-1}\exp[-(2J\rho_0)^{-1}]$ deduced from this series is renormalized downward to $\rho_0{}^{-1}(J\rho_0)^{1/J}$, while for $J < 0$ essentially free-spin behavior was found.

The model may also be used to test the validity of the renormalization-group method.[8] This problem together with several interesting questions concerning impurity-spin dynamics and resistivity is currently being studied.

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