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EXACT RESULTS IN THE KONDO PROBLEM: EQUIVALENCE TO A CLASSICAL ONE-DIMENSIONAL COULOMB GAS

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We demonstrate an exact equivalence between a Kondo problem and the thermodynamics of a classical one-dimensional gas with alternating charges and a logarithmic potential. This classical gas has a critical point.

We demonstrate an asymptotically exact equivalence[1] between the simplest Kondo problem, the ground state of a spin $S=\frac{1}{2}$ interacting with an otherwise free electron gas, and the thermodynamics of a certain one-dimensional classical gas. The central point is an asymptotic expression (i.e., for $E_F t \gg 1$) for the probability amplitude for a succession of spin flips. The interaction in the classical gas is of logarithmic (two-dimensional Coulomb) type for which simpler cases have been solved exactly by Dyson, Wilson, and Gunson.[2] Some physical results from the classical gas problem are available already—e.g., that the antiferromagnetic case has no mean spin—and these will be discussed in a succeeding communication. Generalizations to finite T, higher spin, and more physical models seem not forbidding.

We divide the Hamiltonian as follows:

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1, \tag{1}$$

$$\mathcal{H}_0=\sum_{k,\sigma}\epsilon_k n_{k\sigma}+JS_z\sum_{kk'\sigma\sigma'}c_{k\sigma}^{\dagger}(s_z)_{\sigma\sigma'}c_{k'\sigma'}, \tag{2}$$

$$\mathcal{H}_1=J\sum_{k,k'}c_{k\sigma}^{\dagger}c_{k'\sigma'}[S_+(s_-)_{\sigma\sigma'}+S_-(s_+)_{\sigma\sigma'}]. \tag{3}$$

The eigenstates of $\mathcal{H}_0$ are

$$\Psi_\uparrow=\alpha\prod_k c_{k\uparrow}^{\dagger}\prod_{k'}d_{k'\downarrow}^{\dagger}|\mathrm{vac}\rangle,\quad \Psi_\downarrow=\beta\prod_k d_{k\downarrow}^{\dagger}\prod_{k'}c_{k'\uparrow}^{\dagger}|\mathrm{vac}\rangle, \tag{4}$$

where $c_k^{\dagger}$ are scattering states appropriate to the potential $+\frac{1}{4}J$ [phase shift $\delta_+\simeq-\frac{1}{4}\pi J\rho(E_F)$] and d_k are scattering states appropriate to $-\frac{1}{4}J$ ($\delta_-\simeq-\delta_+$). For J antiferromagnetic, δ_+ is negative.

The lowest eigenstate with $S_z=+\frac{1}{2}$ we denote by $\alpha\Psi_{0\uparrow}$. We calculate

$$F(t)=\langle\alpha\Psi_{0\uparrow}|\exp(i\mathcal{H}t)|\alpha\Psi_{0\uparrow}\rangle=\sum_\omega|\langle\alpha\Psi_{0\uparrow}|\Psi_\omega\rangle|^2e^{i\omega t}, \tag{5}$$

where Ψ_ω are the exact eigenstates. We assume that the Fourier transform $F(\omega)$ must have a branch

point or pole singularity at the ground-state energy ω_0. [I.e., states infinitesimally close to the ground state are assumed not all orthogonal to $\alpha\Psi_{0\uparrow}$. This is not a doubtful assumption; if it appeared so, we could turn on J in (3) slowly, following standard methods, and ensure nonorthogonality.] t can be complex; note that if $t=i\beta$, the least rapidly decaying part of F, which is now real, refers exclusively to the ground state and those infinitesimally close to it.

In the interaction representation we may write

$$F(t)=\langle\alpha\Psi_{0\uparrow}|\exp(+i\mathcal{H}_0 t)T\{\exp[i\int_0^t\mathcal{H}'(t')dt']\}|\alpha\Psi_{0\uparrow}\rangle, \tag{6}$$

where

$$\mathcal{H}'(t')=\exp(-i\mathcal{H}_0 t')\mathcal{H}'\exp(+i\mathcal{H}_0 t'). \tag{7}$$

Thus a typical term of $F(t)$, for example the second order which is the lowest nontrivial one, is

$$\langle\alpha\Psi_{0\uparrow}|\int_0^t dt_2\int_0^{t_2}dt_1\exp[i\mathcal{H}_0(t-t_2)](i\mathcal{H}')\exp[i\mathcal{H}_0(t_2-t_1)](i\mathcal{H}')\exp[i\mathcal{H}_0(t_1)]|\alpha\Psi_{0\uparrow}\rangle. \tag{8}$$

If we measure energies from $\langle\alpha\Psi_{0\uparrow}|\mathcal{H}_0|\alpha\Psi_{0\uparrow}\rangle=\Omega_0$, $\exp(i\mathcal{H}_0 t_1)=1$. Then the effect of $\mathcal{H}'$ is to flip the local spin ($\alpha\to\beta$) at t_1, at the same time destroying an electron of down spin and creating an up spin, both at the local spin site [in $\Psi(0)$]; then from t_1 to t_2 all particles propagate under the new potential $-\frac{1}{2}Js_z(0)$ but at t_2 we get a reverse flip and at t measure the amplitude that the system is still in the original state.

The method is based on Nozières and de Dominicis'[3] exact solution of the x-ray intensity problem, which we had earlier observed[4] was closely related to the Kondo problem. Nozières and de Dominicis have calculated the ground-state–to–ground-state amplitude $F_N(t)$ for a process involving creation of a particle and simultaneous application of a scattering potential such that the phase shift changes by δ at $t=0$, the particle to be destroyed at t as the scattering is turned off again. We see that the first nontrivial term (8) for the Kondo problem is just the product of two x-ray problems, one for each spin, integrated over appropriate time intervals:

$$-J^2\int_0^t dt_1\int_0^{t_1}dt_2 F_{N\uparrow}(t_1-t_2)F_{N\downarrow}(t_1-t_2), \tag{9}$$

where F_N is the appropriate Nozières correlation function,

$$F_{N\pm}(t)=\left(\frac{it}{\tau}\right)^{-\pi^{-2}(\pm\pi+2\delta_\pm)^2}=\left(\frac{it}{\tau}\right)^{-1+\epsilon}. \tag{10}$$

Here we define

$$\epsilon=-\frac{4\delta_+}{\pi}-\frac{4\delta_+^2}{\pi^2}\cong J\rho; \tag{11}$$

ϵ is small and positive for the antiferromagnetic case. In choosing the phase of F_N we have followed Nozières; it essentially appears in his calculation as part of the somewhat arbitrary cutoff parameter $\tau\sim E_F^{-1}$, but it is necessarily as given in order that $F(i\beta)$ be real. As in the ground-state–to–ground-state problem,[5] only the relative phase shift 2δ is relevant for the asymptotic behavior. For symmetry reasons, there is no $e^{i\Delta t}$ term.

The general term T_n of (6) involves a sequence of $2n$ spin reversals occuring at $t_1, t_2, \cdots, t_{2n}$. The ground-state–to–ground-state amplitude for this process is what we need, and is clearly the product of amplitudes for two generalized Nozières-Mahan processes with a sequence of n emissions and reabsorptions and n changes in the scattering phase shift by $2\delta_+$.

This amplitude is calculated by a generalization of their method, as the product of three factors: (a) the unscattered amplitude $G_0(t)$ for n emissions and reabsorptions, summed over

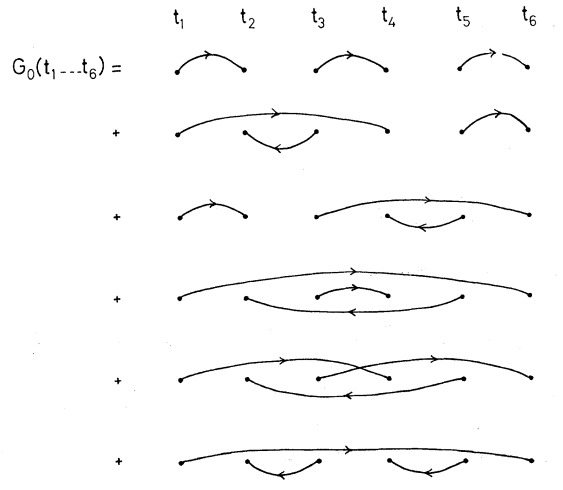

FIG. 1. Example of diagrams contributing to G_0: The contribution of one set of times.

all possible ways of connecting the emissions t_{2n-1} and reabsorptions t_{2n} (see Fig. 1); (b) a correction factor $\varphi(\delta,t)/G_0(t)$ for the single-particle scattering in these diagrams; and (c) the ground-state-to-ground-state amplitude $e^{C(\delta,t)}$ given by exponentiating the sum of all loops $C(\delta,t)$.

Once we have calculated either (a) or (c) the total answer becomes very plausible. Let us do the former. As Nozières observes, G_0 for a single emission at t_1 and reabsorption at t_2 is

$$(G_0)_1 = i\tau/|t_1-t_2|; \tag{12}$$

we do not want to use Nozière's time-ordering convention—since the sequence of times in (8) is predetermined—so we observe that if t_2 is later than t_1 the sign does not change.

There are two second-order diagrams corresponding to pairing of t_1 with t_2 or t_4. For the second case one of the time sequences is reversed: Thus

$$(G_0)_2 = \left(\frac{i\tau}{t_1-t_2}\right)\left(\frac{i\tau}{t_3-t_4}\right) - \left(\frac{i\tau}{t_1-t_4}\right)\left(\frac{i\tau}{t_3-t_2}\right)$$

$$= (i\tau)^2 \begin{vmatrix} \frac{1}{t_1-t_2} & \frac{1}{t_1-t_4} \\ \frac{1}{t_3-t_2} & \frac{1}{t_3-t_4} \end{vmatrix}.$$

In high orders it is necessary to observe that when we add an extra pair of times to a given loop, we add either a reversed time sequence or a pair of crossed lines, corresponding to a reversal in the ordering of a pair of fermions; thus it is possible to show

$$(G_0)_{2n}(t_1\cdots t_{2n}) = (i\tau)^n \det\left|\left|\frac{1}{t_{2j-1}-t_{2k}}\right|\right| = (i\tau)^n \prod_{\substack{j>j' \\ k>k'}} (t_{2j-1}-t_{2j'-1})(t_{2k}-t_{2k'})\left[\prod(t_{2j-1}-t_{2k})\right]^{-1}$$

$$= \exp\left\{\sum_{j>k}(-)^{j-k}\ln\left(\frac{t_j-t_k}{i\tau}\right)\right\}. \tag{13}$$

The second identity is the consequence of the fact that the determinant is of Cauchy form.[6]

Now if we study the Muskhelishvili equation[7] which Nozières and de Dominicis solve to obtain the simple solution for $\varphi(\delta,t)$, we find that it amounts to finding that function for which the poles at 0 and t are replaced by a branch cut joining them. Generalization of this result to the n pairs of poles in (13)—the second form is the clearest—immediately shows us that the only function with all the right analytic properties is

$$F_{2n}(t) = G_0^{1-\epsilon}. \tag{14}$$

A full derivation has been carried out and will be published later.

It is interesting to check this by means of perturbation theory. As pointed out previously[8] the emission process is simply equivalent, physically as well as mathematically, to a sudden phase shift of π (e.g., to the sudden destruction of a bound state). Thus the true weak-potential limit corresponds to $\Delta(\delta)=\pi$, or $1-\epsilon\to 0$. In this limit direct calculation of the necessary overlap determinant using an identity suggested to us by Thouless,

$$(\det|U_{ij}|)^2 = \exp\ln(U\tilde{U}^\dagger + 1 - 1) \simeq \exp\Big[-\sum_{i<k_F,\, j>k_F}|U_{ij}|^2\Big],$$

leads to (14).

For pure imaginary t, the formulas become somewhat easier to handle. Thus we may write the required amplitude for pure imaginary time, $F(i\beta)$, exactly (in the asymptotic limit of large βE_F) as

$$F(i\beta) = \sum_{n=0,2}^{\infty} J^{2n}\int_0^\beta d\beta_{2n}\int^{\beta_{2n}} d\beta_{2n-1}\cdots\int_0^{\beta_2} d\beta_1 \exp\Big[(2-2\epsilon)\sum_{n>n'}(-1)^{n-n'}\ln\Big(\frac{\beta_n-\beta_{n'}}{\tau}\Big)\Big] \tag{15}$$

(divergences when $\beta_n\to\beta_{n-1}$ are to be cut off at τ). This equation may be exactly interpreted as the grand partition function of a classical one-dimensional gas of charged hard rods constrained to be

alternately + and −, on a line of length β. Their interaction is the two-dimensional Coulomb force

$$\frac{V(x-x')}{T} = \pm 2(1-\epsilon)\ln\left(\frac{x_n - x_{n'}}{\tau}\right)$$
$$= \infty \quad (|x_n - x_{n'}| < \tau). \tag{16}$$

The chemical potential is given by

$$e^{-\mu} = J; \tag{17}$$

and the free energy $f(T)$ per unit length determines the ground-state energy according to

$$F(i\beta) \sim e^{+\beta\omega_0} \sim e^{-\beta f(T)/T}. \tag{18}$$

In a subsequent Letter we will show that the point $\epsilon = 0$ (for small J) is a critical point of this system, separating the region where the charged pairs are all associated from that where some are ionized, the latter being the region of zero net spin. It is fascinating that the simple-appearing Kondo system is isomorphous with one which certainly has at least one critical point and possible more. (It is a commonplace that one-dimensional systems with long-range interactions often have critical points.)

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THEORY OF ITINERANT FERROMAGNETS EXHIBITING LOCALIZED-MOMENT BEHAVIOR ABOVE THE CURIE POINT*

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By using a functional integral formulation of the theory of itinerant ferromagnets above the Curie point, we show that for strong Coulomb interaction U, there are localized moments exhibiting a characteristic Curie-law susceptibility with the correct free spin-$\frac{1}{2}$ limiting value of the Curie constant. For weak U the same formulation gives a Pauli-like susceptibility, again with the proper limit, while for intermediate values the theory gives a smooth interpolation between the extreme cases.

The presence of local-moment aspects in band ferromagnetism has long been a baffling problem. The most striking example of this is iron. The high-temperature susceptibility, neutron scattering, alloy experiments, etc., all point to the presence of localized moments, while transport properties show unambiguously the itinerant character of the d electrons.[1] We report here on the first results of a new theoretical approach to such systems. The theory is based on an exact transformation of Stratonovich[2] and Hubbard[3] which eliminates the two-body interaction in favor of a Gaussian average over fluctuating one-body potentials. We concentrate here on the paramagnetic phase, leaving cooperative effects for future publication.

Since there is little short-range order at high temperatures, we expect the problem to be equivalent to an aggregation of one-center problems. The one-center problem can be represented by an Anderson model[4] of an "impurity" atom immersed in an effective band. While orbital degeneracy (Hund's rule) is important in practice, most of the essential features are already contained in the nondegenerate orbital model treated here.

The Hamiltonian is $H_0 + H_1$, where if $\sigma \equiv \pm 1$,

$$H_0 = \sum_{k,\sigma} \epsilon_{k\sigma} n_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} n_{d\sigma} + \sum_{k,\sigma} [V_k c_{k\sigma}^{\dagger} c_{d\sigma} + \text{H.c.}], \tag{1a}$$

$$H_1 = U n_{d\uparrow} n_{d\downarrow} = -\tfrac{1}{2} U (n_{d\uparrow} - n_{d\downarrow})^2 + \tfrac{1}{2} U (n_{d\uparrow} + n_{d\downarrow}). \tag{1b}$$