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PATH INTEGRAL THEORY OF MAGNETIC ALLOYS

by D. R. HAMANN

Bell Telephone Laboratories, Incorporated Murray Hill, New Jersey

**Résumé.** — On étudie, par la méthode du « path integral » appliquée au modèle d'Anderson, la formation de moment localisé et les anomalies à basse température. Chaque chemin représente une histoire différente pour le potentiel fluctuant sur l'atome magnétique. La contribution de chaque chemin à la fonction de partition est calculée explicitement en utilisant la méthode asymptotique exacte de Nozières et De Dominicis. On identifie un ensemble principal de chemins, et on montre que leur contribution correspond exactement à une expression dérivée récemment par Anderson et Yuval pour le modèle d'échange s-d. Une évaluation approximative de ce « path integral » restreint donne la température de Kondo caractéristique, et des prédictions qualitativement correctes pour les diverses propriétés des alliages.

**Abstract.** — Local moment formation and low temperature anomalies are studied by a path integral approach to Anderson's model. Each path represents a particular history for the fluctuating potential on the magnetic atom. A path's contribution to the partition function is calculated explicitly using the asymptotically exact method of Nozières and De Dominicis. A dominant set of paths is identified, and their contribution is shown to correspond exactly to an expression recently derived for the s-d exchange model by Anderson and Yuval. Approximate evaluation of this restricted path integral yields the characteristic Kondo temperature, and qualitatively correct predictions for various alloy properties.

Two key problems are presented by the interaction of a transitional impurity atom with a non-magnetic host metal. One is reconciling the collective theory of local moment formation, such as given by Anderson [1] with the experimental observation that such impurities simulate truly localized quantum-mechanical spins. The second is understanding the consequences of the infrared divergence discovered by Kondo [2] in the low temperature limit. The author [3] has introduced a path-integral formulation of Anderson's model [1] which offers certain advantages over conventional methods of many body theory in coping with these problems.

The Hamiltonian for the Anderson model is

$$H_0 = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} n_{d\sigma} + \sum_{k\sigma} (V_{kd} C_{k\sigma}^{\dagger} C_{d\sigma} + V_{kd}^* C_{d\sigma}^{\dagger} C_{k\sigma}) \quad (1)$$

$$H_1 = U n_{d+} n_{d-} \quad (2)$$

In our results, we will take  $\epsilon_d = -U/2$  for simplicity. By applying the method of Stratonovich [4] and Hubbard [5] the partition function may be written as

$$Z = Z_0 \int \delta x \delta y \times \langle T_{\tau} \exp \left\{ - \int_0^{\beta} d\tau \left[ \frac{\pi x^2}{\beta} + \frac{\pi y^2}{\beta} + \tilde{H}_1 \right] \right\} \rangle, \quad (3)$$

where

$$\tilde{H}_1 = (\pi U/\beta)^{1/2} \{ x(\tau) [n_{d+}(\tau) - n_{d-}(\tau)] + iy(\tau) [n_{d+}(\tau) + n_{d-}(\tau)] \}. \quad (4)$$

In the above,  $Z_0$  is the partition function and  $\langle \rangle$  the thermal average with respect to  $H_0$ .  $T_{\tau}$  is the ordering operator with respect to the imaginary time  $\tau$  which runs from 0 to  $\beta = 1/kT$ . The outside integral is over the c-number functions  $x$  and  $y$ , and the operators  $n_{d\sigma}$  are in the interaction representation defined by  $H_0$ .  $\tilde{H}_1$  can be interpreted as the Hamiltonian for

a time-dependent external d-state potential acting on the electrons. According to (3), we are to compute the partition function of the noninteracting electrons in the presence of each possible fluctuating potential, and add the results with a Gaussian weighting factor. Expanding (3) in powers of  $U$ , we could do the functional integrals trivially term-by-term and recover ordinary diagrammatic perturbation theory. The advantage of the present formulation is that it enables us to isolate the infrared divergence, which occurs in the low frequency response of an electron gas to any localized fluctuating potential.

In studying X-ray absorption, Nozières and De Dominicis [6] treated the corresponding infrared divergence simply and exactly. To use their method, we write the equation satisfied by the d state Green's function in the presence of the potential  $v_{\sigma}(\tau)$ ,

$$G_{d\sigma}(\tau, \tau') = G_{d\sigma}^0(\tau, \tau') + g \int_0^{\beta} d\tau'' G_{d\sigma}^0(\tau, \tau'') v_{\sigma}(\tau'') G_{d\sigma}(\tau'', \tau'). \quad (5)$$

Instead of the exact  $G_d^0$ , we use the approximation

$$G_d^0(\tau) \approx \frac{-\Delta}{\epsilon_d^2 + \Delta^2} \left[ \frac{P}{\beta \sin(\pi\tau/\beta)} + \frac{\epsilon_d}{\Delta} \delta(\tau) \right], \quad (6)$$

where  $\Delta$  is the d resonance width and  $P$  denotes principal value. This expression is asymptotically exact for  $\tau\epsilon_d \gg 1$ , and thus gives an accurate solution of (5) provided the maximum frequency in  $v_{\sigma}(\tau)$  is limited. Using (6), (5) can be solved in closed form and the contribution to the partition function calculated for any arbitrary  $v_{\sigma}$ .

The resulting expression for the partition function is

$$Z = Z_0 \int \delta\xi Z(\xi), \quad (7)$$

where  $\xi = x(\pi U/\Delta)^{1/2}$ , and

$$Z(\xi) = \exp \left\{ - \int_0^{\beta} d\tau [V(\xi) + T(\xi)] \right\}. \quad (8)$$

We have replaced the  $y$  component of the potential, which couples to the  $d$  state number density, with its mean value because we expect its fluctuations to be small and of high frequency. The «partition functional»  $Z(\xi)$  for each «path»  $\xi$  has the contributions

$$V = (\Delta^2/U) \xi^2 - (2\Delta/\pi) \left[ \xi \tan^{-1} \xi - \frac{1}{2} \ln(1 + \xi^2) \right], \quad (9)$$

which depends only on the instantaneous value of  $\xi$ , and

$$T = \frac{P}{\pi^2} \int_0^\beta d\tau' \left( \frac{\pi}{\beta} \right) \text{ctn} \left[ \pi \left( \frac{\tau - \tau'}{\beta} \right) \right] \xi(\tau) \frac{d\xi(\tau')}{d\tau'} \times \\ \times \frac{1}{\xi^2(\tau) - \xi^2(\tau')} \ln \frac{1 + \xi^2(\tau)}{1 + \xi^2(\tau')}, \quad (10)$$

which contains the effects of the infrared divergence.

Since  $Z(\xi)/Z$  is the probability of the path  $\xi$ , we may study (9) and (10) to determine which paths are important.  $V(\xi)$  is shown in figure 1 for several values

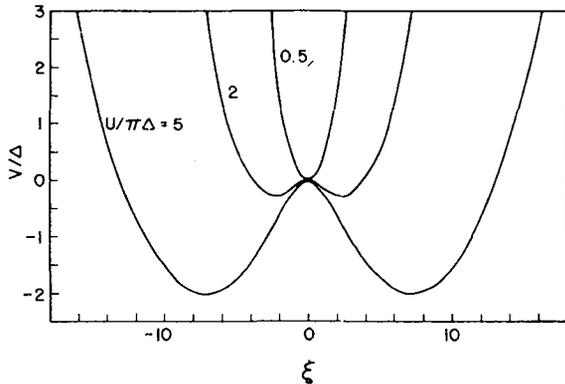


FIG. 1. — The function  $V(\xi)$ , Eq. 9, for  $U/\pi\Delta = 5, 2$  and  $5$ .

of  $U$ . The effect of  $T$  is to decrease the probability of a path in proportion to the amount it fluctuates from a constant value. The most probable path is  $\tau$ -independent, sits at a minimum of  $V$ , and corresponds exactly to Anderson's Hartree-Fock solution [1]. Small fluctuations about one of these extremal solutions would customarily be studied as the «next correction». In the large  $U$  case, however, it is clear that there are a great number of «hopping» paths such as shown in figure 2 which may be almost as probable as the extremal paths. Small fluctuations will make essentially the same contribution to the free energy whether added to an extremal path or one of the hopping

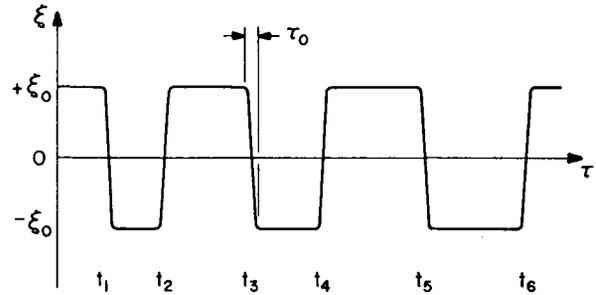


FIG. 2. — A typical «hopping» path.  $\pm \xi_0$  are the positions of the minima of  $V(\xi)$ , and the positions of the hops are arbitrary, except for the obvious requirement  $t_{i+1} - t_i > \tau_0$ .

paths, and are thus of little interest. The partition functional  $Z(\xi)$  can be evaluated explicitly for hopping paths if  $\xi_0 \approx U/2\Delta \gg 1$ , and we obtain

$$Z = \sum_{n=0}^{\infty} \xi_0^{-2n} \int_0^\beta \frac{dt_{2n}}{\tau_0} \int_0^{t_{2n}-\tau_0} \frac{dt_{2n-1}}{\tau_0} \dots \int_0^{t_2-\tau_0} \frac{dt_1}{\tau_0} \times \\ \times \exp \left[ \left( \frac{2 \tan^{-1} \xi_0}{\pi} \right)^2 \sum_{i \neq j} (-1)^{i+j} \times \right. \\ \left. \times \ln \left| \left( \frac{\beta}{\pi \tau_0} \right) \sin \left[ \frac{\pi(t_i - t_j)}{\beta} \right] \right| \right] \quad (11)$$

where the hop width  $\tau_0$  has been chosen variationally as  $6/U$ . This corresponds precisely to an expression for the partition function of the  $s$ - $d$  exchange model recently derived by Anderson and Yuval [7].

The evaluation of (eq. (11)) is itself a difficult problem in one-dimensional classical statistical mechanics. However an approximate evaluation has been carried out [8] yielding the following results:  $\xi(\tau)$  is found to have a correlation range equal to  $1/kT_K$ , where  $T_K$  is the Kondo temperature. Thus for  $T \gg T_K$ ,  $\xi = \pm \xi_0$  is a good approximation and the impurity is essentially a two-state system with a Curie law susceptibility. For  $T \ll T_K$ , typical paths have no long-range correlation, so that the susceptibility is of order  $\mu_B^2/kT_K$  and there is no zero-temperature singularity in the thermodynamic functions.

The resistivity can be examined by expressing the complete  $d$  state Green's function as the path average, weighted by  $Z(\xi)/Z$ , of the Green's function for particular paths. The resulting expression can be evaluated for periodic hopping paths. For  $T \ll T_K$ , this yields the maximum scattering permitted by unitarity, while for  $T \gg T_K$  the scattering falls to a value equal to that computed from the Hartree-Fock approximation.

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