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PERTURBATION TECHNIQUE FOR THE ANDERSON HAMILTONIAN*

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(Received 6 July 1970)

A new strong-coupling diagrammatic perturbation treatment of the Anderson Hamiltonian confirms in finite order Kondo divergencies for the partition function, associated with an effective s-d coupling J as predicted by the Schrieffer-Wolff transformation. This holds true also for the symmetric case. By summing the diagrams with two conduction-electron intermediate states in the limit $U\to\infty$, a Kondo temperature with J near diverging is obtained.

Similarities between the physical properties of the Anderson[1] and the s-d exchange Hamiltonians for dilute magnetic alloys were suggested when Schrieffer and Wolff[2] established the approximate equivalence of the two models most elegantly by means of a canonical transformation. Other approaches, confirming this equivalence, have been based on finite-order perturbation theory.[3,4] However, recent treatments of the Anderson model by means of the Green's functions equations-of-motion decoupling scheme[5,6] seem to show some important differences between the two models. In particular, Ref. 5 obtains a value for the effective s-d coupling J which is half the value of the J in the Schrieffer-Wolff transformation.[7] In Ref. 6 it is proven that the decoupled equations of motion lead to vanishing of all Kondo singularities in the symmetric case $\epsilon_d+\frac{1}{2}U=0$.[8] Since for that particular case the Green's function perturbation theory carried out in Ref. 4 breaks down, while the functional-integral approach leads to the usual Kondo effect,[9] the situation is sufficiently unclear to be re-examined from the viewpoint of direct perturbation theory.

For that purpose we follow Scalapino[3] up to his Eq. (4), which we rewrite as

$$Z/Z_0=1+\sum_{n=1}^{\infty}\int_0^{\beta}d\lambda_1\int_0^{\lambda_1}d\lambda_2\cdots\int_0^{\lambda_{n-1}}d\lambda_n\sum\cdots V_{kd}{}^{*}\cdots V_{k'd}$$
$$\times\langle k\text{-electron operators}\rangle\langle d\text{-electron operators}\rangle. \qquad (1)$$

where the second sum extends over momenta, spins, and all sequences of n d-electron and n k-electron operators. The first bracket, representing the normalized thermodynamic expectation value of the k-electron operators written in the interaction representation, can be evaluated in the usual way, using Wick's theorem for thermodynamic averages. Wick's theorem cannot be used for the second bracket since the zero-order d-electron Hamiltonian $H_d{}^0$ contains the part $Un_{d\uparrow}n_{d\downarrow}$. Evaluating the trace in the second bracket in the representation where $H_0{}^d$ is diagonal, we obtain

$$\langle d\text{-electron operators}\rangle=n_0\langle 00|\cdots c_{ds}(\lambda_j)\cdots c_{ds'}{}^{\dagger}(\lambda_k)\cdots|00\rangle+n_{d\uparrow}\langle 01|\cdots c_{ds}(\lambda_j)\cdots c_{ds'}{}^{\dagger}(\lambda_k)\cdots|10\rangle$$
$$+n_{d\downarrow}\langle 10|\cdots c_{ds}(\lambda_j)\cdots c_{ds'}{}^{\dagger}(\lambda_k)\cdots|01\rangle$$
$$+n_{dd}\langle 11|\cdots c_{ds}(\lambda_j)\cdots c_{ds'}{}^{\dagger}(\lambda_k)\cdots|11\rangle. \qquad (2)$$

Here n_0, $n_{d\uparrow}$, $n_{d\downarrow}$, n_{dd} are the occupation probabilities for the corresponding d states (see Scalapino[3]).

Taking the set of d-electron operators $c_{d\downarrow}(\lambda_1)c_{d\uparrow}{}^{\dagger}(\lambda_2)c_{d\downarrow}{}^{\dagger}(\lambda_3)c_{d\downarrow}(\lambda_4)c_{d\uparrow}(\lambda_5)c_{d\downarrow}{}^{\dagger}(\lambda_6)$ as an example in

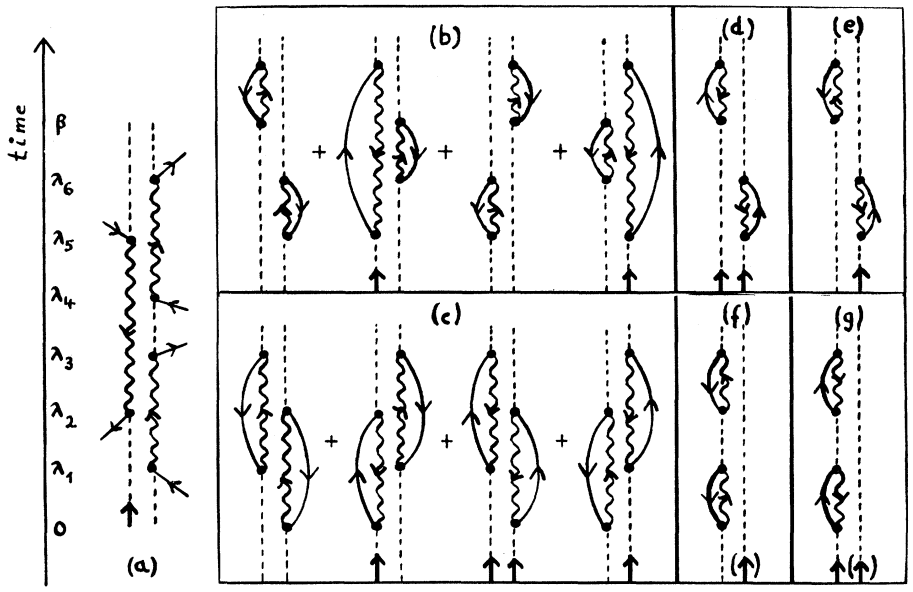

FIG. 1. (a) Graphical representation of the example discussed in the text. (b), (c) Two families of diagrams rotated on a cylinder; (d), (g) representatives R, each one standing for a family. The second d level in (f) and (g) may be occupied or not (arrow in brackets). We get all fourth-order diagrams from (b)-(g), if we add to (c), (e), (f), and (g) the corresponding diagrams in which the $d\uparrow$ and $d\downarrow$ levels are interchanged.

(2), we obtain a nonvanishing matrix element only for the state $|10\rangle$. We indicate the two d levels by two parallel dotted vertical lines (the left one for spin up), and specify the initial state by drawing an arrow if the corresponding d level is occupied. In our example at the "time-vertex" λ_6 a $d_\downarrow$ electron is produced and propagates (wiggly line) until it is annihilated at the later time λ_4 [see Fig. 1(a)], another $d_\downarrow$ electron propagates from λ_3 to λ_1, while a $d_\uparrow$ hole propagates from λ_5 to λ_2. Then the matrix element of the above operators between the $|10\rangle$ states is given by $\exp\{-(\epsilon_\downarrow+U)\lambda_1+(\epsilon_\uparrow+U)\lambda_2+\epsilon_\downarrow\lambda_3-\epsilon_\downarrow\lambda_4-(\epsilon_\uparrow+U)\lambda_5+(\epsilon_\downarrow+U)\lambda_6\}$. We obtain analogous diagrams for other processes.

From these diagrams we get the partition-function diagrams by adding the k-electron contributions. For example, we represent $c_{k\sigma}^{\dagger}(\lambda_i)$ by a full line with an arrow on it, pointing away from the vertex at λ_i on the dotted line σ, carrying momentum k and spin σ. According to Wick's theorem the contraction of the k-electron operators can be represented by closing the full lines belonging to the same spin in all possible ways (there are two possibilities for our example). An ascending line (particle) carrying $k\sigma$ then stands for $|V_{kd}|^2(1-f_{k\sigma})$, where the statistical factor refers to the states available to the particle; a descending line $(k'\sigma')$ for $|V_{k'd}|^2 f_{k'\sigma'}$. We get an exponential factor containing the times and energies, and an overall sign of the diagram $(-1)^c$, where, provided that all $\downarrow$-spin electron lines are closed to the right of the dotted $\downarrow$ line, and all $\uparrow$-spin electron lines are closed to the left of the dotted $\uparrow$ line, c is the number of crossings of full lines.

It is convenient to carry out the time integrations not for a single diagram, but for a family of diagrams "rotated on a cylinder,"[10] for which examples are given in Figs. 1(b) and 1(c). We then obtain

$$Z/Z_0-1=\sum_R(-1)^c N\sum_{\text{all } k} MS\frac{l}{n}\frac{(-\beta)}{2\pi i}\oint dz\, e^{-\beta z}[z(z-E_1)\cdots(z-E_{n-1})]^{-1}. \tag{3}$$

Here the sum extends over all diagrams R, each one arbitrarily chosen as a representative for a family; N denotes the occupation probability of its initial d level (indicated by arrows on the dotted lines); M and S stand for matrix elements $V_{kd}\cdots V_{k'd}^*$ and statistical factors $(1-f_{k\sigma})f_{k'\sigma'}\cdots$, respectively; l is the length of the cycle, n is the number of interactions in R, and the integration path encircles all poles of the integrand. The $n-1$ excitation energies (some of them may be zero or identical) can be read off R by performing $n-1$ horizontal cuts between two subsequent vertices and subtracting the sum of all descending full and wiggly lines from the sum of all ascending ones, where a d-electron energy in an intermediate state is shifted by $+U$, if the other d level is occupied; two d electrons or d holes

in an intermediate state always get the energy $\pm(\epsilon_\uparrow+\epsilon_\downarrow+U)$. Instead of choosing one representative R of each family of diagrams rotated on a cylinder, we can draw all diagrams and assign to the representative diagram the residue at $z=0$ in (3), to the first rotated one the residue at $z=E_1$, etc.

We state our results briefly for a finite-order perturbation expansion of the susceptibility. In second order in V_{kd} we reproduce Scalapino's result [his Eq. (7)] for the free energy, and obtain a slightly different expression for the second-order susceptibility, which is independent of the bandwidth W,

$$\chi^{(2)}=2\beta\mu^2N(0)|V|^2[\epsilon_d^{-1}-(\epsilon_d+U)^{-1}]. \tag{4}$$

While our perturbation technique, in contrast to that in Ref. 4, holds true for all values of ϵ_d, this and all following calculations are valid only for $-\beta\epsilon_d$ and $\beta(\epsilon_d+U)\gg1$, [If, e.g., $|\beta\epsilon_d|\ll1$, one finds free-energy terms proportional to $N(0)|V|^2\ln(\beta W)$, reflecting the anomalously large density of states in the unperturbed system ($V_{kd}\to0$) near the Fermi level, if $\epsilon_d\to0$.]

In fourth order we obtain the first Kondo terms for χ from "small" energy denominators $\epsilon_k-\epsilon_{k'}$ in the "overlapping" diagrams Figs. 1(b) and 1(c) [and in the corresponding diagrams in the family represented by 1(d)]. These, together with the product of the occupation probability $n_{d-\sigma}$ and the statistical factors $1-f_{k\sigma}$ and $f_{k'\sigma}$ expanded up to second order in the magnetic field, lead to $\ln(\beta W)$ terms in the susceptibility. The dominant fourth-order susceptibility contribution, given by Scalapino's result [Eq. (14)], comes from diagrams with singly occupied, "magnetic" initial d states and does not show any peculiarities in the symmetric case (this holds true for any order in V_{kd}). We mention incidentally that in the a priori negligible "nonmagnetic" d-state contributions we find small energy denominators only in the symmetric case which, however, do not lead to Kondo terms.

The concept of looking for diagrams with a magnetic initial d state and a large number of small intermediate-state energy denominators can be used to isolate the leading terms in every order of perturbation theory. In sixth order in V_{kd} we have calculated explicitly all relevant terms and found Scalapino's guess [Eq. (16)] justified with the correct Schrieffer-Wolff value $J=2|V|^2N(0)[\epsilon_d^{-1}-(\epsilon_d+U)^{-1}]$ for the effective s-d coupling. Generally the leading χ contributions turn out to be

$$\chi^{(2n)}=\sum_{m=0}^{n}a_{nm}[\ln(\beta W)]^{n-1}|V|^{2n}\epsilon_d^{m-n}(\epsilon_d+U)^{-m}+\cdots. \tag{5}$$

If we assume a series in $\epsilon_d^{-1}-(\epsilon_d+U)^{-1}$ (in agreement with all references), we can check the coefficient a_{n0} in (4) from the limit $U\to\infty$. Proceeding to the order $|V|^8$, we find the dominant terms given by a very simple set of diagrams with not more than two conduction electrons in an intermediate state. Unfortunately other diagrams (with more than two conduction electrons in the intermediate state) also contain leading logarithmic terms which, however, sum to zero.

Summarizing our results from finite-order perturbation theory, we emphasize two facts: (1) The effective s-d coupling J is the one predicted by the Schrieffer-Wolff transformation,[2] and (2) the logarithmic terms do not disappear in the symmetric case $\epsilon_d+\frac{1}{2}U=0$ in contrast to the result in Ref. 6.

We next sum the infinite series of most divergent diagrams, given in Fig. 2. Based on our calculations in eighth order, we assume that in all orders diagrams which have more than two k electrons in intermediate states contribute only to logarithmic terms two orders lower than the leading ones. The

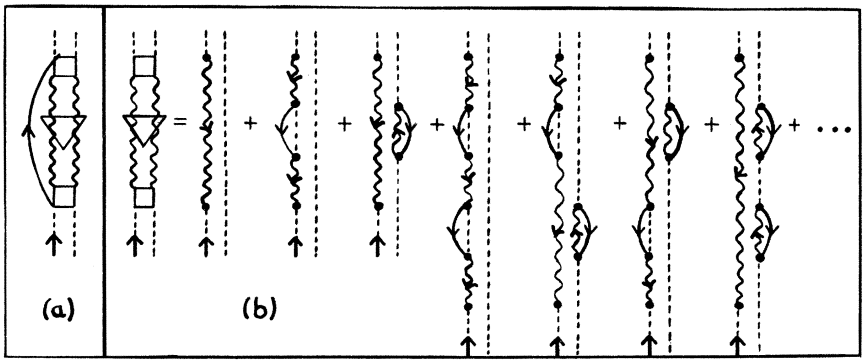

FIG. 2. The infinite diagram summation leading to Eq. (5) shown for $\sigma=\uparrow$ ($d_\uparrow$ level occupied).

zero-field susceptibility from the diagrams in Fig. 2 is given by

$$\chi = 2\beta\mu^2 \sum_k |V_{kd}|^2 \frac{\partial f_k}{\partial \epsilon_k} [\epsilon_k - \epsilon_d - \sum_{k'\sigma'} |V_{k'd}|^2 f_{k'\sigma'} (\epsilon_k - \epsilon_{k'})^{-1}]^{-1}. \quad (6)$$

This is in agreement with the result from various theories for the s-d model.[11] It is tempting to interpret the Kondo term in the denominator in (6) as a strongly temperature-dependent energy renormalization, evaluated in Born's approximation, and to go to higher orders, including the next leading logarithmic terms for $U \to \infty$. We have achieved this by summing diagrams which consist of sequential repetitions of Fig. 2(a) [for the simplest example see Fig. 1(g)] and the corresponding diagrams rotated on a cylinder. We obtain formally the same expression for the susceptibility as above, but with ϵ_k replaced by $\epsilon_k - M(E+\epsilon_k) + M(E)$ and ϵ_d replaced by $\epsilon_d - E$. Here we get $M(E)$, which is a sum of irreducible diagrams, in which an external energy is fed in, from the integral equation

$$M(E) = \sum_k |V_{kd}|^2 (1-f_{k\sigma}) \{E + \epsilon_k - \epsilon_d - \sum_{k'\sigma'} |V_{k'd}|^2 (1-f_{k'\sigma'}) [E + \epsilon_k + \epsilon_{k'} - M(E+\epsilon_k+\epsilon_{k'})]^{-1}\}^{-1}, \quad (7)$$

and E is determined by the self-consistency condition $E = M(E)$. For small ϵ_d, where Schrieffer-Wolff $J = 2|V|^2 N(0) \epsilon_d^{-1}$ diverges, the first iteration of Eq. (7) leads to the simplified self-consistency condition

$$EN(0) = \exp\{-E[|V|^2 N(0)]^{-1}\}. \quad (8)$$

This has a positive solution for E, and thus the new s-d coupling $J' = 2|V|^2 N(0)(\epsilon_d - E)^{-1}$ never diverges, in qualitative agreement with Toulouse and Coqlin.[12]

The authors would like to thank Professor J. R. Schrieffer for helpful discussions.

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*Work supported in part by the National Science Foundation.

†On leave from Institut für Theoretische Physik, Köln, Germany, with a research grant from the Deutsche Forschungsgemeinschaft.

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