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Path-Integral Approach to the Magnetic-Impurity Problem. I

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The Anderson model is treated using a functional-integral technique. A systematic approach is described which does not resort to expansions in the amplitudes of the oscillating components of the random field, nor in the parameters of the model. The first leg of the program, which selects a given temperature interval, is carried out in detail, and the resulting distribution functions and thermodynamic quantities are calculated. The results are discussed and compared with other approaches to the magnetic-impurity problem.

I. INTRODUCTION

Recently, the problem of a single impurity inside a conduction band was vigorously attacked in a series of articles[1-6] using the path-integral method. This method, which was originally introduced by Stratonovich and Hubbard,[7] consists of replacing the electrostatic interaction of two electrons on the impurity with a time-dependent field (or two fields) acting only on the electrons which are on the impurity site. To obtain the exact partition function of the problem, one must carry out a functional average with a Gaussian weight over the auxiliary fields.[1-5]

The above-mentioned replacement is exact, and the one-particle problem in the presence of the time-dependent fields can be formally solved.[1-5] Nevertheless, concrete results have been obtained only in certain approximations. Most of the approximations to date[1-6] have consisted of treating the oscillating part of the field as a small quantity. In this paper we present an approach which treats each Fourier component of the oscillating field exactly to all orders, but approximates interactions between different oscillating components.

To put our contribution in perspective, we review briefly the approximations that have been used in previous work. The simplest approximation is the "static" one.[1-5] Here, the fields are time independent and all thermodynamic quantities can be fully calculated. In this approximation one obtains exact results in two limiting cases: (i) when there is finite electrostatic repulsion U and vanishing width Γ of the impurity level, and (ii) when $U=0$ and $\Gamma>0$.[1-4] The first-order corrections (in Γ/U or U/Γ) to these limits do not agree with the static approximation.

The static approximation to the partition function as a function of the time-independent field ξ_0 (before the Gaussian average) develops maxima at

some $\xi_0 \neq 0$ when

$$y = U/\pi\Gamma \tag{1.1}$$

is greater than y_c. Wang, Evenson, and Schrieffer (WES) find $y_c = \frac{1}{2}$ while Hamman[5] finds $y_c = 1$. When $y > y_c$ the susceptibility χ diverges linearly with $\beta = (k_B T)^{-1}$ as $T \to 0$. This is a serious shortcoming of the static approximation because it is reasonable to have χ finite at $T = 0$.[8] For smaller values of y the partition function is peaked about $\xi_0 = 0$ and the localized impurity enhances the Pauli susceptibility of the band.

A better approximation proposed by WES keeps terms up to second order in the Fourier components of the random field. This approximation, named RPA′, amounts to including small oscillations about the constant field. Such oscillations are stable only for $y < y_c$. As a by-product of RPA′ the susceptibility is obtained correctly to first order in y as $U \to 0$ for fixed Γ.[1,2,6] In Sec. VI we will show that RPA′ overestimates the effects of fluctuations and gives too large a value for the susceptibility.

In order to treat the intermediate coupling region, defined by $\frac{1}{2} < y \lesssim 1$, Schrieffer, Evenson, and Wang[3] included quartic terms in the Fourier components of the random field in their expansion for the free energy for a given field function. They further argued that since the lifetime of an electron in the d state is of the order of $(\beta\Gamma)^{-1}$, one can neglect oscillations in the random field which have frequency higher than $\beta\Gamma$.[3] To calculate the thermodynamic functions, further simplifying approximations were made. The quartic terms were replaced by quadratic ones multiplied by the average of quadratic terms which were then determined self-consistently. The advantage of this approach, which is analogous to a Hartree-Fock treatment, is that the oscillations are stabilized in the intermediate coupling region. Moreover, the zero-temperature susceptibility is finite. However, as one further increases y, the zero-temperature susceptibility decreases as a function of y, which indicates that the approximation is no longer adequate.

For very large values of y (y so large that a well-developed local moment is present) one expects the Anderson model[9] to behave essentially like an s-d model.[10] The susceptibility should exhibit a Kondo effect[11] and flatten out to a finite zero-temperature value.[8] Hamann[5] and Schrieffer *et al.*[3] suggest that in this region it is advantageous to assume that the electron on the impurity probes the instantaneous value of the field. The probability distribution for the instantaneous field is given by the static approximation, i.e., it is local in time. They proceed to insert the time-dependent field, smoothed on a scale $(\beta\Gamma)^{-1}$, into the expression for the static approximation and include quadratic oscillations about it. Hamann showed that this becomes equivalent to Anderson and Yuval's[12] treatment of the Kondo problem.[11]

Keiter[6] analyzed these and other failings of the various approximations in the functional-integral method which uses only one random field.[1-4] His parallel development of the functional approximations and standard perturbation expansion makes some shortcomings apparent. Furthermore, his parallel treatment provides a tool for improving the approximations of Refs. 1–4. In particular, he obtains the first-order correction to χ for large y and derives the logarithmic term,[13] which is of order y^{-2}, after revoking the approximation of a constant level width. On a pessimistic note, Keiter concluded[6] that the amount of effort involved in the renormalization associated with the functional-integral paradigm casts serious doubts as to its advantages over the usual many-body perturbation expansions.

The picture that emerges from the above treatment is not very clear. What may be concluded is that as y increases beyond the value $\frac{1}{2}$, one must include in the partition function anharmonic terms in the random field as well as their dependence on their frequency. Interactions between the various modes of the field also become important.[14] As y becomes greater than 1, the anharmonic terms have to be kept to all orders.

In this paper we present the first part of an effort to avoid expansions in the amplitudes of the field components. We treat the problem of the thermodynamics of the Anderson model using the single random field method.[1-4] For a given value of $\beta\Gamma$ we include field frequencies Ω_ν which satisfy

$$\Omega_\nu = 2\pi\nu \leq \beta\Gamma\,, \tag{1.2}$$

where ν is an integer. We calculate exactly the contribution to the partition function of each of the field amplitudes with these frequencies and either spin projection. This procedure omits interactions between the various modes of the field for a given spin except that all modes interact fully with the zero-frequency mode. The up- and down-spin contributions, when multiplied together, provide the partition function of the localized impurity for the given random field before the Gaussian average is performed. Thus, interactions between the modes of the random field with different spins are included to all orders.

The mathematical formulation of this approach is presented together with the analytical and numerical results for the case $\beta\Gamma \leq 2\pi$ (that is, when only the first oscillating Fourier component of the random field is included). Our results for lower temperatures (that is, larger $\beta\Gamma$) will be described elsewhere.

II. DEFINITION OF NOTATION

We adopt the approach of WES in which the Coulomb repulsion of the electrons on the impurity is replaced by a single random external field, and the energy of the free impurity state is shifted by $\frac{1}{2}U$. The random field

$$\xi(\tau)=\sum_{\nu=-\infty}^{\infty}\xi_\nu e^{i\Omega_\nu\tau} \tag{2.1}$$

is defined in the interval $0\le\tau\le 1$ and the frequencies Ω_ν are defined in Eq. (1.2). In terms of complex field amplitudes ξ_ν, the partition function for the system is given by WES as

$$Z=\int_{-\infty}^{\infty}d\xi_0\prod_{\nu>0}2\int d^2\xi_\nu\exp\left[-\pi\sum_{\nu'=-\infty}^{\infty}|\xi_{\nu'}|^2+\sum_\sigma \mathrm{Tr}\ln(1-K^\sigma)\right]Z_0(\xi_0). \tag{2.2}$$

In the above equation we have

$$Z_0(\xi_0)=Z^0Z_0'(\xi_0)\ . \tag{2.3}$$

Z^0, the partition function for the Anderson model with no Coulomb interaction term and with the impurity levels shifted by $\frac{1}{2}U$, is given by

$$Z^0=\mathrm{Tr}e^{-\beta(\bar H_0+H_v)}\ , \tag{2.4}$$

where

$$\bar H_0=\sum_{k,\sigma}\epsilon_{k\sigma}n_{k\sigma}+\sum_\sigma(\epsilon_{d\sigma}+\tfrac{1}{2}U)n_{d\sigma} \tag{2.5}$$

and

$$H_v=\sum_{k,\sigma}(V_kc_{k\sigma}^\dagger c_{d\sigma}+V_k^*c_{d\sigma}^\dagger c_{k\sigma})\ , \tag{2.6}$$

where $\epsilon_{k,\sigma}$ and $\epsilon_{d\sigma}$ are the energies of an electron in the band and on the impurity with spin projection $\sigma=\pm1$, respectively. $c_{k\sigma}^\dagger$, $c_{k\sigma}$, $c_{d\sigma}^\dagger$, and $c_{d\sigma}$ are, respectively, the creation and destruction operators of electrons with spin projection σ in the band and in the localized d state. U, the strength of the Coulomb interaction, is the coefficient in the term

$$H_U=Un_dn_d\ , \tag{2.7}$$

where $n=c^\dagger c$.

$Z_0'(\xi_0)$ is the correction to Z^0 due to a time-independent external magnetic field $C\xi_0$ which acts only on the d electron. ξ_0 is just the zero-frequency Fourier component of $\xi(\tau)$ in Eq. (2.1) and

$$C^2=2\pi\beta U. \tag{2.8}$$

WES termed $Z_0(\xi_0)$ the static approximation and wrote

$$Z_0'(\xi_0)=\exp\left(\sum_{n,\sigma}\ln(1+\sigma CG_n^\sigma)\right)\ , \tag{2.9}$$

in which G_n^σ is the Fourier component of the two-time d-d Green's function belonging to the Hamiltonian $\bar H_0+H_V$. In the "wide-band" approximation we have

$$G_n^\sigma=(i\omega_n-\beta\bar\epsilon_{d\sigma}+i\beta\Gamma\,\mathrm{sgn}\omega_n)^{-1}\ , \tag{2.10}$$

where

$$\omega_n=(2n+1)i\pi\ ,\quad n=0,\ \pm1,\ \pm2,\ \ldots \tag{2.11}$$

and Γ is the width of the virtual d state. Note that the Green's function is diagonal in Fourier space. With G_n^σ given by Eq. (2.10), Z_0' can be evaluated and is found to be

$$Z_0'(\xi_0)\equiv\prod_\sigma\left(\frac{\beta\Gamma}{2\pi}+\frac{1}{2}+\frac{\beta\bar\epsilon_d}{2\pi}i\ ,\ \frac{\beta\Gamma}{2\pi}+\frac{1}{2}-\frac{\beta\bar\epsilon_d}{2\pi}i\right)\left[B\left(\frac{\beta\Gamma}{2\pi}+\frac{1}{2}+\frac{\beta\bar\epsilon_{d\sigma}-\sigma C\xi}{2\pi}i\ ,\ \frac{\beta\Gamma}{2\pi}+\frac{1}{2}-\frac{\beta\bar\epsilon_{d\sigma}-\sigma C\xi}{2\pi}i\right)\right]^{-1}\ . \tag{2.12}$$

B is the Eulerain integral of the first kind.[15]

A special case that is most often considered is the symmetric case, where

$$\bar\epsilon_{d\sigma}=\epsilon_d+\tfrac{1}{2}U=0\ . \tag{2.13}$$

Under this condition the asymptotic behavior of Z_0' as $\beta\Gamma\to\infty$ was shown by WES to be

$$\ln Z_0'(\xi_0)\sim\left(\frac{2C\xi_0}{\pi}\right)\tan^{-1}\left(\frac{C\xi_0}{\beta\Gamma}\right)-\left(\frac{\beta\Gamma}{\pi}\right)\ln\left[1+\left(\frac{C\xi_0}{\beta\Gamma}\right)^2\right]. \tag{2.14}$$

Returning to Eq. (2.2) we note that the matrix elements of $1-K^\sigma$ are given by

$$1-K_{m,n}^\sigma\begin{cases}=\sigma C\xi_{m-n}G_n^{0\sigma}\ , & m\neq n\\ =1, & m=n\end{cases} \tag{2.15}$$

where $G_n^{0\sigma}$ is the d Green's function for $\bar H_0+H_V$ in the symmetric case; in the presence of a magnetic field $C\xi_0$

$$G_n^{0\sigma}=(i\omega_n+\sigma C\xi_0+i\beta\Gamma\,\mathrm{sgn}\omega_n)^{-1}\ . \tag{2.16}$$

III. STATEMENT OF GENERAL APPROXIMATION

The quantity that has to be approximated is

$$\exp[\mathrm{Tr}\ln(1-K^\sigma)]\ . \tag{3.1}$$

In order to develop the approximation, this quantity is expressed as an infinite determinant using the

identity

$$\exp[\mathrm{Tr}\ln(1-K^\sigma)]=\mathrm{Det}(1-K^\sigma)\equiv D^\sigma\ . \tag{3.2}$$

The static approximation consists of keeping only the diagonal, i.e., in the static approximation

$$D^\sigma=1\ . \tag{3.3}$$

With some effort, it can be shown that as $\Gamma\to 0$, $D^\sigma\to 1$. It is obvious that as U or C vanishes $D^\sigma\to 1$ because in this case all off-diagonal elements are zero.

In the matrix D^σ [16] every diagonal is proportional to one Fourier component of the field ξ [see Eq. (2.15)]. Specifically, the diagonal which is ν diagonals above the main one is proportional to ξ_ν. No other diagonal depends on ξ_ν although there is one diagonal below the main one which is proportional to

$$\xi_{-\nu}=\xi_\nu^*\ . \tag{3.4}$$

Equation (3.4) states the reality of the field.

The determinant D^σ is expressed as the limit of a $(2N+2)$-dimensional determinant D_N^σ:

$$D^\sigma=\lim_{N\to\infty}D_N^\sigma\ . \tag{3.5}$$

For a given value of $\beta\Gamma$ we define M (an integer) by

$$2\pi(M-1)<\beta\Gamma\le 2\pi M\ , \tag{3.6}$$

and set

$$\xi_\nu=0\quad\text{for}\quad|\nu|>M\ . \tag{3.7}$$

In other words, we assume that oscillations of the field with frequency which is greater than the inverse "time" that an electron spends on the impurity are unimportant. This assumption, which we feel is a rather safe one, is similar to the one made by Schrieffer *et al.*[3] D_N^σ, for $N>M$, becomes a matrix with M nonzero diagonals above and below the main diagonal. We denote it by $D_N^\sigma(M)$, where

$$D^\sigma(M)\equiv\lim_{N\to\infty}D_N^\sigma(M)\ . \tag{3.8}$$

The elements along the main diagonal are 1.

Our main approximation consists of disentangling the various modes of the field from each other. This is done by writing $D_N^\sigma(M)$ as a sum of M terms, each of which involves only one ξ_ν:

$$D_N^\sigma(M)\approx 1+\sum_{j=1}^{M}[d_N(j)-1]\ , \tag{3.9}$$

where $d_n(j)$ is a determinant whose elements are given by Eq. (2.15) with the restriction (3.6), except that

$$\xi_\nu=0\quad\text{for}\quad|\nu|\neq j\ . \tag{3.10}$$

Thus, $d_N(j)$ is a tridiagonal determinant with a principal diagonal of ones and one diagonal j removed above it and one j removed below it. Our approximation to $D^\sigma(M)$ is then

$$D^\sigma(M)=1+\sum_{j=1}^{M}(d_j-1) \tag{3.11}$$

and

$$d_j=\lim_{N\to\infty}d_N(j)\ . \tag{3.12}$$

Before concluding this section the following comments on the approximation are in order: (i) Every term that appears on the right-hand side of Eq. (3.11) appears once, and only once, in $D_N^\sigma(M)$. (ii) All terms in $D_N^\sigma(M)$ which involve only one amplitude $\xi_\nu(\nu\neq 0)$ and its complex conjugate $\xi_{-\nu}$ are included in our approximations. (iii) Each one of the terms in the sum in Eq. (3.9) vanishes as $\Gamma\to 0$ or $U\to 0$.

IV. EXACT EVALUATION OF $D^\sigma(1)$

At this point we specialize in the case $M=1$. According to the discussion following Eq. (3.7), one expects the results of this approximation to give a good description as long as $\beta\Gamma\le 2\pi$. From Eq. (3.11) we have

$$D^\sigma(1)=d_1=\lim_{N\to\infty}d_N(1). \tag{4.1}$$

The evaluation of d_1 will be described in detail because it will be the cornerstone for the extensions of the present theory to $M>1$. These extensions will be described in a subsequent paper.

The calculation of $d_N(1)$ is difficult because $i\beta\Gamma$ (in the denominators of the off-diagonal terms) changes sign when ω_n changes sign. Thus, we start by expressing $d_N(1)$ in terms of subdeterminants for each sign of $i\beta\Gamma$. We write

$$d_N(1)=|B_N|^2-\frac{C^2|\xi_1|^2}{|i\pi-\sigma C\xi_0+i\beta\Gamma|^2}\,|\tilde{B}_N|^2\ . \tag{4.2}$$

That is, we expand $d_N(1)$ about its central two rows. B_N and $\tilde{B}_N$ are subdeterminants whose elements are given by Eq. (2.15) with the restrictions that $0\le m$ and $n\le N$, respectively. In addition, of course, $\xi_\nu=0$ for $|\nu|>1$.

From the definition of B_N and $\tilde{B}_N$ it follows that

$$\tilde{B}_{N+1}(\sigma C\xi_0)=B_N(\sigma C\xi_0-2\pi i)\ . \tag{4.3}$$

Expanding B_N about its first and second rows gives a second-order difference equation for B_N

$$B_N=B_{N-1}+\frac{C^2|\xi_1|^2}{4\pi^2(A_\sigma+N)(A_\sigma+N+1)}B_{N-2}\ , \tag{4.4}$$

and boundary conditions

$$B_0=1, \tag{4.5}$$

$$B_1 = 1 + \frac{C^2 |\xi_1|^2}{4\pi^2(A_\sigma+1)(A_\sigma+2)} , \tag{4.6}$$

where, in the symmetric case,

$$A_\sigma = -\tfrac{1}{2} + \tfrac{1}{2}\delta - i\sigma C\xi_0/2\pi , \tag{4.7}$$

$$\delta = \beta\Gamma/\pi . \tag{4.8}$$

As is shown in Appendix A, repeated iteration of Eq. (4.4) leads to

$$\lim_{N\to\infty} B_N = \Gamma(A_\sigma+1)\left(\frac{iC|\xi_1|}{2\pi}\right)^{-A_\sigma} J_{A_\sigma}\left(\frac{iC|\xi_1|}{\pi}\right) , \tag{4.9}$$

where J is a Bessel function.

Finally, inserting Eq. (4.2) in (4.1) and using Eqs. (4.3) and (4.9) we find

$$D^\sigma(1) = |\Gamma(A_\sigma+1)|^2\left(\frac{iC\xi_1}{2\pi}\right)^{1-\delta}\left[J_{A_\sigma}\left(\frac{iC|\xi_1|}{\pi}\right)J_{A_\sigma}^*\left(\frac{iC|\xi_1|}{\pi}\right) J + J_{A_\sigma+1}\left(\frac{iC|\xi_1|}{\pi}\right) J_{A_\sigma+1}^*\left(\frac{iC|\xi_1|}{\pi}\right)\right] . \tag{4.10}$$

Equation (4.10) is exact and has the following properties:

$$D^\sigma(1) = [D^\sigma(1)]^* , \tag{4.11}$$

$$D^\dagger(1) = D^\dagger(1) = D(1) , \tag{4.12}$$

$$\lim_{\xi_1\to 0} D(1) = 1 . \tag{4.13}$$

V. PARTITION FUNCTION

In the present approximation the result (4.10) provides us with the partition function. Since $Z_0(\xi_0)$ and $e^{\sum_\sigma \mathrm{Tr}(1-K^\sigma)}$ in Eq. (2.2) depend on ξ_0 and $|\xi_1|$ only, the integration over the Gaussian weights for all other Fourier components can be carried out. Since they all integrate to unity, we have

$$Z = 4\pi \int_{-\infty}^{\infty} d\xi_0 \int_0^\infty \xi_1\, d\xi_1\, e^{-\pi\xi_0^2 - 2\pi\xi_1^2} Z_0(\xi_0)[D(1)]^2 , \tag{5.1}$$

where ξ_1 stands for the absolute value of ξ_1. In the nonsymmetric case, $\epsilon_d + \frac{1}{2}U \neq 0$, and $[D(1)]^2$ should be replaced by $D^\dagger(1)\cdot D^\dagger(1)$.

Two quantities are now of interest. The first is the probability distribution of various field amplitudes for different values of the parameters y and $\delta = \beta\Gamma/\pi$. For a selected set of pairs (y, δ) we plot in Figs. 1–4 the ratio of the integrand as a function of ξ_1 to its value at $\xi_1 = 0$ for several values of ξ_0.

In order to plot these curves, we use a rapidly convergent series representation for $D(1)$, which we derive in Appendix B, as follows:

$$D(1) = |\Gamma(A_\sigma+1)|^2\,\delta \times \sum_{k=0}^{\infty} \frac{\Gamma(\delta+2k)}{k!\,\Gamma(\delta+k+1)\Gamma(A_\sigma+k+1)}\left(\frac{C\xi_1}{2\pi}\right)^{2k} . \tag{5.2}$$

The second quantity of interest is the distribution of ξ_0 after the Gaussian average over ξ_1 has been carried out. As shown in Appendix C, this can be written as

$$\frac{Z}{Z^0} = \delta^2 \int_{-\infty}^{\infty} d\xi_0\, e^{-\pi\xi_0^2} \sum_{m=0}^{\infty}\left(\frac{C^2}{8\pi^3}\right)^m \sum_{p=0}^{m}\binom{m}{p} \times \frac{\Gamma(\delta+2p)\Gamma(\delta+2m-2p)}{\Gamma(\delta+p+1)\Gamma(\delta+m-p+1)} \times \frac{\Gamma[(\delta+1)/2]^4}{|\Gamma(A_\sigma+1+p)|^2\,|\Gamma(A_\sigma+1+m-p)|^2} \equiv \int_{-\infty}^{\infty} d\xi_0\, Z_1(\xi_0) , \tag{5.3}$$

where Z^0 is defined in Eq. (2.3). Setting $\epsilon_{d\sigma} = 0$ in Eq. (2.12) one finds that $Z_0'(\xi_0)$ is just the $m = p = 0$ term of the double sum in Eq. (5.3).

In Figs. 5–8 we plot $\log Z_1(\xi_0)$ as a function of ξ_0 for a set of values of y and δ. For comparison, on each figure we also plot the static approximation result. [Note that the curve for the static approximation vanishes exactly at $\xi_0 = 0$ as a consequence of Eq. (2.12). However, $\log Z_1(0)$ is a nonvanishing function of the parameters y and δ. To aid in the above comparison, we have shifted the value of $\log Z_1(0)$ on Figs. 5–8 so that $\log Z_1(0)$ also vanishes.]

A general characteristic of the approximation is that for small values of $y = U/\pi\Gamma$ the first term in

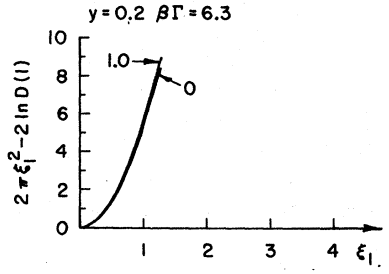

FIG. 1. Logarithm of the distribution of ξ_1 vs ξ_1 [see Eq. (5.1)]. The numbers marking the curves are the values of $\pi\xi_0/C$.

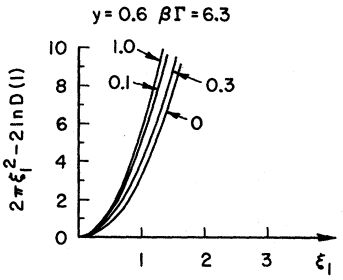

FIG. 2. Logarithm of the distribution of ξ_1 vs ξ_1 [see Eq. (5.1)]. The numbers marking the curves are the values of $\pi\xi_0/C$.

the series representing Z_1 is dominant. Hence, the results are essentially the same as in the static approximation.

As y increases beyond $y=\frac{1}{2}$ the static approximation develops maxima at values of $\xi_0 \neq 0$. The positions of these maxima tend to the limit $\pm\frac{1}{2}C\pi$ as $y\to\infty$. Furthermore, the RPA′ corrections to the static approximation become unstable. The RPA′ corresponds in the present approach to the replacement

$$D(1) \to \exp\{(\delta/2)[(\pi\delta+\pi)^2+(C\xi_0)^2]^{-1}(C\xi_1)^2\}\,, \tag{5.4}$$

the exponential of the ratio of the first two terms. For small ξ_0 and large y this approximation to $D(1)$ diverges like $e^{a\xi_1^2}$, where a is arbitrarily large. In fact, $D(1)$ in Eq. (5.2) is an entire function of ξ_1 which diverges as $\xi_1\to\infty$ slower than $e^{a\xi_1^2}$ for any a. [$D(1)$ behaves asymptotically like $e^{b\xi_1}$ for some b.]

As can be seen from Fig. 4, for $y>\frac{1}{2}$ and $\xi_0\approx 0$, the function $-2\pi\xi_1^2+2\ln D(1)$ does tend to increase for small ξ_1, where its behavior is the same as in the RPA′. However, as ξ_1 increases on the scale of $C/2\pi$ this increase is rapidly quelled by the decrease of the term $-2\pi\xi_1^2$. For larger ξ_0, even the small ξ_1 increase disappears, as can be seen from Eq. (5.4).

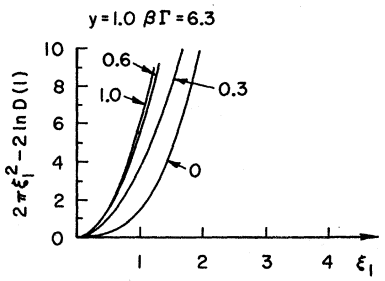

FIG. 3. Logarithm of the distribution of ξ_1 vs ξ_1 [see Eq. (5.1)]. The numbers marking the curves are the values of $\pi\xi_0/C$.

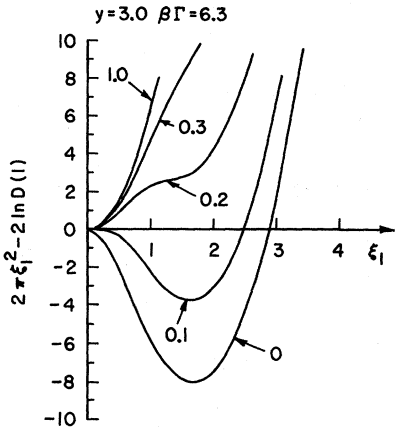

FIG. 4. Logarithm of the distribution of ξ_1 vs ξ_1 [see Eq. (5.1)]. The numbers marking the curves are the values of $\pi\xi_0/C$.

As far as $Z_1(\xi_0)$, which is defined in Eq. (5.3), we find that the inclusion of ξ_1 weakens the symmetry breaking. Specifically, for a given y, the maxima in Z_1 appear at higher values of $\beta\Gamma$ or at lower temperatures. These maxima are less pronounced than in the static approximation. This is quite an important feature since, as we show in Sec. VI, it brings about a reduction and possible leveling off of the static local susceptibility.

The RPA′ expression for $Z_1(\xi_0)$ amounts to factorization of the term with $m=p=0$ in Eq. (5.3) (which is just the static approximation) and a replacement of the infinite series multiplying it by a geometric series with a quotient equal to the ratio of the first two terms.

VI. SUSCEPTIBILITY AND ENTROPY

It was shown by Schrieffer *et al.*[3] that the in-

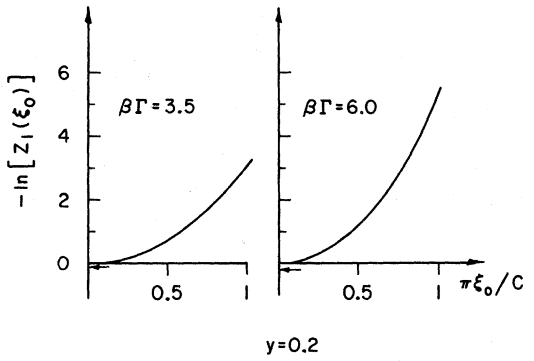

FIG. 5. Logarithm of the distribution of ξ_0 vs ξ_0 [see Eq. (5.3)]. The solid curve represents the static approximation, the dashed curve represents the present calculation. (In this figure the two curves are overlapping.) The arrow represents the position of $-\ln[Z_1(0)]$ for the dashed curve.

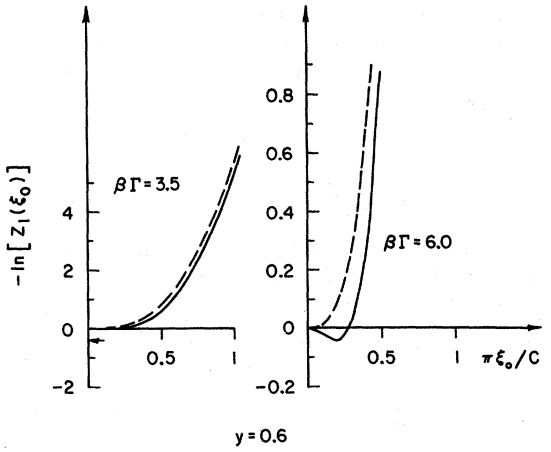

FIG. 6. Logarithm of the distribution of ξ_0 vs ξ_0 [see Eq. (5.3)]. The solid curve represents the static approximation, the dashed curve represents the present calculation. The arrow represents the position of $-\ln[Z_1(0)]$ for the dashed curve.

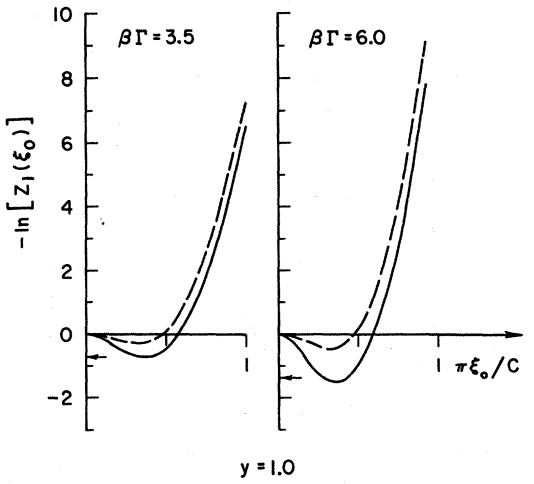

FIG. 8. Logarithm of the distribution of ξ_0 vs ξ_0 [see Eq. (5.3)]. The solid curve represents the static approximation, the dashed curve represents the present calculation. The arrow represents the position of $-\ln[Z_1(0)]$ for the dashed curve.

clusion of a local external magnetic field, which varies in time according to

$$h(t) = h_\nu e^{i\Omega_\nu t} + h_{-\nu} e^{-i\Omega_\nu t}, \tag{6.1}$$

with $0 \le t \le 1$ and $h_{-\nu} = h_\nu^*$ leads to a partition function which is identical in form to Eq. (2.2); however, there is the exception of

$$C\xi_\nu \to C\xi_\nu + \beta\mu_B h_\nu \tag{6.2}$$

in K and $Z_0(\xi_0)$. The Gaussian weights are not affected. The corresponding local susceptibility can then, by a change of integration variable, be shown to be[4]

$$\chi_{1oc}(\nu) = \frac{\mu_B^2}{U}\,(2\pi < |\,\xi_\nu\,|^2 > - 1)\,, \tag{6.3}$$

where μ_B is the magnetic moment of the electron on the impurity and $\langle\,|\,\xi_\nu\,|^2\,\rangle$ is the average of $|\,\xi_\nu\,|^2$ using the integrand in Eq. (2.2) as a weight after normalization.

We are concerned here with the static susceptibility $\chi_{1oc}(0)$. WES showed that $\chi_{1oc}(0)$ is just the excess susceptibility due to the localized impurity over and above the susceptibility of the band when a uniform static field is applied to the system.

In Fig. 9 we plot $\Delta\chi_s = \chi_{1oc}(0)\ \Gamma/\mu_B^2$ as a function of $\beta\Gamma$ for various values of y. The static approximation is included for comparison. The values of the temperature are limited to $\beta\Gamma \le 2\pi$ (see Sec. IV). The arrow next to each curve indicates the point at which $\beta U = 2\pi$.

In this temperature interval and for small values of $y \le 0.2$ the susceptibility is essentially indistinguishable from that calculated in the static approximation. The relatively large increase in χ in RPA[17] is due to the slow decrease of the distribution function as a function of ξ_1 for large ξ_1. This behavior brings about a very slow decrease of the distribution function as a function of ξ_0 for large ξ_0 (see, e.g., Sec. V). The quartic approximation has the opposite effect. Due to the rapid decrease of the distribution function for large ξ_ν (as $e^{-a|\xi_\nu|^4}$) large values of ξ_ν and, consequently, of ξ_0 are too severely repressed. This brings

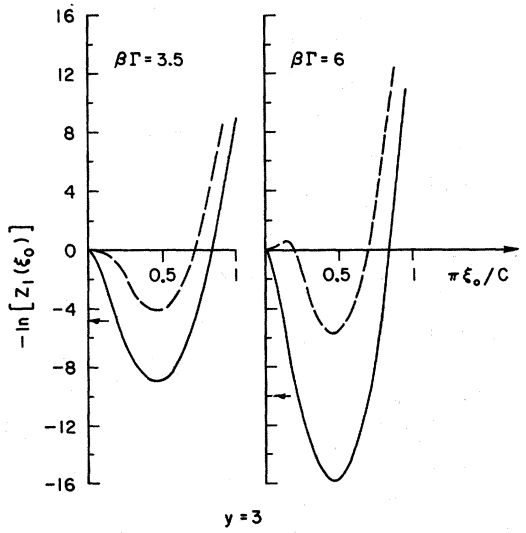

FIG. 7. Logarithm of the distribution of ξ_0 vs ξ_0 [see Eq. (5.3)]. The solid curve represents the static approximation, the dashed curve represents the present calculation. The arrow represents the position of $-\ln[Z_1(0)]$ for the dashed curve.

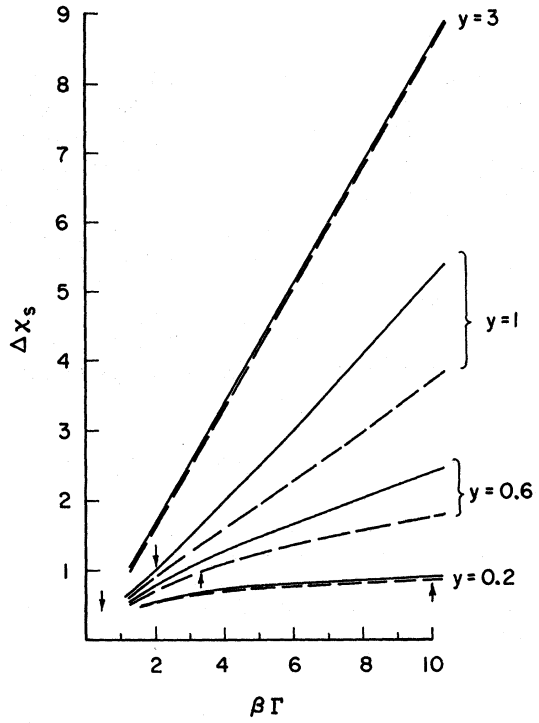

FIG. 9. Excess susceptibility due to the impurity vs $\beta\Gamma$. Solid curves represent the static approximation. Dashed curves represent the present calculation. The arrow next to each pair of susceptibility curves marks the value of $\beta\Gamma$ for which $\beta U = 2\pi$.

about a decrease in the second moments of the distribution and, in turn, of the susceptibility [see Eq. (6.3)]. The present calculation suggests that the distribution function behaves asymptotically like $e^{a|\xi_\nu|}$. This conjecture is corroborated by the static approximation and by the extensions of the present approximation to higher ν's.[18]

For greater values of y, namely for $0.5 \le y \le 1$, $\Delta\chi_s$ tends to saturate in the temperature interval $\beta\Gamma \le 2\pi$. If the present approximation is extended to temperatures much lower than $2\pi/\Gamma$, $\Delta\chi_s$ increases rapidly and eventually approaches the static approximation to $\Delta\chi_s$. However, such an extension would be unwarranted according to the discussion in Sec. IV. In order to obtain reliable results in the next temperature interval, which is

$$2\pi \le \beta\Gamma \le 4\pi\,, \tag{6.4}$$

ξ_2 must be included in the calculation.

As y increases far beyond one (such as $y = 3$ in Fig. 9), $\Delta\chi_s$ behaves linearly with $\beta\Gamma$ in the interval $\beta\Gamma \le 2\pi$. The slope becomes closer and closer to that of $\Delta\chi_s$ which was calculated in the static approximation. This behavior is quite reasonable. As $y \to \infty$ the value of $\Delta\chi_s$ at $T = 0$ increases to infinity. Hence, the saturation of $\Delta\chi_s$ takes place at higher and higher values as y increases. Since the slope of $\Delta\chi_s$, as a function of $\beta\Gamma$, is bounded by its free-spin value, which is unity in the variable of Fig. 9, saturation must occur at lower temperatures.

In Fig. 10, we plot the excess free energy due to the impurity

$$\Delta F = (\beta\Gamma)^{-1} \ln(Z/Z^0) \tag{6.5}$$

as a function of $\beta\Gamma$ for various values of y. The value of ΔF evaluated in the static approximation is included for comparison. The excess entropy is then given simply in terms of ΔF by the following:

$$\Delta S = \left(\frac{\partial \Delta F}{\partial T}\right)_{\mu,\Omega} \tag{6.6}$$

where μ is the chemical potential and Ω is the volume.

ΔF and ΔS are contributions to the total free energy and to the total entropy of order unity. The conduction band contributes a quantity of order N, the number of electrons in the band. Thus, the smooth behavior of ΔF as a function of temperature (Fig. 10) implies that the localized impurity has a negligible effect on the total entropy and hence, on the specific heat of the system. This is to be contrasted with the case of the susceptibility which varies rather rapidly with the temperature for large values of y.

VII. DISCUSSION

Much is still to be desired from the approach presented in this paper. We list below some of

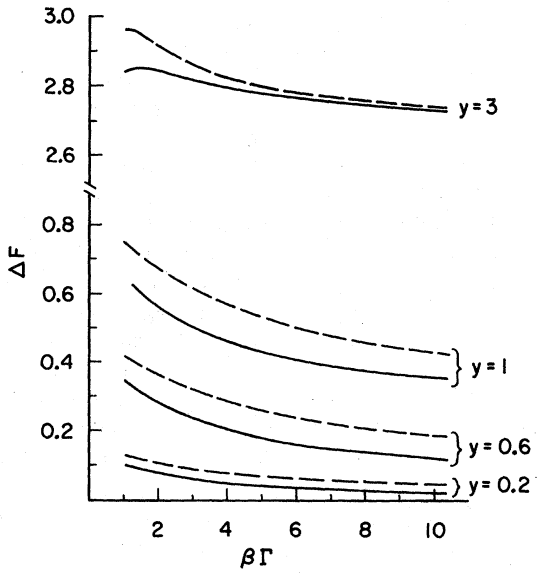

FIG. 10. Excess free energy due to the impurity vs $\beta\Gamma$ [see Eq. (6.1)].

the obvious needs and we discuss them in relation to other approaches.

One has yet to determine the nature of the terms which are preserved in the approximation out of the totality of terms in the full expansion of $Z(\xi)$ in a series in ξ_ν. Such an expansion was performed by Keiter.[6] A criterion which justifies the selection of the particular set of terms treated above is clearly missing. However, we feel that neither the RPA′ nor the quartic approximation provide a good criterion for this selection, except in the extreme limits of very small or very large y. As Keiter[6] pointed out, the usual argument of cancellations due to random phases does not apply in the case of a localized impurity. We feel that the asymptotic behavior of our approximation, namely, $Z(\xi)$ diverges like $\exp(a_\nu | \xi_\nu |)$, speaks strongly in favor of the present choice. This behavior persists when field amplitudes with $\nu > 1$ are included.[18] It should be contrasted with the attempts of Herz[14] to renormalize the coefficients of the $| \xi_\nu |^2$ for low values of ν by integrating over higher-order terms in ξ_ν for higher values of ν.

Irrespective of the outcome of the investigation proposed above, one can ask whether there is, within the present approach, a saturation of $\Delta\chi_s$ at low temperature and whether a Kondo-type logarithmic dependence on temperature appears for large y. Since in the above we limited ourselves to $\nu \leq 1$ we cannot pursue the calculation of $\Delta\chi_s$ to low enough temperatures to answer these questions. We are presently analyzing the effect of including Fourier components of the field with $\nu > 1$ on the various thermodynamic quantities.

An important attraction of the scheme proposed here is that, as in the static approximation,[1-4] one obtains a systematic calculation in the whole continuous range of parameters. If one is to accept Keiter's conclusions[6] then this possibility has to be abandoned, as it was before the introduction of the functional integral method by WES. In such a case, the most reasonable approach would be that of Mattis[19] who considers the Anderson model with a finite number of shells of atoms around the impurity. This problem can be solved, as a linear chain, to any desired accuracy. With four shells, Mattis obtains convergence of the thermodynamic quantities as a function of the size of the system. The only drawback of such an approach is that the Anderson model for a single impurity is just the first step in understanding conducting magnets which show localized moment behavior. The Hartree-Fock[20] and functional-integral[3] methods are easily generalizable to the two-center problem. The identifications made in the one-center problem are helpful for gaining insight into the more complicated multicenter problems. Mattis's approach does not have this virtue.

ACKNOWLEDGMENTS

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APPENDIX A

To derive Eq. (4.9) from Eqs. (4.4)–(4.6) we write

$$B_\infty = \lim_{N\to\infty} B_N = 1 + \sum_{n=0}^{\infty} (B_n - B_{n-1}) , \tag{A1}$$

where we have used the difference equation to extend the sequence of B's to

$$B_{-1} = 1 . \tag{A2}$$

The sequence further extends to

$$B_{-2} = 0 . \tag{A3}$$

Inserting Eq. (4.4) into the right-hand side of Eq. (A1) and using (A2) and (A3) gives

$$\begin{aligned} B_\infty &= 1 + \sum_{n=1}^{\infty} \frac{K^2}{(A+n)(A+n+1)} B_{n-2} \\ &= 1 + \sum_{n=1}^{\infty} K^2 \left(\frac{1}{A+n} - \frac{1}{A+n+1} \right) B_{n-2} \\ &= 1 + \frac{K^2}{A+1} + K^2 \sum_{n=0}^{\infty} \frac{1}{A+n+2} (B_n - B_{n-1}) , \end{aligned} \tag{A4}$$

where $K^2 = C^2 | \xi_1 |^2 / 4\pi^2$. Once again $B_n - B_{n-1}$ is substituted from Eq. (4.4), the coefficient written as the difference of two partial fractions, and one more term separates from the sum. Iterating this procedure gives

$$B_\infty = \sum_{j=0}^{\infty} \frac{K^{2j}}{j!(A+1)(A+2)\cdots(A+j+1)} . \tag{A5}$$

Equation (A5) is identified[21] as

$$B_\infty = \Gamma(A+1)(iK)^{-A} J_A(2iK) , \tag{A6}$$

which is just Eq. (4.9).

APPENDIX B

The integral representation for the product of two Bessel functions[22] implies that

$$R = J_A(Z) J_A^*(Z) + J_{A+1}(Z) J_{A+1}^*(Z)$$

$$= \frac{2}{\pi} \int_0^{\pi/2} [J_{A+A^*}(2Z\cos\theta)$$

$$+ J_{A+A^*+2}(2Z\cos\theta)]\cos[(A-A^*)\theta]d\theta \ . \qquad \text{(B1)}$$

From Eq. (4.7) one has

$$A_\sigma + A_\sigma^* = \delta - 1 \ , \qquad \text{(B2)}$$

$$A_\sigma - A_\sigma^* = -i\sigma C\xi_0/\pi \ . \qquad \text{(B3)}$$

Inserting (B2) and (B3) in (B1) gives

$$R = \frac{2}{\pi} \int_0^{\pi/2} [J_{\delta-1}(2Z\cos\theta) + J_{\delta+1}(2Z\cos\theta)]$$

$$\times \cosh\left(\frac{\sigma C\xi_0}{\pi}\,\theta\right) d\theta \qquad \text{(B4)}$$

$$= \frac{2\delta}{\pi Z} \int_0^{\pi/2} J_\delta(2Z\cos\theta)\, \frac{\cosh(\sigma C\xi_0\theta/\pi)}{\cosh\theta}\, d\theta \ , \qquad \text{(B5)}$$

where the recursion relation for Bessel functions[23] was used. Finally, the series expansion for J_δ is substituted into (B5). Performing the integral over θ term by term leads to Eq. (5.2).

APPENDIX C

When $D(1)$, in Eq. (5.2), is inserted into Eq. (5.1) and the Gaussian average over ξ_1 is performed term by term one obtains

$$\frac{Z}{Z^0} = \int_{-\infty}^{\infty} d\xi_0\, e^{-\pi\xi_0^2} Z_0'(\xi_0) \,|\, \Gamma(A_\sigma + 1) \,|^4 \delta^2$$

$$\times \sum_{k,l=0}^{\infty} \binom{k+l}{k} \frac{\Gamma(\delta+2k)\Gamma(\delta+2l)}{\Gamma(\delta+k+1)\Gamma(\delta+l+1)}$$

$$\times \frac{1}{|\Gamma(A_\sigma+1+k)|^2\, |\,\Gamma(A_\sigma+1+l)\,|^2} \left(\frac{C^2}{8\pi^3}\right)^{k+l} \ , \qquad \text{(C1)}$$

where we have used the formula

$$\int_0^\infty \xi^{2s+1} e^{-2\pi\xi^2} d\xi = \tfrac{1}{2}(2\pi)^{-s-1}\,\Gamma(s+1) \ . \qquad \text{(C2)}$$

Transforming the summation indices in Eq. (C1) according to

$$k + l = m \ , \quad k = p \ , \qquad \text{(C3)}$$

and inserting $Z_0'(\xi_0)$ from Eq. (2.12) in the symmetric case leads to Eq. (5.3).

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[23]See Ref. 16, Sec. 3.2.