Low-temperature properties of the Kondo Hamiltonian

V. J. Emery*
Brookhaven National Laboratory, Upton, New York 11973
and Nordita, Copenhagen, Denmark†

A. Luther*
Lyman Laboratory, Harvard University, Cambridge, Massachusetts 02138
(Received 5 May 1972)

The equilibrium properties of a magnetic impurity in a metal are discussed in the long-time approximation introduced by Nozières and de Dominicis for the x-ray threshold problem. It is shown that the free energy satisfies an exact homogeneity condition, from which it is possible to display explicitly the structure of the singularities of perturbation theory in the exchange coupling J as the magnetic field $H \to 0$ and the temperature $T \to 0$. The nature of the Kondo problem is made clear and it is shown that, for antiferromagnetic coupling, when $H = 0$ and $T = 0$, physical properties are expected to be nonanalytic functions of J. To resolve those problems, the partition function is first shown to be exactly the same as that of a spin-1/2 interacting with a certain boson field. The ground-state properties are then studied by finding a new division of the spin-boson Hamiltonian into two parts, such that perturbation theory is finite term by term. For antiferromagnetic coupling, the moment vanishes at $T = 0$ and for weak ferromagnetic coupling, the free moment is only slightly renormalized. The partition function is also shown to be equivalent to that of an unusual one-dimensional Ising model. For $T \neq 0$, the free energy is intensive. For $T = 0$, the free energy is extensive and the interaction follows an inverse-square law at large distances but is infinitely strong for neighboring spins. The method of solving the spin-boson problem is worked out explicitly for the Ising model and in this way extended to finite temperatures.

I. INTRODUCTION

This paper is concerned with equilibrium properties of magnetic impurities in metals at low temperatures. For low concentrations, it is sufficient to study the properties of a single impurity, and the discussion will be based upon the Kondo Hamiltonian,[1] although the conclusions may also be applied to the Anderson model,[1] by changing the interpretation of constants. It is well known[1] that the characteristic difficulty of this Hamiltonian stems from the fact that, for derivatives of the free energy, perturbation theory in the coupling between the impurity and the electrons diverges term by term as the magnetic field H and the temperature T tend to zero. The problem is to find a divergence-free theory from which the limiting behavior may be obtained. Many elegant partial-summation schemes have been applied to this problem,[1] but they omit some singularities and the results are suspect at low temperatures. Our approach is to work with a scheme which aims to include all singularities, so that their structure may be studied in a general way. We shall show that this scheme is equivalent to the use of a simplified Hamiltonian for which it is possible to construct a new form of perturbation theory with every term finite.

The starting point will be the series for the partition function Z derived from the Kondo Hamiltonian by Yuval and Anderson[2] and from the Anderson model by Hamann.[3] The fundamental assumption in both approaches is the "long-time approximation" used in the x-ray-threshold problem by Nozières and de Dominicis,[4] and its significance is discussed in Sec. II. Our first result concerns the structure of this perturbation series, which is an expansion in powers of the transverse coupling constant $J_\perp$. In Sec. II we derive an exact homogeneity property of the partition function which enables us to display the singularities in every order. It is found that the perturbation theory is finite for ferromagnetic coupling and a moment exists in the ground state. For antiferromagnetic coupling the free energy, as well as its derivatives, becomes infinite term by term in sufficiently high-order perturbation theory as $H \to 0$ and $T \to 0$.

In order to proceed further, it is shown in Sec. IV that a spin-$\frac{1}{2}$ interacting with a certain boson field has a partition function exactly equal to that derived by Yuval and Anderson[2] and Hamann.[3] Thus, its Hamiltonian $\mathcal{H}_B$ is a complete summary of the content of the long-time approximation in the Kondo problem, and it allows us to study ground-state properties directly, without having to take the tricky limit $T \to 0$. In effect, $\mathcal{H}_B$ is a simpler representation of a magnetic impurity in a metal, and it allows us to imagine different approximation schemes which avoid the singularities.

The solution of the spin-boson problem is considered in Sec. V. It is argued that the singulari-

ties are consequences of using the wrong starting point for perturbation theory. An alternative division of the Hamiltonian into two parts is proposed. For antiferromagnetic coupling, the optimum choice removes all divergences and gives the expected nonanalytic character of physical quantities. Every order of perturbation theory is an analytic function of H^2 and the moment is zero when $H=0$. For weak ferromagnetic coupling the optimum choice gives ordinary perturbation theory and a moment which is not very different from the free value. As the transverse coupling is increased, a point is reached at which the moment jumps to zero, and the new division of the Hamiltonian is required. This "phase diagram" is different from the one obtained by Anderson, Yuval, and Hamann[5] by an approximate scaling argument, and we believe that the difference is related to the use of the long-time approximation, which is essential to the spin-boson equivalence but not the scaling method. This will be discussed further in Sec. VII.

In evaluating corrections to the new unperturbed Hamiltonian, it is found that the series for the susceptibility or the moment (whichever is finite) are finite term by term but are not rapidly convergent. The method is thus capable of determining the "phase diagram" but requires a partial summation of perturbation theory to evaluate experimentally determined quantities.

In the course of deriving the relationship between $\mathcal{H}_B$ and the long-time approximation for the Kondo partition function Z, it is shown that Z is also the partition function of a certain one-dimensional Ising model. This has previously been pointed out by Yuval and Anderson[2] and was of interest because the coupling followed an inverse-square law at large distances, and was a case which had not been solved.[2] In Sec. VI this problem is studied in some detail. First it is shown to have the peculiarity that for $T\neq 0$, the free energy is intensive. It can be turned into an extensive problem at $T=0$, but only in a limit which is of crucial importance for the relationship to the Kondo problem. This limit shows that there is an infinitely strong near-neighbor coupling which dominates the problem. Thus we conclude that the equivalence of the Kondo problem and the ordinary inverse-square Ising model suggested by Anderson and Yuval[6] requires a further assumption, which is discussed in detail in Sec. VI. Finally, we show how the approximation of Sec. V may be derived directly from the Ising model and, at the same time, extended to finite temperatures. This work has been described briefly in two earlier publications.[7,8]

II. SERIES FOR PARTITION FUNCTION

The Kondo Hamiltonian $\mathcal{H}_K$ is given by

$$\mathcal{H}_K = T + \frac{J_\parallel}{4N_0}(a_+^\dagger a_+ - a_-^\dagger a_-)\sigma_z + \frac{J_\perp}{4N_0}(a_+^\dagger a_-\sigma_- + a_-^\dagger a_+\sigma_+) + H\left(\sigma_z + \sum_i S_{iz}\right) , \tag{2.1}$$

where T is the electron kinetic-energy operator measured relative to the chemical potential, $a_{\vec{k},\alpha}$ annihilates electrons of momentum $\vec{k}$ and spin up ($\alpha=+$) or down ($\alpha=-$), and $a_\alpha=\sum_{\vec{k}} a_{\vec{k}\alpha}$, with the sum being taken over a band of width $2/\tau$ ($\hbar$ is taken to be unity). The impurity is assumed to have a spin $=\frac{1}{2}$ and its Pauli matrix vector is $\vec{\sigma}$, with $\sigma_\pm=\sigma_x\pm i\sigma_y$. The S_{iz} are the Pauli matrices for the z component of the electrons' spin, and N_0 is the number of electrons of each spin in the s wave. With this choice of signs, $J_\parallel>0$ corresponds to antiferromagnetic coupling and the sign of $J_\perp$ is irrelevant, since it may be changed by a proper rotation.[5] Usually one sets $J_\parallel=J_\perp=J$, but the distinction is made here because the two couplings play rather different roles, and this is not clearly seen in the special case of isotropic coupling. Furthermore, Yuval and Anderson[2] exploited the fact that, when $J_\perp=0$, $\mathcal{H}_K$ is exactly soluble, since it then describes an independent-electron problem, with the potential depending on the value of σ_z, which becomes a c number. If the part of $\mathcal{H}_K$ which is proportional to $J_\perp$ is treated as a perturbation, it induces transitions between $\sigma_z=+1$ and $\sigma_z=-1$, thereby switching from one potential to the other. This is reminiscent of the transition produced by an x ray when it knocks an electron from a low-lying atomic level of a solid, and Yuval and Anderson[2] exploited this analogy to derive a power series for the partition function Z:

$$\frac{Z}{Z_0} = e^{\beta H}\sum_m \left(\frac{J_\perp\rho}{2\tau}\right)^{2m}\int_0^\beta dt_{2m}\int_0^{t_{2m}} dt_{2m-1}\cdots\int_0^{t_2} dt_1 \exp\left\{-\sum_{i>j}^{2m}(-1)^{i-j}\phi(t_i-t_j) + H\sum_{i=1}^{2m} 2t_i(-1)^{i+1}\right\} + \{H\leftrightarrow -H\}, \tag{2.2}$$

where

$$e^{\phi(t)} \to \left(\frac{\pi T\tau}{\sin\pi Tt}\right)^{2-\epsilon} \quad \text{for } t,\ \beta-t \text{ large.} \tag{2.3}$$

Here H is the magnetic field, T the temperature, $\beta=T^{-1}$ (Boltzmann's constant has been set equal to 1), ρ is the density of states, and

$$\epsilon = -8\delta/\pi - 8\delta^2/\pi^2 , \tag{2.4}$$

where δ is the one-particle phase shift calculated from $\mathcal{H}_K$ with $J_\perp = 0$, $H = 0$, $J_\parallel > 0$, $\sigma_z = 1$. For weak coupling we have

$$\epsilon \approx 2J_\parallel \rho \ . \tag{2.5}$$

The partition function for $J_\perp = 0$, $H = 0$ is denoted by $2Z_0$. In Eq. (2.2) the integrands were evaluated for long times by using the approximation introduced by Nozières and de Dominicis[4] for the x-ray-threshold problem. This gave the specific form of Eq. (2.3) and was also responsible for the simple form of the exponent in Eq. (2.2), which is a sum of "pair potentials." The form of $\phi(t)$ for short times depends upon details of the band structure and, when any of the $t_i - t_j$ are small, the exponent in Eq. (2.2) becomes quite complicated. All of this is buried in a cutoff t_0 such that

$$e^{\phi(t)} = 0, \quad t < t_0 \text{ or } \beta - t < t_0 \ . \tag{2.6}$$

It is assumed that the same cutoff may be used in every term of every order of perturbation theory. Since ρ, τ, and t_0 are expected to have the same order of magnitude, Yuval and Anderson[2] used the same symbol τ for all of them. We have chosen to distinguish among them, so that the sensitivity to density of states, bandwidth, and cutoff may be studied separately.

Hamann[3] derived Eq. (2.2) from the Anderson Hamiltonian, also making use of the long-time approximation. We shall interpret our results in terms of $\mathcal{H}_K$, but our conclusions can be applied equally to the Anderson Hamiltonian by reinterpreting the constants $J_\perp$ and ϵ.

The important assumption in deriving Eq. (2.2) is the long-time approximation. Its qualitative basis is that, for weak coupling, only low-energy excitations are important in the series for Z, and they correspond to the long-time behavior of the integrands. Quantitatively, it is necessary to show that no singularities of importance have been omitted. In general, the approximation is accurate when $t_0 \to 0$ and it should be good for those quantities which are insensitive to t_0, although, even then, it may prove necessary to include in $\phi(t)$ terms which tend to a constant as $t \to \infty$, since they effectively renormalize $J_\perp$. These are points which will be considered in the course of the discussion.

First, however, we shall take Eqs. (2.2) and (2.6) for granted and derive some exact consequences which will enable us to discuss the singularities of the perturbation theory.

III. HOMOGENEITY AND SINGULARITIES OF PERTURBATION THEORY

In this section we shall show that Z/Z_0, given by Eq. (2.2), is a homogeneous function of degree zero in the variables H, T, t_0^{-1}, and $(J_\perp \rho)^{2/\epsilon}$. This result allows us to analyze the structure of perturbation theory, to show directly that the series for the ground-state energy and its derivatives are asymptotic, and to anticipate the form of the ground-state energy and susceptibility.

The homogeneity may be obtained quite simply from Eqs. (2.2), (2.3), and (2.6). If T, t_0^{-1}, and H are multiplied by a constant λ, and integration variables are changed from t_i to $x_i = \lambda t_i$, then the only changes in Eq. (2.2) are that $(J_\perp \rho/\tau)^{2m}$ is multiplied by $\lambda^{-\epsilon m}$ and that the integration variables are renamed. The latter change is irrelevant and the former may be compensated for by multiplying $J_\perp$ by $\lambda^{\epsilon/2}$. It follows at once that the impurity free energy $F = -T \ln(Z/Z_0)$ is a homogeneous function of degree one and that the magnetization $M = \partial F/\partial H$, entropy $S = \partial F/\partial T$, and specific heat $C = T(\partial S/\partial T)$ are all homogeneous functions of degree zero, in the same variables.

First consider the consequences of this result for $T = 0$. If the ground-state energy E_g is expanded as a series in $J_\perp$, it must take the form

$$E_g = \sum_{m=1}^{\infty} a_m(H, t_0^{-1}) J_\perp^{2m} \ , \tag{3.1}$$

and a_m has to be a homogeneous function of degree $(1 - m\epsilon)$. Thus we can rewrite

$$a_m(H, t_0^{-1}) = a_m(1, 1/Ht_0) H^{1-m\epsilon} \ , \tag{3.2}$$

which diverges as $H \to 0$, when $m\epsilon > 1$, unless $a_m(1, \infty) = 0$. This latter requirement is not satisfied in general, since it is equivalent to saying that integrals become zero when the lower cutoff t_0 is set equal to zero. Thus we may conclude that, for $\epsilon > 0$, perturbation theory for the ground state in zero field is infinite in every order above $2/\epsilon$. A similar argument for M, S, and C, which are of degree zero, would give coefficients proportional to $H^{-m\epsilon}$ and hence, for $\epsilon > 0$, every order is singular. These are infrared divergences and an understanding of their significance is the essence of the Kondo problem.

The coefficient $a_m(H, t_0^{-1})$ may also be rewritten

$$a_m(H, t_0^{-1}) = a_m(Ht_0, 1)\, t_0^{m\epsilon - 1} \ , \tag{3.3}$$

and this diverges as $t_0 \to 0$ when $m\epsilon < 1$, unless a_m is zero for $H = 0$, which would mean that the term is missing from perturbation series in zero field. A corresponding argument shows that M, S, and C have these ultraviolet divergences in every order, when $\epsilon < 0$ (ferromagnetic coupling). These are not real divergences, since t_0 is kept finite, but, where they exist, it is clear that integrals are sensitive to high-energy excitations and that the long-time approximation is inadequate.

The above discussion may be repeated for $H = 0$, $T \neq 0$ by simply substituting T for H. This dis-

plays the singularities in the zero-field free energy as zero temperature is approached.

It is clear that, for $m\epsilon > 1$, $a_m(Ht_0, 1)$ has to diverge as Ht_0 tends to zero, in order to produce the singularity shown in Eq. (3.2). In the same way, $a_m(1, 1/Ht_0)$ must diverge for $m\epsilon < 1$. The general argument does not exclude the possibility that these coefficients diverge for all $m\epsilon$ and so produce stronger divergences than the simple powers shown in Eqs. (3.2) and (3.3). However, a number of calculations indicate that this does not happen; in particular, low-order perturbation theory for all ϵ, perturbation theory to all orders for $\epsilon = 1, 2$, and the results of Sec. V support this assertion. In other words, E_g has only infrared divergences when $m\epsilon < 1$ and only ultraviolet divergences when $m\epsilon > 1$. For M, S, and C, the dividing line occurs at $\epsilon = 0$, and there are no infrared singularities for ferromagnetic coupling.

The divergences in the ground-state energy have not previously been discussed, because it is traditional to expand in powers of ϵ as well as $J_\perp$. Equation (3.2) shows that such an expansion would be finite term by term as $H \to 0$, since the singularities are of the form $H(\ln H)^n$. Treating ϵ exactly makes it clear that for $\epsilon > 0$ E_g cannot be expanded in powers of $J_\perp$ and that there should be a nonanalytic contribution of order $J_\perp^p$, where p is the smallest power for which a divergence occurs. Thus we expect a nonanalyticity $J_\perp^{2/\epsilon}$, and this is exactly what we shall find in Sec. V.

For $\epsilon > 0$, $t_0 = 0$, homogeneity implies that the magnetization series is

$$M = 1 + \sum_{n=1}^{\infty} b_n(\epsilon) \left(\frac{J_\perp^2}{H^\epsilon}\right)^n . \tag{3.4}$$

The reason for the Kondo problem is now clear—M is a function of $J_\perp^2/H^\epsilon$ and perturbation theory in $J_\perp$ is quite inappropriate for determining the behavior in zero field. The method described in Sec. V effectively "inverts" this series to a function of $H/J_\perp^{2/\epsilon}$. Equation (3.4) also shows that the value of M in the $H \to 0$ limit is independent of $J_\perp$ and, if it were possible to solve the problem for a particular value of $J_\perp$, with ϵ arbitrary, then $M(H = 0)$ would be known for all $J_\perp$. It is tempting, for example, to consider large $J_\perp$, but this is not strong coupling in the usual sense and care is needed in taking the limits $t_0 \to 0$ and $J_\perp \to \infty$.

These considerations are well illustrated by second-order perturbation theory for the free energy which may be derived from Eqs. (2.2) and (2.3):

$$F = -T \ln \cosh\beta H - T(J_\perp \rho/2\tau)^2 \int_{t_0}^{\beta - t_0} dt(\beta - t) \times \left(\frac{\pi T \tau}{\sin \pi T t}\right)^{2-\epsilon} \frac{\cosh H(\beta - 2t)}{\cosh \beta H} . \tag{3.5}$$

The susceptibility may be obtained by differentiating F twice with respect to H, setting $t_0 = 0$, and writing $x = Tt$ to give, for $\epsilon > 0$,

$$\chi = \beta \left(1 - \frac{(J_\perp \rho)^2}{(T\tau)^\epsilon} \pi^{2-\epsilon} \int_0^1 dx \frac{(1-x)^2 x}{(\sin \pi x)^{2\epsilon}}\right) . \tag{3.6}$$

For ferromagnetic coupling ($\epsilon < 0$) the second-order term tends to zero as $T \to 0$ and χ is not very different from a Curie law. Treating ϵ exactly has removed the Kondo divergences. For antiferromagnetic coupling the second-order term diverges as $T \to 0$ and is of order unity when $T = T_c \equiv (J\rho)^{2/\epsilon}/I\tau$, where $I^{-\epsilon}$ is $\pi^{2-\epsilon}$ times the integral in Eq. (3.6). For $J\rho = 0.2$, for example, this temperature is about 10% of the Kondo temperature T_K and, for $T = T_K$, Eq. (3.6) is a good approximation to the numerical values obtained by Schotte and Schotte.[9] For very much smaller $J\rho$, higher-order terms in the series are expected to build up and modify the scale.

Setting $T = 0$ in Eq. (3.5) gives the second-order ground-state energy:

$$E_g = -H - \left(\frac{J_\perp \rho}{2\tau}\right)^2 \int_{t_0}^{\infty} dt\, e^{-2Ht} \left(\frac{\tau}{t}\right)^{2-\epsilon} , \tag{3.7}$$

which explicitly shows the infrared divergence for $\epsilon > 1$ and the ultraviolet divergence for $\epsilon < 1$. When $\epsilon < 0$ the magnetization in zero field is, for $t_0 = \tau$,

$$M = 1 + \frac{J_\perp^2 \rho}{4J_\parallel} . \tag{3.8}$$

It may be verified that the terms of order $J_\perp^{2n}$ have a coefficient proportional to ϵ^{1-2n} for small ϵ, so that, for weak isotopic coupling, they are of order J, and can be summed[5,6] to give $M = 1 + \frac{1}{2} J\rho$.

It is clearly essential to have a method of solution which does not depend on perturbation theory in $J_\perp$, when $H \to 0$ and $T \to 0$. In Sec. IV it will be shown that there is a Hamiltonian for which Eq. (2.2) gives the exact partition function. This will enable us directly to introduce a nonperturbative approximation for the ground state while still retaining the simplicity of the long-time approximation.

IV. SPIN-BOSON REPRESENTATION OF PARTITION FUNCTION

In this section it will be shown that a spin interacting with a certain boson field has the series (2.2) as its exact partition function. The Hamiltonian $\mathcal{H}_B$ of such a system therefore is a complete statement of the long-time approximation as applied to the series. The Hamiltonian is

$$\mathcal{H}_B = \sum_k \omega_k b_k^\dagger b_k + \sum_k V_k (b_k^\dagger + b_k)\sigma_z - \Delta\sigma_x - H\sigma_z , \tag{4.1}$$

where $b_k^\dagger$ creates a one-dimensional boson of momentum k and

$$\omega_k = k/\rho \ ,$$
$$V_k^2\rho^2 = (1-\tfrac{1}{2}\epsilon)\,k/2N_0 \quad (k<\rho/\tau)\,, \tag{4.2}$$
$$V_k^2\rho^2 = 0 \qquad\qquad (k>\rho/\tau)\,.$$

It will be shown that if $Z_B = \mathrm{Tr}\, e^{-\beta\mathcal{H}_B}$ and Z_{B0} is the value of Z_B when $\Delta = 0 = H$, then Z_B/Z_{B0} is equal to the right-hand side of Eq. (2.2) with $\phi(t)$ given by Eq. (2.3) for large t. The coefficient Δ is $J_\perp$ multiplied by a constant to be determined later. For small t, $\phi(t)$ will be different from Eq. (2.6), but that was in any event just one of several possible ways of cutting off. A derivation of this equivalence has been given by Blume, Emery, and Luther[8] and the argument will be repeated here for completeness. In the course of the derivation, it will be shown that Z/Z_0 is also the partition function of a peculiar one-dimensional Ising model, whose properties may also be discussed together with those of the Kondo problem. This will be considered in some detail in Sec. VI.

A physical feeling for $\mathcal{H}_B$ may be obtained by considering the Tomonaga model,[10] which treats longitudinal spin-density operators as bosons. If this model is applied to $\mathcal{H}_K$, it may be canonically transformed,[8,10] into Eq. (4.1), except that the boson operators have a polarization index α. As shown in Ref. 8, α may be omitted if a factor $\sqrt{2}$ is included in V_k. However, we emphasize that we do not rely in any way upon the assumed validity of the Tomonaga model; it is merely used to give a physical picture. Our procedure is to give a formal evaluation of Z_B/Z_{B0} and to relate it directly to Eq. (2.2).

To evaluate Z_B, we first introduce a discrete ordering label[11] n such that

$$Z_B = \lim_{N\to\infty} Z_N \ , \tag{4.3}$$

where

$$Z_N = \mathrm{Tr}\,\hat{T}\exp\left[-\left(\frac{\beta}{N}\right)\sum_{n=1}^{N}(K_n + V_n\sigma_{zn} - \Delta\sigma_{xn} - H\sigma_{zn})\right] \tag{4.4}$$

and $\hat{T}$ is an ordering symbol which requires operators with larger n to stand to the left. We have written $K = \sum_k \omega_k b_k^\dagger b_k$ and $V = \sum_k V_k(b_k^\dagger + b_k)$. When $N\to\infty$, Eq. (4.4) becomes the more familiar time-ordered product. Now Z_N may be rewritten

$$Z_N = \mathrm{Tr}\,\hat{T}\exp\left[-\left(\frac{\beta}{N}\right)\sum_n k_n\right] M_N M_{N-1}\cdots M_1, \tag{4.5}$$

where

$$M_n = \exp\left[-\left(\frac{\beta}{N}\right)(V_n\sigma_z - \Delta\sigma_x)\right] \ . \tag{4.6}$$

In Eq. (4.5) the spin operators have been ordered explicitly and $\hat{T}$ has only to ensure that the relative orders of K_n and V_n are correct. Thus the ordering labels have been omitted from σ_x and σ_z in Eq. (4.6).

Since we shall ultimately let $N\to\infty$, it is sufficient to work to leading order in N in the exponent and to rewrite

$$M_n \approx \left(1+\frac{\beta\Delta}{N}\sigma_x\right)\exp-\left[\left(\frac{\beta}{N}\right)V_n\sigma_z\right] = \exp\left(\tfrac{1}{2}\ln\frac{\beta\Delta}{N}\right)\begin{bmatrix}\exp\left(-\frac{1}{2}\ln\frac{\beta\Delta}{N}\right) & \exp\left(\frac{1}{2}\ln\frac{\beta\Delta}{N}\right)\\ \exp\left(\frac{1}{2}\ln\frac{\beta\Delta}{N}\right) & \exp\left(-\frac{1}{2}\ln\frac{\beta\Delta}{N}\right)\end{bmatrix}\exp\left[-\left(\frac{\beta}{N}\right)V_n\sigma_z\right]. \tag{4.7}$$

The sign of Δ is unimportant and it has been assumed to be positive. Apart from the factor $\exp[\frac{1}{2}\ln(\beta\Delta/N)]$, the right-hand side of Eq. (4.7) is just the unsymmetrized form of the transfer matrix[12] for a one-dimensional Ising model with temperature set equal to unity. There is a site-dependent magnetic field $(-\beta V_n/N)$ and a near-neighbor interaction $\frac{1}{2}\ln(\beta\Delta/N)$. Therefore Eq. (4.5) may be rewritten as an Ising partition function:

$$Z_N = \mathrm{Tr}\,\hat{T}\exp\left(\frac{-\beta}{N}\sum_n K_n\right)$$
$$\times \sum_{(\mu_n)}\exp\left(-\frac{\beta}{N}\sum_{n=1}^{N}V_n\mu_n + \sum_{n=1}^{N}\frac{1}{2}(1-\mu_n\mu_{n+1})\ln\frac{\beta\Delta}{N}\right), \tag{4.8}$$

where the trace is now to be carried out over the boson variables, the μ_i takes values ± 1, and periodic boundary conditions are imposed so that $\mu_{N+1} = \mu_1$.

Since V_N is linear in the b_k and $b_k^\dagger$, it is straightforward to carry out the remaining trace over boson variables[13] to obtain

$$\frac{Z_N}{Z_{B0}} = \sum_{(\mu_i)}\exp\left[\frac{\beta^2}{N^2}\sum_{m,n}^{N}B\left(\frac{\beta(m-n)}{N}\right)\mu_m\mu_n + \sum_{n=1}^{N}\frac{1}{2}(1-\mu_n\mu_{n+1})\ln\left(\frac{\beta\Delta}{N}\right) + \frac{\beta H}{N}\sum_{n=1}^{N}\mu_n\right] \ , \tag{4.9}$$

where $Z_{B0} = \mathrm{Tr}\, e^{-\beta K}$ and

$$B(t) = \frac{1}{2}\sum_k V_k^2 (e^{-\omega_k |t|} + 2n_k \cosh\omega_k t) \ . \tag{4.10}$$

The right-hand side of Eq. (4.9) is the Ising-model partition function. This will be discussed in detail in Sec. VI and, for the present, we shall continue with the derivation of Eq. (2.2).

We wish to rearrange Eq. (4.9) as a power series in Δ. For this purpose, we specify a configuration of spins by introducing

$$\begin{aligned} \Phi_M(t) &= 1 \quad (t_{2\nu} < t \leq t_{2\nu+1}, \quad \nu = 0, 1, 2, \ldots M) \\ &= -1 \quad (t_{2\nu+1} < t \leq t_{2\nu+2}, \quad \nu = 0, 1, 2, \ldots M-1) \end{aligned} \tag{4.11}$$

and $t_\nu = (\beta n_\nu / N)$, $t_{2M+1} = [\beta(N+1)/N]$. Then,

$$\mu_n = \Phi_M\left(\frac{\beta n}{N}\right) \tag{4.12}$$

is a configuration in which $\mu_1 = +1$ and the n_ν give the positions at which the spin changes sign. The periodic boundary conditions require that there is an even number of sign changes, as assumed in Eq. (4.11). The sum over configurations is now completed by summing over all M and over all sets n_ν for each M. For every M

$$\sum_n \tfrac{1}{2}(1 - \mu_n \mu_{n+1}) = 2M \ , \tag{4.13}$$

so that the near-neighbor term in Eq. (4.9) reduces to a factor $(\beta\Delta/N)^{2M}$ and, as $N \to \infty$, the rest of the exponent in Eq. (4.9) becomes

$$E[\Phi_M] = \int_0^\beta dt \int_0^\beta dt' B(t-t')\Phi_M(t)\Phi_M(t') + H\sum_{\nu=1}^{2M}(-1)^{\nu+1} 2t_\nu + \beta H \ . \tag{4.14}$$

Then,

$$\begin{aligned} \frac{Z_B}{Z_{B0}} &= \sum_{M=0}^{\infty} \lim_{N\to\infty} \sum_{n_1 < n_2 < \cdots < n_{2m}} \left(\frac{\beta\Delta}{N}\right)^{2M} e^{E[\Phi_M]} + (H \leftrightarrow -H) \\ &= \sum_{M=0}^{\infty} \int_0^\beta dt_{2M} \int_0^{t_{2m}} dt_{2M-1} \cdots \int_0^{t_2} dt_1 \, \Delta^{2M} e^{E[\Phi_M]} \ , \end{aligned} \tag{4.15}$$

where we have added in the set of configurations in which $\mu_1 = -1$.

Now, integrating by parts,

$$\int_0^\beta dt \int_0^\beta dt' B(t-t')\Phi_M(t)\Phi_M(t') = \beta\sum_k \frac{V_k^2}{\omega_k} - \int_0^\beta dt \int_0^\beta dt' C(t-t')\Phi'_M(t)\Phi'_M(t') \ , \tag{4.16}$$

where

$$C(t) = \frac{1}{2}\sum_k \left(\frac{V_k^2}{\omega_k^2}\right)(e^{-\omega_k|t|} + 2n_k \cosh\omega_k t) \tag{4.17}$$

and

$$\begin{aligned} \Phi'_M(t) &= \frac{d\Phi_M}{dt} \\ &= 2\sum_{\nu=1}^{2m} (-1)^\nu \delta(t - t_\nu) \ . \end{aligned} \tag{4.18}$$

Now perform the t and t' integration on the right-hand side of Eq. (4.16), and convert the resulting double sum over the time indices to an ordered sum as in Eq. (2.2). This leads to

$$\tfrac{1}{8}\phi(t) = C(t) - C(0) \tag{4.19}$$

and establishes the identity between Z and Z_B, provided Δ is properly related to $J_\perp$. Changing sums to integrals, $(1/N_0)\sum_k \to \int dk$, and evaluating the result for long times,[14] it can be shown that the time dependence of Eq. (4.19) agrees with Eq. (2.3). For $T = 0$, Eqs. (4.2), (4.17), and (4.19) give

$$\frac{\phi(t)}{2-\epsilon} = -\gamma + \ln\left(\frac{t}{\tau}\right) + \mathrm{Ei}\left(\frac{-t}{\tau}\right) \ , \tag{4.20}$$

where γ is Euler's constant and $\mathrm{Ei}(-x)$ is the exponential integral. Thus, to agree with Eqs. (2.2) and (2.4), it is necessary to take

$$\Delta = e^{\gamma(1-\epsilon/2)}\left(\frac{J_\perp \rho}{2\tau}\right) \ . \tag{4.21}$$

The existence of the factor $e^{-\gamma\epsilon/2}$ is partly a consequence of the fact that similar terms were dropped in the original derivation of Eq. (2.2), in making the long-time approximation. With this factor, of course, we have $Z = Z_B$ and we retain it to assess the possible importance of such terms which are properly beyond the long-time approximation.

This completes the derivation of the relationship between $\mathcal{H}_B$ and $\mathcal{H}_K$ in the long-time approximation. In Sec. V we shall carry out a direct calculation of the ground-state properties of $\mathcal{H}_B$.

V. ZERO-TEMPERATURE SOLUTION OF SPIN-BOSON PROBLEM

In this section we shall consider the solution of the spin-boson problem introduced in Sec. IV. As shown in Sec. III, the interesting singularities occur when $H \to 0$ and $T \to 0$, so we shall calculate the ground-state energy. The object will be to find a division of the Hamiltonian into two parts which gives a finite and rapidly convergent perturbation theory.

A. Zero-Order Solution

If $\Delta = 0$, $\mathcal{H}_B$ may be diagonalized by a canonical transformation,

$$\mathcal{H}_B' = e^{-S\sigma_z}\mathcal{H}_B e^{S\sigma_z} , \tag{5.1}$$

where

$$S = \sum_k f_k(b_k - b_k^\dagger) \tag{5.2}$$

and $f_k = V_k/\omega_k$. This would be the first step in carrying out perturbation theory in Δ, which would lead to all of the divergences described in Sec. III. On the other hand, when $V_k = 0$, but $\Delta \neq 0$, the Hamiltonian is diagonalized (so far as the bosons are concerned) by $f_k = 0$. This suggests that, in general, it may be more advantageous to choose f_k somewhere between 0 and V_k/ω_k.

It should be stressed that our objective is to obtain a convergent perturbation theory and not necessarily to obtain a good approximation in lowest order. The choice of canonical transformation has been restricted to functions of $(b_k - b_k^\dagger)\sigma_z$, which preserve the invariance of $\mathcal{H}_B$ under simultaneous change of sign of σ_z and the b_k. It may be possible to obtain a lower zero-order ground-state energy by violating this symmetry, but this is unacceptable and fails to deal with the problem of divergences, which requires that the proper relationship between $\sigma_z = +1$ and $\sigma_z = -1$ be maintained. This is confirmed by the solution of the Ising model in Sec. VI, since it treats the bosons exactly.

The transformed Hamiltonian may be written

$$\mathcal{H}_B' = \mathcal{H}_0' + \mathcal{H}_1' , \tag{5.3}$$

where

$$\mathcal{H}_0' = \sum_k(\omega_k f_k^2 - 2V_k f_k) + \sum_k \omega_k b_k^\dagger b_k - H\sigma_z , \tag{5.4}$$

$$\mathcal{H}_1' = \sum_k (V_k - \omega_k f_k)(b_k^\dagger + b_k)\sigma_z - \frac{\Delta}{2}(e^{-2S}\sigma_+ + e^{2S}\sigma_-) . \tag{5.5}$$

We should like to choose f_k so that perturbation theory in $\mathcal{H}_1'$ converges as rapidly as possible. Also, for $H = 0$, the ground state of $\mathcal{H}_0'$ is degenerate, since it is independent of the spin part of the wave function, so (if $\mathcal{H}_1'$ splits the degeneracy in lowest order) we must take part of $\mathcal{H}_1'$ into the unperturbed Hamiltonian. All of this may be achieved automatically by choosing a trial state equal to the boson vacuum $|0\rangle$ multiplied by an arbitrary spin state, and minimizing the expectation value of $\mathcal{H}_B'$. The trial state is the general ground state of $\mathcal{H}_0'$. Minimization with respect to the spin state solves first-order degenerate perturbation theory, and the higher-order corrections are then made as small as possible by minimizing with respect to f_k, since the trial energy is then as close as possible to the true energy.

Using Eqs. (5.4) and (5.5), the vacuum expectation value of $\mathcal{H}_B'$ is

$$\langle 0|\mathcal{H}_B'|0\rangle = \sum_k(\omega_k f_k^2 - 2V_k f_k) - H\sigma_z - \sigma_x\Delta\exp\left(-2\sum_k f_k^2\right), \tag{5.6}$$

and the variation of the spin state is equivalent to diagonalizing this (2×2) matrix. Its lowest eigenvalue is

$$E = \sum_k(\omega_k f_k^2 - 2V_k f_k) - \left[H^2 + \Delta^2\exp\left(-4\sum_k f_k^2\right)\right]^{1/2} . \tag{5.7}$$

Minimization with respect to f_k now shows that f_k has the general form

$$f_k = V_k/(\omega_k + D) . \tag{5.8}$$

When $D \neq 0$, Eqs. (4.2) and (5.8) show that $\exp(-2\sum_k f_k^2) \neq 0$, which means that the degeneracy is split and, for $H = 0$, the spin points in the x direction. This does not imply a broken symmetry for $\mathcal{H}_K$, because comparison with the Tomonaga model shows that the ground-state wave function $|\psi_K\rangle$ of $\mathcal{H}_K$ is analogous to

$$|\psi_K\rangle = \exp\left[\sigma_z\sum_k\left(\frac{2}{N_0 k}\right)^{1/2}(b_k^\dagger - b_k)\right]|\psi_B\rangle , \tag{5.9}$$

where $|\psi_B\rangle$ is the ground state of $\mathcal{H}_B$. Taking $|\psi_B\rangle$ equal to $\exp(S\sigma_z)|0\rangle$ times an eigenvalue of σ_x, Eq. (5.9) shows that $\langle\psi_K|\sigma_x|\psi_K\rangle$ is $\exp\{-2\sum_k[f_k - (2/kN_0)^{1/2}]^2\}$, which is zero because the sum in the exponent diverges.

When $D \neq 0$, the ground state of $\mathcal{H}_0'$ is orthogonal to the ground state for $D = 0$, which is the starting point for ordinary perturbation theory. Their overlap is proportional to $\exp[-\frac{1}{2}\sum_k(f_k - V_k/\omega_k)^2]$ and the sum in the exponent diverges. This is yet another indication of the singular nature of the problem.

Minimization of Eq. (5.7) with respect to f_k also gives an expression for D but, if there are several solutions, the simplest way to find the one which gives the lowest energy is to substitute Eq. (5.8) into Eq. (5.7) and to consider the energy as a function of the single parameter D. If E_0 is the energy at $D = 0$, $H = 0$ then Eqs. (4.2), (5.7), and (5.8) give

$$\Delta E = E(D) - E_0$$

$$= \left(\frac{2-\epsilon}{4}\right)\frac{D}{1+D\tau} - \left[H^2 + \Delta^2\left(\frac{D\tau}{1+D\tau}e^{(1+D\tau)^{-1}}\right)^{2-\epsilon}\right]^{1/2} . \tag{5.10}$$

1. Antiferromagnetic coupling $\epsilon > 0$

First consider $H = 0$ and assume $D\tau$ is small. To lowest order, Eq. (5.10) becomes

$$\Delta E = \tfrac{1}{4}(2-\epsilon)D - \Delta(D\tau e)^{1-\epsilon/2} , \tag{5.11}$$

which has a minimum at $D = D_0$, where

$$D_0 = (2e\Delta\tau)^{2/\epsilon}/\tau e \tag{5.12}$$

or, from Eq. (4.21),

$$D_0 = (J_\perp \bar{\rho})^{2/\epsilon}/\bar{\tau} , \tag{5.13}$$

where $\bar{\rho} = \rho e^{(1+\gamma)}$ and $\bar{\tau} = \tau^{(1+\gamma)}$. Thus $D_0\tau$ is indeed small for weak coupling and Eq. (5.11) is a good approximation to Eq. (5.10). If the factor $e^{-\gamma\epsilon/2}$ had been omitted from Eq. (4.21), then D_0 in Eq. (5.13) would have been bigger by a factor e^{γ}. This indicates that, to obtain accurate numerical results, it is necessary to include constant terms in the evaluation of $\phi(t)$ for Eq. (2.2).

Substituting Eq. (5.12) into Eq. (5.11) gives

$$\Delta E = -\tfrac{1}{4}\epsilon D_0 , \tag{5.14}$$

which is the nonanalytic function of $J_\perp$ anticipated in Sec. III.

Since E is stationary with respect to variations of D, it is not necessary to determine D for $H \neq 0$ in order to obtain the magnetization $M = -(\partial E/\partial H)_{H=0}$, and from (5.10) it follows at once that $M = 0$. Similarly, the susceptibility is given by

$$\chi = -\left(\frac{\partial^2 E}{\partial H^2}\right) \quad \chi = \frac{2}{D_0} . \tag{5.15}$$

However, we shall see later that this is not an accurate calculation of χ, since there are important corrections coming from higher orders.

To consider $H \neq 0$, we again work to lowest order in $D\tau$ and so simply restore H to Eq. (5.11) and write it in the form

$$\Delta E/D_0 = \tfrac{1}{4}(2-\epsilon)\bar{D} - (\bar{H}^2 + \tfrac{1}{4}\bar{D}^{2-\epsilon})^{1/2} , \tag{5.16}$$

where

$$\bar{D} = D/D_0, \quad \bar{H} = H/D_0 . \tag{5.17}$$

In this form, the homogeneity discussed in Sec. III is evident, and it is possible to expand in powers of ϵ and $\bar{H}$. For small $\bar{H}$ the minimum occurs when

$$\bar{D} = 1 - 4\bar{H}^2/\epsilon + O(\bar{H}^4) \tag{5.18}$$

and, for this value of $\bar{D}$,

$$\Delta E/D_0 = -\tfrac{1}{4}\epsilon - \bar{H}^2 . \tag{5.19}$$

On the other hand, for $\bar{D} = 0$, $\Delta E/D_0 = -\bar{H}$, and this gives the lowest energy when $\bar{H}$ exceeds the critical value $\bar{H}_c$, where

$$\bar{H}_c \equiv \tfrac{1}{4}\epsilon + O(\epsilon^2) . \tag{5.20}$$

At this field, D jumps discontinuously to zero, and in this lowest order, M jumps from zero to unity. However, it will be seen that it is necessary to include all orders in perturbation theory to determine the magnetization at finite field. There is then no reason to believe that M is discontinuous; rather, it is the optimum starting point for perturbation theory which changes. Since $H \neq 0$, there are no infrared divergences when D becomes zero.

2. Ferromagnetic coupling

When $\epsilon < 0$, Eq. (5.11) shows that $\partial E/\partial D > 0$ as $D \to 0+$. Since $D > 0$, there is a local minimum at $D = 0$, and, for weak coupling, this gives the lowest energy. This will lead to ordinary perturbation theory in Δ, as anticipated in Sec. III. For $D = 0$, Eq. (5.10) gives $M = 1$. It is also of interest to consider mathematically what happens when $\Delta\rho$ is not small. In that case, band-structure effects are important, but the results should be qualitatively correct. For this purpose, it is necessary to use the full equation (5.10) for ΔE. This has a second minimum and, for each ϵ, there is a critical value Δ_c above which the second minimum gives a lower energy. The phase diagram is shown in Fig. 1. The critical line $\Delta = \Delta_c(\epsilon)$ is AB and above that line $D \neq 0$ and $M = 0$. This is quite similar to the phase diagram for a second-order phase transition which becomes first order.[15] D changes continuously across OB but discontinuously across the line AB. The value of $\Delta_c(0)$ may be obtained analytically, since it is the value of Δ for which

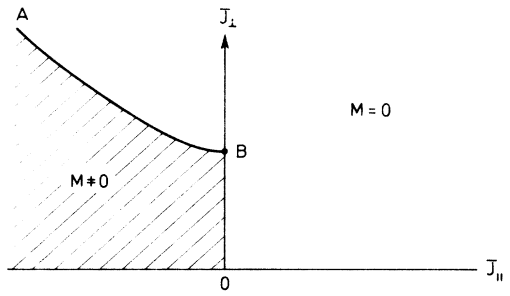

FIG. 1. Phase diagram in $[J_\parallel, J_\perp]$ plane using variational solution of Sec. V. For antiferromagnetic coupling, $J_\parallel > 0$. The shaded region corresponds to a finite moment. The point B occurs for $J_\perp\rho = \exp-[1+\gamma]$. The transition from $M = 0$ to $M \neq 0$ is continuous across OB but discontinuous across AB. $J_\parallel$, $J_\perp$ are defined in Eqs. (2.4) and (4.19).

$D=0$ becomes an unstable solution at $\epsilon=0$. Equation (5.11) gives $\Delta_c(0)=(2e\tau)^{-1}$. Although most of the line AB depends upon the details of the band structure, $\Delta_c(0)$ does not. From Eq. (4.21) the critical value of $J_\perp\rho$ at B is $e^{-(1+\gamma)}=0.21$, which is about the value expected experimentally, although B is not a physical point since one expects the coupling to be isotropic. The phase diagram differs from that obtained by Anderson, Yuval, and Hamann[5] by an approximate scaling technique. They found that the dividing line between $M=0$ and $M=$ finite was the isotropic ferromagnetic line. However, both agree that, for *isotropic coupling*, there is a moment for $\epsilon<0$ but not for $\epsilon>0$.

B. Perturbation theory for ground-state energy

When $D\neq 0$, $\mathcal{H}_1'$ splits the $H=0$ degeneracy of the ground state of $\mathcal{H}_0'$, and this is why the magnetization is zero. We shall now see that it also removes the infrared divergences in perturbation theory by putting a gap between the initial-state and intermediate-state energies. The unperturbed Hamiltonian is $\mathcal{H}_0'-\Delta\langle 0|e^{2S}|0\rangle\sigma_x$, which is solved exactly by the trial wave function $|\psi_0\rangle$, and the perturbation is $\mathcal{H}_1'+\Delta\langle 0|e^{2S}|0\rangle\sigma_x$, which has no diagonal matrix elements in $|\psi_0\rangle$. Using Eqs. (5.4) and (5.5), the contribution to the energy from second-order perturbation theory is

$$E_2=-\frac{H^2}{\Lambda^2}\sum_k\frac{(V_k-\omega_k f_k)^2}{\omega_k}+\left(1-\frac{H^2}{\Lambda^2}\right)\sum_k(V_k-\omega_k f_k)\left(f_k-\frac{V_k}{\omega_k+2\Lambda}\right)-\left(1-\frac{H^2}{\Lambda^2}\right)\frac{\Delta^2}{2}\int_0^\infty dt\,C_+(t)$$
$$+\frac{\Delta^2}{2}\int_0^\infty dt\,e^{-2\Lambda t}\left(C_-(t)-\frac{H^2}{\Lambda^2}C_+(t)\right)\ , \tag{5.21}$$

where

$$\Lambda^2=H^2+\Delta^2\,(D\tau e)^{2-\epsilon} \tag{5.22}$$

and

$$C_\pm(t)=\langle 0|e^{2S(t)}e^{2S}|0\rangle\pm\langle 0|e^{2S(t)}\times e^{-2S}|0\rangle-|\langle 0|e^{2S}|0\rangle|^2(1\pm 1). \tag{5.23}$$

Here $S(t)$ is the operator S, time evolved with the free boson Hamiltonian $\sum_k\omega_k b_k^\dagger b_k$, so that, using Eqs. (4.2), (5.2), and (5.8),

$$\langle 0|e^{2S(t)}e^{\pm 2S}|0\rangle=\exp\left(-(2-\epsilon)\int_0^{\rho/\tau}dk\,\frac{k}{(k+D\rho)^2}\,(1\pm e^{-kt/\rho})\right). \tag{5.24}$$

When $D\neq 0$, $C_-(t)\sim t^{-2}$, and $C_+(t)\sim t^{-4}$ for large t, and the time integrals in Eq. (5.21) converge for all ϵ. Thus the divergence in E_2 which occurs for $D=0$, $\epsilon>1$, as shown in Sec. III has been removed. At $\epsilon=1$, $E_2\approx\Delta_0^2\rho_0\ln D_0\tau$ for small Δ in agreement with the exact solution,[5] which is known for small τ. Near to $\epsilon=2$, E_2 is negligible, and it may be verified that the variational energy is correct by comparison with perturbation theory in V_k or with Wigner-Brillouin perturbation theory in Δ, evaluating all orders for small values of $(\epsilon-2)$. When $\epsilon\ll 1$, the variational energy is quite small, and E_2 is the dominant term. In fact, one can set $D=0$ in evaluating E_2 in this range of ϵ, since there are no infrared divergences and the correction produced by D_0 is negligible. However, $D\neq 0$ is essential in evaluating any infrared divergent term. In the energy, this means every order greater than $2/\epsilon$, and in M, S, and C, all orders for $\epsilon>0$. In calculating any property of the system, it is essential to evaluate terms in the perturbation series to see which order gives a good approximation. Since the energy requires second order when $\epsilon\ll 1$, the variational wave function is not necessarily a good approximation to the true wave function; it is merely a good starting point for pertubation theory.

C. Magnetic properties at $T=0$

The second-order contribution to the magnetization is given by $-\partial E_2/\partial H$ and, for $D=0$, this agrees with Eq. (3.9). However, for $D\neq 0$, $C_-(t)\sim t^{-2}$ and $C_+(t)\sim t^{-4}$ for large t and this, together with the factors $e^{-D_0 t}$, ensures that there is no divergence. This feature persists in higher orders of perturbation theory: Every order is finite and is an analytic function of H^2. Thus the zero-field magnetization vanishes, term by term, and the zero-order conclusion that the moment vanishes is unchanged.

Corrections to the susceptibility, however, are not small. In zero field, the second-order contribution to χ is given by $\chi_2=2(\partial E_2/\partial H^2)_{H=0}$, and it is easy to see from Eqs. (5.21)–(5.24), by changing variables of integration, that X_2 is of the form $\psi_1(\epsilon)(2/D_0)$, which is $\psi_2(\epsilon)$ times the zero-order susceptibility. A similar result is obtained in each order of perturbation theory, and these corrections cannot be neglected unless the $\psi_n(\epsilon)$ are small. In fact, $\psi_2(\epsilon)$ will contain terms proportional to ϵ^{-1} for small ϵ. They come both from the variation of D with H, as shown in Eq. (5.18)

and the time integrals in Eq. (5.21). Thus, when ϵ is small, the correction is bigger than the leading term [given by Eq. (5.15)]. This could have been anticipated from the discussion of Sec. III, since there are additional factors like $\epsilon^{1/\epsilon}$, which do not occur in Eq. (5.15) and must come from perturbation corrections, so that successive terms in the perturbation series will become larger and larger. It should be stressed that, in contrast to the original perturbation theory, each term of the series is finite and the problem is to get an accurate value for the coefficient of D_0^{-1}.

VI. ISING MODEL

In this section we wish to discuss the one-dimensional Ising model derived in Sec. IV and given in Eq. (4.9). The solution of the spin-boson problem described in Sec. V will be formulated directly for the Ising model. This will enable us at the same time to illustrate the general nature of the Ising model and to obtain the finite-temperature version of the variational solution. This latter could, of course, be derived directly from $\mathcal{H}_B$, but that is unnecessary since it will appear as a natural by-product of the discussion of the Ising model.

First, however, we consider two limiting cases to illustrate the peculiarities of the problem. The Ising Hamiltonian corresponding to Eq. (4.9) has a near-neighbor coupling $\frac{1}{2}\ln\beta\Delta/N$ and a long-range interaction $(\beta^2/N^2)\,B[\beta(m-n/N]$. From Eqs. (2.3), (4.17), and the fact that $B(t)=d^2C/dt^2$, it is clear that, when $T=0$,

$$\frac{\beta^2}{N^2}B\left(\frac{\beta(m-n)}{N}\right)\approx-\left(\frac{2-\epsilon}{8}\right)\frac{1}{(m-n)^2}$$

for
$$\frac{\beta|m-n|}{N}\gg\tau; \tag{6.1}$$

i.e. for sufficiently long range, we have an inverse-square interaction.

However, this is not the usual kind of Ising model for finite β, since the free energy has to be finite in the limit $N\to\infty$. This follows from the fact that the exponent in Eq. (4.4) simply becomes an integral in this limit. As an example, if $V_k=0$, the right-hand side of Eq. (4.7) is simply $1+(\beta\Delta/N)\sigma_x$, which has eigenvalues $1\pm\beta\Delta/N$. In the usual way the partition function is given by

$$\mathrm{Tr}\,M^N=\left(1+\frac{\beta\Delta}{N}\right)^N+\left(1-\frac{\beta\Delta}{N}\right)^N\xrightarrow[N\to\infty]{}e^{\beta\Delta}+e^{-\beta\Delta}. \tag{6.2}$$

In contrast to the usual extensive Ising model, both eigenvalues of the transfer matrix contribute in the thermodynamic limit, and the free energy is independent of N. The significance of the near-neighbor term may be seen in another way. Suppose $\Delta\to0$, with V_k finite. Since the result must be finite, it is necessary to have $\mu_n=+1$ for all n or $\mu_n=-1$ for all n to make the coefficient of $\ln\beta\Delta/N$ vanish in Eq. (4.9). In either case the sum involving B becomes $\int_0^\beta dt\int_0^\beta dt'\,B(t-t')$ as $N\to\infty$, and again this is independent of N. Both of these results may be obtained directly from $\mathcal{H}_B$.

If $\beta\to\infty$, it is possible, with some care, to rearrange the Ising model to an extensive form. Care is necessary because there are two limits, $\beta\to\infty$ and $N\to\infty$, and, since the ratio β/N occurs, we have the classical example of limits which cannot be interchanged. From the derivation it is necessary to let $N\to\infty$ first, because for fixed β the manipulations with the aid of the discrete ordering label are exact only if $N\to\infty$. This order may be achieved by setting $\beta=\alpha N$, taking $N\to\infty$, and finally $\alpha\to0$. The exponent in Eq. (4.9) becomes $-\mathcal{K}_I(\alpha)$, where

$$\mathcal{K}_I(\alpha)=-\alpha^2\sum_{m,n}^{N}B\,(\alpha(m-n))\;\mu_m\,\mu_n$$
$$-\frac{1}{2}\sum_n(1-\mu_n\mu_{n+1})\ln\alpha\Delta\,, \tag{6.3}$$

which is an extensive Ising Hamiltonian. If the free energy per spin is $f_I(\alpha)$, then the ground-state energy shift in the Kondo problem is given by

$$\lim_{\alpha\to0}\frac{N}{\beta}f_I(\alpha)=\lim_{\alpha\to0}\frac{f_I(\alpha)}{\alpha}\,. \tag{6.4}$$

Now the essential role of the $\alpha\to0$ limit may be seen. From Eq. (6.1) the long-range term is an inverse-square law only if $|m-n|\gg\tau/\alpha$, i.e., at infinitely long range when $\alpha\to0$. Also the near-neighbor coupling $\ln\alpha\Delta\to-\infty$ as $\alpha\to0$; i.e., it is ferromagnetic and infinitely strong. Clearly then, the near-neighbor term is likely to dominate the problem and one is far from a simple inverse-square interaction. In fact, we shall see that both terms come into play and the limit has to be taken with some care.[15]

We now turn to a derivation of the solution given in Sec. V, directly from the Ising model, where these points may be illustrated more explicitly.

We make use of the thermodynamic variation principle,[16] which states that the free energy F_I of the Ising Hamiltonian $\mathcal{H}_I$ satisfies

$$F_I\leqq F_{I0}+\langle\langle\,\mathcal{H}_I-\mathcal{H}_{I0}\,\rangle\rangle_0\,, \tag{6.5}$$

where $\mathcal{H}_{I0}$ is a trial Ising Hamiltonian, F_{I0} is the corresponding free energy, and $\langle\langle\,\hat{O}\,\rangle\rangle_0$ $=\mathrm{Tr}\,\hat{O}\,e^{-(\mathcal{H}_{I0}-F_{I0})}$ for any operator $\hat{O}$. (The "temperature" in the one-dimensional problem is set equal to unity.) We now consider $H=0$, for simplicity, and take

$$\mathcal{H}_{I0}=-\sum_{n=1}\frac{1}{2}(1-\mu_n\mu_{n+1})\ln\frac{\beta D}{2N}\,; \tag{6.6}$$

that is, it is the Hamiltonian $\mathcal{H}_I$ with B set equal

to zero and Δ replaced by $\frac{1}{2}D$. This says that it is a good starting point (and, for some ϵ, a good approximation) to keep only the near-neighbor interaction and to ignore the long-range term. The free energy F_{I0} may be obtained by the standard transfer matrix method[12]:

$$F_{I0}/N = -(1/N)\ln[\lambda_+^N + \lambda_-^N] \ , \tag{6.7}$$

where

$$\lambda_\pm = 1 \pm (\beta D/2N) \tag{6.8}$$

are the eigenvalues of the transfer matrix [set $V_n = 0$ in Eq. (4.7)]. As explained above, for the nonextensive case (β finite) it is necessary to keep both roots. To evaluate Eq. (6.5), we need the correlation function

$$\ll \mu_i \mu_j \gg_0 = \frac{(\lambda_-/\lambda_+)^{j-i} + (\lambda_-/\lambda_+)^{N+i-j}}{1+(\lambda_-/\lambda_+)^N}, \quad j > i. \tag{6.9}$$

We first consider the extensive case, $\beta/N = \alpha$ and β and $N \to \infty$. From Eqs. (4.7) and (6.5)–(6.9),

$$\frac{F_I}{N} \leqq -\ln\left(1+\frac{\alpha D}{2}\right) - \frac{\alpha^2}{N}\sum_{m,n}^{N} B[\alpha(m-n)] \times \left(\frac{1+\frac{1}{2}\alpha D}{1-\frac{1}{2}\alpha D}\right)^{-|m-n|} - \frac{\alpha D}{2+\alpha D}\ln\frac{2\Delta}{D} \ . \tag{6.10}$$

Then by Eq. (6.4) the ground-state energy in the Kondo problem is

$$\lim_{\alpha\to 0}\frac{F_I}{\alpha N} \leqq \frac{-D}{2}\left(1+\ln\frac{2\Delta}{D}\right) - 2\int_0^\infty dt\, e^{-Dt}B(t) \tag{6.11}$$

and minimizing with respect to D,

$$D = 2\Delta \exp\left(-4\int_0^\infty dt\, e^{-Dt} t\, B(t)\right) . \tag{6.12}$$

Using Eq. (4.10) with $T = 0$, this is the same equation for D as obtained by minimizing Eq. (5.7) with $H = 0$, and the ground-state energies are the same at minimum. From Eq. (6.12) it can be seen that it is the large-t behavior of $B(t)$ which determines how the right-hand side varies for small D. This supports the use of the long-time approximation. Furthermore, since B depends upon V_k^2, it follows that, for $D = 2\Delta$, the right-hand side of Eq. (6.11) is just second-order perturbation theory in V_k and Eq. (6.11) shows that it is an upper bound for the ground-state energy. Of course, by varying D it is possible to obtain a much better bound, in general.

The derivation of Eq. (6.12) illustrates the essential nature of the limit $\alpha \to 0$. Without it, we should not obtain the same energy as the spin-boson Hamiltonian and, furthermore, the approximation on the Ising model would not be believable. This is because we have assumed that the near-neighbor correlation functions give a good trial density matrix, which is plausible in the limit $\alpha \to 0$, since the near-neighbor coupling becomes infinite [see Eq. (6.3)].

For $T \neq 0$, it is necessary to let $N \to \infty$ in Eqs. (6.5)–(6.9), keeping β finite. Both eigenvalues of the transfer matrix must be kept, since the Ising model is intensive. The free energy F for the spin-boson Hamiltonian is $F_{I/\beta}$ and, from Eqs. (6.5)–(6.9),

$$\frac{F_I}{\beta} = F_K \leqq -\frac{1}{\beta}\ln\left(2\cosh\frac{\beta D}{2}\right) - \left(\frac{D}{2}\right)\ln\frac{2\Delta}{D} - \int_0^\beta dt\, B(t)\frac{e^{-Dt}+e^{-(\beta-t)D}}{1+e^{-\beta D}} \ , \tag{6.13}$$

which reduces to Eq. (6.11) as $\beta \to \infty$. This is a finite-temperature form of the variational principle of Sec. V.

Equation (6.13) may be rewritten

$$F_K \leqq -\frac{1}{\beta}\ln\left(2\cosh\frac{\beta D}{2}\right) - \left(\frac{D}{2}\right)\ln\frac{2\Delta}{D} - \frac{1}{2}\sum_k V_k^2\left(\frac{1-\coth\frac{1}{2}\beta\omega_k\tanh\frac{1}{2}\beta D}{\omega_k - D} + \frac{1+\coth\frac{1}{2}\beta\omega_k\tanh\frac{1}{2}\beta D}{\omega_k + D}\right), \tag{6.14}$$

from which the finite-temperature properties may be calculated. A similar derivation of the connection between the Kondo problem and a one-dimensional Ising model was given by Anderson and Yuval.[6] However, they set $\alpha = \tau$ and then, by choice of $J_\perp$, were able to remove the near-neighbor term and obtain the particularly interesting case of an inverse-square interaction. We have shown here that the limit $\alpha \to 0$ is required by the proof, and hence the Kondo problem and the inverse-square Ising model are equivalent only if *the existence of a phase transition* as well as its associated singular behavior are independent of the value of α even when $\alpha \to 0$. Arguments based upon "universality" lead one to believe that, *if a transition occurred*, the associated singular behavior would be independent of α for finite α. In other words, on scaling and eliminating the short-range couplings,[6] one is eventually led to a limiting Hamiltonian which is independent of the details of the short-range couplings. However, it is also necessary to show that this limiting process can be interchanged with the limit $\alpha \to 0$. Since, when $\alpha \to 0$, there is an infinite near-neighbor coupling and also the point $m - n = \tau/\alpha$ (at which the inverse-square law begins) tends to infinity [see Eq. (6.1)], then the Hamiltonian is drastically different from that for finite α and it

seems unlikely that the required universality exists in the limit $\alpha \to 0$.

VII. CONCLUSIONS

We have shown how the general nature of the singularities of Kondo problem may be displayed explicitly with the aid of the long-time approximation. By considering the equivalent spin-boson problem, we have determined the phase diagram, shown in Fig. 1, which gives the regions in the $(J_\parallel, J_\perp)$ plane in which the zero-temperature moment M is finite or zero. In contrast to the usual perturbation theory, we obtain series which are finite term by term for M (when $M \neq 0$) and for χ (when $M = 0$). However, in both cases, it is necessary to do a partial summation of perturbation theory in order to obtain an accurate value for these quantities.

Our phase diagram is not the same as that obtained by Anderson, Yuval, and Hamann.[5] The difference appears to lie in the use of the long-time approximation. This is quite essential for the derivation of the spin-boson Hamiltonian, and the equivalence of $\mathcal{K}_K$ and $\mathcal{K}_B$ requires that the cutoff $t_0 \to 0$. On the other hand, the scaling method of Ref. 5 was based upon Eq. (2.2) but made no essential use of the long-time approximation, since it has been shown to be equivalent to the renormalization-group equations for $\mathcal{K}_K$ in lowest-order perturbation theory.[17] Now the homogeneity relation derived in Sec. III shows that, for $H = 0$, $T = 0$, $J_\perp \rho$ and t_0 occur in the combination $(J_\perp \rho) \times (t_0 \rho)^{\epsilon/2}$, so that if one let $t_0 \to 0$, keeping ρ and τ fixed, the phase diagram[5] for $\mathcal{K}_K$ would become the same as Fig. 1 for small $J_\perp$. Thus the phase diagrams are the same in the limit in which $\mathcal{K}_K$ and $\mathcal{K}_B$ are equivalent but appear to be different for $t_0 = \tau$. It should be emphasized that the comparison with the scaling theory refers only to the phase diagram. No calculation of the susceptibility, specific heat, resistivity, etc., was made in Ref. 5.

ACKNOWLEDGMENTS

We wish to acknowledge helpful discussions with P. W. Anderson, G. A. Baker, M. Blume, B. Buck, D. C. Mattis, and S. Kahana.

---

*Work carried out mainly at Brookhaven National Laboratory, Upton, N. Y., under the auspices of the U.S. Atomic Energy Commission.

†Visiting Professor.

[1]J. Kondo, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969), Vol. 23, p. 184.

[2]G. Yuval and P. W. Anderson, Phys. Rev. B **1**, 1522 (1970).

[3]D. R. Hamann, Phys. Rev. B **2**, 1373 (1970).

[4]P. Nozières and C. T. de Dominicis, Phys. Rev. **178**, 1097 (1969).

[5]P. W. Anderson, G. Yuval, and D. R. Hamann, Phys. Rev. B **1**, 4464 (1970); and Solid State Commun. **8**, 1033 (1970).

[6]P. W. Anderson and G. Yuval, J. Phys. C **4**, 607 (1971).

[7]V. J. Emery and A. Luther, Phys. Rev. Lett. **26**, 1547 (1971).

[8]M. Blume, V. J. Emery, and A. Luther, Phys. Rev. Lett. **25**, 450 (1970).

[9]K. D. Schotte and U. Schotte, Phys. Rev. B **4**, 2228 (1971).

[10]K. D. Schotte and U. Schotte, Phys. Rev. **182**, 479 (1969); K. D. Schotte, Z. Phys. **230**, 99 (1970).

[11]R. P. Feynman, Phys. Rev. **84**, 108 (1951).

[12]T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. **36**, 856 (1964).

[13]See, for example, Appendix A of A. C. Zemach and R. J. Glauber, Phys. Rev. **101**, 118 (1956).

[14]See, for example, R. A. Ferrell, Phys. Rev. **186**, 399 (1969).

[15]L. D. Landau and E. M. Lifschitz, *Statistical Physics*, 2nd ed. (Addison-Wesley, Reading, Mass., 1969), p. 424.

[16]See, for example, H. Falk, Am. J. Phys. **38**, 858 (1970), Eq. (64).

[17]M. Fowler and A. Zawadowski, Solid State Commun. **9**, 471 (1971).