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Exact Results in the Kondo Problem. II. Scaling Theory, Qualitatively Correct Solution, and Some New Results on One-Dimensional Classical Statistical Models

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The simplest Kondo problem is treated exactly in the ferromagnetic case, and given exact bounds for the relevant physical properties in the antiferromagnetic case, by use of a scaling technique on an asymptotically exact expression for the ground-state properties given earlier. The theory also solves the $n=2$ case of the one-dimensional Ising problem. The ferromagnetic case has a finite spin, while the antiferromagnetic case has no truly singular $T\to 0$ properties (e.g., it has finite χ).

I. INTRODUCTION

A previous paper[1] showed that the simplest Kondo problem is equivalent to a certain class of problems in the classical statistical mechanics of one-dimensional systems. One limit of the problem of the Anderson model of a magnetic impurity also leads to the same classical problem.[2] This problem was stated in Ref. 1 as the statistical mechanics of a set of alternating hard rods on a line interacting via logarithmic ("two-dimensional Coulomb") potentials:

$$\langle 0|e^{-\beta\mathcal{H}}|0\rangle = Z' = \sum_n \left(\frac{J_\pm}{2}\right)^{2n} \int_0^\beta d\beta_{2n} \int_0^{\beta_{2n}-\tau} d\beta_{2n-1} \times \cdots \int_0^{\beta_2-\tau} d\beta_1 \exp\sum_{i>j} (-1)^{i-j}(2-\epsilon) \times \ln\left(\frac{\beta_i-\beta_j}{\tau}\right). \quad (1)$$

Here $\mathcal{H}$ is the Hamiltonian of the Kondo system:

$$\mathcal{H} = \text{K. E.} + 2J_\pm(S_+s_- + S_-s_+) + J_z s_z S_z, \quad (2)$$

S being the local spin ($S=\frac{1}{2}$) and s the spin of the free electrons at the local site. τ is a cutoff of order $1/E_F$, and

$$\epsilon = 8\delta/\pi - 8\delta^2/\pi^2 \simeq 2J_z\tau, \quad (3)$$

where δ is the scattering phase shift of antiferromagnetic sign caused by the $J_z s_z S_z$ term. $|0\rangle$ is the unperturbed ground state of $\mathcal{H}_0 = \text{K. E.} + JS_z s_z$.

Since we depend so completely here on the result Eq. (1) of Ref. 1, let us outline the argument of that paper and try to clarify the meaning of Eq. (1). In that paper we go to the Feynman space-time formalism (actually space-imaginary time = temperature) and, since the Kondo problem of the magnetic impurity treats only a single-point impurity, the question reduces to a sum over paths in only the one ("time") dimension. In addition, the perturbation [which we take as the $J_\pm$ term of Eq. (2)] has the effect of flipping the local spin at each application, so that the problem reduces to calculating the amplitude for a succession of spin flips at times $\beta_1, \beta_2, \ldots$ and the sum over histories is just the sum over all possible numbers and positons of flips. Thus, formally we can write a ground-state average such as Eq. (1) as a grand partition function of an effective one-dimensional gas of spin flips. The one difficult step of Ref. (1) is that of showing that the effective interaction in this one-dimensional gas is a simple logarithmic pair interaction, and it is only at long enough distances $\beta_i - \beta_j$ that the proof we used is precise. Fortunately, the classic Kondo problem has been defined as the calculation of the limiting behavior for small J, in which case the gas of spin flips becomes increasingly rarified and the behavior for large distances must be controlling; as we shall see, this statement has a precise meaning in the context of the present paper. This corresponds to the fact that the Kondo effect has always been assumed to involve only electrons near the Fermi surface. But because of the singular nature at small $\beta_i - \beta_j$ of the asymptotic expression valid for large $\beta_i - \beta_j$, at several stages of the problem the behavior for small $\beta_i - \beta_j$ must be handled in some way such as to avoid ultraviolet divergences; and cutoffs of various shapes [of which Eq. (1) is

an example] must be introduced. It is easy to see that such a cutoff must be present physically; energy bands are not infinitely wide, and J's involve form factors of physical wave functions. In the derivation of Eq. (1), the "origin-to-origin unperturbed Green's function"

$$G_0(t) = \langle 0 | T\psi(0)\psi^\dagger(t) | 0 \rangle ,$$

where ψ is the normalized wave function coupled to the local spin, enters. G_0 behaves like τ/t at large times, where τ is the density of states $\sim 1/E_F$, and has an easily computed cutoff at short times for any given ψ and band structure. Of Eq. (1) we know only that the relevant τ is closely related to the cutoff in G_0, a relationship which may be computed precisely only in certain limiting cases.

Let us also remark that only a slight modification of Eq. (1) gives the finite-temperature partition function of the Kondo problem, which will be the subject of a later paper. Essentially, one replaces $\ln[(\beta_i - \beta_j)/\tau]$ by

$$\ln\{(\beta/2\pi\tau)\sin[(\beta_i - \beta_j)/2\pi\beta]\} ,$$

where $\beta = 1/T$.[3]

One important thing to note is that a transformation $S_x \to -S_x$, $S_y \to -S_y$, $S_z \to +S_z$ leaves the dynamics of the spin unchanged (it is simply a proper rotation of the coordinate system) so that the sign of $J_\pm$ is irrelevant. The sign of J_z, and thus of ϵ, determines whether the coupling is ferromagnetic or antiferromagnetic. As we have it, $\epsilon > 0$ is antiferromagnetic. Thus by varying ϵ with $J_\pm$ fixed (i.e., varying the effective "temperature" of the statistical problem) we can go continuously from ferromagnetic to antiferromagnetic coupling. Manifestly, the quantity (1) is a function only of three parameters, β/τ, $J_\pm\tau$, and $\epsilon \simeq 2J_z\tau$. As $\beta \to \infty$ we expect $Z = e^{\beta F}$, and $F\tau$ is now a function only of $J_\pm\tau$ and ϵ. We may think of these two parameters as the exponential of the chemical potential for spin flips, and as the effective temperature of the classical problem (which is to be carefully distinguished from the real temperature β^{-1}, which is the inverse of the "volume" and goes to zero as the length of the line increases to ∞). The quantity F is the negative of the ground-state energy relative to that of $\mathcal{H}_0$; in the one-dimensional problem, however, it plays the role of a "pressure," conjugate to the "volume" β. All $\beta \to \infty$ problems may be plotted on a diagram [Fig. 1(a)] on which two lines, radiating from $\epsilon = 0$ to left and right, represent the manifold of physical (isotropic) Kondo problems of ferromagnetic and antiferromagnetic sign.

It is commonly believed that the ferromagnetic Kondo system has a mean spin moment at absolute zero, while the antiferromagnetic one does not. It is easy to see that the possession of a spin moment at 0 corresponds to a long-range order of the classical system in which + and − charges are all associated in pairs pointing in one direction, either left or right. This type of order is clearer if we partially integrate the interaction twice and write Eq. (1) as an integral over all possible paths of a function $S_z(\beta')$:

$$\langle 0 | e^{-\beta\mathcal{H}} | 0 \rangle = \int d(\text{paths}) \exp\left[\frac{2-\epsilon}{2}\int_0^\beta\int_0^\beta d\beta'\, d\beta'' \frac{S_z(\beta')S_z(\beta'')}{(\beta'-\beta'')^2+\gamma^2} - (\ln J_\pm)\times(\text{number of jumps})\right] . \quad (4)$$

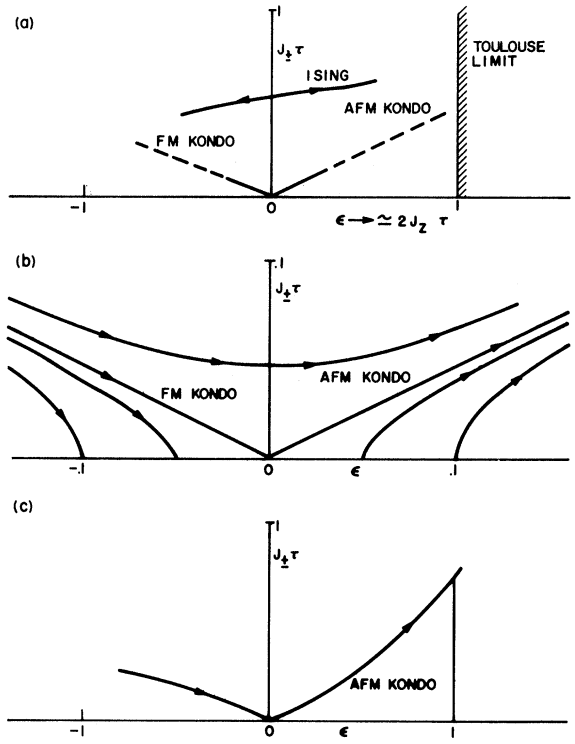

FIG. 1. Space of possible Ising models and Kondo Hamiltonians. The Kondo Hamiltonians are characterized by $J_z\tau$ and $J_\pm\tau$, the former being roughly proportional to ϵ, the horizontal axis, and the latter being the vertical axis. (a) Relationships among various cases. The coefficient of long-range forces in the corresponding Ising model is $2-\epsilon = V_{1r}/T_{\text{Ising}}$ and of short-range forces $(\text{const}\times V_{1r} + V_{sr})/T_{\text{Ising}} = \ln(1/J_\pm\tau)$. Isotropic Kondo models are on the lines $\epsilon = \pm 2J_\pm\tau$ as $J \to 0$. The soluble Toulouse limit is $\epsilon = 1$. (b) Exact scaling curves for small J. Scaling is unidirectional in the direction of the arrows. The Ising transition is at the line FM Kondo. (c) Approximate scaling curves for strong interactions according to "upper limit" of Fig. 5. "Best guess" would be almost indistinguishably lower.

Here $S_z(\beta)$ is a function of the form of Fig. 2; it takes on only the values $\pm\frac{1}{2}$ and jumps (with either a minimum jump time or a form factor of order τ) between these two values at will. Then the long-range order which implies magnetization is the long-range order of $S_z(\beta')$. This last expression is, in turn, essentially equivalent to an Ising model with a long-range ferromagnetic interaction with form $1/(i-j)^2$ and strength $(1-\epsilon/2)$, and a short-range ferromagnetic interaction $\ln(1/J_\pm\tau)$ + const.

It may be best to make a pedagogic point about the meaning of the asymptotic validity of (1) on this Ising-model version of the problem. It is recognized universally, for sound but not generally explicitly stated reasons, that the qualitative behavior, at least, of such Ising models is entirely controlled by the long-range forces. The basic reason is that short-range forces cannot lead to long-range order, or even to short-range order decaying more slowly than exponentially. Thus, the nature of all long-range singularities (corresponding to low-temperature or low-frequency singularities in the Kondo effect) is entirely determined by the long-range interaction, for which the asymptotic theory that we use is accurate.

Incidentally, a theorem of Griffith[4] shows that the correlations cannot be weaker than the long-range forces themselves in the Ising model, thus, than $1/\beta^2$. We shall show that this is indeed the correlation behavior in the antiferromagnetic case,

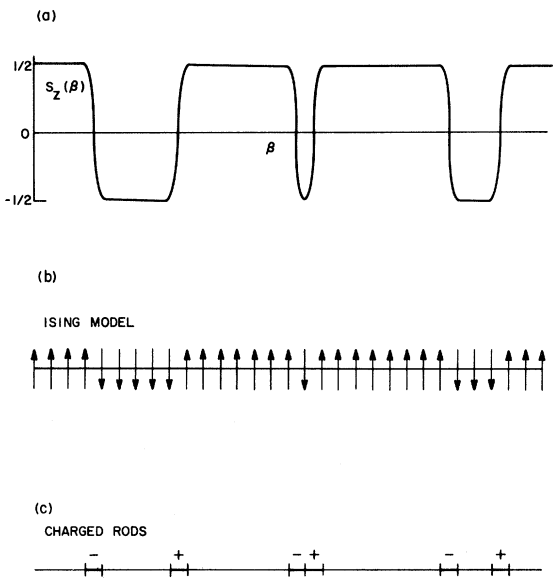

FIG. 2. Corresponding one-dimensional statistical models. (a) Path integral of $S_z(\beta)$, (b) Ising model, (c) charged rod model. Corresponding configurations as a function of β are shown.

since we derive also an upper limit to the correlations in that case.

Dyson has been unable to determine whether or not this Ising model has a phase transition.[5] One purpose of this paper is to show that it does [actually on the original model (1)] and that at least for small $J_\pm$ this does indeed occur at the ferromagnetic-antiferromagnetic boundary point $\epsilon = 0$. We also throw considerable further light on the Kondo problem (though, unfortunately, without achieving a completely exact solution of the interesting antiferromagnetic case) by showing that there is a rigorous scaling technique which reduces the two-dimensional manifold of Fig. 1 to a one-dimensional one. In particular, we can map the entire ferromagnetic line on the point at the origin ($\epsilon = 0$), thus solving the ferromagnetic case really exactly and showing that it has finite magnetization. All cases to the left of the ferromagnetic ones can be mapped on the $J_\pm = 0$ line, and thus are soluble and ordered.

The same scaling laws map all antiferromagnetic cases onto each other, the scale factor being the Kondo temperature. Unfortunately, the direction is in the sense of increasing $J_\pm\tau$, which carries one eventually into the region where the scaling equations are form-factor dependent numerically. Nonetheless, the meaning of the Kondo temperature, the fact that the state is unpolarized, and the connection with perturbation theory are all clear. Inequalities can be found which show that the renormalization procedure is qualitatively valid up to $\epsilon = 1$. Thus, since all cases with $\epsilon = 1$ are exactly soluble (a remark due independently to Toulouse[6]), we can give a solution with parameters correct to logarithmic accuracy. We believe this solution to be at least qualitatively right; in particular, it gives correlation functions which indicate nonsingular properties at absolute zero, in contradiction to most previous theories.[7]

II. SCALING THEORY OF THE COULOMB GAS MODEL

The technique we use is a "renormalization" of the cutoff parameter τ, which leads to a set of scaling laws connecting a given problem to ones with different parameter values. We show that all pairs of flips closer than $\tau_1 > \tau$ can be eliminated, leaving a problem of precisely the same form but with modified parameters $\tilde{J}_\pm\tau_1$ and $\tilde{\epsilon}(\tau_1)$, and a modified F:

$$Z'(J_\pm\tau, \epsilon) = Z'(\tilde{J}_\pm\tau_1, \tilde{\epsilon})\exp\Delta F_{\tau_1}\beta \ . \qquad (5)$$

These scaling laws are exact for small $J_\pm\tau$ and ϵ, and are subject to precise inequalities in any case.

First we observe that if $J_\pm\tau$ is small enough, there will be few spin flips + or −: Our "Coulomb gas" of spin flips is a rarified one. On the other

hand, in the presence of the strong $\ln(\beta_i - \beta_j)$ interaction, those which are present will tend to appear as close pairs. Clusters of more than two will not form with high probability because the + and − members of a pair attract and repel a third flip with equal intensity:

$$-\ln(\beta_i + \Delta\beta - \beta_j) + \ln(\beta_i - \beta_j) \simeq -[\Delta\beta/(\beta_i - \beta_j)] .$$

Thus, pairs attract singles with a weak $1/x$ potential, which cannot overwhelm the large $(-\ln J_\pm)$ extra energy required to make a group of three. Thus, close pairs of flips form reasonably self-contained systems whose behavior is mostly determined by the internal force between the pair. It is easy to calculate that the mean distance between pairs is

$$\frac{1}{l_0} = N = \frac{1}{\beta}\frac{\partial \ln Z'}{\partial \mu} = \frac{\partial E_g}{\partial[\ln(\frac{1}{2}J_\pm)^2]} , \tag{6}$$

where we note (see Ref. 1) that Z' as defined in Eq. (1) is a constant times $e^{-\beta E_g}$, and E_g is the ground-state energy relative to $\langle 0|\mathcal{H}|0\rangle$. Second-order perturbation theory gives an estimate for E_g adequate for our purposes:

$$E_g \simeq \tfrac{1}{4}J_\pm^2\tau , \quad l_0 \sim 2\tau/(J_\pm\tau)^2 . \tag{7}$$

We can also estimate that the separation of spin flips tends to be of the order

$$\bar{X} \sim \tau/\epsilon , \tag{8}$$

although the actual mean value is dependent on the precise treatment of long-range forces and is not well defined. In any case for ϵ and $J_\pm\tau$ small

$$l_0 \gg \bar{X} \gg \tau . \tag{9}$$

The physical picture we have is of many close pairs of flips which change the mean magnetization slightly, interspersed between pairs of isolated flips which are real reversals of M over a larger timescale. This suggests that we might consider the isolated flips as operating in a medium where the close pairs merely modify the mean magnetization (see Fig. 3). It is this idea which we now give a rigorous form.

Consider only "close pairs," so close that their separation is between the limits $\tau \le \beta_{i+1} - \beta_i < \tau + d\tau$. If $d\tau$ is infinitesimal, such a pair occurs very rarely, so we may completely neglect the possibility of two successive close pairs occurring. Then we can rewrite the integrals in Eq. (1) as follows:

$$\cdots \int_0^{\beta_5-\tau} d\beta_4 \int_0^{\beta_4-\tau} d\beta_3 \int_0^{\beta_3-\tau} d\beta_2 \int_0^{\beta_2-\tau} d\beta_1$$

$$= \int_0^{\beta_5-\tau-d\tau} d\beta_4 \int_0^{\beta_4-\tau-d\tau} d\beta_3$$

$$\times \int_0^{\beta_3-\tau-d\tau} d\beta_2 \int_0^{\beta_2-\tau-d\tau} d\beta_1 \quad \text{(all "free")}$$

$$+ \int_0^{\beta_5-\tau-d\tau} d\beta_4 \int_0^{\beta_4-\tau-d\tau} d\beta_3$$

$$\times \int_0^{\beta_3-\tau} d\beta_2 \int_{\beta_2-\tau-d\tau}^{\beta_2-\tau} d\beta_1 \quad \text{(1, 2 paired)}$$

$$+ \int_0^{\beta_5-\tau-d\tau} d\beta_4 \int_0^{\beta_4-\tau} d\beta_3$$

$$\times \int_{\beta_3-\tau-d\tau}^{\beta_3-\tau} d\beta_2 \int_0^{\beta_2-\tau-d\tau} d\beta_1 \quad \text{(2, 3 paired)}$$

$$+ \cdots , \tag{10}$$

and between any pair of free flips (such as 4 and 1 in the second version above) there may be only one close pair; two only occur $\sim (d\tau)^2 = 0$.

We rearrange the sum (10) in a familiar way: We group together all terms with $2n$ free β's, between each pair of which there may be either zero or one close pair with separation $\sim\tau$. Consider one particular pair of free β's, β_i and β_{i+1}. We now have

$$Z = \sum_n \int^\beta \cdots \int_0^{\beta_{i+2}-\tau-d\tau} d\beta_{i+1} \int_0^{\beta_{i+1}-\tau-d\tau} d\beta_i$$

$$\cdots (\tfrac{1}{2}J_\pm)^{2n} \exp[-V_0(\beta_{2n}\cdots\beta_{i+1}, \beta_i \cdots)]$$

$$\times \prod_i \{1 + \tfrac{1}{4}J_\pm^2 \int_{\beta_i+2\tau}^{\beta_{i+1}} d\beta' \int_{\beta'-\tau-d\tau}^{\beta'-\tau} d\beta'' \exp[-V$$

$$\times (\beta' - \beta_{2n}, \beta' - \beta_{2n-1}\cdots, \beta'' - \beta_2 \cdots, \beta' - \beta'')]\} . \tag{11}$$

The β'' integral just multiplies by a factor $d\tau$. Now let us examine $V(\beta', \beta'')$ which expresses the dependence of the amplitude on β' and β'':

$$\exp(-V) = \left[\left(\frac{\beta_{i+1} - \beta''}{\beta_{i+1} - \beta'}\right)\left(\frac{\beta_{i+2} - \beta'}{\beta_{i+2} - \beta''}\right)\left(\frac{\beta_{i+3} - \beta''}{\beta_{i+3} - \beta'}\right)\cdots \right.$$

$$\left. \times \left(\frac{\beta' - \beta_i}{\beta'' - \beta_i}\right)\left(\frac{\beta'' - \beta_{i-1}}{\beta' - \beta_{i-1}}\right)\cdots\right]^{2-\epsilon} .$$

We have $\beta' - \beta'' = \tau$, so this may be written

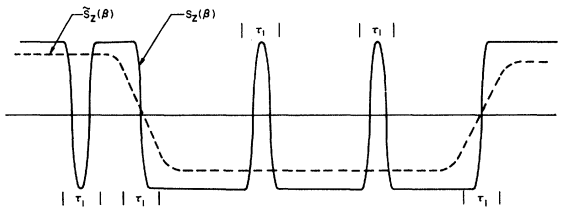

FIG. 3. Visualization of the renormalization process: We replace $S_z(\beta)$ by a long-term average including the effect of all spin-flip pairs closer together than τ_1.

$$\exp(-V)=\left[\left(1+\frac{\tau}{\beta_{i+1}-\beta}\right)\left(1+\frac{\tau}{\beta''-\beta_i}\right)\times\left(1+\frac{\tau}{\beta_{i+2}-\beta'}\right)^{-1}\left(1+\frac{\tau}{\beta''-\beta_{i-1}}\right)^{-1}\cdots\right]^{2-\epsilon} \tag{12}$$

and our basic approximation is simply to write the integral of this over the permitted range of β' as (we denote the integral by an average $\langle\ \rangle$ to save writing)

$$\langle\exp(-V)-1\rangle\cong(2-\epsilon)\tau\left\langle\frac{1}{\beta_{i+1}-\beta'}+\frac{1}{\beta''-\beta_i}-\frac{1}{\beta_{i+2}-\beta'}-\frac{1}{\beta''-\beta_{i-1}}+\cdots\right\rangle\ . \tag{13}$$

Let us make some comments about this approximation, which is much better than it looks. (1) It obviously correctly reproduces the dependence on all β's far from i. (2) The alternating series are rapidly converging as is the product in Eq. (12). (3) For small ϵ even $\tau/(\beta_i-\beta')$ is of order ϵ and thus small. (4) All intervals between β's are $>\tau$ so that $\exp(-V)<4$ and that occurs only with very low probability. In the Appendix, we consider the validity of the approximations in great detail and show that Eq. (12) is exact in a certain asymptotic sense, and that rigorous limits may be set on the behavior.

Inserting Eq. (13) in Eq. (10), we get

$$Z=\sum_n\int_0^{\beta}\cdots\int_0^{\beta_{i+2}-\tau-d\tau}d\beta_{i+1}\cdots(\tfrac{1}{2}J_\pm)^{2n}\exp(-V_0)\times\prod_i\left[1-(\tfrac{1}{2}J_\pm)^2\,d\tau\left\{(\beta_{i+1}-\beta_i-3\tau)\times\left(1+(2-\epsilon)\tau\left\langle\sum\pm\frac{1}{\beta_n-\beta'}\right\rangle\right)\right\}\right]. \tag{14}$$

Since $d\tau$ is infinitesimal, we may exponentiate the $J_\pm^2 d\tau$ terms. The factor involving $\beta_{i+1}-\beta_i$ gives us

$$Z=\exp[(\tfrac{1}{2}J_\pm)^2\beta\,d\tau]\tilde{Z}\ , \tag{15}$$

where $\tilde{Z}$ is formally the same as in Eq. (1) except for modifications of the amplitudes. Calculating these modifications, we distinguish two regions. First, there is the region of small $J_\pm\tau$ and ϵ, where $\beta_{i+1}-\beta_i$ is in general $\sim l_0\gg\tau$, and we neglect corrections of order $\tau/\Delta\beta$. Then we have very simply

$$\int\frac{d\beta'}{\beta_n-\beta'}\cong\ln\frac{\beta_n-\beta_{i+1}}{\beta_n-\beta_i}, \tag{16}$$

with each interval $i\to i+1$ contributing two terms, one for each end; counting in the ones for $n\to n\pm1$ we get four in all. Then we neglect τ relative to the interval and get

$$\tilde{Z}=\sum_n(\tfrac{1}{2}J_\pm)^{2n}\prod_m\int_0^{\beta_{m+1}-\tau-d\tau}d\beta_m\times\exp\{(2-\epsilon)n\ln\tau+[2-\epsilon-J_\pm^2\tau\,d\tau(2-\epsilon)]\times\sum_{i>j}(-1)^{i-j}\ln(\beta_i-\beta_j)\}. \tag{17}$$

Clearly, $\tilde{Z}$ is of the appropriate form of a modified Z with a new interaction $\epsilon\to\tilde{\epsilon}=\epsilon+d\epsilon$

$$d\epsilon=(2-\epsilon)J_\pm^2\tau\,d\tau=(2-\epsilon)(J_\pm\tau)^2\,d(\ln\tau). \tag{18}$$

Although apparently $J_\pm$ is unmodified, we know that, in fact, there will be fewer flips per unit β in $\tilde{Z}$ than in Z. The cutoff has been altered, while the dimensional coefficient $\tau^{(2-\epsilon)n}$ in the amplitude is unchanged. In order to reduce $\tilde{Z}$ to the form of Z in Eq. (1), we must change

$$J_\pm\tau\to\tilde{J}_\pm\tilde{\tau}=J_\pm\tau[(\tau+d\tau)/\tau]^{\epsilon/2} \tag{19}$$

and then it may be verified that

$$\tilde{Z}=Z[\beta/\tilde{\tau},\ (\tilde{J}_\pm\tilde{\tau}),\ \tilde{\epsilon}]\ . \tag{20}$$

Equation (19) may be written in differential form:

$$d(J_\pm\tau)=\tfrac{1}{2}\epsilon(J_\pm\tau)\,d(\ln\tau)\ . \tag{21}$$

Equations (15), (18), and (21) are the basic scaling laws which solve the problem in the small ϵ, $J_\pm$ case.

Let us add a few more words about the validity of Eqs. (15), (18), and (21). It may appear at first that the use of $d\tau$ infinitesimal may make the computation sensitive to the region near the cutoff. Note, however that in the basic laws, Eqs. (18) and (21), the infinitesimal is $d(\ln\tau)$ multiplied by $(J_\pm\tau)^2$. Thus, so long as the latter is even reasonably small, rather large jumps in $\ln\tau$, and thus large *factors* in τ, can be considered to be infinitesimal. (This was, in fact, the route by which we arrived originally at these equations.) Thus the first few steps for any true Kondo problem (defined as small $J\tau$) are cutoff independent. After the first step, the cutoff is an artifact of the method and may be chosen at will as in the Appendix. Note also that the small factors need only be $J_\pm\tau$ in all equations; finite ϵ is still treated as accurately as desired. Thus the scaling laws are exact throughout the lower region of Fig. 1.

Note that Eqs. (21) and (18) are compatible in the isotropic case $J_z=J_\pm$, $\epsilon\cong 2J_z\tau\cong 2J_\pm\tau$, and where ϵ and $J_\pm\tau$ are small. Thus ϵ and $J_\pm\tau$ scale together, and, as should not be entirely unexpected, the isotropic case remains isotropic at every time scale. For anisotropic cases,

$$d\epsilon/d(J_\pm\tau)\cong 4J_\pm\tau/\epsilon,\quad \epsilon^2-4J_\pm^2\tau^2=\text{const.} \tag{22}$$

The scaling lines are a set of hyperbolas with the isotropic cases as asymptotes [see Fig. 1(*b*)]. All ferromagnetic cases below the isotropic one scale

onto the case $J_\pm\tau=0$, which is manifestly ordered, thus locating the transition line at the ferromagnetic case [or above, but we shall argue that all antiferromagnetic cases are disordered and that the two scale into each other according to Fig. 1(b)].

Before going on to further results let us discuss the regime where ϵ and $J_\pm\tau$ are no longer negligible compared to 1. It turns out that for many reasons it is not possible to follow the renormalization in complete detail when it reaches this region (as it obviously shall for the antiferromagnetic cases from Fig. 1). It is not, in fact, even very necessary to do so. What is necessary is to show that there is no tendency for the renormalization process to stop short of $\epsilon=1$, the case where an exact solution exists as we shall see. To alter the actual parameters by numerical constants which are not exponentially large is physically almost irrelevant. Thus the essential thing is to bound the corrections $d\epsilon/d\tau$ and $dJ_\pm\tau/d\tau$ above (below) some finite numbers. This program is carried out in the Appendix.

III. RESULTS: FERROMAGNETIC CASE

The simple limiting equations (15), (18), (22) suffice to solve the ferromagnetic weak-coupling case. We start at an isotropic case $\tau=\tau_0$, $\epsilon=\epsilon_0$, $J_\pm\tau=\frac{1}{2}\epsilon_0\ll 1$. Equation (18) gives us

$$4d\epsilon/\epsilon^2(2-\epsilon)=d(\ln\tau)\ ,$$

and neglecting ϵ relative to 2,

$$\ln(\tau/\tau_0)=2/|\epsilon|-2/\epsilon_0\ . \tag{23}$$

At the same time Eq. (21) gives

$$\ln(\tau/\tau_0)=1/J_\pm\tau-2/\epsilon_0=1/J_\pm\tau-1/(J_\pm\tau)_0\ . \tag{24}$$

Thus the renormalization takes place toward the origin; events on an ever larger time scale occur according to ever weaker interactions. Equation (24) says that the number of flips farther apart than τ decreases logarithmically with τ; this means an extremely slow decay of fluctuations, but in the end the state is polarized.

We expand on the nature of our solution: At a stage at which we have eliminated all pairs closer together than $\tau\gg\tau_0$, the remaining pairs occur at a mean separation of order $l\sim\tau/\epsilon^2(\tau)\sim\tau\ln^2(\tau/\tau_0)$ and have a length $\sim\tau/\epsilon\sim\tau\ln(\tau/\tau_0)$. Thus averaging over lengths of order $\tau\ln^2(\tau/\tau_0)$ we would see a mean polarization of order

$$\epsilon(\tau)\simeq\frac{2}{\ln(\tau/\tau_0)}\simeq\frac{2}{\ln(l/\tau_0)-2\ln\ln(l/\tau_0)}\ .$$

We have supposed it permissible to rotate in the complex time plane and to interpret this as the qualitative behavior of the time spin-spin correlation function.

$F=E_g$ can be obtained using Eq. (15) with (24).

$$-E_g=F=\tfrac{1}{4}\int_{\tau_0}^{0}J_\pm^2\tau^2\frac{d\tau}{\tau^2}=\tfrac{1}{4}\int_{(J\tau)_0}^{0}\frac{d(J_\pm\tau)}{d}$$

$$=\frac{1}{2\tau_0}\exp\left(\frac{2}{(J_\pm\tau)_0}\right)\int_{(J\tau)_0}dx\exp\left(-\frac{2}{x}\right). \tag{25}$$

This expression has the interesting property that while it is very nonanalytic at $J\tau=0$, it has a perfectly innocent-seeming asymptotic series at that point which agrees term by term with perturbation theory; as Kondo[8] has noted, perturbation theory gives no logarithmically singular terms in the series for the energy (relative to E_0 of course):

$$E_g=-\left[(\tfrac{1}{2}J_\pm)^2\tau_0\right]\left[1-2J_\pm\tau_0+6(J_\pm\tau_0)^2+\cdots\right]\ . \tag{26}$$

Equation (26) is, as we shall see, also the correct asymptotic series in the antiferromagnetic case with appropriate sign changes, but does not in that case represent the answer adequately: A Stokes phenomenon has intervened. The situation here is almost a classic case of the dangers of relying on perturbation-theory methods and of the complicated analytic behavior which may underly the simple and well-known fact that perturbation series are usually asymptotic.

IV. RESULTS: ANTIFERROMAGNETIC CASE AND TOULOUSE LIMIT

As already noted, the antiferromagnetic (AF) case cannot quite be settled in the same conclusive way. In the ferromagnetic case, as we scale $\tau\to\infty$, $\epsilon\to 0$, and $J_\pm\to 0$. All our expressions become more and more accurate and we have a full and exact solution so long as we start from small values of these parameters. In the AF case, ϵ and $J_\pm$ increase starting from any values, no matter how small, and there is no case for which we cannot eventually find a timescale for which $\epsilon\sim 1$. In fact, this is the fundamental expression of the Kondo phenomenon: Solving Eqs. (18) and (21) approximately by neglecting ϵ relative to 2, we have $\epsilon^2-(2J_\pm\tau)^2=\text{const}=0$ for the isotropic case, and

$$2/\epsilon_0-2/\epsilon(\tau)=\ln(\tau/\tau_0)\ . \tag{27}$$

Defining τ_K as the point where $\epsilon=1$, we have

$$2/\epsilon_0-2=\ln(\tau_K/\tau_0)$$

$$\text{or}\quad e^2(\tau_K/\tau_0)=e^2/\epsilon_0\ , \tag{28}$$

the familiar expression for $1/T_K$, T_K being the Kondo temperature. Thus the meaning of the Kondo temperature is merely that it is the scale of "time" = temperature at which the system behaves as though it were strongly coupled. Incidentally,

the fact that our equations are exact as $J_\pm \tau \to 0$ and give a vertical slope at all points except $\epsilon = 0$ on that line shows that the scaling curve cannot reenter the horizontal axis.

Why is $\epsilon = 1$ important? Because it is equivalent to a trivially soluble problem.[6] Consider the Hamiltonian

$$\mathcal{H}_1 = \sum_k \epsilon_k n_k + V_\pm \sum_k (c_d^\dagger c_k + c_k^\dagger c_d) = \mathcal{H}_0 + V \,. \qquad (29)$$

Here n_k, and c_k, $c_k^\dagger$ are Fermi operators for free spinless electrons, while $c_d^\dagger$ is the same for a local resonant state. This can be solved completely in well-known fashion (it is the "Lee model") as we shall do shortly. On the other hand, it is also possible to calculate the quantity

$$\langle 0 | e^{-\beta \mathcal{H}_1} | 0 \rangle = \langle 0 | e^{-\beta \mathcal{H}_0} T \exp\left(-\int_0^\beta V \, d\beta\right) | 0 \rangle$$

$$= \sum_n V_\pm^{2n} \int_0^\beta d\beta_{2n} \int_0^{\beta_{2n}} d\beta_{2n-1} \cdots \int_0^{\beta_2} d\beta_1 \, G(\beta_1 \cdots \beta_{2n}) . \qquad (30)$$

Here G is easily shown to be

$$G = \det_{ij} G_0(\beta_{2i} - \beta_{2j-1}) \,, \qquad (31)$$

where G_0 is the free-particle Green's function, and since we may assume a cutoff form for G_0

$$G_0(\beta) = \tau/\beta, \qquad \beta > \tau \qquad (32)$$

this determinant can be evaluated as a Cauchy determinant, giving

$$\langle 0 | e^{-\beta \mathcal{H}_1} | 0 \rangle = \sum_n V_\pm^{2n} \int\int\int\int \exp\left((-1)^{i-j} \sum_{i>j} \ln \frac{\beta_i - \beta_j}{\tau} \right)$$

$$= Z'(\beta/\tau, 2V_\pm \tau, \epsilon = 1) \,. \qquad (33)$$

(We need not specialize to Eq. (32); Mushkelishvili methods[9] give us the form (33) for any reasonable G_0.)

The ground-state energy of Eq. (29), which is the Hamiltonian of a resonance of width $\Delta = V_\pm^2 \tau$ at the Fermi surface, is easily calculated to be

$$E_{gT} = V_\pm^2 \tau \ln(V_\pm^2 \tau^2) + \text{cutoff-dependent terms}$$

$$\cong V_\pm^2 \tau \ln(V_\pm^2 \tau^2) - (1/\tau) \cot^{-1}(1/V_\pm^2 \tau^2)$$

$$- V_\pm^2 \tau \ln(1 + V_\pm^4 \tau^4)^{1/2} \,, \qquad (34)$$

the latter for the simple assumption of a constant density of states, $G_0 = (\tau/\beta)(1 - e^{-\beta/\tau})$, which is quite close enough to our assumption of the Appendix.

The $S_z - S_z$ correlation function of the real Kondo system with $\epsilon = 1$ obviously corresponds to the $n_d - n_d$ correlation function of Eq. (29). This correlation function is just

$$G_d^2(t) \simeq (\Delta/t)^2 \,.$$

A $1/t^2$ correlation function corresponds to

$$\chi(T=0) = (1/T) \int_0^{1/T} S_z(0) S_z(t) \, dt = \text{finite} \,.$$

Our scheme, then, is to scale by means of the basic equations (15), (18), (21) (or their more accurate counterparts from the Appendix)

$$dF = [(2-\epsilon)/(2-\epsilon_0)] (\tfrac{1}{2} J_\pm) \, d\tau \,, \qquad (35)$$

$$d\epsilon = [(2-\epsilon)^2/(2-\epsilon_0)] J_\pm^2 \tau^2 (d\tau/\tau) \,, \qquad (36)$$

$$d \ln(J_\pm^2 \tau^2) = \epsilon \, (d\tau/\tau) \,. \qquad (37)$$

These equations must be solved starting from their weak-coupling asymptotes [Eq. (27)]. Once integrated up to $\epsilon = 1$, at which we obtain $J_\pm \tau = 0.783$, we obtain the total ground-state energy by adding the Toulouse result Eq. (34)

$$E_g = -\int_{\tau_0}^{\epsilon(\tau)=1} \left(\frac{2-\epsilon}{2-\epsilon_0}\right) \left(\frac{J_\pm \tau}{2}\right)^2 \frac{d\tau}{\tau^2} - E_{gT}\left(\tau_K, \frac{J_\pm \tau_K}{2}\right) . \qquad (38)$$

Both the upper limit and the Toulouse term give results of the order of T_K, while the lower limit term is the series [Eq. (26)]. Further numerical results will be given in succeeding communications.

In what sense is this a complete solution of the antiferromagnetic problem? We believe it is so in a very real sense, just as Fermi liquid theory solves most problems of pure metals even without giving precise numerical parameters. We establish the scaling factor to logarithmic accuracy only, but what is important is to prove that it exists: that all magnetic impurities at *some* scale behave just like ordinary ones.

V. CONCLUSION

In conclusion let us, for one thing, make some remarks about experimental comparisons. The most interesting question on the Kondo effect[10] has been from the start whether it did or did not fit into the structure of usual Fermi gas theory: In particular, does a true infrared singularity occur as in the x-ray problem,[9] or does the Kondo impurity obey phase-space arguments as $T \to 0$ and give no energy dependences more singular than E^2 (or T^2), and is $\chi(T=0)$ finite? The result we find is that the usual antiferromagnetic case in fact *does* fit after the time scale has been revised to τ_K, i.e., that it behaves like a true bound singlet as was conjectured originally by Nagaoka.[7] Thus, experimental results giving singular behavior are, after all, as suggested by Star,[11] probably interaction effects. This is a satisfactory situation from the point of view of many-body theory but a highly unsatisfactory one from the

experimentalists' side.

The ferromagnetic case, on the other hand, exhibits strange enough behavior to satisfy the most particular, with finite S, zero effective J, and logarithmic correlation functions.

The one-dimensional Ising model with $n=2$ is solved en route and Thouless's conjecture[12] that a finite magnetization jump occurs at T_c is verified. Nagle and Bonner[13] have, by means of numerical extrapolations, calculated an approximate transition temperature for this case with no additional nearest-neighbor force (i.e., $J_\pm \tau \simeq 1$) which is consistent with Fig. 1(c). Nagle and Bonner's estimate of the critical exponent β of 0 is consistent with our finite jump of M, also.

But perhaps the most interesting implications of this work are purely theoretical: First, it represents a soluble case of a true many-body problem where one can gain insight into the reality behind approximations of many different kinds; and second, it may throw a very great deal of light onto the formal theory of scaling laws in statistical mechanics.

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APPENDIX: SOFT CUTOFFS – AN APPROXIMATE THEORY AND EXACT LIMITS IN THE STRONG-COUPLING CASE

The "sharp" cutoffs we have used in the bulk of the paper are a strictly artificial representation of the actual physics. The physical effect in any reasonable band structure of bringing two flips together is not to reduce the amplitude to zero but to cancel out the effects of the two flips leaving unit amplitude. (This is just a statement about the algebra of the spin operators at equal times.) Thus, in the initial problem, the cutoff at τ should essentially be to unit amplitude: For $[\tau/(\beta_i-\beta_{i+1})]^{2-\epsilon}$, we should substitute some function such as is shown in Fig. 4(c). For definiteness we pick the simplified "flat-top" cutoff also shown in Fig. 4(b).

$$\begin{aligned}\varphi_{ft}(\beta) &= 1, && \beta<\tau\\ &= (\tau/\beta)^{2-\epsilon}, && \beta>\tau\,.\end{aligned} \tag{A1}$$

The quantity Z' we wish to evaluate, then, now has integrals covering the full region, but whenever any two arguments β_i, β_j come closer than τ we replace the $[(\beta_i-\beta_j)/\tau]$ factor by unity:

$$Z' = \sum_n (\tfrac{1}{2}J_\pm)^{2n}\int_0^\beta d\beta_{2n}\int_0^{\beta_{2n}} d\beta_{2n-1}\cdots\int_0^{\beta_{2i+1}} d\beta_{2i}\times\cdots\int_0^{\beta_2} d\beta_1\times \prod_{i>j}[\varphi(\beta_i-\beta_j)]^{(-1)^{i-j+1}}\,. \tag{A2}$$

Now the process of scaling the cutoff τ may be carried out by making a small change in φ:

$$\varphi = \varphi' + d\varphi\,, \tag{A3}$$

where for the flat-top function we choose to use

$$\begin{aligned}\varphi'_{ft} &= 1-(2-\epsilon)\,d\tau/\tau, && \beta<\tau+d\tau\\ &= (\tau/\beta)^{2-\epsilon}, && \beta>\tau+d\tau\\ d\varphi &= (2-\epsilon)\,d\tau/\tau, && \beta<\tau+d\tau\\ &= 0, && \beta>\tau+d\tau\,.\end{aligned} \tag{A4}$$

[In general, of course, we are simply scaling the parameter in φ. The sharp cutoff function used in the text can be considered from this point of view, see Fig. 4(a).]

Now we insert (A3) into (A2) and rearrange in just the same way, keeping all the terms in which

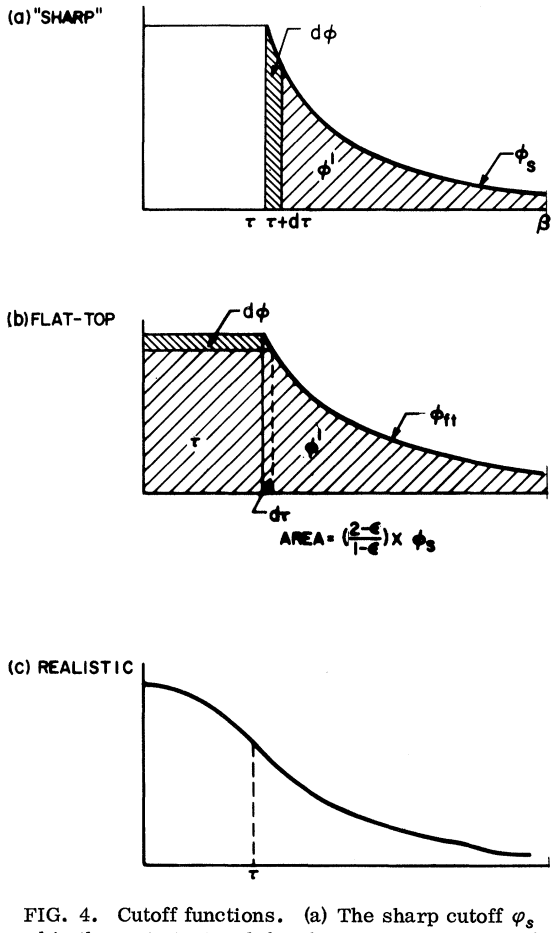

FIG. 4. Cutoff functions. (a) The sharp cutoff φ_s used in the main text and the change in φ_s on a modification of the cutoff by $d\tau$, (b) the flat-top cutoff used in the Appendix and the corresponding rescaling, (c) a possible realistic cutoff function.

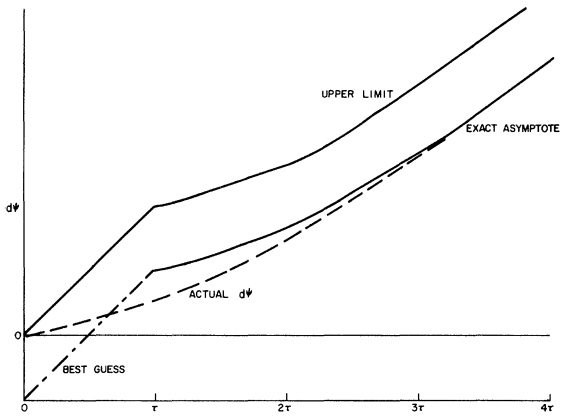

FIG. 5. Changes $d\psi$ in the cutoff function upon modification of τ to $\tau+d\tau$ (arbitrary scale; we have chosen $\epsilon=1$ for illustration). Dotted curve matches exact low-β behavior and exact asymptote; upper limit is a self-reproducing approximation for $d\psi$ which is definitely above the exact curve; and best guess is an approximate self-reproducing estimate.

φ' appears $2n$ times as the new $2n$th term, and in this new term $d\varphi$ may either enter between any pair of β's, β_{2i} and β_{2i+1}, or not. The cutoff properties are now such that it is not impossible, but simply negligibly rare, that β_{2i} and β_{2i+1} are closer together than τ, and certainly even rarer that β_{2i-1} and β_{2i+2} are also within τ of β_{2i+1} or β_{2i}, respectively. Thus without fear of appreciable error and noting that the error is always in the direction of *over*estimating correlations, we expand the dependence on distant β's as in the text, and focus on a particular pair β_{2i} and β_{2i+1} of interest:

$$Z' = \sum (\tfrac{1}{2}J_\pm)^2 \int\cdots\int_{\beta_{2i-1}}^{\beta_{2i+2}} d\beta_{2i+1}\int_{\beta_{2i-1}}^{\beta_{2i+1}} d\beta_{2i} \times[\varphi'(\beta_{2i+1}-\beta_{2i})(1+d\psi(\beta_{2i+1}-\beta_{2i}))] \quad , \tag{A5}$$

where $d\psi$ is the function which results from having a pair of flips β', β'' with a factor $d\varphi(\beta''-\beta')$ between β_{2i+1} and β_{2i}. We can establish three facts about the function $d\psi$:

$$d\psi(\beta) > 0 \quad , \tag{A6a}$$

$$d\psi \le \left(\frac{J_\pm}{2}\right)^2 \frac{d\tau}{\tau}\beta^2\left(\frac{2-\epsilon}{2}\right), \quad \beta\to 0 \tag{A6b}$$

$$d\psi \sim dF\times\beta - d\epsilon\ln\beta - d\gamma + O(1/\beta), \quad \beta\to\infty. \tag{A6c}$$

We sketch the behavior of $d\psi$ in Fig. 5, according to the calculation we shall do shortly, and also the behavior of $d\psi$ which corresponds to the approximations we shall use: (1) We keep only the first three terms of the asymptotic series, corresponding to the three scaling laws we have already introduced, of F, ϵ, and $J_\pm\tau$; and (2) we go on to the next stage with the same $\varphi'(\beta_{2i+1}-\beta_{2i})/\tau$, i.e., we get $d\varphi = \text{const} + dF\beta$ inside τ and $=$ (A6c) outside. It is obvious that this can be made a *lower* limit for $d\psi$, and thus a state which has *stronger* correlation, by setting $d\gamma = 0$. This should be a fair estimate as well. Thus we do not falsify any long-range low-frequency singular behavior by Griffith's inequalities. A limit in the other direction is shown in Fig. 5; numerical calculations show that the two are indistinguishable, in fact.

Next we establish (A6). Equation (A6a) is obvious. Let us, for the other two, write out $d\psi$ in Eq. (A5):

$$d\psi(\beta) = \left(\frac{J_\pm}{2}\right)^2 \int_0^\beta d\beta'' \int_0^{\beta''} d\beta' \times \frac{\varphi(\beta-\beta'')\,d\varphi(\beta''-\beta')\,\varphi(\beta')}{\varphi(\beta-\beta')\,\varphi(\beta'')} \quad . \tag{A7}$$

For (A6b) we note that when $\beta<\tau$ all functions except $d\varphi$ are unity and the integrals give simply the total area $\frac{1}{2}\beta^2$.

To establish the asymptotic behavior it suffices to go to $\beta\gg\tau$ in Eq. (A7). We then write

$$d\psi = \left(\frac{J_\pm}{2}\right)^2 \frac{d\tau}{\tau}(2-\epsilon)\int_0^\beta d\beta'' \times\int_{\beta''-\tau\text{ or }0}^{\beta''} d\beta'\left[1+\left(\frac{\varphi(\beta-\beta')}{\varphi(\beta-\beta')}\frac{\varphi(\beta')}{\varphi(\beta'')}-1\right)\right] \quad .$$

The "1" gives

$$(\tfrac{1}{2}J_\pm)^2(d\tau/\tau)(2-\epsilon)[\tau(\beta-\tau)+\tfrac{1}{2}\tau^2] \quad . \tag{A8}$$

The second term contains, first, the expansion which is valid throughout the interior of the interval,

$$\left(\frac{J_\pm}{2}\right)^2\frac{d\tau}{\tau}(2-\epsilon)\int_\tau^{\beta-\tau} d\beta''\int_{\tau\text{ or }\beta''-\tau}^{\beta''} d\beta' \times(2-\epsilon)(\beta''-\beta')\left(\frac{1}{\beta-\beta'}+\frac{1}{\beta''}\right)+O\left(\frac{1}{\beta^2}\right) \quad ,$$

which may be evaluated by assuming τ always small relative to β's:

$$= -\left(\frac{J_\pm}{2}\right)^2\tau\,d\tau\frac{(2-\epsilon)^2}{2}\times 2\ln\left(\frac{\beta-\tau/2}{\tau}\right) \quad . \tag{A9}$$

Finally, we have contributions from the ends of the interval which are again of order $1/\beta$. Neglecting all $1/\beta$ contributions we get, adding (A8) and (A9),

$$d\psi \sim (2-\epsilon)(J_\pm/2)^2\,d\tau[\beta-(2-\epsilon)\tau\ln(\beta/\tau)-\tau/2] \quad . \tag{A10}$$

We have therefore the new set of scaling laws, setting $(1+d\psi)\simeq e^{d\psi}$, and carrying out the argument as in the main text:

$$dF=(\tfrac{1}{2}J_{\pm})^2\,d\tau(2-\epsilon)\,, \tag{A11}$$

$$d\epsilon=\tfrac{1}{2}(2-\epsilon)^2J_{\pm}^2\tau\,d\tau\,, \tag{A12}$$

$$d\ln(J_{\pm}^2)=-\tfrac{1}{2}(J_{\pm})^2\tau\,d\tau$$
$$+\text{rescaling correction as in text ("best")}$$
$$=0+\text{rescaling ("upper limit").} \tag{A13}$$

We use this latter estimate in the text because it is simpler.

One feature of these laws which is a bit surprising is the extra factor of $2-\epsilon$ in all of them. This comes from the fact that the area of φ_{sharp} and φ_{ft} differs by a factor $(2-\epsilon)$, so that $d\varphi$ must be larger by this factor in order eventually to annihilate φ_{ft}. Second-order perturbation theory gives the total area of $\varphi(=\int G_0^2\,dt)$ as the appropriate energy correction. Thus τ in terms of band parameters is different in (A11)–(A13) by a factor $2-\epsilon$ from that in Eq. (15). Since we choose to renormalize self-consistently with φ_{ft} throughout, this is irrelevant but all of Eqs. (A11)–(A13) should be divided by $(2-\epsilon_0)$ for comparison with the sharp equations (15), (18), and (21).

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