

## Approximate mapping of the two-impurity symmetric Anderson model in the local-moment regime to a classical problem

Sudip Chakravarty

*Department of Physics, State University of New York, Stony Brook, New York 11794*

Jorge E. Hirsch

*Institute for Theoretical Physics, University of California, Santa Barbara, California 93106*

(Received 26 May 1981)

Using a path-integral formulation for the partition function the two-impurity symmetric Anderson model in the local-moment regime is mapped onto a problem of a classical four-component "Coulomb" gas interacting with a logarithmic potential. This can be viewed alternately as a problem of a general four-state spin system with inverse-square interaction in one dimension. The scaling equations for this model are derived and their implications for the properties of the Anderson model are pointed out. This mapping, although approximate, provides an explicit and physically interesting realization of a class of general  $n$ -state inverse-square spin systems in one dimension.

### I. INTRODUCTION

The two-impurity symmetric Anderson model in the local-moment regime<sup>1</sup> is of interest in connection with the properties of dilute magnetic alloys.<sup>2</sup> In this paper, we consider an approximate map of this model to a classical statistical-mechanics problem with long-range interactions. We derive scaling equations for this classical problem and discuss their implications for the behavior of the Anderson model. Analysis of this nature led to a variety of interesting results in the corresponding single-impurity problem. First, the equivalence between the single-impurity Kondo problem and two interacting one-dimensional classical models, namely the two-component charge rods interacting via a logarithmic interaction and the inverse-square Ising model, was pointed out by Anderson and Yuval<sup>3</sup> and Hamann.<sup>4</sup> Second, the scaling equations for this classical problem led to a qualitatively correct understanding of the single-impurity Kondo-Anderson model,<sup>5</sup> and third, from the same equations it was argued that the ferromagnetic inverse-square Ising model in one dimension should have a phase transition at a finite temperature.<sup>6</sup> This inverse-square Ising model is a particularly curious one since it is known that for models with the interaction falling off faster than  $1/r^2$  there is no phase transition,<sup>7</sup> while for those falling off slower

than inverse square there is.<sup>8</sup>  $1/r^2$  is the borderline case for which Thouless<sup>9</sup> has given strong heuristic arguments for the existence of an unusual phase transition at finite temperatures, as verified later by Yuval and Anderson.<sup>6</sup>

In this paper, we show that the two-magnetic-impurity problem maps onto a four-component "Coulomb gas" interacting via a logarithmic potential in one dimension. This can also be viewed as a four-state inverse-square problem in one dimension. Such general  $n$ -state models have interesting properties, as pointed out recently by Cardy.<sup>10</sup> Our work then shows that the two-impurity Anderson model in the local-moment regime is an explicit physical realization of an interesting statistical-mechanics model, although an approximate one. With the help of the scaling equations we obtain some qualitative results pertaining to the two-impurity Anderson model which should shed some light on the properties of dilute magnetic alloys.

This paper is organized as follows: In the following section we formulate the problem in terms of functional integrals. In Sec. III we discuss the long-time approximation for the unperturbed impurity Green's functions. In Secs. IV and V we show how the partition function can be expressed in terms of a functional integral over  $c$  number fields of the exponential of a certain quantum-mechanical action. By choosing a certain class of

important paths in the functional integral we show in Sec. VI that the problem reduces to a four-component Coulomb-gas model. We derive the scaling equations for the model in Sec. VII and discuss the results in Sec. VIII.

## II. THE PATH INTEGRAL

The Hamiltonian of interest is given by

$$H = H_0 + H_1, \quad (2.1)$$

where

$$H_0 = \sum_{\vec{k}, \sigma} \epsilon_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + E_f \sum_{i, \sigma} f_{i\sigma}^\dagger f_{i\sigma} + \sum_{B, i, \sigma} v_k c_{\vec{k}\sigma}^\dagger f_{i\sigma} e^{i\vec{k} \cdot \vec{R}_1} + \text{H.c.} \quad (2.2)$$

and

$$H_1 = \frac{U}{2} \sum_{i, \sigma} f_{i\sigma}^\dagger f_{i\sigma} f_{i-\sigma}^\dagger f_{i-\sigma}. \quad (2.3)$$

The subscript  $i$  labels the two impurities situated at  $\vec{R}_1$  and  $\vec{R}_2$ . The conduction-electron operators are represented by  $c$ 's and local  $f$  electrons by  $f$ 's. The two-impurity model was introduced by Alexander and Anderson,<sup>1</sup> but note that we have dropped the direct hopping of the  $f$  electrons from site to site; we have the case of rare-earth impurities in mind. The extension to the case of  $f$ - $f$  direct hopping is simple but will not be discussed here. We shall further restrict ourselves to the case where  $E_f = -U/2$ , i.e., the symmetric case, and consider the case where charge degrees of freedom can be frozen out, i.e., the local levels will be assumed to lie well below the Fermi level of the conduction band. Note furthermore that there are no orbital degeneracies in the model and  $\sigma$  is the spin index. Since we freeze the charge degrees of freedom, the partition function, following Hamann,<sup>4</sup> can immediately be written down as a functional integral over two  $c$  number variable  $\xi_1(\tau)$  and  $\xi_2(\tau)$  as

$$\frac{Z}{Z_0} = \int \delta[\xi_1] \delta[\xi_2] \exp \left[ -\frac{\Delta^2}{U} \int_0^\beta d\tau [\xi_1^2(\tau) + \xi_2^2(\tau)] \right] \prod_{s=\pm} \tilde{Z}_s, \quad (2.4)$$

where

$$\tilde{Z}_s = \exp \left[ -\Delta \int_0^\beta d\tau \int_0^1 dg \sum_{i=1}^2 \xi_{is}(\tau) G_{ii}^s(\tau, \tau^+, g) \right] \quad (2.5)$$

and

$$\xi_{is}(\tau) = s \xi_i(\tau). \quad (2.6)$$

Here  $\Delta = \pi \rho_0(\epsilon_f) \langle V^2 \rangle$  is the hybridization width of the local levels. The Green's functions  $G_{ij}^s$  obey the coupled Dyson's equations given by

$$G_{ij}^s(\tau, \tau'; g) = G_{ij}^0(\tau, \tau') + g \Delta \sum_{l=1}^2 \int_0^\beta d\tau'' G_{il}^0(\tau, \tau'') \xi_{ls}(\tau'') \times G_{lj}^s(\tau'', \tau'; g). \quad (2.7)$$

## III. GREEN'S FUNCTIONS AND THE LONG-TIME APPROXIMATION

The unperturbed impurity Green's functions are defined by

$$G_{ij}^0(\tau, \tau') = -\langle T_\tau f_i(\tau) f_j^\dagger(\tau') \rangle_0, \quad (3.1)$$

where the average  $\langle \rangle_0$  is defined with respect to  $H_0$  of Eq. (2.2), and we have dropped the irrelevant spin indices. Defining the Fourier series by

$$G_{ij}^0(\tau, \tau') = \frac{1}{\beta} \sum_n e^{-i\omega_n(\tau-\tau')} G_{ij}^0(i\omega_n), \quad (3.2)$$

$$\omega_n = \frac{(2n+1)}{\beta} \pi, \quad (3.3)$$

and computing the equations of motion for the Green's functions one finds

$$G_{11}^0(i\omega_n) = \frac{1}{i\omega_n - \epsilon_1 - F_0 - \frac{F_{12}F_{21}}{i\omega_n - \epsilon_2 - F_0}}, \quad (3.4)$$

$$G_{12}^0(i\omega_n) = \frac{F_{12}}{i\omega_n - \epsilon_2 - F_0} G_{11}^0. \quad (3.5)$$

For generality we have allowed for the possibility of two different energies for the  $f$  levels at sites 1 and 2;  $E_{f1} = \epsilon_1$ ,  $E_{f2} = \epsilon_2$ .  $G_{22}^0$  and  $G_{21}^0$  are easily obtained by interchanging 1 and 2 in the above equations. The quantities  $F_0$  and  $F_{12}$  are given by

the following equations:

$$F_0 = \sum_{\vec{k}} \frac{|V_{\vec{k}}|^2}{i\omega_n - \epsilon_{\vec{k}}}, \quad (3.6)$$

and

$$F_{12} = \sum_{\vec{k}} \frac{|V_{\vec{k}}|^2}{i\omega_n - \epsilon_{\vec{k}}} e^{i\vec{k} \cdot \vec{R}_{12}}.$$

$F_0$  is readily evaluated by taking  $V_{\vec{k}} = V$  and a flat density of states of the wide conduction band yielding

$$F_0 = -i\Delta \operatorname{sgn}(\omega_n). \quad (3.7)$$

$$G_{11}^0(\tau) = \frac{1}{2\pi i} \int_c d\epsilon e^{-\epsilon\tau} [f(\epsilon) - \Theta(\tau)] \frac{\epsilon - \epsilon_2 + i\Delta\eta}{(\epsilon - \epsilon_1 + i\Delta\eta)(\epsilon - \epsilon_2 + i\Delta\eta) - \Delta^2(j_1 + i\eta j_0)^2} \quad (3.11)$$

and

$$G_{12}^0(\tau) = \frac{1}{2\pi i} \int_c d\epsilon e^{-\epsilon\tau} [f(\epsilon) - \Theta(\tau)] \frac{\Delta(j_1 + i\eta j_0)}{(\epsilon - \epsilon_1 + i\Delta\eta)(\epsilon - \epsilon_2 + i\Delta\eta) - \Delta^2(j_1 + i\eta j_0)^2}, \quad (3.12)$$

with  $\eta = \operatorname{sgn}(\operatorname{Im}\epsilon)$ , and the contour encloses the real axis in the counterclockwise sense.  $f(\epsilon)$  is the Fermi function and  $\Theta(\tau)$  is the step function. For the case  $\epsilon_1 = \epsilon_2 = E_f$  the expressions can be written as

$$G_{11}^0(\tau) = -\frac{1}{2} \int_{-\infty}^{+\infty} \frac{d\epsilon}{\pi} e^{-\epsilon\tau} [f(\epsilon) - \Theta(\tau)] \left[ \frac{\Delta(1-j_0)}{(\epsilon - E_f - \Delta j_1)^2 + \Delta^2(1-j_0)^2} + \frac{\Delta(1+j_0)}{(\epsilon - E_f + \Delta j_1)^2 + \Delta^2(1+j_0)^2} \right], \quad (3.13)$$

and

$$G_{12}^0(\tau) = \frac{1}{2} \int_{-\infty}^{+\infty} \frac{d\epsilon}{\pi} e^{-\epsilon\tau} [f(\epsilon) - \Theta(\tau)] \left[ \frac{\Delta(1-j_0)}{(\epsilon - E_f - j_1)^2 + \Delta^2(1-j_0)^2} - \frac{(1+j_0)}{(\epsilon - E_f + j_1)^2 + \Delta^2(1+j_0)^2} \right]. \quad (3.14)$$

The standard long-time approximation<sup>11</sup> for the Green's functions now leads to the following expressions:

$$G_{11}^0(\tau) = -(a_- + a_+) \frac{P}{\pi\tau} + (b_- - b_+) \delta(\tau), \quad (3.15)$$

$$G_{12}^0(\tau) = +(a_- - a_+) \frac{P}{\pi\tau} - (b_- + b_+) \delta(\tau), \quad (3.16)$$

with

$$a_{\pm} = \frac{1}{2\Delta} \frac{1 \pm j_0}{j_1^2 + (1 \pm j_0)^2} \quad (3.17)$$

The evaluation of  $F_{12}$  is slightly more involved and we have found it reasonable to use  $k^2$  dispersion of the conduction band, giving

$$F_{12} = -\Delta j_1 - i\Delta j_0 \operatorname{sgn}(\omega_n) \quad (3.8)$$

with

$$j_1 = \frac{\sin k_F R_{12}}{k_F R_{12}}, \quad (3.9)$$

$$j_0 = \frac{\cos k_F R_{12}}{k_F R_{12}}. \quad (3.10)$$

Using a standard trick it is simple to write down the expressions for  $G_{11}^0(\tau)$  and  $G_{12}^0(\tau)$ :

and

$$b_{\pm} = \frac{1}{2\Delta} \frac{j_1}{j_1^2 + (1 \pm j_0)^2}. \quad (3.18)$$

Substitution of the expressions for the Green's functions given by Eqs. (3.15) and (3.16) in Eq. (2.7) now leads to coupled singular integral equations. The corresponding equation for the single impurity case was solved by Hamann<sup>4</sup> exactly using Muskhelishvili's method.<sup>12</sup> Unfortunately, the method is not easily extended to the case of coupled equations and we have not been able to apply it to (2.7). However, in the next section we show that an explicit solution is not required for our purpose.

## IV. THE QUANTUM-MECHANICAL ACTION

We must now express  $G_{ij}^s(\tau, \tau^+; g)$  explicitly in terms of the  $c$  number fields  $\xi_i(\tau)$ . Since we have not found it possible to solve the coupled Dyson's equations, even within the long-time approximation, we shall follow an indirect route. The argument runs as follows. Assume first that the fields  $\xi_1$  and  $\xi_2$  are constant in time  $\tau$ . Equation (2.7) can then be solved trivially and let the solutions be denoted by  $G_{ij}^{ad}(\tau, \tau^+; \xi_1, \xi_2)$ . When the fields are varying in time, we write for equal times

$$G_{ij}(\tau, \tau^+; [\xi_1, \xi_2]) = G_{ij}^{ad}(\tau, \tau^+; \xi_1(\tau), \xi_2(\tau)) + G_{ij}^{nl}(\tau, \tau^+; [\xi_1, \xi_2]), \quad (4.1)$$

where the first part is the "adiabatic part" obtained from the static solution by simply replacing  $\xi_1, \xi_2$  by  $\xi_1(\tau), \xi_2(\tau)$ , and the second term is a "non-local" part, a *functional* of the time-dependent fields. Equation (4.1) simply defines  $G_{ij}^{nl}$ .  $G_{ij}^{nl}$  must contain the derivatives of the fields  $\xi_1(\tau)$  and  $\xi_2(\tau)$  since it must vanish for constant fields. After performing the coupling constant integration, one must be able to arrange the partition function in the form

$$V(\xi_1, \xi_2) = \frac{\Delta}{u} (\xi_1^2 + \xi_2^2) + \int_0^1 dg \{ \xi_1 [F(g\xi_1, g\xi_2) - F(-g\xi_1, -g\xi_2)] + \xi_2 [F(g\xi_2, g\xi_1) - F(-g\xi_2, -g\xi_1)] \}, \quad (5.1)$$

where

$$F(x, y) = -\frac{1}{\pi} \text{Im} \int_{-\infty}^0 d\epsilon \frac{\epsilon - y\Delta + i\Delta}{(\epsilon - x\Delta + i\Delta)(\epsilon - y\Delta + i\Delta) - \Delta^2(j_1 + j_0)^2}. \quad (5.2)$$

In order to understand the qualitative properties of  $V(\xi_1, \xi_2)$  it is extremely revealing to expand  $V(\xi_1, \xi_2)$  in powers of  $\xi_1$  and  $\xi_2$ , keeping only up to the quartic terms. This yields

$$V(\xi_1, \xi_2) \simeq A_+ (\xi_1 + \xi_2)^2 + A_- (\xi_1 - \xi_2)^2 + B_+ (\xi_1 + \xi_2)^4 + B_- (\xi_1 - \xi_2)^4 + C \xi_1^2 \xi_2^2, \quad (5.3)$$

where the coefficients  $A_{\pm}$ ,  $B_{\pm}$  and  $C$  are functions  $j_0, j_1, \Delta$ , and  $U$ . Although unwieldy looking objects, it is perfectly straightforward to write these coefficients down explicitly. For a qualitative discussion it is not necessary to have the explicit

$$\frac{Z}{Z_0} = \int \delta[\xi_1] \delta[\xi_2] \times \exp \left[ - \int_0^\beta d\tau \{ V(\xi_1, \xi_2) + T[\xi_1, \xi_2] \} \right], \quad (4.2)$$

where  $V(\xi_1, \xi_2)$  arises from  $G_{ii}^{ad}$  and is a *function* of two field variables  $\xi_1(\tau)$  and  $\xi_2(\tau)$ . On the other hand,  $T[\xi_1, \xi_2]$ , a *functional* of field variables arising from  $G_{ii}^{nl}$ , vanishes when the fields are constant in time. The symbols  $V$  and  $T$  are suggestive of potential and kinetic energies for this quantum-mechanical action.

The analysis in this section has been exact and we have not yet invoked any approximations. Furthermore, since it is trivial to evaluate  $G_{ij}^{ad}$ ,  $V(\xi_1, \xi_2)$  can be written down exactly. This is not the case for  $T[\xi_1, \xi_2]$ . In the next section we discuss a well-motivated approximation for  $T[\xi_1, \xi_2]$ .

V. EVALUATION OF  $V(\xi_1, \xi_2)$  AND  $T[\xi_1, \xi_2]$ 

As mentioned in the last section it is easy to obtain an exact expression for  $V(\xi_1, \xi_2)$ . This is given by the following expression:

forms for these coefficients. It is convenient to introduce the following variables in Eq. (5.3). They are

$$\eta_1 = \frac{\xi_1 + \xi_2}{2} \quad (5.4)$$

and

$$\eta_2 = \frac{\xi_1 - \xi_2}{2}. \quad (5.5)$$

One then has

$$V(\eta_1, \eta_2) = \Gamma_1 \eta_1^2 + \mu_1 \eta_1^4 + \Gamma_2 \eta_2^2 + \mu_2 \eta_2^4 + \Gamma_{12} \eta_1^2 \eta_2^2, \quad (5.6)$$

where

$$\Gamma_1 = 2A_+, \quad (5.7)$$

$$\Gamma_2 = 2A_-, \quad (5.8)$$

$$\mu_1 = 4B_+ + \frac{1}{4}C, \quad (5.9)$$

$$\mu_2 = 4B_- + \frac{1}{4}C, \quad (5.10)$$

$$\Gamma_{12} = -\frac{1}{2}C. \quad (5.11)$$

The structure of the energy surface is now clear. For  $\Gamma_1, \Gamma_2 > 0$ ,  $V$  will have a single minimum at  $\eta_1 = \eta_2 = 0$ . If  $\Gamma_1$  or  $\Gamma_2$  is less than zero,  $\eta_1 = \eta_2 = 0$  will be a saddle point and two symmetrical minima will develop in one direction. If both  $\Gamma_1$  and  $\Gamma_2$  are less than zero the origin is a maximum and there are four minima as follows:

(1) Ferromagnetic minima:

$$\eta_2 = 0, \quad \eta_1^F = \pm(-\Gamma_1/2\mu_1)^{1/2}. \quad (5.12a)$$

(2) Antiferromagnetic minima:

$$\eta_1 = 0, \quad \eta_2^F = \pm(-\Gamma_2/2\mu_2)^{1/2}. \quad (5.12b)$$

These four minima correspond to the local-moment regime and occur for  $U > \pi\Delta$ . For an accurate determination of the minima, one must of course use the exact expression for  $V(\xi_1, \xi_2)$  given by Eqs. (5.1) and (5.2). The condition for the formation of ferromagnetic minima is

$$1 - \frac{\Delta\pi}{U} - (j_1^2 - j_0^2) > 0, \quad (5.13a)$$

and for antiferromagnetic minima,

$$1 - \frac{\Delta\pi}{U} - \frac{1}{3}(j_1^2 - j_0^2) > 0. \quad (5.13b)$$

The values of the potential energy at these minima are

$$V_F = -\frac{3[1 - \Delta\pi/U - (j_1^2 - j_0^2)]^2}{1 - 6(j_1^2 - j_0^2)}, \quad (5.14a)$$

$$V_{AF} = -3\frac{[1 - \Delta\pi/U - 1/3(j_1^2 - j_0^2)]^2}{1 - (6/5)(j_1^2 - j_0^2)}, \quad (5.14b)$$

respectively. These expressions are valid for  $k_f R \gg 1$ ; similar expressions can be found in the general case. As  $R \rightarrow \infty$ , the four minima become degenerate and coincide with the solution for a single impurity. The four minima are also degenerate at the special points where  $j_1^2 = j_0^2$ , or

$$2k_f R = \pi(n + \frac{1}{2}). \quad (5.15)$$

In the regions

$$\frac{\pi}{2} + 2n\pi < 2k_f R < \frac{\pi}{2} + (2n+1)\pi \quad (5.16)$$

the ferromagnetic minima are lower, for

$$\frac{\pi}{2} + (2n+1)\pi < 2k_f R < \frac{\pi}{2} + 2(n+1)\pi, \quad (5.17)$$

the antiferromagnetic solutions are favored. Of course, such an oscillatory behavior is what one expects in this problem due to the sharpness of the Fermi surface.

Alexander and Anderson<sup>1</sup> have studied the two-impurity model in the Hartree-Fock approximation. However, they include in the model direct exchange and restrict the discussion to the case where the indirect exchange can be neglected. They also find ferro- and antiferromagnetic minima, depending on the parameters of the Hamiltonian but due to a quite different physical mechanism, the sign of the exchange being determined mainly by the position of the local level relative to the Fermi level. In our case within the static approximation the ferro- and antiferromagnetic solutions alternate as a function of the distance between impurities.

Although  $V(\xi_1, \xi_2)$  can be calculated quite precisely, we approximate  $T[\xi_1, \xi_2]$  by a weak-field limit. For fields that do not vary too rapidly, we expect  $G_{ij}^{ad}$  to be still the dominant contribution to the Green's function. The remaining "nonlocal" term which depends on the values of the fields at different times, we expand to lowest order in the fields using the long-time approximation discussed earlier. After doing the coupling constant integration we obtain

$$T[\xi_1, \xi_2] = \frac{(a_+ + a_-)^2}{\pi^2} \int_0^\beta d\tau \int_0^\beta d\tau' \ln|\tau - \tau'| \left[ \frac{d\xi_1}{d\tau} \frac{d\xi_1}{d\tau'} + \frac{d\xi_2}{d\tau} \frac{d\xi_2}{d\tau'} \right] \\ + \frac{(a_+ - a_-)^2}{\pi^2} \int_0^\beta d\tau \int_0^\beta d\tau' \ln|\tau - \tau'| \left[ \frac{d\xi_2}{d\tau} \frac{d\xi_1}{d\tau'} + \frac{d\xi_1}{d\tau} \frac{d\xi_2}{d\tau'} \right]. \quad (5.18)$$

Note that this approximation has not destroyed the nonlocality of the kernel expressed by the  $\ln|\tau-\tau'|$  factor. This important factor, or more accurately  $\ln\{\beta/\pi\sin[\pi(\tau-\tau')/\beta]\}$  at finite temperatures, reflects the sharpness of the Fermi surface and slow relaxation of the conduction electrons to a time-dependent perturbation. Furthermore, the presence of the derivatives of the fields in the integrand allows for the existence of hopping paths which tunnel between various minima. Such an approximation for the single-impurity case<sup>4</sup> can be verified to change only formally the numerical factors which cannot be obtained by this procedure. This approximation does not, however, change the fact that the single-impurity problem maps on to the inverse-square Ising model. We now turn to a discussion of the dominant paths in the functional integral.

## VI. DOMINANT PATHS

Our next task is to compute the functional integral (4.2) with the potential and kinetic energy given in (5.1) and (5.13), respectively. It is clearly not possible to compute this functional integral exactly. To obtain an approximation to (4.2), one can choose by examination a class of "important paths," that is, field configurations, that make important contributions to the functional integral. A reasonable first approximation consists in choosing a single straight path, (i.e., independent of time) that minimizes the potential-energy term. For this kind of path the kinetic-energy term vanishes and one obtains the Hartree-Fock results. A better approximation consists in taking paths that stay most of the time in one of the energy minima and "hop"

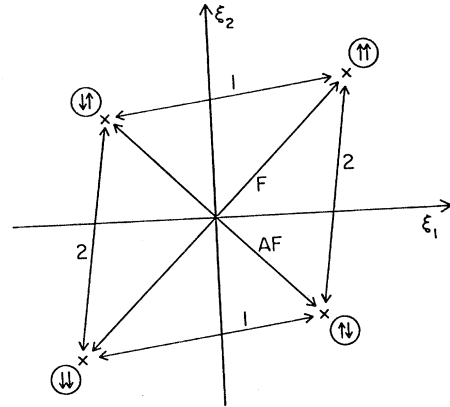


FIG. 1. Schematic diagram of potential-energy minima and different types of hops. 1 and 2 denote a single spin flip of impurity 1 and 2, respectively,  $F$  denotes ferromagnetic hops, and  $AF$  antiferromagnetic hops.

over short time intervals to other energy minima. Such hopping paths were considered by Hamann in his study of the single-impurity problem.<sup>4</sup> The partition function can then be parametrized in terms of these hopping paths, occurring at instants  $t_i$  and lasting over a time interval  $\tau$ . The parameter  $\tau$  plays the role of a high-energy cutoff, and from balancing potential and kinetic energy, it can be shown that  $\tau \sim 1/U$ , as in the single-impurity case.<sup>4</sup> There are four different types of hops to be considered: (1) only impurity-one hops, (2) only impurity-two hops, (3) both impurities flip spin in the same direction (ferromagnetic hops), (4) both impurities exchange spins (antiferromagnetic hops) (see Fig. 1).

The kinetic energy takes the form

$$\begin{aligned}
 T[\xi_1, \xi_2] = & \sum_{i \neq j} \left[ \left( \frac{a_+ + a_-}{\pi} \right)^2 [(\Delta\xi_1)_i (\Delta\xi_1)_j + (\Delta\xi_2)_i (\Delta\xi_2)_j] \right. \\
 & + \left. \left( \frac{a_+ - a_-}{\pi} \right)^2 [(\Delta\xi_1)_i (\Delta\xi_2)_j + (\Delta\xi_1)_j (\Delta\xi_2)_i] \right] \ln |t_i - t_j| \\
 & + \sum_i \int_{t_i}^{t_i+\tau} d\tau \int_{t_i}^{t_i+\tau} d\tau' \ln |\tau - \tau'| \left[ \left( \frac{a_+ + a_-}{\pi} \right)^2 \left[ \frac{d\xi_1}{d\tau} \frac{d\xi_1}{d\tau'} + \frac{d\xi_2}{d\tau} \frac{d\xi_2}{d\tau'} \right] \right. \\
 & \left. + \left( \frac{a_+ - a_-}{2} \right)^2 \left[ \frac{d\xi_1}{d\tau} \frac{d\xi_2}{d\tau'} + \frac{d\xi_2}{d\tau} \frac{d\xi_1}{d\tau'} \right] \right], \quad (6.1)
 \end{aligned}$$

where  $(\Delta\xi_\alpha)_i$  is the change of the  $\alpha$ th impurity field at hop  $i$ . The first term in  $T$  describes logarithmic interactions between the four types of hops (or "charges") described previously. The second term gives the chemical potential for the different charges, and it can be evaluated by assuming a linear time dependence for the field during the time of the hop. The partition function takes the form

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \sum_{n=n_1+n_2+n_F+n_{AF}} y_1^{n_1} y_2^{n_2} y_F^{n_F} y_{AF}^{n_{AF}} \int_0^{\beta} \frac{dt_n}{\tau} \int_0^{t_n-\tau} \frac{dt_{n-1}}{\tau} \int_0^{t_2-\tau} \frac{dt_1}{\tau} \exp \left[ \sum_{i < j} K_{\alpha_i \alpha_j} \ln \frac{|t_i - t_j|}{\tau} + \sum_i (-1)^i (\Delta V)_i t_i \right]. \quad (6.2)$$

This is the partition function for a classical four-component ‘‘Coulomb gas’’ in one dimension with logarithmic interactions. Alternatively, it can be rewritten by partial integrations to describe a four-state spin system with  $1/r^2$  interactions.<sup>10</sup> The term  $(\Delta V)_i$  plays the role of a symmetry-breaking field and gives the difference in the potential energy before and after hop  $i$ . This term is zero whenever the four minima are degenerate. Otherwise, it only appears when one impurity alone flips its spin and thus tends to favor correlated hops between the two lower-energy minima.

In terms of the original parameters of the Hamiltonian,  $\Delta V$  is given by the difference  $V_F$  and  $V_{AF}$  in Eqs. (5.14). The parameters in the Hamiltonian can be written in terms of the quantities

$$J = 4 \left[ \frac{a_+ + a_-}{\pi} \right]^2 \xi_0^2, \quad (6.3)$$

$$J_{12} = 4 \left[ \frac{a_+ - a_-}{\pi} \right]^2 \xi_0^2,$$

where  $(\pm \xi_0, \pm \xi_0)$  are the positions of the energy minima. (We are assuming degenerate minima here; deviations from this give unimportant corrections for these parameters.) In (6.2),  $\alpha_i$  denotes the charge at site  $i$  (1, 2,  $F$ , or  $AF$ ) and the interaction between charges  $K_{\alpha_i \alpha_j}$  is given by

$$\begin{aligned} K_{11} &= K_{22} = \pm J, \\ K_{12} &= \pm J_{12}, \\ K_{1,F} &= K_{2,F} = \pm (J + J_{12}), \\ K_{1,AF} &= K_{2,AF} = \pm (J - J_{12}), \\ K_{F,F} &= \pm 2(J + J_{12}), \\ K_{AF,AF} &= \pm 2(J - J_{12}), \\ K_{F,AF} &= 0. \end{aligned} \quad (6.4)$$

The fugacities in (6.2) are given by

$$\begin{aligned} \ln y_1 &= \ln y_2 = -\frac{3}{4} J, \\ \ln y_F &= -\frac{3}{2} (J + J_{12}), \\ \ln y_{AF} &= -\frac{3}{2} (J - J_{12}), \end{aligned} \quad (6.5)$$

and the energy splitting  $\Delta V = V_F - V_{AF}$  can be obtained by substituting (5.12) into (5.6) in the small-field limit, or more generally by solving numerically for the minima of (5.1).

As discussed earlier, the weak-field expansion for the kinetic energy is not expected to modify the qualitative features of the problem. Thus, we expect only the numerical values of the coefficients to be changed for general values of the fields. To be more precise, in the single-impurity case it is easy to show that by doing the replacement  $\xi_0 \rightarrow \arctan \xi_0$  in the interaction term and  $\xi_0^2 \rightarrow \ln \xi_0$  in the chemical potential term, the weak-field expansion reproduces exactly Hamann’s result obtained for general values of the fields. We expect similar correspondences to hold in the present case.

## VII. SCALING EQUATIONS

We are now faced with the problem of computing the partition function of a four-component Coulomb-gas model in a symmetry-breaking field, Eq. (6.2). We have studied the problem using the scaling approach introduced by Anderson, Yuval, and Hamann in their study of the single-impurity problem.<sup>5</sup> Instead of computing the integrals in the partition function all at once, we do it in steps. In the first step we integrate out only ‘‘close pairs,’’ that is, charges that are within a range between  $\tau$  and  $\tau + d\tau$ . The partition function that results describes a new problem with cutoff  $\tau' = \tau + d\tau$  and, as we will see, no new interactions appear in the partition function; only the original parameters get ‘‘renormalized’’. This allows one to write scaling equations for the various parameters in the model and by studying these equations to obtain insight into its phase structure. Such scaling equations were recently independently derived by Cardy<sup>10</sup> for a more general model. As is well known, the single-component model with logarithmic interactions shows a phase transition from a regime where the charges are bound in close pairs (low temperatures) to a plasma phase where the charges are free (high temperatures). Similar but richer behavior occurs in multicomponent Coulomb-gas models. The scaling technique we have used can only be

rigorously justified in the the "dilute gas limit," i.e., when all the  $y$ 's in (6.2) are small so that the Coulomb gas is a rarefied one. For our problem.

$$\begin{aligned} \frac{Z}{Z_0} = & \sum_{n=0}^{\infty} \sum_{n=n_1+n_2+n_F+n_{AF}} y_1^{n_1} y_2^{n_2} y_F^{n_F} y_{AF}^{n_{AF}} \\ & \times \int_0^\beta \frac{dt_n}{\tau} \cdots \int_0^{t_2-\tau} \frac{dt_1}{\tau} \exp \left[ \sum_{i < j} K_{\alpha_i \alpha_j} \ln \frac{|t_i - t_j|}{\tau} \right] \\ & \times \left\{ 1 + \sum_{a,b} y_a y_b \sum_l \int_{t_l+2\tau}^{t_{l+1}-\tau} \frac{dt'}{\tau} \int_{t'-\tau-d\tau}^{t'-\tau} \frac{dt''}{\tau} \right. \\ & \left. \times \exp \left[ \sum_i \left( K_{\alpha_i a} \ln \frac{|t_i - t'|}{\tau} + K_{\alpha_i b} \ln \frac{|t_i - t''|}{\tau} + K_{ab} \ln \frac{|t' - t''|}{\tau} \right) \right] \right\}. \end{aligned} \quad (7.1)$$

There are now two cases to be considered: If the charges  $a$  and  $b$  are different, it is easy to see that for  $t_i - t' \gg \tau$  we can approximate the  $t_i$ -dependent part in the exponential by

$$\begin{aligned} K_{\alpha_i a} \ln \frac{|t_i - t'|}{\tau} + K_{\alpha_i b} \ln \frac{|t_i - t''|}{\tau} \\ \simeq (K_{\alpha_i a} + K_{\alpha_i b}) \ln \frac{|t_i - t'|}{\tau}. \end{aligned} \quad (7.2)$$

Using the relations (6.4), it is easy to see that

$$K_{\alpha_i a} + K_{\alpha_i b} = K_{\alpha_i c}, \quad (7.3)$$

where  $c$  is the effective hop that results from combining the hops  $a$  and  $b$ . This term then contributes to a renormalization of the chemical potential for the  $c$  charges. The chemical potentials are modified as

$$\begin{aligned} y & \rightarrow y + y(y_F + y_{AF}) \frac{d\tau}{\tau}, \\ y_F & \rightarrow y_F + 2y^2 \frac{d\tau}{\tau}, \\ y_{AF} & \rightarrow y_{AF} + 2y^2 \frac{d\tau}{\tau}. \end{aligned} \quad (7.4)$$

If the charges  $a$  and  $b$  are the same (with opposite sign), this term does not give any contribution to the renormalization of the parameters and one has to go to the next order in  $\tau/(t_i - t')$ . Expanding the exponential it is easy to show, following the procedure of Anderson *et al.*,<sup>5</sup> that one obtains a renormalization of the interaction parameters as follows:

this regime occurs in the limit  $U/\Delta \gg 1$ .

To lowest order in  $d\tau$ , the partition function can be rewritten as (for  $\Delta V = 0$ )

$$\begin{aligned} J & \rightarrow J - [2J(2y^2 + y_F^2 + y_{AF}^2) \\ & \quad + 2J_{12}(y_F^2 - y_{AF}^2)] \frac{d\tau}{\tau}, \\ J_{12} & \rightarrow J_{12} - [2J_{12}(2y^2 + y_F^2 + y_{AF}^2) \\ & \quad + 2J(y_F^2 - y_{AF}^2)] \frac{d\tau}{\tau}. \end{aligned} \quad (7.5)$$

One has also to take into account the modifications in the parameters due to changing  $\tau$  to  $\tau + d\tau$  inside the logarithms in (7.1). It is easy to verify that this modifies the chemical potentials as

$$\begin{aligned} y & \rightarrow y + y \left[ 1 - \frac{J}{2} \right] \frac{d\tau}{\tau}, \\ y_F & \rightarrow y_F + y_F(1 - J - J_{12}) \frac{d\tau}{\tau}, \\ y_{AF} & \rightarrow y_{AF} + y_{AF}(1 - J + J_{12}) \frac{d\tau}{\tau}. \end{aligned} \quad (7.6)$$

Finally, we have to consider how the symmetry-breaking field  $\Delta V$  renormalizes. This occurs similarly as in the single-impurity problem<sup>6</sup> and yields, for  $\tau\Delta \ll 1$ ,

$$\Delta V \rightarrow \Delta V - 8y^2 \Delta V \frac{d\tau}{\tau}. \quad (7.7)$$

Putting all these contributions together we obtain the recursion relations for the parameters in our problem:

$$\begin{aligned} \frac{dJ}{d \ln \tau} & = -2J(2y^2 + y_F^2 + y_{AF}^2) \\ & \quad - 2J_{12}(y_F^2 - y_{AF}^2), \end{aligned} \quad (7.8a)$$



$$\frac{dJ_{12}}{d\ln\tau} = -2J(2y^2 + y_F^2 + y_{AF}^2) - 2J(y_{AF}^2 - y_F^2), \quad (7.8b)$$

$$\frac{dy}{d\ln\tau} = y \left[ 1 - \frac{J}{2} \right] + y(y_F + y_{AF}), \quad (7.8c)$$

$$\frac{dy_F}{d\ln\tau} = y_F(1 - J - J_{12}) + y^2, \quad (7.8d)$$

$$\frac{dy_{AF}}{d\ln\tau} = y_{AF}(1 - J + J_{12}) + y^2, \quad (7.8e)$$

$$\frac{d(\tau\Delta V)}{d\ln\tau} = (1 - 8y^2)(\tau\Delta V), \quad (7.8f)$$

where we emphasize again, that these equations are only valid in the dilute-gas limit, i.e.,  $y, y_F, y_{AF} \ll 1$ . In the next section we discuss the phase diagram resulting from these recursion relations.

### VIII. PHASE STRUCTURE OF THE MODEL

It is clear that a fixed point for the recursion relations (7.8) is given by  $y = y_F = y_{AF} = 0$ . This corresponds to the impurities being decoupled from the conduction band and occurs in the  $U = \infty$  limit. For large but finite  $U$ , the fugacities will be initially small but different from zero. Let us define the following parameters, which appear in the recursion relations for the fugacities,

$$\begin{aligned} \lambda &= 1 - J/2, \\ \lambda_F &= 1 - J - J_{12}, \\ \lambda_{AF} &= 1 - J + J_{12}, \end{aligned} \quad (8.1)$$

and consider first the point where the symmetry-breaking field  $\Delta V = 0$ . We have the following possible phases for the model.

(a)  $\lambda > 0$ . According to the recursion relations, the fugacity  $y$  will grow under iterations and we will obtain an increasing number of single-spin flips. Physically, this corresponds to a situation where the impurity spins are individually Kondo-quenched by the conduction electrons. Note that even if  $\lambda_F, \lambda_{AF} < 0$ , the second term in (7.8) will cause  $y_F$  and  $y_{AF}$  to grow and one will obtain an increasing number of ferro and antiferromagnetic flips too. Depending on whether  $\lambda_F > \lambda_{AF}$  or  $\lambda_{AF} > \lambda_F$  the two-impurity spins will have short-range ferromagnetic or antiferromagnetic correla-

tions. But for long times, the impurities will behave as single Kondo impurities. In particular, this situation arises in the limit  $R \rightarrow \infty$ , where we obtain the single-impurity recursion relations of Anderson *et al.*<sup>5</sup> by putting  $J_{12} = 0$  and  $y_F = y_{AF} = y^2$  in (7.8). This is a consistency check on our recursion relations.

(b)  $\lambda_{AF} > 0, \lambda < 0, \lambda_F < 0$ . Here, the single-spin flips and the ferromagnetic flips are bound in close pairs and disappear from the problem under scaling ( $y, y_F \rightarrow 0$ ) while the number of antiferromagnetic flips grows. Physically, it is a situation where the two-impurity spins are antiferromagnetically correlated via the conduction electrons and form a singlet state.

(c)  $\lambda_F > 0, \lambda < 0, \lambda_F < 0$ . Here  $y_F$  grows while  $y_{AF}, y$  go to zero; the impurity spins are ferromagnetically correlated in a triplet state (forming an effective-spin one impurity) and collectively quenched by the conduction electrons.

We will not discuss the case  $\lambda, \lambda_F, \lambda_{AF} < 0$  since it is not likely to appear in the case of an Anderson model. A similar situation arises in the case of the single-impurity Anderson model, which is always mapped onto the antiferromagnetic side of the Kondo phase diagram.

In the cases where the potential-energy minima are nondegenerate, i.e.,  $\Delta V \neq 0$ , the preceding analysis has to be modified. Equation (7.8f) shows that  $(\tau\Delta V)$  is a *relevant* perturbation always, i.e., it grows under scaling. The term  $\Delta V$  corresponds to the usual RKKY interaction.<sup>13</sup> We can understand qualitatively what happens from the following considerations: Assume we are in regime (a) described above; we can define a Kondo temperature, as in the single-impurity problem, as

$$T_K = 1/\tau_K, \quad (8.2)$$

where  $\tau_K$  is the value of  $\tau$  for which the parameters on the problem have scaled to the strong coupling regime.  $T_K$  is the Kondo temperature and corresponds to the binding energy of the Kondo singlet state. We can also define a time  $\tau_{\Delta V}$  as the value of  $\tau$  for which  $\Delta V$  has become strong, which from (7.8f) is given approximately by

$$\tau_{\Delta V} \sim 1/\Delta V. \quad (8.3)$$

If  $\tau_K < \tau_{\Delta V}$ , the situation will continue as described in (a) above. In other words, if the binding energy of the Kondo singlet state is larger than the RKKY interaction, the Kondo quenching predominates. In the case  $T_K < \Delta V$ , the symmetry-breaking field dominates and there is a

crossover to a regime where only two of the four minima (either ferro- or antiferromagnetic) are present, which will correspond to highly correlated processes. However, this regime cannot be described by our low-order equations (7.8). Note also that one can expect the Kondo temperature (8.2) to have an oscillatory  $R$  dependence due to the  $R$  dependence of the parameters in (6.3) [see Eqs. (3.17), (3.9), and (3.10).]

In summary, we have shown that the problem of a two-impurity symmetric Anderson model in the local-moment regime can be approximately mapped onto a one-dimensional four-component Coulomb-gas model. By studying the scaling equations of this classical statistical-mechanics problem, one can obtain information about the phase diagram of the Coulomb-gas model and the corresponding behavior of the two-impurity Ander-

son model. Although far from providing any quantitative answers, we believe our analysis provides a good qualitative picture of the behavior of a two-magnetic impurity system. In addition, we have provided a physically relevant realization of a multicomponent one-dimensional spin system with inverse-square interaction.

#### ACKNOWLEDGMENTS

We would like to thank Walter Kohn, John Cardy, Steve Shenker, and J. R. Schrieffer for discussions. This work was in part supported by the National Science Foundation, Grant No. PHY77-27084.

---

<sup>1</sup>S. Alexander and P. W. Anderson, *Phys. Rev.* **133**, A1594 (1964).

<sup>2</sup>G. Gruner and A. Zawadowsky, *Progress in Low Temperature Physics* (North-Holland, New York, 1978), Vol. 7B, p. 593.

<sup>3</sup>G. Yuval and P. W. Anderson, *Phys. Rev. B* **1**, 1522 (1970).

<sup>4</sup>D. R. Hamann, *Phys. Rev. B* **2**, 1373 (1970).

<sup>5</sup>P. W. Anderson, G. Yuval, and D. R. Hamann, *Phys. Rev. B* **1**, 4464 (1970).

<sup>6</sup>P. O. Anderson and G. Yuval, *J. Phys. C* **4**, 607 (1971).

<sup>7</sup>D. Ruelle, in *Statistical Mechanics: Rigorous Results*

(Benjamin, New York, 1969).

<sup>8</sup>F. J. Dyson, *Commun. Math. Phys.* **12**, 91 (1969).

<sup>9</sup>D. J. Thouless, *Phys. Rev.* **187**, 732 (1969).

<sup>10</sup>J. Cardy, *J. Phys. A* (in press).

<sup>11</sup>P. Nozières and C. T. de Dominicis, *Phys. Rev.* **178**, 1097 (1969).

<sup>12</sup>N. I. Muskhelishvili, *Singular Integral Equations*, translated by J. R. M. Radok (Noordhoff, Groningen, Holland, 1953).

<sup>13</sup>M. A. Ruderman and C. Kittel, *Phys. Rev.* **96**, 99 (1954).