

## Solution of the two-impurity Kondo model: Critical point, Fermi-liquid phase, and crossover

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An asymptotically exact solution is presented for the two-impurity Kondo model for a finite region of the parameter space surrounding the critical point. This region is located in the most interesting intermediate regime where the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction is comparable to the Kondo temperature. After several exact simplifications involving reduction to one dimension and Abelian bosonization, the critical point is explicitly identified, making clear its physical origin. By using controlled low-energy projection, an effective Hamiltonian is derived for the finite region in the phase diagram around the critical point. The completeness of the effective Hamiltonian is rigorously proved from general symmetry considerations. The effective Hamiltonian is solved exactly not only at the critical point but also for the surrounding Fermi-liquid phase. Analytic crossover functions from the critical to Fermi-liquid behavior are derived for the specific heat and staggered susceptibility. It is shown that applying a uniform magnetic field has negligible effect on the physical behavior inside our solution region. A detailed comparison is made with the numerical renormalization-group and conformal-field-theory results. The excellent agreement is exploited to argue for the universality of the critical point, which in turn implies universal behavior everywhere inside our solution region.

### I. INTRODUCTION

For a vast number of materials with strong electron correlation, the low-energy excitations involve both itinerant electrons and well-localized magnetic moments residing periodically on the lattice sites. This is the case of heavy fermion compounds,<sup>1</sup> and to certain extent it is also the case of high-temperature superconducting cuprates.<sup>2</sup> In such systems, two effects have crucial influence on the low-energy properties and they compete with each other. They are the Kondo effect<sup>3</sup> and Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction,<sup>4</sup> which represent two different tendencies of the system to quench the local moments either with conduction electrons or by themselves. The simplest model capturing both effects is the two-impurity Kondo model.<sup>5-7</sup> It is also believed that possible new physics that may occur in lattice due to the competition between the two effects should be essentially contained in the two-impurity problem.<sup>8</sup>

A simple way to see how the competition arises in the two-impurity Kondo model is to look at the problem from the scaling point of view.<sup>9</sup> For all practical purposes, the bare Kondo coupling constant  $J$  and the bare RKKY interaction  $K$  are much smaller than the Fermi energy  $\epsilon_F$ . Thus, if we form two dimensionless coupling constants with the help of the conduction electron density of states at the Fermi level  $\rho_F(\sim 1/\epsilon_F)$ ,  $\rho_F J$  and  $\rho_F K$ , they are always in the weak coupling regime. However, as soon as we start the scaling procedure to eliminate high-energy conduction electron states near the top and bottom of the conduction band, both dimensionless coupling constants grow under renormalization and they mutually renormal-

ize each other. Simple dimensional counting shows that  $\rho_F J$  has dimension one and is marginally relevant, while  $\rho_F K$  has dimension zero and is relevant. For these two relevant interactions we can define two energy scales, the Kondo temperature  $T_K$  and RKKY temperature  $T_{\text{RKKY}}$ , such that they correspond to the values of the decreasing conduction bandwidth at which the renormalized dimensionless coupling constants  $\rho_F J$  and  $\rho_F K$  reach unity respectively. In either  $T_K \gg T_{\text{RKKY}}$  or  $T_K \ll T_{\text{RKKY}}$  limit, the problem is simple because we can perturb one of the two interactions. The most difficult situation corresponds to  $T_K \sim T_{\text{RKKY}}$ . This is also the situation of most practical interest.

Due to the broad interest in the competition between the Kondo effect and RKKY interaction, extensive investigations have been carried out in the last decade.<sup>5,10-18</sup> As a result, a convincing phase diagram has emerged,<sup>11,14-16</sup> if not yet universally accepted without reservation.<sup>19</sup> This phase diagram is shown in Fig. 1. The model exhibits Fermi-liquid behavior everywhere except at a special point on the particle-hole symmetric axis. At this point, the ratio between the fully renormalized effective RKKY interaction and the Kondo temperature is numerically estimated to be 2.2.<sup>11</sup> The effective RKKY interaction is actually the RKKY temperature whose meaning we have specified in the last paragraph. Although the precise numerical value of the ratio may depend on the individual's convention of defining the coupling constants, the important point is that this critical point is located at  $T_K \sim T_{\text{RKKY}}$ .

Although several asymptotically exact results have been available on the critical point in certain limits,<sup>11,18</sup> the precise physical origin of this critical point had not

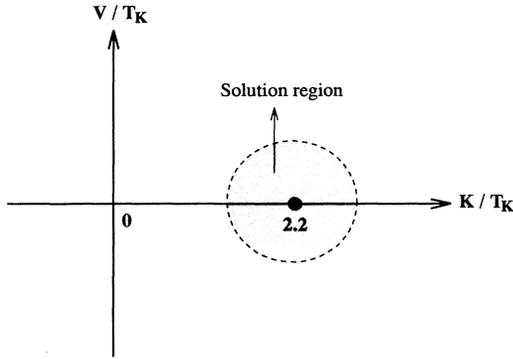


FIG. 1. The phase diagram of the two-impurity Kondo model.  $V$  is the energy scale characterizing particle-hole symmetry breaking strength.  $K$  is the fully renormalized RKKY interaction.  $T_K$  is the Kondo temperature. Except at the critical point marked by the black dot, the low-energy behavior is of Fermi-liquid type everywhere. The area inside the dashed circle is the region where our solution applies. The radius of the solution region is a fraction of  $T_K$ .

been unveiled completely until recently.<sup>20</sup> By an explicit identification of two many-body states whose level crossing being the origin of the critical point, we have rigorously shown how the constraints set by the discrete symmetries of the model ensure the non-Fermi-liquid behavior at the critical point. We have also presented an effective Hamiltonian for the finite solution region as marked in Fig. 1, and listed the low-temperature properties of the critical point. In this paper, we present a detailed derivation of the effective Hamiltonian, and for the first time a full analytic solution for the whole solution region in Fig. 1.

Having admitted the existence of the critical point, we can already present a framework for the solution of the two-impurity Kondo model inside the solution region in Fig. 1 by only invoking general scaling ideas. It is then the task of Sec. IV to fill in concrete results. Since the Kondo effect always takes place in our solution region, the basic energy scale must be the Kondo temperature  $T_K$ , which is much smaller than the Fermi energy. On the scale of  $T_K$ , the system has already lost its memory of microscopic details existing on the energy scale of the Fermi energy. The above-mentioned  $T_{\text{RKKY}}$  is of the same order as  $T_K$ , and therefore does not constitute a new energy scale by itself. However, the competition induces the second energy scale  $T_c$ . Inside our solution region,  $T_c \ll T_K$ , and  $T_c$  vanishes at the critical point. For any physical quantity, its dependence on the bare parameters of the two-impurity Kondo Hamiltonian should be absorbed into these two energy scales. For instance, we can write the specific heat in the form  $C(T) = f(T/T_K, T_c/T_K)$ , where  $f(x, y)$  is some universal two-variable function. The role of  $T_K$  is simply to set an energy unit for the problem. The second energy scale  $T_c$  determines the crossover from the non-Fermi-liquid behavior governed by the critical point at  $T \gg T_c$  to the Fermi-liquid behavior governed by the stable Fermi-liquid fixed point at  $T \ll T_c$ . If we recall how the appear-

ance of the Kondo temperature  $T_K (\ll \epsilon_F)$  in the one-impurity Kondo problem leads to the drastic enhancement of various physical quantities such as the density of states, we can expect additional enhancement from the appearance of  $T_c (\ll T_K)$ . The translation of this effect to the lattice problem will be a new mechanism for the heavy electron mass.

Moving far away from the critical point in the phase diagram of Fig. 1, the accuracy of our solution deteriorates. However, the low-energy exponents for all physical quantities should not change since after all the system is still governed by a Fermi-liquid fixed point as inside the solution region of Fig. 1. What need to be improved are the constant prefactors. Generally, a physical quantity calculated for a Fermi-liquid fixed point contains several contributions with the same exponent. Among them, only a few are associated with the energy scale  $T_c$ , while the others are associated with  $T_K$ . What we calculate in this paper are those contributions associated with the energy scale  $T_c$ . This is enough near the critical point because they are enhanced inside our solution region. As one moves away from the critical point,  $T_c$  increases and eventually reaches the same order as  $T_K$ . Therefore, the other contributions associated with the energy scale  $T_K$  become increasingly significant. Certainly, one can always fit the prefactors for every physical quantity if well-established numerical results or experimental data are available. But it is the merit of the theory to establish the relations between these prefactors in the same spirit as Nozières's Fermi-liquid theory of Kondo effect.<sup>21</sup> A complete solution of the two-impurity Kondo model for the whole parameter space is beyond the scope of this paper.

The layout of the paper is as follows. In Sec. II, we present the preliminary transformations on the two-impurity Kondo model including the reduction to one dimension and bosonization. In Sec. III, we identify the critical point and derive the effective Hamiltonian. Then, we rigorously prove the completeness of the ef-

TABLE I. Definition of frequently used parameters and symbols.

Symbol	Definition (eq. no.)	Symbol	Definition (eq. no.)
$v_F$	Fermi velocity	$g_1$	(46), (49)
$\rho_F$	Density of states	$\tilde{V}$	(47), (50)
$J^z, J^\perp$	Kondo coupling constants	$\alpha_u$	(45), (51)
$K_z, K_\perp$	RKKY interaction	$\alpha_s$	(45), (52)
$S_\pm^{x,y,z}$	(5)	$\delta K$	(68)
$h_u, h_s$	(15)	$\Lambda$	(80)
$J_\pm^{z,\perp}, J_m^{z,\perp}$	(17)	$Z_b$	(86)
$V$	(18)	$T_K$	(88)
$\tilde{J}_\pm^z, \tilde{K}_z$	(38)	$T_c$	(89)
$g_0$	(45), (48)	$\tilde{\alpha}_s$	(90)

fective Hamiltonian. In Sec. IV, we solve the effective Hamiltonian and calculate the low-energy thermodynamics. In Sec. V, we compare our results with those derived from the numerical renormalization-group and conformal-field-theory approaches. The excellent agreement strongly supports the universality of the critical point. We conclude our paper in Sec. VI with a summary and some speculations on the lattice problem. To alleviate cross reference, some frequently used parameters and symbols are collected in Table I.

## II. REDUCTION TO ONE DIMENSION AND BOSONIZATION

In this section, we shall start from the most general two-impurity Kondo model and perform various exact transformations to reduce it to a simplified form, (36)+(37)+(39), suitable for identifying the critical point and uncovering the underlying physics.

The general Hamiltonian for the anisotropic two-impurity Kondo model has the following form:

$$H = \int d^3k \epsilon_k \psi_{\mathbf{k}}^\dagger \psi_{\mathbf{k}} + \int \frac{d^3k d^3k'}{(2\pi)^3} \sum_{\lambda=x,y,z} \frac{J^\lambda}{2} \left[ e^{\frac{i}{2}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}} \psi_{\mathbf{k}}^\dagger \sigma^\lambda \psi_{\mathbf{k}'} S_1^\lambda + e^{-\frac{i}{2}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}} \psi_{\mathbf{k}}^\dagger \sigma^\lambda \psi_{\mathbf{k}'} S_2^\lambda \right] + \sum_{\lambda=x,y,z} K_\lambda S_1^\lambda S_2^\lambda, \quad (1)$$

where  $\psi_{\mathbf{k}}^\dagger = (\psi_{\mathbf{k}\uparrow}^\dagger, \psi_{\mathbf{k}\downarrow}^\dagger)$  are the conduction electron creation operators with dispersion  $\epsilon_k$ ,  $\sigma^\lambda$  with  $\lambda = x, y, z$  are the Pauli matrices,  $\mathbf{S}_1$  and  $\mathbf{S}_2$  are the two impurity-spin-1/2 operators located at  $\pm\mathbf{R}/2$ .  $J^\lambda$  with  $\lambda = x, y, z$  are the bare Kondo coupling constants.  $K_\lambda$  with  $\lambda = x, y, z$  are the bare RKKY interaction constants. It has been shown that the Hamiltonian (1) can be reduced to an equivalent one-dimensional (1D) problem.<sup>11,18</sup> Introducing 1D fermionic operators,

$$\psi_{1,2}(k) = \frac{k}{\sqrt{2}} \left[ \frac{1}{N_e(k)} \int d^2\Omega \cos\left(\frac{\mathbf{k}\cdot\mathbf{R}}{2}\right) \mp \frac{i}{N_o(k)} \int d^2\Omega \sin\left(\frac{\mathbf{k}\cdot\mathbf{R}}{2}\right) \right] \psi_{\mathbf{k}}, \quad (2)$$

with the notations  $d^3k = k^2 dk d^2\Omega$  and

$$N_{e,o}(k) = \sqrt{1 \pm \frac{\sin(kR)}{kR}}, \quad (3)$$

we can completely rewrite the Kondo interactions in terms of these new operators,

$$H_{\text{Kondo}} = \frac{v_F}{2} \sum_{\lambda=x,y,z} \int_0^\infty \frac{dk dk'}{(2\pi)^2} \left\{ J_+^\lambda(k, k') \left[ \psi_1^\dagger(k) \sigma^\lambda \psi_1(k') + \psi_2^\dagger(k) \sigma^\lambda \psi_2(k') \right] S_+^\lambda + J_m^\lambda(k, k') \left[ \psi_1^\dagger(k) \sigma^\lambda \psi_1(k') - \psi_2^\dagger(k) \sigma^\lambda \psi_2(k') \right] S_-^\lambda + J_-^\lambda(k, k') \left[ \psi_1^\dagger(k) \sigma^\lambda \psi_2(k') + \psi_2^\dagger(k) \sigma^\lambda \psi_1(k') \right] S_+^\lambda - J_{ir}^\lambda(k, k') \left[ \psi_1^\dagger(k) \sigma^\lambda \psi_2(k') - \psi_2^\dagger(k) \sigma^\lambda \psi_1(k') \right] S_-^\lambda \right\}. \quad (4)$$

In the last expression, we have introduced the shorthand notation

$$S_\pm^\lambda = S_1^\lambda \pm S_2^\lambda, \quad \lambda = x, y, z. \quad (5)$$

The momentum-dependent coupling constants are, for  $\lambda = x, y, z$ ,

$$J_+^\lambda(k, k') = \frac{J^\lambda k k'}{4\pi v_F} [N_e(k)N_e(k') + N_o(k)N_o(k')], \quad (6)$$

$$J_-^\lambda(k, k') = \frac{J^\lambda k k'}{4\pi v_F} [N_e(k)N_e(k') - N_o(k)N_o(k')], \quad (7)$$

$$J_m^\lambda(k, k') = \frac{J^\lambda k k'}{4\pi v_F} [N_e(k)N_o(k') + N_o(k)N_e(k')], \quad (8)$$

$$J_{ir}^\lambda(k, k') = \frac{J^\lambda k k'}{4\pi v_F} [N_e(k)N_o(k') - N_o(k)N_e(k')]. \quad (9)$$

From the commutation relation  $\{\psi_{\mathbf{k}\sigma}^\dagger, \psi_{\mathbf{k}'\sigma'}\} = \delta^3(\mathbf{k} -$

$\mathbf{k}')\delta_{\sigma,\sigma'}$ , we can verify

$$\{\psi_{i\sigma}^\dagger(k), \psi_{i'\sigma'}(k')\} = 2\pi\delta(k-k')\delta_{i,i'}\delta_{\sigma,\sigma'}. \quad (10)$$

The free conduction electron Hamiltonian can also be written in terms of these 1D fermions, plus completely decoupled extra degrees of freedom,

$$\int d^3k \epsilon_k \psi_{\mathbf{k}}^\dagger \psi_{\mathbf{k}} = \int_0^\infty \frac{dk}{2\pi} \epsilon_k \left[ \psi_1^\dagger(k) \psi_1(k) + \psi_2^\dagger(k) \psi_2(k) \right] + \dots \quad (11)$$

Thus, only 1D fermions defined in (2) are relevant to the two-impurity Kondo problem.

So far, the reduction has been exact. In the next step, we linearize the dispersion  $\epsilon_k$  at  $k = k_F$ ,  $\epsilon_k \simeq v_F(k - k_F)$ , and expand the momentum-dependent coupling constants around  $k = k_F$ . We only need to retain the leading terms of the expansion since others contain

some power of  $k - k_F$ , which have high scaling dimension and are irrelevant at low energy. From  $J_{ir}^\lambda(k_F, k_F) = 0$ , we see that the  $J_{ir}$  interaction only contains irrelevant terms. Denoting  $k - k_F$  by  $k$  again and with implicit understanding of an ultraviolet cutoff, we can introduce the Fourier transforms

$$\psi_i(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \psi_i(k), \quad i = 1, 2. \quad (12)$$

The fermion operators satisfy the standard commutation relation,

$$\{\psi_{i\sigma}^\dagger(x), \psi_{i'\sigma'}(x')\} = \delta(x - x') \delta_{i,i'} \delta_{\sigma,\sigma'}. \quad (13)$$

After linearization, the full two-impurity Kondo Hamiltonian can be cast in the following form:

$$H = H_0 + H_1, \quad (14)$$

$$H_0 = -i v_F \sum_{i=1,2} \int_{-\infty}^{\infty} dx \psi_i^\dagger(x) \partial_x \psi_i(x) + \sum_{\lambda=x,y,z} K_\lambda S_1^\lambda S_2^\lambda + h_u \left[ S_+^z + \frac{1}{2} \sum_{i=1,2} \int_{-\infty}^{\infty} dx \psi_i^\dagger(x) \sigma^z \psi_i(x) \right] + h_s S_-^z, \quad (15)$$

$$H_1 = \frac{v_F}{2} \sum_{\lambda=x,y,z} \left\{ J_+^\lambda \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_1(0) + \psi_2^\dagger(0) \sigma^\lambda \psi_2(0) \right] S_+^\lambda + J_m^\lambda \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_1(0) - \psi_2^\dagger(0) \sigma^\lambda \psi_2(0) \right] S_-^\lambda + J_-^\lambda \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_2(0) + \psi_2^\dagger(0) \sigma^\lambda \psi_1(0) \right] S_+^\lambda \right\}. \quad (16)$$

The coupling constants are, for  $\lambda = x, y, z$ ,

$$J_+^\lambda = \pi J^\lambda \rho_F, \quad J_-^\lambda = \pi J^\lambda \rho_F \frac{\sin(k_F R)}{k_F R}, \quad J_m^\lambda = \pi J^\lambda \rho_F \sqrt{1 - \left( \frac{\sin k_F R}{k_F R} \right)^2}, \quad (17)$$

with  $\rho_F = k_F^2 / (2\pi^2 v_F)$ , denoting the conduction electron density of states per spin at the Fermi energy. Note that we have included both uniform and staggered magnetic fields  $h_u$  and  $h_s$  in (15), with the Bohr magneton and gyromagnetic ratio set equal to one.

At this stage, the 3D two-impurity Kondo model has been successfully reduced to an equivalent 1D problem, up to some terms irrelevant at low energy. However, we must remove two accidental features of (14) resulting from linearization. They are the particle-hole symmetry and a special relation between  $J_\pm^\lambda(k_F, k_F)$  and  $J_m^\lambda(k_F, k_F)$ : that the RKKY interaction generated from them is always ferromagnetic<sup>11</sup>. These accidental features will be spoiled by the corrections generated from the irrelevant terms neglected during the linearization. That an irrelevant interaction can renormalize the coupling constant of a relevant interaction is a well-known fact.<sup>22</sup> An example can also be found in Sec. IV: the last term in expression (83) is the induced correction to the dimension 1/2 relevant operator by the dimension 3/2 leading irrelevant operator in the effective Hamiltonian (44). Usually, the accidental features at the lowest order will not survive if there is no hidden symmetry ensuring them. The accidental relation between  $J_\pm^\lambda(k_F, k_F)$  and  $J_m^\lambda(k_F, k_F)$ , with  $\lambda = x, y, z$ , is removed by treating these coupling constants as *independent* parameters. This is also physically meaningful since these interactions are completely independent and presumably play different roles at low energy. Particle-hole symmetry breaking,

although weak, is always present for a general conduction band. The general particle-hole symmetry breaking term that can be added to the 1D Hamiltonian (14) has the following form:<sup>11,18</sup>

$$H_2 = V \left[ \psi_1^\dagger(0) \psi_2(0) + \psi_2^\dagger(0) \psi_1(0) \right], \quad (18)$$

where  $V$  is the energy scale characterizing the symmetry breaking strength. The operator (18) is marginal. Adding it to the 1D Hamiltonian (14) after dropping irrelevant interactions during the linearization may seem unusual, it is actually the natural thing to do. The reason is again the generation of (18) from the irrelevant interactions in the absence of the particle-hole symmetry. Usually, all possible operators allowed by the symmetry will be generated by irrelevant interactions, and we only need to include relatively more relevant operators. In this case, the lowest dimension operator breaking particle-hole symmetry is (18). In Sec. III and Appendix B, we shall see a similar example where the marginal operator (18) generates a relevant operator (47) when projecting to a subspace relevant for the solution region in Fig. 1.

In the rest of this paper, we shall retain the rotational symmetry around the  $z$  axis by setting  $K_x = K_y = K_\perp$  and  $J_i^x = J_i^y = J_i^\perp$  for  $i = m, \pm$ . Apart from the continuous  $U(1)$  rotational symmetry, the Hamiltonian (14) possesses several discrete symmetries which will be very useful for our analysis. The transformation rules are, omitting unaffected operators,

$$\begin{aligned}
&\text{parity : } \psi_1 \leftrightarrow \psi_2, \quad S_1^\lambda \leftrightarrow S_2^\lambda \text{ for } \lambda = x, y, z, \\
&\text{particle-hole : } \psi_{i\uparrow} \rightarrow \psi_{i\downarrow}^\dagger, \quad \psi_{i\downarrow} \rightarrow -\psi_{i\uparrow}^\dagger, \\
&\pi \text{ rotation around the } x \text{ axis : } \psi_{i\uparrow} \leftrightarrow \psi_{i\downarrow}, \quad S_i^y \rightarrow -S_i^y, \quad S_i^z \rightarrow -S_i^z.
\end{aligned} \tag{19}$$

The particle-hole symmetry exists when  $V = 0$ .

The next step is to reduce the Hamiltonian (14)+(18) to a simple form suitable for identifying the critical point. The reduction involves bosonizing the Hamiltonian which only contains 1D left-moving fermions.<sup>23,24,17</sup> There are four species of fermions, so we need to introduce four Bose fields,

$$\psi_{i\sigma}(x) = \frac{P_{i\sigma}}{\sqrt{2\pi\alpha}} e^{i\Phi_{i\sigma}(x)}, \quad i = 1, 2, \quad \sigma = \uparrow, \downarrow, \tag{20}$$

where  $\alpha$  is the lattice spacing and

$$\Phi_{i\sigma}(x) = \sqrt{\pi} \left[ \phi_{i\sigma}(x) - \int_{-\infty}^x dx' \Pi_{i\sigma}(x') \right]. \tag{21}$$

The Bose fields satisfy the standard commutation relation,

$$[\phi_{j\sigma}(x), \Pi_{j'\sigma'}(x')] = i \delta_{jj'} \delta_{\sigma\sigma'} \delta(x - x'). \tag{22}$$

The phase factors  $P_{i\sigma}$  are introduced to take care of the anticommutation relations between different species of fermions. Our choices are

$$P_{1\uparrow} = P_{1\downarrow} = e^{i\pi \int_{-\infty}^{\infty} dx \psi_{1\uparrow}^\dagger(x) \psi_{1\uparrow}(x)}, \tag{23}$$

$$P_{2\uparrow} = P_{2\downarrow} = e^{i\pi \int_{-\infty}^{\infty} dx [\sum_{\sigma} \psi_{1\sigma}^\dagger(x) \psi_{1\sigma}(x) + \psi_{2\uparrow}^\dagger(x) \psi_{2\uparrow}(x)]}. \tag{24}$$

By substituting (20) into (14) and using the relation  $\psi_{i\sigma}^\dagger(x) \psi_{i\sigma}(x) = \partial_x \Phi_{i\sigma}(x) / (2\pi)$ , the two-impurity Kondo Hamiltonian is expressed in terms of the four Bose fields  $\phi_{i\sigma}(x)$ . Then we make linear transformations to four new Bose fields corresponding to charge, spin, flavor, and spin-flavor degrees of freedom,

$$\begin{aligned}
\phi_c &= (\phi_{1\uparrow} + \phi_{1\downarrow} + \phi_{2\uparrow} + \phi_{2\downarrow})/2, \\
\phi_s &= (\phi_{1\uparrow} - \phi_{1\downarrow} + \phi_{2\uparrow} - \phi_{2\downarrow})/2, \\
\phi_f &= (\phi_{1\uparrow} + \phi_{1\downarrow} - \phi_{2\uparrow} - \phi_{2\downarrow})/2, \\
\phi_{sf} &= (\phi_{1\uparrow} - \phi_{1\downarrow} - \phi_{2\uparrow} + \phi_{2\downarrow})/2.
\end{aligned} \tag{25}$$

The Hamiltonian now acquires the following form:

$$H_0 = \frac{v_F}{2} \sum_{\lambda=c,s,f,ff} \int_{-\infty}^{\infty} dx \{ \Pi_\lambda^2(x) + [\partial_x \phi_\lambda(x)]^2 \} + \sum_{\lambda=x,y,z} K_\lambda S_1^\lambda S_2^\lambda + h_u \left[ S_+^z + \int_{-\infty}^{\infty} \frac{dx}{2\pi} \partial_x \Phi_s(x) \right] + h_s S_-^z, \tag{26}$$

$$\begin{aligned}
H_1 &= \frac{v_F}{2} \left\{ \frac{J_+^z}{\pi} \partial_x \Phi_s(0) S_+^z + \frac{J_m^z}{\pi} \partial_x \Phi_{sf}(0) S_-^z - i \frac{2J_-^z}{\pi\alpha} e^{i\pi\theta} \cos \Phi_{sf}(0) \sin \Phi_f(0) S_+^z + \frac{2J_+^\perp}{\pi\alpha} \right. \\
&\quad \times \cos \Phi_{sf}(0) [\cos \Phi_s(0) S_+^z - \sin \Phi_s(0) S_+^y] - \frac{2J_m^\perp}{\pi\alpha} \sin \Phi_{sf}(0) [\sin \Phi_s(0) S_-^z + \cos \Phi_s(0) S_-^y] \\
&\quad \left. - \frac{2J_+^\perp}{\pi\alpha} e^{i\pi\theta} \sin \Phi_f(0) [\sin \Phi_s(0) S_+^z + \cos \Phi_s(0) S_+^y] \right\}, \tag{27}
\end{aligned}$$

$$H_2 = -i \frac{2V}{\pi\alpha} e^{i\pi\theta} \sin \Phi_{sf}(0) \cos \Phi_f(0), \tag{28}$$

where the phase factor  $\theta$  is

$$\theta = \int_{-\infty}^{\infty} dx [\psi_{1\downarrow}^\dagger(x) \psi_{1\downarrow}(x) + \psi_{2\uparrow}^\dagger(x) \psi_{2\uparrow}(x)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx [\partial_x \Phi_c(x) - \partial_x \Phi_{sf}(x)]. \tag{29}$$

The charge Bose field  $\phi_c(x)$  is decoupled from the interaction (27). It will be omitted from now on, and so will be  $\partial_x \Phi_c$  in the integrand of the phase  $\theta$ . Both  $\cos \Phi_s(0)$  and  $\sin \Phi_s(0)$  factors in (27) can be eliminated by rotating the impurity spins around the  $z$  axis by an angle  $\Phi_s(0)$ ,

$$H \rightarrow \hat{U} H \hat{U}^{-1} \text{ with } \hat{U} = e^{-iS_+^z \Phi_s(0)}, \tag{30}$$

$$\begin{aligned}
\hat{U} H_0 \hat{U}^{-1} &= \frac{v_F}{2} \sum_{\lambda=s,f,ff} \int_{-\infty}^{\infty} dx \{ \Pi_\lambda^2(x) + [\partial_x \phi_\lambda(x)]^2 \} + \sum_{\lambda=x,y,z} K_\lambda S_1^\lambda S_2^\lambda + h_s S_-^z \\
&\quad + h_u \int_{-\infty}^{\infty} \frac{dx}{2\pi} \partial_x \Phi_s(x) - v_F \partial_x \Phi_s(0) S_+^z + \frac{v_F}{\alpha} (S_+^z)^2, \tag{31}
\end{aligned}$$

$$\begin{aligned}
\hat{U} H_1 \hat{U}^{-1} &= \frac{v_F}{2} \left\{ \frac{J_+^z}{\pi} \partial_x \Phi_s(0) S_+^z + \frac{J_m^z}{\pi} \partial_x \Phi_{sf}(0) S_-^z - i \frac{2J_-^z}{\pi\alpha} e^{i\pi\theta} \cos \Phi_{sf}(0) \sin \Phi_f(0) S_+^z \right. \\
&\quad \left. - \frac{2J_+^\perp}{\pi\alpha} (S_+^z)^2 + \frac{2}{\pi\alpha} [J_+^\perp \cos \Phi_{sf}(0) S_+^z - J_m^\perp \sin \Phi_{sf}(0) S_-^z - J_-^\perp e^{i\pi\theta} \sin \Phi_f(0) S_+^y] \right\}. \tag{32}
\end{aligned}$$

The particle-hole symmetry breaking term  $H_2$  is not affected by the above rotation. We note that both  $J_+^z$  and  $K_z$  acquired corrections under the rotation, and  $h_u S_+^z$  is canceled out in (31). Since the spin Bose field  $\phi_s(x)$  only enters (32) in the form  $\partial_x \Phi_s(0)$ , it can be integrated out analytically if needed.

The bosonized Hamiltonian (31)+(32)+(28) can be refermionized by introducing three new species of left-moving fermions,

$$\psi_{sf}(x) = \frac{1}{\sqrt{2\pi\alpha}} e^{i\Phi_{sf}(x)}, \quad (33)$$

$$\psi_f(x) e^{i\pi \int_{-\infty}^x dx \psi_{sf}^\dagger(x) \psi_{sf}(x)} = \frac{1}{\sqrt{2\pi\alpha}} e^{i\Phi_f(x)}, \quad (34)$$

$$\psi_s^\dagger(x) \psi_s(x) = \frac{1}{2\pi} \partial_x \Phi_s(x). \quad (35)$$

Again, a phase factor is included in the definition of the fermion operator  $\psi_f(x)$  to take care of the anticommutation relations between three different species of fermions. Because the interactions in (32) contain only  $\partial_x \Phi_s(0)$  which implies that  $\psi_s$  only appears in the product  $\psi_s^\dagger(0)\psi_s(0)$ , we do not need to specify the phase for  $\psi_s(x)$ . The complete Hamiltonian can be rewritten as

$$\begin{aligned} H_0 &= -iv_F \sum_{i=s,f,sf} \int_{-\infty}^{\infty} dx \psi_i^\dagger(x) \partial_x \psi_i(x) + \tilde{K}_z S_1^z S_2^z + K_\perp \sum_{\lambda=x,y} S_1^\lambda S_2^\lambda + h_u \int_{-\infty}^{\infty} dx \psi_s^\dagger(x) \psi_s(x) + h_s S_-^z, \quad (36) \\ H_1 &= \frac{v_F}{2} \left\{ \tilde{J}_+^z [\psi_s^\dagger(0)\psi_s(0) - \psi_s(0)\psi_s^\dagger(0)] S_+^z + J_m^z [\psi_{sf}^\dagger(0)\psi_{sf}(0) - \psi_{sf}(0)\psi_{sf}^\dagger(0)] S_-^z \right. \\ &\quad \left. + J_-^z [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] [\psi_f(0) - \psi_f^\dagger(0)] S_+^z \right\} + \frac{v_F}{\sqrt{2\pi\alpha}} \left\{ J_+^\perp [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] S_+^x \right. \\ &\quad \left. + iJ_m^\perp [\psi_{sf}(0) - \psi_{sf}^\dagger(0)] S_-^y + iJ_-^\perp [\psi_f(0) - \psi_f^\dagger(0)] S_+^y \right\}, \quad (37) \end{aligned}$$

where

$$\tilde{J}_+^z = J_+^z - 2\pi, \quad \tilde{K}_z = K_z - \frac{2v_F}{\pi\alpha} (J_+^z - \pi). \quad (38)$$

The particle-hole symmetry breaking term becomes

$$H_2 = V [\psi_{sf}(0) - \psi_{sf}^\dagger(0)] [\psi_f(0) + \psi_f^\dagger(0)]. \quad (39)$$

How do the new fermion operators transform under the discrete symmetries of (19)? We can keep track of the transformation rules during the bosonization and subsequent fermionization to derive, omitting unaffected operators,

$$\text{parity: } \psi_{sf} \leftrightarrow \psi_{sf}^\dagger, \quad \psi_f \leftrightarrow -\psi_f^\dagger, \quad S_1^\lambda \leftrightarrow S_2^\lambda$$

for  $\lambda = x, y, z$ ,

$$\text{particle-hole: } \psi_f \leftrightarrow -\psi_f^\dagger, \quad (40)$$

$$\pi \text{ rotation, } x \text{ axis: } \psi_{sf} \leftrightarrow \psi_{sf}^\dagger, \quad \psi_s \leftrightarrow \psi_s^\dagger, \quad \psi_f \leftrightarrow -\psi_f,$$

$$S_i^y \rightarrow -S_i^y, \quad S_i^z \rightarrow -S_i^z.$$

Alternatively, one can directly verify (40) from (36), (37), and (39).

### III. EFFECTIVE HAMILTONIAN NEAR THE CRITICAL POINT

In this section, we shall identify the critical point from (36)+(37) and then derive an effective Hamiltonian around the critical point from the full interaction Hamiltonian (36)+(37)+(39) using second-order projection. Finally, we shall prove the completeness of the effective Hamiltonian.

To search for the critical point, we need only consider the particle-hole symmetric case,  $V = 0$ . At first glance the Hamiltonian (36)+(37) still looks too complicated to provide any intuition. On the other hand, from the conformal field theory results it is known that the critical point exists in a restricted Hamiltonian with  $J_-^z = J_-^\perp = 0$ , and around the critical point both  $J_-^z$  and  $J_-^\perp$  interactions are irrelevant. Thus, our task is greatly reduced by searching the critical point in this restricted Hamiltonian. An important step is to verify the irrelevance of the  $J_-^z$ ,  $J_-^\perp$  interactions after we find the critical point.

We have noted before that only the product  $\psi_s^\dagger(0)\psi_s(0)$  appears in (37). This is because only  $\partial_x \Phi_s(0)$  appears in (32) and both  $\cos \Phi_s(0)$  and  $\sin \Phi_s(0)$  have been eliminated by the canonical transformation (30). Thus, the  $\tilde{J}_+^z$  term containing the Bose field  $\phi_s(x)$  can be integrated out analytically. Although  $\partial_x \Phi_s(0)$  couples to an operator  $S_+^z$  in (31) and (32), the integration can be done formally in the bosonic path integral formalism, yielding the following two terms to the action:

$$\begin{aligned} & -\frac{v_F (\tilde{J}_+^z)^2}{4\pi^2 \alpha} \int_0^\beta d\tau [S_+^z(\tau)]^2 \\ & + \frac{(\tilde{J}_+^z)^2}{8\pi} \sum_n |\nu_n| S_+^z(-\nu_n) S_+^z(\nu_n), \end{aligned}$$

$$\text{with } \nu_n = 2n\pi/\beta. \quad (41)$$

The first term is a correction to the RKKY interaction, so it is absorbed into  $\tilde{K}_z$ . The second term has higher

scaling dimension and is expected to be less important. The point we want to make here is that the  $\tilde{J}_+^z$  interaction does not affect the critical point and can be ignored during the search for the critical point.

When  $J_-^z = J_-^\perp = 0$  and neglecting  $\tilde{J}_+^z$ , the remaining Kondo interactions only contain three local impurity spin operators,  $S_+^x$ ,  $S_+^y$ , and  $S_-^z$ , which only act on three (out of four) local impurity spin states. The impurity spin state  $(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)/\sqrt{2}$  is decoupled from the Kondo interactions. Together with the RKKY interactions, we derive an energy level scheme for the impurity spin states in Fig. 2. We have to keep in mind that these so-called local impurity spin states are actually many-body states because of the canonical transformation (30). The critical point corresponds to the special case when the two lowest levels become degenerate. Specifically, the  $z$  component of the RKKY interaction, i.e., the  $-\tilde{K}_z(S_-^z)^2/2$  term in (36), raises the energy of the states  $|\uparrow\downarrow\rangle$  and  $|\downarrow\uparrow\rangle$  by an amount  $-\tilde{K}_z/2$  (assuming  $-\tilde{K}_z > 0$ ) with respect to the other two states  $|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle$ . These two states,  $|\uparrow\downarrow\rangle$  and  $|\downarrow\uparrow\rangle$ , are further split symmetrically by the transverse part of the RKKY interaction,  $K_\perp(S_1^+S_2^- + S_1^-S_2^+)/2$ . When  $-\tilde{K}_z = K_\perp$ ,  $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$  and  $(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$  become degenerate and form a doublet. Because there is almost no Kondo interaction in the state  $(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)/\sqrt{2}$  when  $J_-^z = J_-^\perp = 0$  and neglecting  $\tilde{J}_+^z$ , the superficial degeneracy between this state and the doublet is lifted by the Kondo interactions in the doublet which lower the energy of the doublet by a finite amount  $T_K$ , equal to the ground state energy gain at the critical point. Turning on  $\tilde{J}_+^z$ ,  $J_-^z$ , and  $J_-^\perp$  will not change the energy level scheme as long as  $v_F\tilde{J}_+^z < T_K$ ,  $v_FJ_-^z < T_K$  and  $v_FJ_-^\perp < T_K$ .

Now, we have identified the critical point. To describe the low-energy physics, it is sufficient to project the full interaction Hamiltonian (36)+(37)+(39) onto the lowest energy doublet. When all coupling constants, possibly except  $J_m^\perp$ , are much smaller than one, the projection can be done accurately. Let  $\hat{Q}$  be the projection operator onto the doublet, the effective Hamiltonian to the second order is

$$H_{\text{eff}} = \hat{Q}H\hat{Q} + \hat{Q}H(1 - \hat{Q}) \frac{1}{E_0 - \hat{Q}H\hat{Q} - (1 - \hat{Q})H(1 - \hat{Q})} \times (1 - \hat{Q})H\hat{Q}, \quad (42)$$

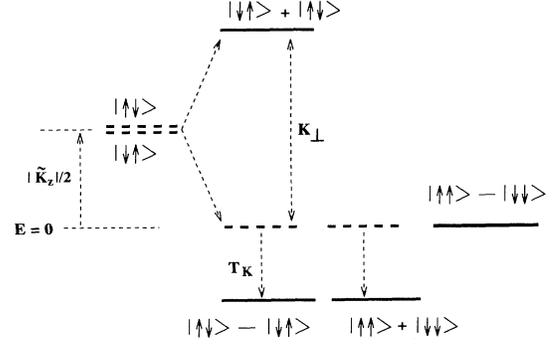


FIG. 2. The energy level scheme of the four impurity spin states. The up and down spin states refer to the eigenstates of the operators  $S_1^z$  and  $S_2^z$ . At  $-\tilde{K}_z = K_\perp$ , the two levels  $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$  and  $(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$  become degenerate, forming a doublet. The superficial degeneracy between the doublet and  $(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)/\sqrt{2}$  is lifted by the Kondo interaction term  $J_m^\perp$ .

where  $E_0$  is ground state energy. The doublet can be described by local fermion operators  $d$  and  $d^\dagger$  such that  $(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$  and  $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$  correspond to  $d^\dagger d = 0$  and  $d^\dagger d = 1$  states, respectively. From Fig. 3, it is not difficult to verify  $\hat{Q}S_-^y\hat{Q} = i(d - d^\dagger)$ ,  $\hat{Q}S_+^y\hat{Q} = \hat{Q}S_+^x\hat{Q} = \hat{Q}S_-^z\hat{Q} = 0$ . These relations are used in the first-order projection. In the second order, nonvanishing terms may contain  $\hat{Q}(S_-^z)^2\hat{Q} = d^\dagger d$ ,  $\hat{Q}(S_+^x)^2\hat{Q} = \hat{Q}(S_+^z)^2\hat{Q} = dd^\dagger$ ,  $\hat{Q}S_+^xS_-^z\hat{Q} = d$ , and  $\hat{Q}S_-^zS_+^x\hat{Q} = d^\dagger$ . Since the extended fermions commute with the impurity spin operators, we need to install anticommutation relations between the local fermion operators  $d$ ,  $d^\dagger$  and the extended fermion operators  $\psi_\lambda(x)$  with  $\lambda = s, f, sf$ . This is accomplished by a simple transformation,

$$\psi_\lambda(x) = \tilde{\psi}_\lambda(x) e^{i\pi d^\dagger d}, \quad \lambda = s, f, sf. \quad (43)$$

The commutation relations between  $d$  and  $\psi_\lambda(x)$  are converted to anticommutation relations between  $d$  and  $\tilde{\psi}_\lambda(x)$ . The effective Hamiltonian will be represented in terms of  $d$  and  $\tilde{\psi}_\lambda(x)$ . But we shall omit the tilde signs on  $\psi_\lambda(x)$  in the following. With the help of the above-mentioned results, it is straightforward to evaluate (42). The details are captured in Appendix B. The results are

$$H_{\text{eff}} = H_{\text{fp}} + H_{\text{pert}} + H_{\text{phb}}, \quad (44)$$

$$H_{\text{fp}} = -iv_F \sum_{i=f, sf} \int_{-\infty}^{\infty} dx \psi_i^\dagger(x) \partial_x \psi_i(x) + v_F g_0 [\psi_{sf}(0) - \psi_{sf}^\dagger(0)] (d + d^\dagger) + \alpha_u h_u [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] [\psi_f(0) - \psi_f^\dagger(0)] + \alpha_s h_s [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] (d - d^\dagger), \quad (45)$$

$$H_{\text{pert}} = - \left( \frac{K_z + K_\perp}{2} - K^* \right) d^\dagger d - iv_F g_1 (d - d^\dagger) \partial_x [\psi_{sf}(x) - \psi_{sf}^\dagger(x)]_{x=0}, \quad (46)$$

$$H_{\text{phb}} = \tilde{V} [\psi_f(0) + \psi_f^\dagger(0)] (d - d^\dagger), \quad (47)$$

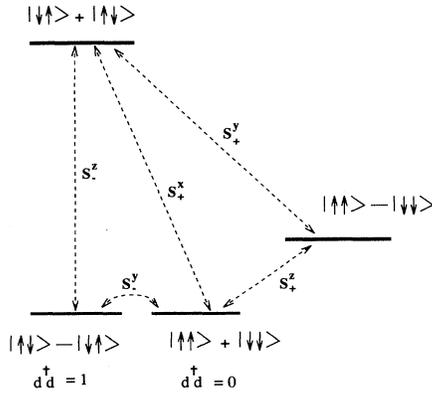


FIG. 3. The four impurity-spin states and the impurity spin operators connecting them,  $S_{\pm}^{\lambda} = S_1^{\lambda} \pm S_2^{\lambda}$  for  $\lambda = x, y, z$ .

where  $K^*$  is the critical value of  $(K_z + K_{\perp})/2$ . We have separated the Hamiltonian into the fixed point part, perturbation part, and particle-hole symmetry breaking part. We note that (45) in the absence of the external magnetic fields  $h_u$  and  $h_s$  has the same form as that of the two-channel Kondo model.<sup>24</sup> To the second order, the coefficients in  $H_{\text{eff}}$  are given by

$$g_0 = -\frac{J_m^{\perp}}{\sqrt{2\pi\alpha}} \left[ 1 + \frac{v_F J_+^{\perp} J_m^z}{4\pi\alpha(K_{\perp} + T_K)J_m^{\perp}} \right], \quad (48)$$

$$g_1 = \frac{v_F^2 J_+^{\perp} J_m^z}{8(K_{\perp} + T_K)^2 (2\pi\alpha)^{3/2}}, \quad (49)$$

$$\tilde{V} = \frac{v_F^2 J_+^{\perp} J_m^z V}{2(K_{\perp} + T_K)^2 (2\pi\alpha)^{5/2}}, \quad (50)$$

$$\alpha_u = \frac{v_F J_-^z \tilde{J}_+^z}{8\pi T_K}, \quad (51)$$

$$\alpha_s = -\frac{v_F J_+^{\perp}}{(K_{\perp} + T_K)\sqrt{2\pi\alpha}}. \quad (52)$$

The projection induces corrections to the RKKY interactions, so the critical value  $K^*$  is slightly shifted from  $v_F(J_+^z - \pi)/(\pi\alpha)$ , as determined by the condition  $-\tilde{K}_z = K_{\perp}$  in (B4). The energy  $T_K$  in the above expressions is the ground state energy gain in (45) from the hybridization term with coefficient  $v_F g_0$ . From the study of the two-channel Kondo problem, we know (as it will also be calculated later)

$$T_K \simeq 2v_F g_0^2 \simeq \frac{v_F (J_m^{\perp})^2}{\pi\alpha}. \quad (53)$$

As it is well known that the ground state energy is not universal, it depends on the conduction band cut-off scheme.<sup>9</sup> Thus, the energy gain  $T_K$  given by (53) is only determined up to a numerical factor of the order of unity. As we shall rigorously prove the completeness of the effective Hamiltonian (44) in the following, the validity of (44) will be extended far beyond the validity of the expressions for the coefficients (48)–(53). Since all these coefficients will eventually be lumped into the

two energy scales  $T_K$  and  $T_c$ , we only need to fit the two energy scales in case we do not know how to determine these coefficients in terms of the parameters in the original Hamiltonian (1). In fact, this is the virtue of our solution. Otherwise, the strict constraint imposed by requiring a valid perturbative projection as detailed in Appendix B would render our solution of little practical value.

The spin degrees of freedom are completely decoupled and their Hamiltonian is, parallel to (44),

$$H_s = -iv_F \int_{-\infty}^{\infty} dx \psi_s^{\dagger}(x) \partial_x \psi_s(x) + h_u \int_{-\infty}^{\infty} dx \psi_s^{\dagger}(x) \psi_s(x) + \frac{v_F (\tilde{J}_+^z)^2 h_u}{4\pi T_K} \psi_s^{\dagger}(0) \psi_s(0). \quad (54)$$

Since this piece of Hamiltonian does not contain any interesting physics, we shall not discuss it hereafter.

The effective Hamiltonian (44) is the central result of this paper. The rest of this section is to prove the completeness of (44) from general symmetry considerations. For a certain region of the parameter space, the projection is controllable in a sense that high-order corrections to the coefficients of  $H_{\text{eff}}$  are too small to alter its critical behavior. However, the projection is not done exactly. One may ask how do we know that there are no other operators which could arise from high orders in the projection and spoil the critical behavior determined by (44)? Fortunately, it turns out that all other operators up to dimension 3/2 inclusive can be eliminated by the three discrete symmetries of (40). We recall that the marginal dimension for a quantum impurity problem is one. To proceed, we first determine how the operators  $d$  and  $d^{\dagger}$  transform under parity and the rotation by an angle  $\pi$  around  $x$  axis. The particle-hole transformation does not involve the impurity spins, so will not affect  $d$  and  $d^{\dagger}$ . Since the two states of the doublet have different parity and  $d^{\dagger}$ ,  $d$  connect them, we conclude that under parity,  $d^{\dagger} \rightarrow -d^{\dagger}$  and  $d \rightarrow -d$ . This could also be seen from  $\hat{Q} S_z^{\pm} S_{\mp}^{\pm} \hat{Q} = d^{\dagger}$  and  $\hat{Q} S_{\mp}^{\pm} S_z^{\pm} \hat{Q} = d$ . From these relations, we also see that under the  $\pi$  rotation around  $x$  axis,  $d^{\dagger} \rightarrow -d^{\dagger}$  and  $d \rightarrow -d$ . Combining these results with (40), we derive all “elementary operators” and their transformation rules in the projected Hilbert space comprised of the local doublet and the extended fermions  $\psi_{\lambda}(x)$  with  $\lambda = s, f, sf$ . They are listed in Table II.

Some explanations are necessary at this point. First, it is well known that 1D extended fermion operators have scaling dimension 1/2. This can be easily seen from the free fermion action  $S(\psi, \psi^{\dagger}) = \int_0^{\beta} d\tau \int_{-\infty}^{\infty} dx \psi^{\dagger}(x, \tau) (\partial_{\tau} - iv_F \partial_x) \psi(x, \tau)$ . Second, we have noted before that  $\psi_s$  and  $\psi_s^{\dagger}$  can only appear in the product  $\psi_s^{\dagger} \psi_s$ . Therefore, the spin degrees of freedom do not bring in the dimension-1/2 operators  $\psi_s$  and  $\psi_s^{\dagger}$  as additional building blocks in Table II. Third, usual local fermion operators have scaling dimension zero. As can be seen from the free fermion action  $S(d, d^{\dagger}) = \int_0^{\beta} d\tau d^{\dagger}(\tau) \partial_{\tau} d(\tau)$ , we need not change  $d$  and  $d^{\dagger}$  under a rescaling of the imaginary time  $\tau$ . This would imply that both combinations  $d \pm d^{\dagger}$  have scaling dimension zero. However, the dimension of the operator combina-

TABLE II. The building blocks for constructing operators in the effective Hamiltonian around the critical point.

Operator	Dimension	Parity	Particle hole	$\pi$ $x$ axis
$\psi_{sf}(0) - \psi_{sf}^\dagger(0)$	1/2	-	+	-
$\psi_{sf}(0) + \psi_{sf}^\dagger(0)$	1/2	+	+	+
$\psi_f(0) + \psi_f^\dagger(0)$	1/2	-	-	-
$\psi_f(0) - \psi_f^\dagger(0)$	1/2	+	+	-
$d + d^\dagger$	1/2	-	+	-
$d - d^\dagger$	0	-	+	-
$\psi_s^\dagger(0)\psi_s(0) - \psi_s(0)\psi_s^\dagger(0)$	1	+	+	-
$\partial_x$	1	+	+	+

tion  $d + d^\dagger$  is raised to 1/2 by the hybridization term in (45) with coefficient  $v_{FG0}$ . This follows immediately from the requirement of preserving scale invariance of this hybridization term under a rescaling of  $x$  and  $\tau$ . Lastly, because both  $d$  and  $d^\dagger$  are odd under parity and  $\pi$  rotation around the  $x$  axis, only  $\psi_{sf}(0) - \psi_{sf}^\dagger(0)$  could hybridize with them to give rise to a term in the effective Hamiltonian that is even under all discrete symmetries, as can be seen from Table II. Of the two linear independent combinations of  $d$  and  $d^\dagger$ ,  $\psi_{sf}(0) - \psi_{sf}^\dagger(0)$  could only hybridize with one. From the hermiticity requirement, the hybridizing combination could be either  $d + d^\dagger$  or  $d - d^\dagger$ . Thus, once  $[\psi_{sf}(0) - \psi_{sf}^\dagger(0)](d + d^\dagger)$  is generated in (45),  $[\psi_{sf}(0) - \psi_{sf}^\dagger(0)](d - d^\dagger)$  is forbidden. This guarantees that the dimension of  $d - d^\dagger$  will remain zero, as usual local operators.

To construct operators for the effective Hamiltonian in the projected Hilbert space, we only need to multiply together the building blocks in Table II and keep products of even number of fermionic operators. We list all dimension-1/2 operators in Table III, all dimension 1 operators in Table IV, and all dimension 3/2 operators in Table V.

Let us first consider the particle-hole symmetric case. Any operator that could appear in the effective Hamil-

TABLE III. All dimension-1/2 operators. The first one is the relevant operator. The second one can couple to the staggered magnetic field. The third one could become the second relevant operator if the particle-hole symmetry is broken. As explained in the text,  $[\psi_{sf}(0) - \psi_{sf}^\dagger(0)](d - d^\dagger)$  does not exist. This is because  $[\psi_{sf}(0) - \psi_{sf}^\dagger(0)]$  could hybridize with either  $d + d^\dagger$  or  $d - d^\dagger$ , but not both.  $[\psi_{sf}(0) - \psi_{sf}^\dagger(0)](d + d^\dagger)$  has dimension one and is included in Table IV.

Operator	Parity	Particle hole	$\pi$ $x$ axis
$(d + d^\dagger)(d - d^\dagger)$	+	+	+
$[\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d - d^\dagger)$	-	+	-
$[\psi_f(0) + \psi_f^\dagger(0)](d - d^\dagger)$	+	-	+
$[\psi_f(0) - \psi_f^\dagger(0)](d - d^\dagger)$	-	+	+

tonian must be even under all three discrete symmetry operations (40). We can explicitly verify that all allowed operators up to dimension 3/2 that could appear in the effective Hamiltonian have been included in (45) and (46). In order to couple to the uniform magnetic field, an operator has to be even under parity and particle-hole transformations but odd under  $\pi$  rotation around the  $x$  axis. From Tables III and IV, we also verify that the only allowed operator up to dimension 1 inclusive is the one appearing in (45). As for the operators that could couple to the staggered magnetic field, they must be even under particle-hole transformation but odd under parity transformation and  $\pi$  rotation around the  $x$  axis. Apart from the dimension-1/2 operator that couples to the staggered field in (45), two more dimension-1 operators are allowed by the symmetries. They are the third and fourth operators in Table IV. Thus, including marginal operators we could have the following additional staggered field coupling terms added to (44):

$$H'_{\text{stag}} = \alpha'_s h_s [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] [\psi_{sf}(0) - \psi_{sf}^\dagger(0)] + i\alpha''_s h_s [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] (d + d^\dagger), \quad (55)$$

where  $\alpha'_s$  and  $\alpha''_s$  are two dimensionless parameters depending on the original coupling constants of (14). Nevertheless, the contributions to the staggered susceptibility from (55) are negligible as we shall see in Appendix D.

A subtle point arises here. We have used the argument that  $\psi_{sf}(0) - \psi_{sf}^\dagger(0)$  could hybridize with either one of  $d \pm d^\dagger$  but not both to rule out possible hybridization between  $\psi_{sf}(0) - \psi_{sf}^\dagger(0)$  and  $d - d^\dagger$  in (45). Since we already have  $[\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d - d^\dagger)$  in (45), why could we not make the same argument to eliminate  $[\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d + d^\dagger)$  in (55)? The reason is as follows. For an arbitrary hybridization, we can rewrite it in the following way:

$$i [\psi_{sf}(0) - \psi_{sf}^\dagger(0)] [\alpha(d - d^\dagger) + i\beta(d + d^\dagger)] = i\sqrt{\alpha^2 + \beta^2} [\psi_{sf}(0) - \psi_{sf}^\dagger(0)] (d e^{i\varphi} - d^\dagger e^{-i\varphi}),$$

TABLE IV. All dimension-1 operators. The first one is the hybridization term. The second one can couple to the uniform magnetic field  $h_u$ . The third and fourth operators could couple to the staggered field  $h_s$ . The fifth and ninth are the marginal particle-hole symmetry breaking operators.

Operator	Parity	Particle hole	$\pi$ $x$ axis
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)](d + d^\dagger)$	+	+	+
$[\psi_{sf}(0) + \psi_{sf}^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)]$	+	+	-
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_{sf}(0) + \psi_{sf}^\dagger(0)]$	-	+	-
$[\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d + d^\dagger)$	-	+	-
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)]$	+	-	+
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)]$	-	+	+
$[\psi_{sf}(0) + \psi_{sf}^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)]$	-	-	-
$[\psi_f(0) + \psi_f^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)]$	-	-	+
$[\psi_f(0) + \psi_f^\dagger(0)](d + d^\dagger)$	+	-	+
$[\psi_f(0) - \psi_f^\dagger(0)](d + d^\dagger)$	-	+	+
$\psi_s^\dagger(0)\psi_s(0) - \psi_s(0)\psi_s^\dagger(0)$	+	+	-

where  $\alpha$ ,  $\beta$  are two arbitrary real constants, and  $\varphi = \tan^{-1}(\beta/\alpha)$ . The imaginary number  $i$  in the last formula is needed to meet the hermiticity requirement. Redefining the operators  $d$  and  $d^\dagger$  to absorb the phase  $\varphi$ , we reduce the hybridizing combination to either  $d - d^\dagger$  or

$d + d^\dagger$ . In other words, we can always choose a proper definition for  $d$  and  $d^\dagger$  so that only one of  $d \pm d^\dagger$  hybridizes with  $\psi_{sf}(0) - \psi_{sf}^\dagger(0)$ . But we can only perform phase absorption once. A redefinition of  $d$  and  $d^\dagger$  to absorb a

TABLE V. All dimension-3/2 operators. The first one is the only allowed leading irrelevant operator in the presence of particle-hole symmetry.

Operator	Parity	Particle hole	$\pi$ $x$ axis
$\partial_x[\psi_{sf}(0) - \psi_{sf}^\dagger(0)](d - d^\dagger)$	+	+	+
$\partial_x[\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d - d^\dagger)$	-	+	-
$\partial_x[\psi_f(0) + \psi_f^\dagger(0)](d - d^\dagger)$	+	-	+
$\partial_x[\psi_f(0) - \psi_f^\dagger(0)](d - d^\dagger)$	-	+	+
$[\psi_s^\dagger(0)\psi_s(0) - \psi_s(0)\psi_s^\dagger(0)][\psi_{sf}(0) - \psi_{sf}^\dagger(0)](d - d^\dagger)$	+	+	-
$[\psi_s^\dagger(0)\psi_s(0) - \psi_s(0)\psi_s^\dagger(0)][\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d - d^\dagger)$	-	+	+
$[\psi_s^\dagger(0)\psi_s(0) - \psi_s(0)\psi_s^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)](d - d^\dagger)$	+	-	-
$[\psi_s^\dagger(0)\psi_s(0) - \psi_s(0)\psi_s^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)](d - d^\dagger)$	-	+	-
$[\psi_s^\dagger(0)\psi_s(0) - \psi_s(0)\psi_s^\dagger(0)](d + d^\dagger)(d - d^\dagger)$	+	+	-
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_{sf}(0) + \psi_{sf}^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)](d - d^\dagger)$	-	-	-
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_{sf}(0) + \psi_{sf}^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)](d - d^\dagger)$	+	+	-
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d + d^\dagger)(d - d^\dagger)$	-	+	-
$[\psi_{sf}(0) + \psi_{sf}^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)](d - d^\dagger)$	+	-	-
$[\psi_{sf}(0) + \psi_{sf}^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)](d + d^\dagger)(d - d^\dagger)$	-	-	-
$[\psi_f(0) + \psi_f^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)](d + d^\dagger)(d - d^\dagger)$	-	-	+
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)](d - d^\dagger)$	-	-	+
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)](d + d^\dagger)(d - d^\dagger)$	+	-	+
$[\psi_{sf}(0) - \psi_{sf}^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)](d + d^\dagger)(d - d^\dagger)$	-	+	+
$[\psi_{sf}(0) + \psi_{sf}^\dagger(0)][\psi_f(0) - \psi_f^\dagger(0)](d + d^\dagger)(d - d^\dagger)$	+	+	-

second phase to eliminate  $[\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d + d^\dagger)$  from the staggered field coupling terms in (45)+(55) is not possible without spoiling the simple hybridization form of the fixed point Hamiltonian (45).

When the particle-hole symmetry is broken, another relevant operator becomes allowed, as can be seen from Table III. This is the dimension-1/2 operator in (47). There are two more dimension-1 operators breaking only particle-hole symmetry. From Table IV, they are

$$H'_{\text{phb}} = V [\psi_{sf}(0) - \psi_{sf}^\dagger(0)] [\psi_f(0) + \psi_f^\dagger(0)] + i\alpha_v V [\psi_f(0) + \psi_f^\dagger(0)] (d + d^\dagger), \quad (56)$$

where  $\alpha_v$  is a dimensionless coefficient depending on the original coupling constants of (14). The first term in (56) is the original particle-hole symmetry breaking term (39), surviving the first-order projection. The second term is a generated one from high orders and cannot be eliminated by a simple phase absorption in  $d$  and  $d^\dagger$  for the same reason as in the last paragraph.

Summarizing this section, (44)+(55)+(56) constitutes the most general effective Hamiltonian for the solution region in Fig. 1, even allowing particle-hole symmetry breaking. What are omitted up to dimension 3/2 only include the following.

(1) A dimension-1 operator  $[\psi_{sf}(0) + \psi_{sf}^\dagger(0)][\psi_f(0) + \psi_f^\dagger(0)]$ , which could couple to the staggered field  $h_s$  but breaks the particle-hole symmetry. Thus, the coefficient of this operator must be proportional to the particle-hole symmetry breaking potential  $V$ . Near the critical point, we expect this coefficient to be significantly suppressed. This term should be even less important than those in (55).

(2) Two dimension-3/2 operators breaking only particle-hole symmetry, as can be seen from Table V. They could appear as additional irrelevant operators in the effective Hamiltonian. Again, we expect they are significantly suppressed near the critical point.

(3) Several dimension-3/2 operators which could couple to the uniform or staggered magnetic fields. Their contributions to the susceptibilities vanish according to high powers of temperature as  $T \rightarrow 0$ .

The above proof of the completeness of the effective

Hamiltonian ensures that the physical results calculated from it are asymptotically exact in the low-energy limit. It is worth pointing out that up to dimension 3/2 the number of allowed operators around the critical point and their dimensions are in complete agreement with the conformal theory results.<sup>18</sup>

#### IV. LOW-ENERGY THERMODYNAMICS

In this section, we shall calculate low-energy thermodynamic properties of the effective Hamiltonian (44) for the solution region of Fig. 1. The marginal operators (56) will be considered in Appendix C where we shall show that their effect is to slightly renormalize the Kondo and crossover temperatures. The contribution to the staggered susceptibility from the marginal operators (55) will be considered in Appendix D and shown to be negligible. The way we adopt to carry out calculations is to represent the partition function as a path integral in which every fermion operator becomes a Grassmann variable. Then we perform linear transformations on the Grassmann variables to bring the action to a diagonal form.

The partition function in the path integral formalism can be written as

$$Z = \int \mathcal{D}[\psi_{sf}, \bar{\psi}_{sf}, \psi_f, \bar{\psi}_f, d, \bar{d}] e^{-\int_0^\beta d\tau (\mathcal{L}_0 + H_{\text{eff}})}, \quad (57)$$

$$\mathcal{L}_0 = \int_{-\infty}^{\infty} dx [\bar{\psi}_{sf}(x) \partial_\tau \psi_{sf}(x) + \bar{\psi}_f(x) \partial_\tau \psi_f(x)] + \bar{d} \partial_\tau d, \quad (58)$$

where  $H_{\text{eff}}$  is the effective Hamiltonian given by (44). By making linear transformations to new Grassmann variables,

$$a_{sf} = \frac{1}{\sqrt{2}}(\psi_{sf} + \bar{\psi}_{sf}), \quad b_{sf} = -\frac{i}{\sqrt{2}}(\psi_{sf} - \bar{\psi}_{sf}), \quad (59)$$

$$a_f = \frac{1}{\sqrt{2}}(\psi_f + \bar{\psi}_f), \quad b_f = -\frac{i}{\sqrt{2}}(\psi_f - \bar{\psi}_f), \quad (60)$$

$$a = \frac{1}{\sqrt{2}}(d + \bar{d}), \quad b = -\frac{i}{\sqrt{2}}(d - \bar{d}), \quad (61)$$

we write the total Lagrangian in (57) as

$$\mathcal{L} = \mathcal{L}_0 + H_{\text{eff}} = \mathcal{L}_1(a_{sf}, b) + \mathcal{L}_2(b_{sf}, a, b) + \mathcal{L}_3(a_f, b) + \mathcal{L}_4(b_f, a_{sf}) + \mathcal{L}_{\text{loc}}(a, b), \quad (62)$$

$$\mathcal{L}_1(a_{sf}, b) = \frac{1}{2} \int_{-\infty}^{\infty} dx a_{sf}(\tau, x) (\partial_\tau - iv_F \partial_x) a_{sf}(\tau, x) + 2i\alpha_s h_s a_{sf}(\tau, 0) b(\tau), \quad (63)$$

$$\mathcal{L}_2(b_{sf}, a, b) = \frac{1}{2} \int_{-\infty}^{\infty} dx b_{sf}(\tau, x) (\partial_\tau - iv_F \partial_x) b_{sf}(\tau, x) + 2iv_F [g_0 b_{sf}(\tau, 0) a(\tau) + g_1 b(\tau) \partial_x b_{sf}(\tau, 0)], \quad (64)$$

$$\mathcal{L}_3(a_f, b) = \frac{1}{2} \int_{-\infty}^{\infty} dx a_f(\tau, x) (\partial_\tau - iv_F \partial_x) a_f(\tau, x) + 2i\tilde{V} a_f(\tau, 0) b(\tau), \quad (65)$$

$$\mathcal{L}_4(b_f, a_{sf}) = \frac{1}{2} \int_{-\infty}^{\infty} dx b_f(\tau, x) (\partial_\tau - iv_F \partial_x) b_f(\tau, x) + 2i\alpha_u h_u a_{sf}(\tau, 0) b_f(\tau, 0), \quad (66)$$

$$\mathcal{L}_{\text{loc}}(a, b) = \frac{1}{2} [a(\tau) \partial_\tau a(\tau) + b(\tau) \partial_\tau b(\tau)] + i\delta K a(\tau) b(\tau), \quad (67)$$

where

$$\delta K = K^* - \frac{1}{2}(K_z + K_\perp). \quad (68)$$

Introducing the Fourier transform,

$$a_{sf}(\tau, x) = \frac{1}{\beta} \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} a_{sf}(\omega_n, k) e^{-i\omega_n \tau + ikx}, \quad \omega_n = (2n+1)\pi/\beta, \quad (69)$$

and similar ones for the other Grassmann variables, we can write the actions corresponding to the Lagrangians (63)–(67) as

$$\mathcal{S}_1(a_{sf}, b) = \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[ -\frac{1}{2}(i\omega_n - v_F k) a_{sf}(-\omega_n, -k) a_{sf}(\omega_n, k) + 2i\alpha_s h_s a_{sf}(\omega_n, k) b(-\omega_n) \right], \quad (70)$$

$$\mathcal{S}_2(b_{sf}, a, b) = \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left\{ -\frac{1}{2}(i\omega_n - v_F k) b_{sf}(-\omega_n, -k) b_{sf}(\omega_n, k) - 2iv_F [g_0 a(-\omega_n) - ig_1 k b(-\omega_n)] b_{sf}(\omega_n, k) \right\}, \quad (71)$$

$$\mathcal{S}_3(a_f, b) = \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[ -\frac{1}{2}(i\omega_n - v_F k) a_f(-\omega_n, -k) a_f(\omega_n, k) + 2i\tilde{V} a_f(-\omega_n, -k) b(\omega_n) \right], \quad (72)$$

$$\mathcal{S}_4(b_f, a_{sf}) = \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[ -\frac{1}{2}(i\omega_n - v_F k) b_f(-\omega_n, -k) b_f(\omega_n, k) + 2i\alpha_u h_u a_{sf}(-\omega_n, -k) b_f(\omega_n, k) \right], \quad (73)$$

$$\mathcal{S}_{\text{loc}}(a, b) = \sum_n \left\{ -\frac{i\omega_n}{2} [a(-\omega_n) a(\omega_n) + b(-\omega_n) b(\omega_n)] + i\delta K a(-\omega_n) b(\omega_n) \right\}. \quad (74)$$

The uniform magnetic field term in (73) is an exactly marginal operator. This is most easily seen by setting  $h_s = 0$  in (70) and combining it with (73). From the real Grassmann variables  $a_{sf}$  and  $b_f$ , we can make a linear transformation to

$$\psi = \frac{1}{\sqrt{2}}(a_{sf} + ib_f), \quad \bar{\psi} = \frac{1}{\sqrt{2}}(a_{sf} - ib_f).$$

The Grassmann variables  $\psi$  and  $\bar{\psi}$  correspond to the usual fermion annihilation and creation operators. When  $h_s = 0$ , (70)+(73) is completely decoupled from the rest of the action responsible for the critical behavior. Moreover, the  $h_u$  term in (73) is simply a potential scattering term in terms of the fermion operators corresponding to  $\psi$  and  $\bar{\psi}$ ,

$$\begin{aligned} & \mathcal{S}_1(a_{sf}, b) + \mathcal{S}_4(b_f, a_{sf}) \\ &= \int_0^\beta d\tau \left[ \int_{-\infty}^{\infty} dx \bar{\psi}(x) (\partial_\tau - iv_F \partial_x) \psi(x) + 2\alpha_u h_u \bar{\psi}(0) \psi(0) \right]. \end{aligned} \quad (75)$$

Thus, not only the uniform susceptibility is well behaved but also applying a uniform external magnetic field has negligible effect on the physical behavior of the system

inside the solution region of Fig. 1. From now on, we shall set  $h_u = 0$  and drop (73) from further discussion.

We can diagonalize (70) to (72) simply by shifting the Grassmann variables corresponding to the extended degrees of freedom,

$$\tilde{a}_{sf}(\omega_n, k) = a_{sf}(\omega_n, k) - \frac{2i\alpha_s h_s}{i\omega_n - v_F k} b(\omega_n), \quad (76)$$

$$\begin{aligned} \tilde{b}_{sf}(\omega_n, k) &= b_{sf}(\omega_n, k) \\ &\quad - \frac{2iv_F}{i\omega_n - v_F k} [g_0 a(\omega_n) + ig_1 k b(\omega_n)], \end{aligned} \quad (77)$$

$$\tilde{a}_f(\omega_n, k) = a_f(\omega_n, k) - \frac{2i\tilde{V}}{i\omega_n - v_F k} b(\omega_n). \quad (78)$$

Upon inserting the results for the following integrals,

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{1}{i\omega_n - v_F k} = -\frac{i \operatorname{sgn} \omega_n}{2v_F}, \quad (79)$$

$$\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi} \frac{k}{i\omega_n - v_F k} = -\frac{1}{v_F^2} \left( \frac{v_F \Lambda}{\pi} - \frac{|\omega_n|}{2} \right), \quad (80)$$

$$\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi} \frac{k^2}{i\omega_n - v_F k} = -\frac{i\omega_n}{v_F^3} \left( \frac{v_F \Lambda}{\pi} - \frac{|\omega_n|}{2} \right), \quad (81)$$

where  $\Lambda$  is the ultraviolet cutoff, the actions (70) to (72) become

$$\mathcal{S}_1(a_{sf}, b) = - \sum_n \int_{-\infty}^{\infty} \frac{dk}{4\pi} (i\omega_n - v_F k) \tilde{a}_{sf}(-\omega_n, -k) \tilde{a}_{sf}(\omega_n, k) - \frac{i(\alpha_s h_s)^2}{v_F} \sum_n \operatorname{sgn} \omega_n b(-\omega_n) b(\omega_n), \quad (82)$$

$$\begin{aligned}
\mathcal{S}_2(b_{sf}, a, b) = & - \sum_n \int_{-\infty}^{\infty} \frac{dk}{4\pi} (i\omega_n - v_F k) \tilde{b}_{sf}(-\omega_n, -k) \tilde{b}_{sf}(\omega_n, k) \\
& - i v_F g_0^2 \sum_n \text{sgn} \omega_n a(-\omega_n) a(\omega_n) + \frac{i g_1^2}{v_F} \sum_n \omega_n \left( |\omega_n| - \frac{2v_F \Lambda}{\pi} \right) b(-\omega_n) b(\omega_n) \\
& + 2i g_0 g_1 \sum_n |\omega_n| a(-\omega_n) b(\omega_n) - \frac{4i}{\pi} v_F g_0 g_1 \Lambda \sum_n a(-\omega_n) b(\omega_n), \tag{83}
\end{aligned}$$

$$\mathcal{S}_3(a_f, b) = - \sum_n \int_{-\infty}^{\infty} \frac{dk}{4\pi} (i\omega_n - v_F k) \tilde{a}_f(-\omega_n, -k) \tilde{a}_f(\omega_n, k) - \frac{i \tilde{V}^2}{v_F} \sum_n \text{sgn} \omega_n b(-\omega_n) b(\omega_n). \tag{84}$$

The last term in (83) is a correction to the relevant operator  $\delta K$  term of (74) and can be absorbed into the critical value of the RKKY interaction  $K^*$ . Collecting the local terms containing Grassmann variables  $a, b$  from (82) to (84) and combining them with (74), we obtain the effective local action,

$$\mathcal{S}_{\text{loc}}^{\text{eff}} = -i \sum_{n>0} [a(-\omega_n), b(-\omega_n)] \begin{pmatrix} |\omega_n| + 2v_F g_0^2 & -(\delta K + 2g_0 g_1 |\omega_n|) \\ \delta K + 2g_0 g_1 |\omega_n| & |\omega_n|/Z_b + 2(\alpha_s^2 h_s^2 + \tilde{V}^2 - g_1^2 \omega_n^2)/v_F \end{pmatrix} \begin{pmatrix} a(\omega_n) \\ b(\omega_n) \end{pmatrix}. \tag{85}$$

The factor  $Z_b$  is defined by

$$Z_b = \frac{1}{1 + 4g_1^2 \Lambda/\pi}, \tag{86}$$

and can be interpreted as the wave function renormalization factor for the Grassmann variable  $b$  (or Majorana fermion). The  $\omega_n^2$  term in the matrix element of (85) can be safely neglected since it is highly irrelevant and satisfies  $g_1^2 \omega_n^2/v_F \ll |\omega_n|$  for the whole energy range of practical interest. All interesting thermodynamics is contained in (85). From (85) we obtain the free energy shift due to the impurity spins,

$$\begin{aligned}
F(T, h_s) = & -T \ln 2 - T \sum_{n>0} \ln \left\{ (\delta K + 2g_0 g_1 |\omega_n|)^2 \right. \\
& + (|\omega_n| + 2v_F g_0^2) \left[ \frac{|\omega_n|}{Z_b} \right. \\
& \left. \left. + \frac{2}{v_F} (\alpha_s^2 h_s^2 + \tilde{V}^2) \right] \right\}, \tag{87}
\end{aligned}$$

where  $-T \ln 2$  is the entropy term of the two lowest degenerate levels in Fig. 3. Defining several convenience notations,

$$T_K = 2v_F g_0^2 + 2Z_b \left( \frac{\tilde{V}^2}{v_F} + 2g_0 g_1 \delta K \right), \tag{88}$$

$$T_c = \frac{Z_b [4g_0^2 \tilde{V}^2 + (\delta K)^2]}{T_K}, \tag{89}$$

$$\tilde{\alpha}_s = 2g_0 \alpha_s \sqrt{Z_b}, \tag{90}$$

we can recast the free energy in a very simple form,

$$\begin{aligned}
F(T, h_s) = & -T \ln 2 + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{e^{\beta\omega} + 1} \\
& \times \tan^{-1} \left\{ \frac{\omega [T_K + \tilde{\alpha}_s^2 h_s^2 / (2v_F g_0^2)]}{\omega^2 - T_c T_K - \tilde{\alpha}_s^2 h_s^2} \right\}. \tag{91}
\end{aligned}$$

The roles of the parameters in (91) can be read off.  $T_K$  is the fundamental energy scale of the problem and should be identified as the Kondo temperature. We note that  $T_K \simeq 2v_F g_0^2$ , as can be seen from (88).  $T_c$  vanishes approaching the critical point, and satisfies  $T_c \ll T_K$  inside the solution region of Fig. 1. The same  $T_c$  defines the crossover energy scale above which the behavior of the system is controlled by the critical point. Below  $T_c$ , it is controlled by the Fermi-liquid fixed point. Accompanying the staggered magnetic field is an involved coefficient  $\tilde{\alpha}_s$  because  $h_s$  couples to an unconserved operator, unlike the uniform magnetic field. Because of this factor, it is not possible to define a universal Wilson ratio from the staggered susceptibility.

For all practical purposes, the  $h_s^2$  term in the numerator inside  $\tan^{-1}$  in (91) can be dropped since it only shifts  $T_K$  to  $T_K + \tilde{\alpha}_s^2 h_s^2 / T_K$ . After some rearrangement, we finally obtain

$$\begin{aligned}
F(T, h_s) = & -T \ln 2 - \int_0^{\infty} \frac{d\omega}{2\pi} \tanh \left( \frac{\beta\omega}{2} \right) \\
& \times \tan^{-1} \left( \frac{\omega T_K}{\omega^2 - T_c T_K - \tilde{\alpha}_s^2 h_s^2} \right). \tag{92}
\end{aligned}$$

This nice looking expression gives us the complete crossover functions for the specific heat and staggered susceptibility.

### A. Specific heat

Setting  $h_s = 0$  in (92) and performing some minor manipulation, we obtain

$$\begin{aligned}
F(T) - F(0) = & -T \ln 2 + T \int_0^{\infty} \frac{dx}{\pi} \frac{1}{e^x + 1} \\
& \times \tan^{-1} \left( \frac{x \beta T_K}{x^2 - \beta^2 T_c T_K} \right). \tag{93}
\end{aligned}$$

Two limiting behaviors follow immediately. At  $T_c \ll$

$T \ll T_K$ ,

$$\begin{aligned} F(T) - F(0) &= -T \ln 2 + T \int_0^\infty \frac{dx}{\pi} \frac{1}{e^x + 1} \left( \frac{\pi}{2} - \frac{x}{\beta T_K} \right) \\ &= -\frac{T}{2} \ln 2 - \frac{\pi}{12} \frac{T^2}{T_K}. \end{aligned} \quad (94)$$

We see a residual entropy  $(\ln 2)/2$ , reduced from the original  $\ln 2$ . At  $T \ll T_c \ll T_K$ ,

$$\begin{aligned} F(T) - F(0) &= -T \ln 2 + T \int_0^\infty \frac{dx}{\pi} \frac{1}{e^x + 1} \left( \pi - \frac{x}{\beta T_c} \right) \\ &= -\frac{\pi}{12} \frac{1}{T_c} T^2. \end{aligned} \quad (95)$$

The limiting behaviors of the specific heat are obvious from (94) and (95),

$$\frac{C(T, T_c)}{T} = \begin{cases} \frac{\pi}{6T_K}, & T \gg T_c, \\ \frac{\pi}{6T_c}, & T_c \gg T. \end{cases} \quad (96)$$

The general crossover function for the specific heat is obtained from (93),

$$\begin{aligned} \frac{C(T)}{T} &= 2T_K^2 \beta^4 \int_0^\infty \frac{dx}{\pi} \frac{x}{e^x + 1} \\ &\quad \times \frac{x^4 T_K - T_c(x^2 - \beta^2 T_c T_K)(3x^2 + \beta^2 T_c T_K)}{[(x^2 - \beta^2 T_c T_K)^2 + (x\beta T_K)^2]^2}. \end{aligned} \quad (97)$$

This crossover function is plotted in Fig. 4. We also plot the crossover function for the entropy (93) in Fig. 5, which may be more instructive.

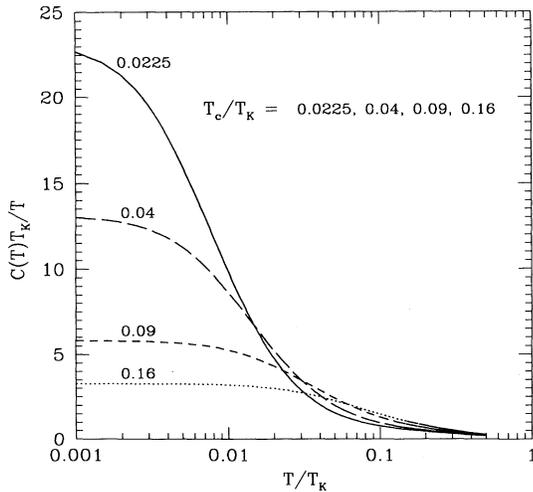


FIG. 4. The crossover function for the specific heat, Eq. (97), for various values of  $T_c/T_K$ .  $T_K$  is the Kondo temperature, and  $T_c$  is the crossover temperature.

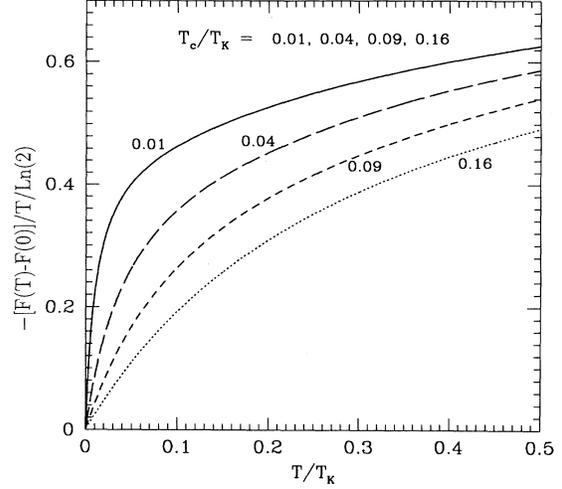


FIG. 5. The crossover function for the entropy, Eq. (93), for various values of  $T_c/T_K$ .

### B. Staggered susceptibility

From (92), the staggered susceptibility is given by

$$\begin{aligned} \chi_s(T, T_c) &= - \left[ \frac{\partial^2}{\partial h_s^2} F(T, h_s) \right]_{h_s=0} \\ &= \tilde{\alpha}_s^2 \int_0^\infty \frac{d\omega}{\pi} \tanh \left( \frac{\beta\omega}{2} \right) \\ &\quad \times \frac{\omega T_K}{(T_c T_K - \omega^2)^2 + (\omega T_K)^2}. \end{aligned} \quad (98)$$

The limiting behaviors are found to be

$$\chi_s(T, T_c) = -\frac{\tilde{\alpha}_s^2}{\pi T_K} \times \begin{cases} \ln T, & T \gg T_c, \\ \ln T_c, & T \ll T_c. \end{cases} \quad (99)$$

The crossover behavior for the function (98) is plotted in Fig. 6.

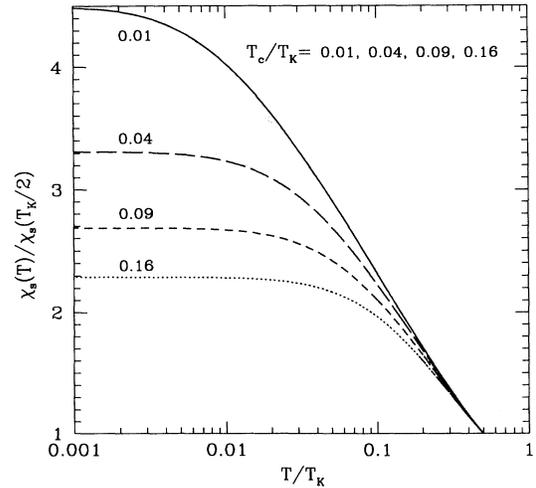


FIG. 6. The crossover function for the staggered susceptibility, Eq. (98), for various values of  $T_c/T_K$ , normalized to its value at  $T_K/2$ .

### C. Impurity spin correlation $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$

Projecting the operator  $(\mathbf{S}_+)^2$  onto the doublet, we find

$$\hat{Q} \mathbf{S}_+^2 \hat{Q} = \hat{Q} (S_+^x)^2 \hat{Q} + \hat{Q} (S_+^y)^2 \hat{Q} + \hat{Q} (S_+^z)^2 \hat{Q} = 2dd^\dagger. \quad (100)$$

Thus, the calculation of the impurity spin correlation is reduced to evaluating  $\langle dd^\dagger \rangle$ . From (85), we have

$$\langle dd^\dagger \rangle - \frac{1}{2} = i\langle ba \rangle = T \sum_n \frac{\delta K + 2g_0g_1|\omega_n|}{(\delta K + 2g_0g_1|\omega_n|)^2 + (|\omega_n| + T_K) \left( |\omega_n|/Z_b + 2\tilde{V}^2/v_F \right)}. \quad (101)$$

The impurity spin correlation is

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -\frac{1}{4} + \frac{Z_b}{\beta} \sum_n \frac{\delta K + 2g_0g_1|\omega_n|}{\omega_n^2 + T_c T_K + |\omega_n| T_K}. \quad (102)$$

At the critical point,  $\delta K = T_c = 0$ , and as  $T \rightarrow 0$ ,

$$\begin{aligned} \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle &\simeq -\frac{1}{4} + Z_b \int_0^{v_F \Lambda} \frac{d\omega}{\pi} \frac{2g_0g_1}{\omega + T_K} \\ &\simeq -\frac{1}{4} + \frac{2g_0g_1 Z_b}{\pi} \ln \frac{v_F \Lambda}{T_K}. \end{aligned} \quad (103)$$

The leading irrelevant operator induces a small nonuniversal correction to the impurity spin correlation. Although the fixed point itself has an extra symmetry between the two states of the doublet,  $d \leftrightarrow d^\dagger$ , which implies  $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -1/4$ , it is broken by the leading irrelevant operator, as can be seen from (46).

We can also calculate the slope of the impurity spin correlation with respect to the RKKY interaction. From (102), we find

$$\begin{aligned} \frac{\partial}{\partial (\delta K)} \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle &= \frac{Z_b}{\beta} \sum_n \frac{1}{\omega_n^2 + |\omega_n| T_K + T_c T_K} \\ &= Z_b \int_0^\infty \frac{d\omega}{\pi} \tanh \left( \frac{\beta \omega}{2} \right) \\ &\quad \times \frac{\omega T_K}{(T_c T_K - \omega^2)^2 + (\omega T_K)^2}. \end{aligned} \quad (104)$$

Comparing the last expression with (98), we find

$$\frac{\partial}{\partial (\delta K)} \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = \text{const} \times \chi_s(T, T_c). \quad (105)$$

In particular, they should have the same limiting behaviors as given by (99). Since

$$\frac{\partial}{\partial (\delta K)} \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle \sim \int_0^\beta d\tau \langle \hat{T}(\mathbf{S}_1 \cdot \mathbf{S}_2)(\tau) (\mathbf{S}_1 \cdot \mathbf{S}_2)(0) \rangle, \quad (106)$$

the result (105) should not be too surprising.

## V. COMPARISON WITH OTHER RESULTS AND UNIVERSALITY

There are two kinds of asymptotically exact limiting results with which we can compare our solution. These

are the conformal-field-theory results at  $T \gg T_c$  and the numerical renormalization-group results at  $T = 0$ . First of all, we would like to emphasize that all our results are also asymptotically exact up to some numerical coefficients  $g_0$ ,  $g_1$ , and  $\tilde{V}$  in (44) even if we do not know how to express them in terms of the parameters of the original Hamiltonian (1). Or eventually the possible uncertainty boils down to the two basic energy scales  $T_K$  and  $T_c$ .

In order to make a comparison, we first need to determine whether or not the critical point we have studied is the same one, and whether or not the spin anisotropy we have introduced in (1) is irrelevant. The answer to both questions is a convincing yes, if not rigorous. A detailed comparison of the finite size spectrum of the critical point between the conformal-field-theory and numerical renormalization-group approaches has been made.<sup>18</sup> Excellent agreement has been found which implies the same critical point in those two approaches. Thus, we shall take the agreement between our results and that obtained from either one of those two approaches as a positive evidence. The conformal-field theory tells us that there is only one non-Fermi-liquid fixed point, i.e., conformally invariant boundary condition.<sup>18</sup> This is supported by the failure of finding other critical points in our approach by considering other impurity spin states as the lowest degenerate levels rather than the doublet in Fig. 2. The strongest evidence for the universality of the critical point is the exact same operator content around the critical point we find in our approach and in the conformal-field-theory approach. In other words, we have the same number of operators with the same symmetry and same dimension. Specifically, there is one dimension-1/2 relevant operator and one dimension-3/2 leading irrelevant operator in the presence of the particle-hole symmetry, as can be seen from (45) and (46). Breaking the particle-hole symmetry introduces another dimension-1/2 relevant operator, as can be seen from (47). Furthermore, the dimension-3/2 leading irrelevant operator in the conformal-field theory is a descendant of the relevant operator. In our approach, we consistently find that the leading irrelevant operator contains the spatial derivative  $\partial_x$ . This is the crucial difference from the two-channel Kondo problem, resulting in different low-temperature behavior of the specific heat [see (96) and Ref. 24]. While in both cases there is a dimension-3/2 leading irrelevant operator, only the one at the critical point of the two-impurity Kondo problem contains  $\partial_x$ . As to the spin anisotropy, it is found

in the conformal-field-theory approach that a small spin anisotropic perturbation around the critical point is irrelevant.<sup>18</sup> Although this does not prove the irrelevance of the spin anisotropy introduced in our approach because the introduced anisotropy is not small, it does indeed point to the right direction. It is worthwhile recalling that the spin anisotropy is irrelevant for all kinds of one-impurity Kondo problem, including the exactly screened<sup>23</sup> and overscreened cases.<sup>25,26</sup> These early experiences in related Kondo problems give us considerable confidence in the universality of the critical point.

Since the behavior of the system above  $T_c$  and the way the system flows to the stable Fermi-liquid fixed point below  $T_c$  are all governed by the critical point, the universality of the critical point also implies the universal behavior everywhere inside the solution region of Fig. 1, as well as all crossover functions. In particular, the crossover functions we have derived for the specific heat and staggered susceptibility are expected to be universal. For a comparison of the results derived from different approaches, the only freedom left is to match the two basic energy scales  $T_K$  and  $T_c$ . For the staggered susceptibility, or any other response function of a nonconserved operator, there may also be an undetermined overall constant prefactor.

At the critical point  $T_c = 0$ , or more generally in the limit  $T \gg T_c$ , the critical properties of all thermodynamic quantities as a function of temperature that we have calculated in the last section completely agree with the conformal-field-theory results, as expected on the grounds of the same operator content. These include the residual entropy  $(\ln 2)/2$ , linear temperature dependent specific heat,  $\ln T$  singularity in the staggered susceptibility, constant uniform susceptibility, and  $\ln T$  singularity in the correlation function of the composite operator  $\mathbf{S}_1 \cdot \mathbf{S}_2$ , as can be seen from (104) and (106). The complete agreement of the critical behavior further ensures us the universality of the critical point.

As to compare with the numerical renormalization-group results at  $T = 0$ , we first note that the empirical observation<sup>11</sup> of an additional hidden symmetry between the singlet and triplet impurity spin states at the critical point becomes crystal clear after our identification of the critical point, as can be seen from Fig. 2. So is its consequence about the value of the impurity spin correlation at the critical point,  $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -1/4$ . However, this hidden symmetry is broken by the leading irrelevant operator as we have noted before. In consistency with the numerical renormalization-group result, we also find that the linear coefficient of the specific heat diverges quadratically in  $\delta K$  on the particle-hole symmetric axis, as can be seen from (96). Our result (105), that the slope of the impurity spin correlation with respect to the variation of RKKY interaction is logarithmically divergent, is broadly consistent with the numerical renormalization-group result which also found it singular.

The only disagreement with the reported numerical renormalization-group results is the behavior of the staggered susceptibility at  $T = 0$ . While  $\chi_s(T = 0, T_c) \sim 1/T_c$  has been claimed, we only find  $\chi_s(T = 0, T_c) \sim (1/T_K) \ln T_c$ , as can be seen from (99). Note that the other limiting behavior of (99),  $\chi_s(T, T_c) \sim \ln T$  at

$T \gg T_c$ , is not disputed. Even if one takes a cautious view about the numerically fitted critical exponent 2 for the staggered susceptibility, i.e.,  $\chi_s \sim (\delta K)^{-2}$ , the original numerical divergence seems to us much stronger than a logarithmic singularity. The reason for this discrepancy is unknown at this moment. But at least the easy explanation of differently adopted definitions for the staggered susceptibility is unlikely. In this paper, we only couple the staggered field  $h_s$  to  $S_z^-$  in (15). One could also couple  $h_s$  to  $[\psi_1^\dagger(0)\sigma^z\psi_1(0) - \psi_2^\dagger(0)\sigma^z\psi_2(0)]/2$  in (15), or even to  $\int dx [\psi_1^\dagger(x)\sigma^z\psi_1(x) - \psi_2^\dagger(x)\sigma^z\psi_2(x)]/2$ . In any case, the contributions to the staggered susceptibility after subtracting out the free Fermi sea contribution should only come from the local operators which are odd under parity and  $\pi$  rotation around the  $x$  axis. Since we only have one such relevant operator, as can be seen from Table III, we do not expect qualitative change of the behavior of the staggered susceptibility as a result of different definitions. A careful reexamination in the numerical renormalization-group approach should be very helpful to clarify this point.

## VI. CONCLUSION

We have presented an asymptotically exact solution for the two-impurity Kondo model for a finite region of the parameter space surrounding the critical point, as shown in Fig. 1. We have also derived the analytic crossover functions for the specific heat and staggered susceptibility. This solution is made possible by an explicit identification of the critical point. As we have explained in Sec. III, the condition for the criticality is the degeneracy between the two lowest impurity spin states,  $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$  and  $(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$ , in the dynamical reference frame. Using the canonical transformation (30), we can rewrite them in the static reference frame: one is the RKKY singlet  $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$  while the other one is a Kondo screened singlet  $e^{iS_z^+ \Phi_s(0)}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$ . By varying RKKY interaction across the critical point, these two levels cross each other. However, level crossing does not necessarily imply a non-Fermi-liquid critical point. That it is so in this case is a consequence of the fact that in the presence of the particle-hole symmetry only half of the degrees of freedom of the doublet can be compensated by the extended degrees of freedom associated with the conduction electrons. Out of four species of spinless fermions or eight species of Majorana fermions associated with all conduction electron degrees of freedom, only one Majorana fermion,  $\psi_{sf} - \psi_{sf}^\dagger$ , is allowed by the symmetry to compensate the local degrees of the freedom of the doublet. This is the same physics responsible for the non-Fermi-liquid behavior of the two-channel one-impurity Kondo model.<sup>24</sup> However, the doublet at the critical point of the two-impurity problem has different symmetry from the simple impurity spin up and down states of the two-channel problem. Therefore, the operator contents around the fixed points (one unstable, the other stable) are different. The nearly complete agreement of our results with those derived from the nu-

merical renormalization-group or conformal-field-theory approaches, except one limiting behavior of the staggered susceptibility, convincingly establishes the universality of the critical point. Thus, the crossover functions we have derived in Sec. IV are also expected to be universal. The calculation of dynamical correlation functions such as the conduction electron Green's function is currently under way.

What have we learned about the lattice problem from the study of the two-impurity Kondo model? An obvious lesson is learned from the striking difference between the uniform and staggered susceptibilities. This difference is solely due to the competition between RKKY interaction and the Kondo effect. A direct and primitive translation to the Kondo lattice problem would be the strong momentum  $\mathbf{q}$  dependence of the spin susceptibility  $\chi''(\omega, \mathbf{q})$ . As a result of the competition, we should expect drastically different enhancement at different momentum transfer  $\mathbf{q}$ . From this perspective, the picture of a periodic array of coherent Kondo scattering centers for the heavy fermion compounds is surely oversimplified. Nonperturbatively incorporating RKKY interaction into the Kondo effect in the lattice is an outstanding problem on which the impact of the insight from the two-impurity Kondo model has to be fully realized.

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#### APPENDIX A: DERIVATION OF (31) AND (32)

Under the transformation  $\hat{U}H\hat{U}^{-1}$ , only two terms in  $H_0$  are affected. They are  $h_u/(2\pi) \int_{-\infty}^{\infty} dx \partial_x \Phi_s(x)$  and

$$H_0^{(s)} = \frac{v_F}{2} \int_{-\infty}^{\infty} dx \{ \Pi_s^2(x) + [\partial_x \phi_s(x)]^2 \}. \quad (\text{A1})$$

As for  $H_1$ , the transformation affects the term containing  $\partial_x \Phi_s(0) S_+^z$  apart from eliminating  $\cos \Phi_s(0)$  and  $\sin \Phi_s(0)$ . Using the mode expansion,

$$\phi_s(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi\sqrt{2|p|}} [\phi_s(p)e^{ipx} + \phi_s^\dagger(p)e^{-ipx}] e^{-\alpha|p|/2}, \quad (\text{A2})$$

$$\Pi_s(x) = \int_{-\infty}^{\infty} \frac{dp|p|}{2\pi\sqrt{2|p|}} [-i\phi_s(p)e^{ipx} + i\phi_s^\dagger(p)e^{-ipx}] \times e^{-\alpha|p|/2}, \quad (\text{A3})$$

we can write

$$H_0^{(s)} = v_F \int_{-\infty}^{\infty} \frac{dp}{2\pi} |p| \phi_s^\dagger(p) \phi_s(p), \quad (\text{A4})$$

$$\partial_x \Phi_s(x) = i \int_0^\infty dp \sqrt{\frac{p}{2\pi}} e^{-\alpha p/2} [\phi_s(p)e^{ipx} - \phi_s^\dagger(p)e^{-ipx}]. \quad (\text{A5})$$

The commutation relation for the Fourier components is

$$[\phi_s(p), \phi_s^\dagger(p')] = 2\pi\delta(p-p'). \quad (\text{A6})$$

Next, let us introduce a generalized transformation operator

$$\hat{U}(\lambda) = e^{-i\lambda S_+^z \Phi_s(0)} = e^{-i\lambda S_+^z \int_0^\infty dp e^{-\alpha p/2} [\phi_s(p) + \phi_s^\dagger(p)] / \sqrt{2\pi p}}, \quad (\text{A7})$$

and define two  $\lambda$ -dependent functions,

$$f_1(\lambda) = \hat{U}(\lambda) H_0^{(s)} \hat{U}^{-1}(\lambda), \quad (\text{A8})$$

$$f_2(\lambda) = \hat{U}(\lambda) \partial_x \Phi_s(x) \hat{U}^{-1}(\lambda). \quad (\text{A9})$$

We note that  $\hat{U}(\lambda=1) = \hat{U}$ . Using the commutation relation (A6), it is straightforward to verify

$$\frac{d^2}{d\lambda^2} f_1(\lambda) = \frac{2v_F}{\alpha} (S_+^z)^2, \quad (\text{A10})$$

$$\frac{d}{d\lambda} f_1(\lambda)|_{\lambda=0} = -v_F \partial_x \Phi_s(0) S_+^z, \quad (\text{A11})$$

$$\frac{d}{d\lambda} f_2(\lambda) = -2 \int_0^\infty dp e^{-\alpha p} \cos(px) S_+^z. \quad (\text{A12})$$

From (A10) and (A11), we obtain

$$\hat{U} H_0^{(s)} \hat{U}^{-1} = H_0^{(s)} - v_F \partial_x \Phi_s(0) S_+^z + \frac{v_F}{\alpha} (S_+^z)^2. \quad (\text{A13})$$

From (A12), we obtain

$$\hat{U} \partial_x \Phi_s(x) \hat{U}^{-1} = \partial_x \Phi_s(x) - 2 \int_0^\infty dp e^{-\alpha p} \cos(px) S_+^z. \quad (\text{A14})$$

This implies

$$\hat{U} \partial_x \Phi_s(0) \hat{U}^{-1} = \partial_x \Phi_s(0) - \frac{2}{\alpha} S_+^z, \quad (\text{A15})$$

$$\hat{U} \int_{-\infty}^{\infty} dx \partial_x \Phi_s(x) \hat{U}^{-1} = \int_{-\infty}^{\infty} dx \partial_x \Phi_s(x) - 2\pi S_+^z. \quad (\text{A16})$$

Substituting (A13), (A15), and (A16) into  $\hat{U}H\hat{U}^{-1}$ , we obtain the results (31) and (32).

#### APPENDIX B: DERIVATION OF THE EFFECTIVE HAMILTONIAN IN THE SECOND-ORDER PROJECTION

In this appendix, we shall derive the coefficients  $g_0$ ,  $g_1$ ,  $\tilde{V}$ ,  $\alpha_u$ , and  $\alpha_s$  in the effective Hamiltonian (44) from the second-order projection (42). The Hamiltonian to be projected is (36) + (37) + (39).

The first-order contributions to the effective Hamiltonian are

$$\begin{aligned} \hat{Q}H\hat{Q} &= -iv_F \int_{-\infty}^{\infty} dx \sum_{\lambda=s,f,sf} \psi_{\lambda}^{\dagger}(x) \partial_x \psi_{\lambda}(x) \\ &+ i \frac{v_F J_m^{\perp}}{\sqrt{2\pi\alpha}} \left[ \psi_{sf}(0) - \psi_{sf}^{\dagger}(0) \right] \hat{Q} S_y^{\perp} \hat{Q} \\ &+ h_u \int_{-\infty}^{\infty} dx \psi_s^{\dagger}(x) \psi_s(x) + H_2. \end{aligned} \quad (\text{B1})$$

In terms of the local fermion operators  $d$  and  $d^{\dagger}$ , we have  $\hat{Q}S_y^{\perp}\hat{Q} = i(d - d^{\dagger})$ . Performing the transformation (43) to install the anticommutation relations between the extended and local fermion operators, the hybridization term between the extended and local fermion operators in (B1) becomes

$$- \frac{v_F J_m^{\perp}}{\sqrt{2\pi\alpha}} \left[ \tilde{\psi}_{sf}(0) - \tilde{\psi}_{sf}^{\dagger}(0) \right] (d + d^{\dagger}). \quad (\text{B2})$$

In the second order of the projection (42), the local impurity spin state is virtually excited from one of the doublet to either  $(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)/\sqrt{2}$  or  $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ , then returns back to the doublet. From Fig. 3, the mixing terms between the doublet and the excited states are those in (36) + (37) which contain  $S_+^x$  and  $S_{\pm}^z$ . If the lo-

cal impurity spins leave and return to the same state of the doublet, the generated contributions to the effective Hamiltonian have the form of either  $d^{\dagger}d$  or  $dd^{\dagger}$ . These are simply the renormalizations to the RKKY interaction, shifting its critical value determined by

$$-\tilde{K}_z = K_{\perp} + \dots, \quad (\text{B3})$$

where the omitted extra terms stand for the above-mentioned renormalizations. The relevant term in the effective Hamiltonian around the critical point is, like the mass term in the usual critical phenomenon,

$$\begin{aligned} &- \left( \frac{K_z + K_{\perp}}{2} - K^* \right) d^{\dagger}d \\ &\text{with } K^* = \frac{v_F}{\pi\alpha} (J_+^z - \pi) + \dots \end{aligned} \quad (\text{B4})$$

The more important contributions come from the situations when the local impurity spins start from one state but return to the other state of the doublet. From Fig. 3, we see that these contributions must come from the projection of the product of  $S_+^x$  and  $S_{\pm}^z$ ,

$$\begin{aligned} &\hat{Q} \left\{ \frac{v_F J_m^z}{2} \left[ \psi_{sf}^{\dagger}(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^{\dagger}(0) \right] S_{\pm}^z \right\} \\ &\times \frac{1 - \hat{Q}}{-(K_{\perp} + T_K) + iv_F \int_{-\infty}^{\infty} dx \psi_{sf}^{\dagger}(x) \partial_x \psi_{sf}(x) - V \left[ \psi_{sf}(0) - \psi_{sf}^{\dagger}(0) \right] \left[ \psi_f(0) + \psi_f^{\dagger}(0) \right]} \\ &\times \left\{ \frac{v_F J_{\pm}^{\perp}}{\sqrt{2\pi\alpha}} \left[ \psi_{sf}(0) + \psi_{sf}^{\dagger}(0) \right] S_{\pm}^x \right\} \hat{Q} + \hat{Q} \left\{ \frac{v_F J_{\pm}^{\perp}}{\sqrt{2\pi\alpha}} \left[ \psi_{sf}(0) + \psi_{sf}^{\dagger}(0) \right] S_{\pm}^x \right\} \\ &\times \frac{1 - \hat{Q}}{-(K_{\perp} + T_K) + iv_F \int_{-\infty}^{\infty} dx \psi_{sf}^{\dagger}(x) \partial_x \psi_{sf}(x) - V \left[ \psi_{sf}(0) - \psi_{sf}^{\dagger}(0) \right] \left[ \psi_f(0) + \psi_f^{\dagger}(0) \right]} \\ &\times \left\{ \frac{v_F J_m^z}{2} \left[ \psi_{sf}^{\dagger}(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^{\dagger}(0) \right] S_{\pm}^z \right\} \hat{Q}. \end{aligned} \quad (\text{B5})$$

Besides the energy gap  $K_{\perp} + T_K$  between the doublet and the local excited state  $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ , we have also kept the intraband terms in the intermediate denominator which will be expanded as

$$\begin{aligned} &\left\{ -(K_{\perp} + T_K) + iv_F \int_{-\infty}^{\infty} dx \psi_{sf}^{\dagger}(x) \partial_x \psi_{sf}(x) - V \left[ \psi_{sf}(0) - \psi_{sf}^{\dagger}(0) \right] \left[ \psi_f(0) + \psi_f^{\dagger}(0) \right] \right\}^{-1} \\ &\simeq - \frac{1}{K_{\perp} + T_K} - \frac{iv_F}{(K_{\perp} + T_K)^2} \int_{-\infty}^{\infty} dx \psi_{sf}^{\dagger}(x) \partial_x \psi_{sf}(x) + \frac{V}{(K_{\perp} + T_K)^2} \left[ \psi_{sf}(0) - \psi_{sf}^{\dagger}(0) \right] \left[ \psi_f(0) + \psi_f^{\dagger}(0) \right]. \end{aligned} \quad (\text{B6})$$

Substituting (B6) into (B5), we obtain three contributions to the effective Hamiltonian.

The first contribution is

$$\begin{aligned} &- \frac{v_F^2 J_{\pm}^{\perp} J_m^z}{2(K_{\perp} + T_K) \sqrt{2\pi\alpha}} \left\{ \left[ \psi_{sf}(0) + \psi_{sf}^{\dagger}(0) \right] \left[ \psi_{sf}^{\dagger}(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^{\dagger}(0) \right] \hat{Q} S_{\pm}^x S_{\pm}^z \hat{Q} \right. \\ &\quad \left. + \left[ \psi_{sf}^{\dagger}(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^{\dagger}(0) \right] \left[ \psi_{sf}(0) + \psi_{sf}^{\dagger}(0) \right] \hat{Q} S_{\pm}^z S_{\pm}^x \hat{Q} \right\}. \end{aligned} \quad (\text{B7})$$

Using the fact  $\hat{Q}S_-^z S_+^x \hat{Q} = d^\dagger$  and  $\hat{Q}S_+^x S_-^z \hat{Q} = d$ , and carrying out the transformation (43), we simplify (B7) to

$$-\frac{v_F^2 J_+^\perp J_m^z}{2(K_\perp + T_K)(2\pi\alpha)^{3/2}} \left[ \tilde{\psi}_{sf}(0) - \tilde{\psi}_{sf}^\dagger(0) \right] (d + d^\dagger). \quad (\text{B8})$$

In deriving (B8), we have used the relation

$$\left\{ \psi_{sf}(0), \psi_{sf}^\dagger(0) \right\} = \delta(0) = \frac{1}{2\pi\alpha}. \quad (\text{B9})$$

Note that (B8) is a renormalization to (B2).

The second contribution to the effective Hamiltonian from (B5) is

$$\begin{aligned} & -i \frac{v_F^3 J_+^\perp J_m^z}{2(K_\perp + T_K)^2 \sqrt{2\pi\alpha}} \left\{ \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \int_{-\infty}^{\infty} dx \psi_{sf}^\dagger(x) \partial_x \psi_{sf}(x) \right. \\ & \times \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \hat{Q} S_+^x S_-^z \hat{Q} + \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \\ & \times \left. \int_{-\infty}^{\infty} dx \psi_{sf}^\dagger(x) \partial_x \psi_{sf}(x) \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \hat{Q} S_-^z S_+^x \hat{Q} \right\}. \quad (\text{B10}) \end{aligned}$$

Commuting all fermion operators evaluated at  $x = 0$  to one side and simplifying the products using anticommutation relations, we find that (B10) contains a term

$$\frac{v_F^3 J_+^\perp J_m^z}{8(K_\perp + T_K)^2 (2\pi\alpha)^{3/2}} i \partial_x \left[ \tilde{\psi}_{sf}(0) - \tilde{\psi}_{sf}^\dagger(0) \right] (d - d^\dagger). \quad (\text{B11})$$

This is the leading irrelevant operator and has dimension 3/2. Note that the combination of local fermion operators appearing in (B11) is  $d - d^\dagger$ , not  $d + d^\dagger$ . This is a vital difference.

The third contribution to the effective Hamiltonian from (B5) is

$$\begin{aligned} & \frac{V v_F^2 J_+^\perp J_m^z}{2(K_\perp + T_K)^2 \sqrt{2\pi\alpha}} \left\{ \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] \left[ \psi_f(0) + \psi_f^\dagger(0) \right] \right. \\ & \times \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \hat{Q} S_+^x S_-^z \hat{Q} + \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \\ & \times \left. \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] \left[ \psi_f(0) + \psi_f^\dagger(0) \right] \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \hat{Q} S_+^x S_-^z \hat{Q} \right\}. \quad (\text{B12}) \end{aligned}$$

This contribution can be reduced to

$$\frac{V v_F^2 J_+^\perp J_m^z}{2(K_\perp + T_K)^2 (2\pi\alpha)^{5/2}} \left[ \tilde{\psi}_f(0) + \tilde{\psi}_f^\dagger(0) \right] (d - d^\dagger). \quad (\text{B13})$$

Again, we note that it is  $d - d^\dagger$  appearing in (B13). This is the second relevant operator which is present only when the particle-hole symmetry is broken, i.e., when  $V \neq 0$ .

The staggered magnetic field coupling term comes from

$$\hat{Q} \{ h_s S_-^z \} \frac{1 - \hat{Q}}{-(K_\perp + T_K)} \left\{ \frac{v_F J_+^\perp}{\sqrt{2\pi\alpha}} \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] S_+^x \right\} \hat{Q} + \hat{Q} \left\{ \frac{v_F J_+^\perp}{\sqrt{2\pi\alpha}} \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \right\} \frac{1 - \hat{Q}}{-(K_\perp + T_K)} \{ h_s S_-^z \} \hat{Q}. \quad (\text{B14})$$

This term is simplified to

$$-\frac{h_s v_F J_+^\perp}{(K_\perp + T_K) \sqrt{2\pi\alpha}} \left[ \tilde{\psi}_{sf}(0) + \tilde{\psi}_{sf}^\dagger(0) \right] (d - d^\dagger). \quad (\text{B15})$$

To obtain the uniform magnetic field coupling term, we restore the Bose field  $\phi_s(x)$  through  $\psi_s^\dagger(x) \psi_s(x) = \partial_x \Phi_s(x)/(2\pi)$  in (36) and (37). Then we integrate out  $\phi_s(x)$  exactly. This is carried out as follows. First, we notice that the terms in (31) and (32) containing  $\phi_s$  can be rewritten as, upon inserting  $\partial_x \Phi_s(x) = \sqrt{\pi} [\partial_x \phi_s(x) - \Pi_s(x)]$ ,

$$\begin{aligned} & \frac{v_F}{2} \int_{-\infty}^{\infty} dx \left\{ \Pi_s^2(x) + [\partial_x \phi_s(x)]^2 + \frac{h_u}{\pi v_F} \partial_x \Phi_s(x) + \frac{\tilde{J}_+^z}{\pi} \delta(x) \partial_x \Phi_s(x) S_+^z \right\} \\ &= \frac{v_F}{2} \int_{-\infty}^{\infty} dx \left\{ \left[ \Pi_s(x) - \frac{h_u}{2\sqrt{\pi} v_F} \right]^2 + \left[ \partial_x \phi_s(x) + \frac{h_u}{2\sqrt{\pi} v_F} \right]^2 + \frac{\tilde{J}_+^z}{\pi} \delta(x) \partial_x \Phi_s(x) S_+^z \right\}, \end{aligned} \quad (\text{B16})$$

up to an additive constant. By introducing

$$\tilde{\phi}_s(x) = \phi_s(x) + \frac{h_u}{2\sqrt{\pi} v_F} x, \quad (\text{B17})$$

we can recast (B16) in the form

$$\frac{v_F}{2} \int_{-\infty}^{\infty} dx \left\{ \tilde{\Pi}_s^2(x) + [\partial_x \tilde{\phi}_s(x)]^2 + \frac{\tilde{J}_+^z}{\pi} \delta(x) \partial_x \tilde{\Phi}_s(x) S_+^z - \frac{h_u \tilde{J}_+^z}{\pi v_F} S_+^z \delta(x) \right\}, \quad (\text{B18})$$

where  $\tilde{\Pi}_s(x)$  and  $\partial_x \tilde{\Phi}_s(x)$  are correspondingly defined as, in consistency with (21) and the relation  $\tilde{\Pi}_s = \partial_t \tilde{\phi}_s$ ,

$$\tilde{\Pi}_s(x) = \Pi_s(x) - \frac{h_u}{2\sqrt{\pi} v_F}, \quad (\text{B19})$$

$$\partial_x \tilde{\Phi}_s(x) = \partial_x \Phi_s(x) + \frac{h_u}{v_F}. \quad (\text{B20})$$

Since the uniform field  $h_u$  only appears in the last term of (B18), we only need to project it onto the lowest doublet in the next step. The contribution is

$$\begin{aligned} & \hat{Q} \left\{ \frac{v_F J_-^z}{2} [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] [\psi_f(0) - \psi_f^\dagger(0)] S_+^z + v_F \tilde{J}_+^z \psi_s^\dagger(0) \psi_s(0) S_+^z \right\} \\ & \times \frac{1 - \hat{Q}}{-T_K} \left\{ -\frac{h_u \tilde{J}_+^z}{2\pi} S_+^z \right\} \hat{Q} + \hat{Q} \left\{ -\frac{h_u \tilde{J}_+^z}{2\pi} S_+^z \right\} \frac{1 - \hat{Q}}{-T_K} \\ & \times \left\{ \frac{v_F J_-^z}{2} [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] [\psi_f(0) - \psi_f^\dagger(0)] S_+^z + v_F \tilde{J}_+^z \psi_s^\dagger(0) \psi_s(0) S_+^z \right\} \hat{Q}. \end{aligned} \quad (\text{B21})$$

With a little algebra, one can show that (B21) contains

$$\begin{aligned} & \frac{h_u v_F \tilde{J}_+^z J_-^z}{8\pi T_K} [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] [\psi_f(0) - \psi_f^\dagger(0)] \\ & + \frac{h_u v_F (\tilde{J}_+^z)^2}{4\pi T_K} \psi_s^\dagger(0) \psi_s(0). \end{aligned} \quad (\text{B22})$$

Combining the results (B2), (B8), (B11), (B13), (B15), (B22) together and omitting the tilde signs on  $\psi$ 's, we obtain the effective Hamiltonian (45), (46), and (47). It should be kept in mind that the obtained expressions, (48)–(52), for the numerical coefficients of the effective Hamiltonian should not be taken too literally in general cases where the second-order projection may not be sufficient. However, the validity of the effective Hamiltonian and the relations between the operators in the effective Hamiltonian and those in the original one (1) will not be affected. The purpose of this appendix is to illustrate how each term in the effective Hamiltonian arises from the projection rather than accurately determining the coefficients of the effective Hamiltonian. A practical way to determine them probably is to fit numerical results or experimental data.

### APPENDIX C: EFFECT OF THE MARGINAL OPERATORS (56)

In this appendix, we shall show that the only effect of including the marginal particle-hole symmetry breaking operators (56) is to slightly renormalize the two basic energy scales  $T_K$  and  $T_c$ .

The marginal operators (56) correspond to the following terms in the action:

$$\begin{aligned} \mathcal{S}'_{\text{phb}}(b_{sf}, a_f, a) &= 2iV \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} a_f(\omega_n, k) \\ & \times \left[ \alpha_v a(-\omega_n) - \int_{-\infty}^{\infty} \frac{dk'}{2\pi} b_{sf}(-\omega_n, k') \right]. \end{aligned} \quad (\text{C1})$$

Setting  $h_s = 0$ , our task now is to diagonalize

$$\begin{aligned} \mathcal{S}(b_{sf}, a_f, a, b) &= \mathcal{S}_2(b_{sf}, a, b) + \mathcal{S}_3(a_f, b) \\ & + \mathcal{S}'_{\text{phb}}(b_{sf}, a_f, a), \end{aligned} \quad (\text{C2})$$

where  $\mathcal{S}_2(b_{sf}, a, b)$  and  $\mathcal{S}_3(a_f, b)$  are given by (71) and (72), respectively. More specifically, we need to find new linear transformations other than (77) and (78) such that

the hybridizing terms in (C2) are canceled out. The desired transformations are

$$\begin{aligned} \tilde{b}_{sf}(\omega_n, k) &= b_{sf}(\omega_n, k) + \xi_1(\omega_n, k) a(\omega_n) \\ &\quad + \xi_2(\omega_n, k) b(\omega_n), \end{aligned} \quad (\text{C3})$$

$$\begin{aligned} \tilde{a}_f(\omega_n, k) &= a_f(\omega_n, k) + \xi_3(\omega_n, k) a(\omega_n) \\ &\quad + \xi_4(\omega_n, k) b(\omega_n), \end{aligned} \quad (\text{C4})$$

where the four transformation coefficients are given by

$$\xi_1(\omega_n, k) = -\frac{2iv_F}{i\omega_n - v_F k} \frac{g_0 + \text{sgn}\omega_n \alpha_v V^2/v_F^2}{1 + V^2/v_F^2}, \quad (\text{C5})$$

$$\begin{aligned} \xi_2(\omega_n, k) &= \frac{2v_F}{i\omega_n - v_F k} \left[ g_1 k - \frac{iV \text{sgn}\omega_n}{v_F^2 + V^2} \left( \tilde{V} - \frac{2Vg_1\Lambda}{\pi} \right. \right. \\ &\quad \left. \left. + \frac{Vg_1}{v_F} |\omega_n| \right) \right], \end{aligned} \quad (\text{C6})$$

$$\xi_3(\omega_n, k) = -\frac{2iV}{i\omega_n - v_F k} \frac{\alpha_v - g_0 \text{sgn}\omega_n}{1 + V^2/v_F^2}, \quad (\text{C7})$$

$$\xi_4(\omega_n, k) = -\frac{2i}{i\omega_n - v_F k} \frac{\tilde{V} - 2Vg_1\Lambda/\pi + Vg_1|\omega_n|/v_F}{1 + V^2/v_F^2}. \quad (\text{C8})$$

The ultraviolet cutoff  $\Lambda$  enters the transformation coefficients through the integrals (80) and (81). In terms of the shifted Grassmann variables, the action (C2) becomes

$$\begin{aligned} \mathcal{S}(b_{sf}, a_f) &= -\sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left\{ \frac{1}{2} (i\omega_n - v_F k) [\tilde{a}_f(-\omega_n, -k) \tilde{a}_f(\omega_n, k) + \tilde{b}_{sf}(-\omega_n, -k) \tilde{b}_{sf}(\omega_n, k)] \right. \\ &\quad \left. + 2iV \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \tilde{a}_f(\omega_n, k) \tilde{b}_{sf}(-\omega_n, k') \right\} + \mathcal{S}_{\text{gen}}(a, b). \end{aligned} \quad (\text{C9})$$

The last term inside the curly bracket is a potential scattering term for the extended fermions. The generated local terms are

$$\begin{aligned} \mathcal{S}_{\text{gen}}(a, b) &= -i \sum_n \left\{ \frac{\text{sgn}\omega_n}{2} [\mathcal{M}_{aa}(|\omega_n|) a(-\omega_n) a(\omega_n) \right. \\ &\quad + \mathcal{M}_{bb}(|\omega_n|) b(-\omega_n) b(\omega_n)] \\ &\quad \left. + \mathcal{M}_{ab}(\omega_n) a(-\omega_n) b(\omega_n) \right\}, \end{aligned} \quad (\text{C10})$$

with

$$\mathcal{M}_{aa}(|\omega_n|) = \frac{2v_F}{1 + V^2/v_F^2} \left[ g_0^2 + \left( \frac{\alpha_v V}{v_F} \right)^2 \right], \quad (\text{C11})$$

$$\begin{aligned} \mathcal{M}_{bb}(|\omega_n|) &= \frac{2}{1 + V^2/v_F^2} \left\{ \frac{1}{v_F} \left( \tilde{V} - \frac{2Vg_1\Lambda}{\pi} \right)^2 \right. \\ &\quad + |\omega_n| \left[ \frac{2g_1^2\Lambda}{\pi} \left( 1 - \frac{V^2}{v_F^2} \right) + \frac{2g_1 V \tilde{V}}{v_F^2} \right] \\ &\quad \left. - \frac{g_1^2}{v_F} \omega_n^2 \right\}, \end{aligned} \quad (\text{C12})$$

$$\begin{aligned} \mathcal{M}_{ab}(\omega_n) &= \frac{2}{1 + V^2/v_F^2} \left[ g_0 \left( \frac{V\tilde{V}}{v_F} + \frac{2v_F g_1 \Lambda}{\pi} - g_1 |\omega_n| \right) \right. \\ &\quad \left. + \text{sgn}\omega_n \frac{\alpha_v V}{v_F} \left( \tilde{V} - \frac{2Vg_1\Lambda}{\pi} + \frac{Vg_1}{v_F} |\omega_n| \right) \right]. \end{aligned} \quad (\text{C13})$$

To obtain the total effective local action, we add the generated terms (C10) to (74). Introducing a new local Grassmann variable,

$$\tilde{b}(\omega_n) = b(\omega_n) + \frac{\alpha_v V}{\tilde{V} - 2Vg_1\Lambda/\pi} a(\omega_n), \quad (\text{C14})$$

we can compactly write the effective local action as, upon neglecting  $\omega_n^2$  terms in the matrix elements,

$$\begin{aligned} \mathcal{S}_{\text{loc}}^{\text{eff}} &= -i \sum_{n>0} \left( a(-\omega_n), \tilde{b}(-\omega_n) \right) \\ &\quad \times \begin{pmatrix} \omega_n/Z_a + 2v_F \tilde{g}_0^2 & -(\delta\tilde{K} + 2\tilde{g}_0 \tilde{g}_1 \omega_n) - \eta\omega_n \\ \delta\tilde{K} + 2\tilde{g}_0 \tilde{g}_1 \omega_n - \eta\omega_n & \omega_n/Z_b + 2\tilde{V}'^2/v_F \end{pmatrix} \begin{pmatrix} a(\omega_n) \\ \tilde{b}(\omega_n) \end{pmatrix}. \end{aligned} \quad (\text{C15})$$

The renormalized parameters are

$$\tilde{g}_0 = \frac{g_0}{\sqrt{1 + V^2/v_F^2}}, \quad (\text{C16})$$

$$\tilde{g}_1 = \frac{g_1}{\sqrt{1 + V^2/v_F^2}}, \quad (\text{C17})$$

$$\tilde{V}' = \frac{\tilde{V} - 2Vg_1\Lambda/\pi}{\sqrt{1 + V^2/v_F^2}}, \quad (\text{C18})$$

$$\delta\tilde{K} = \delta K - \frac{2v_F g_0}{1 + V^2/v_F^2} \left( \frac{V\tilde{V}}{v_F^2} + \frac{2g_1\Lambda}{\pi} \right), \quad (\text{C19})$$

$$\frac{1}{Z_a} = 1 + \left( \frac{\alpha_v V}{\tilde{V} - 2Vg_1\Lambda/\pi} \right)^2 \left( 1 + \frac{4g_1^2\Lambda}{\pi} \right), \quad (\text{C20})$$

$$\frac{1}{Z_b} = 1 + \frac{2}{1 + V^2/v_F^2} \left[ \frac{2g_1^2\Lambda}{\pi} \left( 1 - \frac{V^2}{v_F^2} \right) + \frac{2g_1V\tilde{V}}{v_F^2} \right], \quad (\text{C21})$$

$$\eta = \frac{\alpha_v V}{\tilde{V} - 2Vg_1\Lambda/\pi} \left[ 1 + \frac{2(2g_1^2\Lambda/\pi + g_1V\tilde{V}/v_F^2)}{1 + V^2/v_F^2} \right]. \quad (\text{C22})$$

The effective action (C15) has essentially the same form as (85) except for a wave function renormalization factor  $Z_a$  and a new type term,  $\eta\omega_n$ , in the off-diagonal matrix elements. However, this new type term is irrelevant since it can only generate a  $(\eta\omega_n)^2$  term in physical quantities such as free energy. At this point, it is clear that including the marginal particle-hole symmetry breaking terms with the coefficients  $V$  and  $\alpha_v V$  only slightly renormalizes the coefficients in the effective Hamiltonian (44), so will only renormalize the two energy scales, the Kondo temperature  $T_K$  and the crossover temperature  $T_c$ .

#### APPENDIX D: CONTRIBUTION OF THE MARGINAL OPERATORS (55) TO THE STAGGERED SUSCEPTIBILITY

In this appendix, we show that the contributions to the staggered susceptibility from the marginal operators (55) are negligible.

The marginal operators (55) have the following corresponding terms in the action:

$$\begin{aligned} S'_{\text{stag}} &= 2ih_s \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} a_{sf}(-\omega_n, k) \\ &\times \left[ \alpha'_s \int_{-\infty}^{\infty} \frac{dk'}{2\pi} b_{sf}(\omega_n, k') + \alpha''_s a(\omega_n) \right]. \quad (\text{D1}) \end{aligned}$$

Combining the last expression with the staggered field coupling term in (70) and inserting the transformation (77), we can write the complete staggered field coupling terms in the following form:

$$\begin{aligned} S_{\text{stag}} &= 2ih_s \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} a_{sf}(-\omega_n, k) \\ &\times \left[ \alpha'_s \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \tilde{b}_{sf}(\omega_n, k') \right. \\ &+ (\alpha''_s + \alpha'_s g_0 \text{sgn}\omega_n) a(\omega_n) \\ &\left. + \left( \alpha_s + \frac{2\alpha'_s g_1 \Lambda}{\pi} - \frac{\alpha'_s g_1 |\omega_n|}{v_F} \right) b(\omega_n) \right]. \quad (\text{D2}) \end{aligned}$$

The staggered susceptibility is obtained by calculating the second-order perturbation of  $S_{\text{stag}}$ ,

$$\chi_s = -\frac{\partial^2}{\partial h_s^2} \left[ -\frac{1}{2\beta} \langle S_{\text{stag}} S_{\text{stag}} \rangle \right], \quad (\text{D3})$$

where the average is weighted by an action consisting of the free and decoupled extended Grassmann variables  $a_{sf}$ ,  $\tilde{b}_{sf}$ , and the effective local action (85). The first term in (D2) is a potential scattering term and does not mix with the other terms of  $S_{\text{stag}}$  in the second-order perturbation. It thus gives a finite contribution to the staggered susceptibility and can be treated separately. Carrying out the calculation for (D3), we find that the singular part of the staggered susceptibility is

$$\chi_s = \frac{2}{v_F} \left( \alpha_s + \frac{2\alpha'_s}{\pi} g_1 \Lambda \right)^2 \frac{1}{\beta} \sum_n i \text{sgn}\omega_n \langle b(-\omega_n) b(\omega_n) \rangle. \quad (\text{D4})$$

The propagator is given by, from (85),

$$\langle b(-\omega_n) b(\omega_n) \rangle = -i \text{sgn}\omega_n \frac{Z_b (|\omega_n| + T_K)}{\omega_n^2 + T_c^2 + |\omega_n| T_K}, \quad (\text{D5})$$

where we have taken  $2v_F g_0^2 \simeq T_K$  in the numerator of (D5) for simplicity. The singularity of the staggered susceptibility comes from the fact that at the critical point,  $T_c = 0$ ,  $\langle b(-\omega_n) b(\omega_n) \rangle \sim 1/(i\omega_n)$  which gives rise to a logarithmic singularity in the Matsubara frequency summation in (D4). From (D4), we see that the only effect of the marginal operators (55) is to shift  $\alpha_s$  to  $\alpha_s + 2\alpha'_s g_1 \Lambda/\pi$ . Actually, one should be able to see this result from (D2) without doing calculation.

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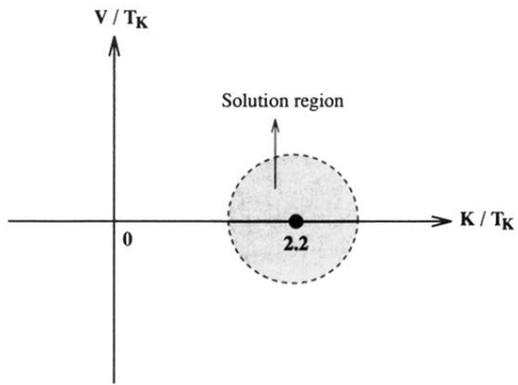


FIG. 1. The phase diagram of the two-impurity Kondo model.  $V$  is the energy scale characterizing particle-hole symmetry breaking strength.  $K$  is the fully renormalized RKKY interaction.  $T_K$  is the Kondo temperature. Except at the critical point marked by the black dot, the low-energy behavior is of Fermi-liquid type everywhere. The area inside the dashed circle is the region where our solution applies. The radius of the solution region is a fraction of  $T_K$ .