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

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Abstract

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 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 mapped out 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 critical behavior. A detailed comparison is made with the numerical renormalization group

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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.

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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 [1], and to certain extent it is also the case of high temperature superconducting cuprates [2]. In such systems, two effects have crucial influence on the low energy properties and they compete with each other. They are the Kondo effect [3] and RKKY interaction [4], which represent two different tendencies of the system to quench the local moments with conduction electrons or by themselves. The simplest model capturing both effects is the two-impurity Kondo model [5–7]. It is also believed that any possible new physics that may occur in lattice due to the competition between the two effects should be contained in the two-impurity problem [8].

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 [9]. The complexity of the problem will be fully realized this way and the concrete task we are facing will be defined. For all practical purposes, the bare Kondo coupling constant $J_0$ and the RKKY interaction $K_0$ 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 $\rho_F(\sim 1/\epsilon_F)$, $\rho_F J_0$ and $\rho_F K_0$, they are always in the weak coupling regime. However, as we start 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 renormalize each other. Simple dimensional counting shows that $\rho_F J_0$ has dimension one and is marginally relevant, while $\rho_F K_0$ 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 $T_{RKKY}$, 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 the unity respectively. In either $T_K \gg T_{RKKY}$ or $T_K \ll T_{RKKY}$ limit, the problem is simple because we can perturb one of the two interactions. The most difficult situation corresponds to $T_K \sim T_{RKKY}$. 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 [3, 14, 18]. As a result, a convincing phase diagram has emerged [11, 14, 16], if not yet universally accepted without reservation [19]. This phase diagram is shown in Figure 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 $2.2^{[1]}$. The effective RKKY interaction is actually the RKKY temperature whose meaning we have explained in the above. But for some reason it has been confusingly called RKKY interaction. Although the precise numerical value of the ratio may depend on the individual’s convention of defining the coupling constants, the important message is that this critical point is located at $T_K \sim T_{RKKY}$.

Although several asymptotically exact results have been available about the critical point in certain limits [11, 18], the exact physical origin of this critical point had not been unveiled until recently [20]. By an explicit identification of two local impurity spin 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 ensures the occurrence of a non-Fermi-liquid critical point. We have also presented an effective Hamiltonian for the finite solution region as marked in Figure 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 of Figure 1.

Having admitted the existence of the critical point, we can already present a framework for the solution inside that solution region in Figure 1, by only invoking general scaling ideas. It is then the task of section IV to fill in concrete results. Since 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 existed on the energy scale of the Fermi
energy. The above mentioned $T_{RKKY}$ 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 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 appearance of the Kondo temperature $T_K(\ll \epsilon_F)$ in the one-impurity Kondo problem leads to the drastic enhancement of various physical quantities including specific heat, 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, 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 in the solution region of Figure 1 near the critical point. What need to be improved are the constant prefactors. Usually, a physical quantity calculated for a Fermi-liquid fixed point is a sum of 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 of Figure 1. As one moves away from the critical point, 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 of Nozières’s Fermi-liquid theory of Kondo effect [21]. 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 the following. In section II, we present the preliminary transformations on the two-impurity Kondo model including the reduction to one dimension and bosonization. In section III, we identify the critical point and derive the effective Hamiltonian. A rigorous proof of the completeness of the effective Hamiltonian is included. In section IV, we solve the effective Hamiltonian and calculate the low energy thermodynamics. In section V, we compare our results with those derived from the numerical renormalization group and conformal field theory approaches. The universality of the critical point is strongly argued for. We conclude our paper in section VI with a summary and some speculations on the lattice problem. To alleviate cross-referencing, some frequently used parameters and symbols are gathered 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,

\[
H = \int d^3k \epsilon_k \psi_k^\dagger \psi_k + \int \frac{d^3k \, d^3k'}{(2\pi)^3} \sum_{\lambda=x,y,z} \frac{j_\lambda}{2} \left[ e^{\frac{i}{2}(\vec{k} - \vec{k}') \cdot \vec{R}} \psi_k^\dagger \sigma^\lambda \psi_{k'} S^\lambda_{1} + e^{-\frac{i}{2}(\vec{k} - \vec{k}') \cdot \vec{R}} \psi_k^\dagger \sigma^\lambda \psi_{k'} S^\lambda_{2} \right] + \sum_{\lambda=x,y,z} K^\lambda S^\lambda_{1} S^\lambda_{2},
\]

where \( \psi_k^\dagger = (\psi_{k1}^\dagger, \psi_{k2}^\dagger) \), \( \sigma^\lambda \) with \( \lambda = x, y, z \) are the Pauli matrices, \( \vec{S}_1 \) and \( \vec{S}_2 \) are the two impurity spin 1/2 operators located at \( \pm \vec{R}/2 \). It has been shown that the Hamiltonian (1) can be reduced to an equivalent one-dimensional(1D) problem \( (11,18) \). Introducing 1D fermionic operators,

\[
\psi_{1,2}(k) = \frac{k}{\sqrt{2}} \left[ \frac{1}{N_v(k)} \int d^2\Omega \cos \left( \frac{\vec{k} \cdot \vec{R}}{2} \right) \mp \frac{i}{N_o(k)} \int d^2\Omega \sin \left( \frac{\vec{k} \cdot \vec{R}}{2} \right) \right] \psi_k,
\]
with the notations \( d^3k = k^2 dk d\Omega \) and

\[
N_{e,o}(k) = \sqrt{1 \pm \frac{\sin(kR)}{kR}},
\]

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

\[
H_{\text{Kondo}} = \frac{v_F}{2} \sum_{\lambda=x,y,z} \int_0^\infty \frac{dk \, dk'}{(2\pi)^2} \left\{ J^\lambda_{+}(k, k') \left[ \psi'^{\dagger}_1(k) \sigma^{\lambda} \psi_1(k') + \psi'^{\dagger}_2(k) \sigma^{\lambda} \psi_2(k') \right] S^\lambda_+ \right. \\
+ J^\lambda_{m}(k, k') \left[ \psi'^{\dagger}_1(k) \sigma^{\lambda} \psi_1(k') - \psi'^{\dagger}_2(k) \sigma^{\lambda} \psi_2(k') \right] S^\lambda_- + J^\lambda_{rr}(k, k') \left[ \psi'^{\dagger}_1(k) \sigma^{\lambda} \psi_2(k') - \psi'^{\dagger}_2(k) \sigma^{\lambda} \psi_1(k') \right] S^\lambda_- \right\}. 
\]

(4)

In the last expression, we have introduced the short-hand notation,

\[
S^\lambda_\pm = S^\lambda_1 \pm S^\lambda_2, \quad \lambda = x, y, z.
\]

(5)

The momentum dependent coupling constants are, for \( \lambda = x, y, z, \)

\[
J^\lambda_{+}(k, k') = \frac{J^\lambda k k'}{4\pi v_F} \left[ N_{e}(k)N_{e}(k') + N_{o}(k)N_{o}(k') \right],
\]

(6)

\[
J^\lambda_{-}(k, k') = \frac{J^\lambda k k'}{4\pi v_F} \left[ N_{e}(k)N_{e}(k') - N_{o}(k)N_{o}(k') \right],
\]

(7)

\[
J^\lambda_{m}(k, k') = \frac{J^\lambda k k'}{4\pi v_F} \left[ N_{e}(k)N_{o}(k') + N_{o}(k)N_{e}(k') \right],
\]

(8)

\[
J^\lambda_{rr}(k, k') = \frac{J^\lambda k k'}{4\pi v_F} \left[ N_{e}(k)N_{o}(k') - N_{o}(k)N_{e}(k') \right].
\]

(9)

From the commutation relation \( \{ \psi'^{\dagger}_{k\sigma}, \psi^\dagger_{k'\sigma'} \} = \delta^3(\vec{k} - \vec{k}') \delta_{\sigma\sigma'} \), we can verify

\[
\{ \psi^\dagger_{i\sigma}(k), \psi_{i'\sigma'}(k') \} = 2\pi \delta(k - k') \delta_{i,i'} \delta_{\sigma,\sigma'}.
\]

(10)

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

\[
\int d^3k \, \epsilon_k \psi'^{\dagger}_k \psi^\dagger_k = \int_0^\infty \frac{dk}{2\pi} \epsilon_k \left[ \psi'^{\dagger}_1(k) \psi_1(k) + \psi'^{\dagger}_2(k) \psi_2(k) \right] + \cdots.
\]

(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 \( k = k_F, \epsilon_k \approx v_F(k - k_F) \), and expand the momentum dependent coupling constants around
We only need to retain the leading terms of the expansion since other terms contain some power of \( k - k_F \), which have high scaling dimension and are irrelevant at low energy. From \( J^\lambda_{ir}(k_F, k_F) = 0 \), we see that \( J_{ir} \) interaction only contains irrelevant terms. Denoting \( k - k_F \) by \( k \) again and with implicit understanding of an ultraviolet cutoff, we can introduce Fourier transformations

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

(12)

The fermion operators satisfy the standard commutation relation,

\[
\{\psi_i^\dagger \sigma(x), \psi_{i'}^\sigma(x')\} = \delta(x - x')\delta_{i,i'}\delta_{\sigma,\sigma'}.
\]

(13)

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

\[
H = H_0 + H_1,
\]

(14)

\[
H_0 = -iv_F \sum_{i=1,2} \int_{-\infty}^{\infty} dx \psi_i^\dagger(x) \partial_x \psi_i(x) + \sum_{\lambda=x,y,z} K_{i\lambda} S_1^\lambda S_2^\lambda
\]

\[
+ h_u \left[ S_+^z + \frac{1}{2} \sum_{\lambda=x,y,z} \int_{-\infty}^{\infty} dx \psi_1^\dagger(x) \sigma^\lambda \psi_1(x) \right] + h_s S_-^z,
\]

(15)

\[
H_1 = \frac{v_F}{2} \sum_{\lambda=x,y,z} \left\{ J^\lambda_+ \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_1(0) + \psi_2^\dagger(0) \sigma^\lambda \psi_2(0) \right] S_+^\lambda
\]

\[+ J^\lambda_m \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_2(0) - \psi_2^\dagger(0) \sigma^\lambda \psi_1(0) \right] S_-^\lambda + J^\lambda_\pm \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_2(0) + \psi_2^\dagger(0) \sigma^\lambda \psi_1(0) \right] S_\pm^\lambda \right\}.
\]

(16)

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

\[
J^\lambda_+ = \pi J^\lambda \rho_F, \quad J^\lambda_- = \pi J^\lambda \rho_F \frac{\sin(k_F R)}{k_F R}, \quad J^\lambda_m = \pi J^\lambda \rho_F \sqrt{1 - \left( \frac{\sin k_F R}{k_F R} \right)^2},
\]

(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. Noting that we have included both uniform and staggered magnetic fields \( h_u \) and \( h_s \) in (15), with 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

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To summarize, the 3D two-impurity Kondo Hamiltonian has been reduced to a 1D problem by retaining only the leading terms of the expansion, discarding higher-order terms that are irrelevant at low energy. The full Hamiltonian is given by

\[
H = H_0 + H_1,
\]

where

\[
H_0 = -iv_F \sum_{i=1,2} \int_{-\infty}^{\infty} dx \psi_i^\dagger(x) \partial_x \psi_i(x) + \sum_{\lambda=x,y,z} K_{i\lambda} S_1^\lambda S_2^\lambda
\]

\[+ h_u \left[ S_+^z + \frac{1}{2} \sum_{\lambda=x,y,z} \int_{-\infty}^{\infty} dx \psi_1^\dagger(x) \sigma^\lambda \psi_1(x) \right] + h_s S_-^z,
\]

and

\[
H_1 = \frac{v_F}{2} \sum_{\lambda=x,y,z} \left\{ J^\lambda_+ \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_1(0) + \psi_2^\dagger(0) \sigma^\lambda \psi_2(0) \right] S_+^\lambda
\]

\[+ J^\lambda_m \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_2(0) - \psi_2^\dagger(0) \sigma^\lambda \psi_1(0) \right] S_-^\lambda + J^\lambda_\pm \left[ \psi_1^\dagger(0) \sigma^\lambda \psi_2(0) + \psi_2^\dagger(0) \sigma^\lambda \psi_1(0) \right] S_\pm^\lambda \right\}.
\]

The coupling constants are given by

\[
J^\lambda_+ = \pi J^\lambda \rho_F, \quad J^\lambda_- = \pi J^\lambda \rho_F \frac{\sin(k_F R)}{k_F R}, \quad J^\lambda_m = \pi J^\lambda \rho_F \sqrt{1 - \left( \frac{\sin k_F R}{k_F R} \right)^2},
\]

with \( \rho_F = k_F^2/(2\pi^2 v_F) \).
two accidental features of (14) resulting from linearization. They are the particle-hole sym-
metry and a special relation between $J_{\mp}^\lambda(k_F, k_F)$ and $J_m^\lambda(k_F, k_F)$: that the RKKY interaction
generated from them is always ferromagnetic [11]. These accidental features will be spoiled
by the generated corrections from irrelevant terms neglected during the linearization. That
an irrelevant interaction can renormalize the coupling constant of a relevant interaction is
a well known fact [22]. An example can also be found in section IV, expression (82), where
the dimension $3/2$ leading irrelevant operator in the effective Hamiltonian (14) induces a
correction to the dimension $1/2$ relevant operator. Usually, the accidental features at the
lowest order will not survive if there is no hidden symmetry ensuring them. The accidental
relation between $J_{\mp}^\lambda(k_F, k_F)$ 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.
For a general conduction band, particle-hole symmetry breaking, although weak, is always
present. The general particle-hole symmetry breaking term that can be added to the 1D
Hamiltonian (14) has the following form [11,18],

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

where $V$ is the energy scale characterizing the strength of particle-hole symmetry break-
ing. Adding the marginal operator (18) to the 1D Hamiltonian after dropping irrelevant
interactions in the linearization may seem unusual, actually it is the natural thing to do.
The reason is again the generation of (18) from 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 only non-irrelevant operator breaking particle-hole symmetry
is (18). In section IV 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 of Figure 1.

In the rest of this paper, we shall retain the rotational symmetry around $z$-axis by setting
$K_x = K_y = K_\perp$ and $J_i^x = J_i^y = J_i^z$ 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,

Parity: $\psi_1 \leftrightarrow \psi_2$, $S_1^\lambda \leftrightarrow S_2^\lambda$ for $\lambda = x, y, z$,  
Particle—hole: $\psi_{i\uparrow} \to \psi_{i\downarrow}^\dagger$, $\psi_{i\downarrow} \to -\psi_{i\uparrow}^\dagger$,  
$\pi$ rotation around $x$—axis: $\psi_{i\uparrow} \leftrightarrow \psi_{i\downarrow}$, $S_i^y \to -S_i^y$, $S_i^z \to -S_i^z$.

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 [23,24,17]. There are four species of fermions, so we need to introduce four bose fields,

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

where $\alpha$ is the lattice spacing and

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

The bose fields satisfy the standard commutation relation,

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

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

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

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

By substituting (21) into (14) and using the relation $\psi_{1\sigma}(x) \psi_{1\sigma}(x) = \partial_x \Phi_{i\sigma}(x)/(2\pi)$, the two-impurity Kondo Hamiltonian is expressed in terms of 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,

\[
\begin{align*}
\phi_c &= (\phi_{1\uparrow} + \phi_{1\downarrow} + \phi_{2\uparrow} + \phi_{2\downarrow})/2, \\
\phi_s &= (\phi_{1\uparrow} - \phi_{1\downarrow} + \phi_{2\uparrow} - \phi_{2\downarrow})/2, \\
\phi_f &= (\phi_{1\uparrow} + \phi_{1\downarrow} - \phi_{2\uparrow} - \phi_{2\downarrow})/2, \\
\phi_{sf} &= (\phi_{1\uparrow} - \phi_{1\downarrow} - \phi_{2\uparrow} + \phi_{2\downarrow})/2.
\end{align*}
\]

(25)

The Hamiltonian now acquires the following form,

\[
\begin{align*}
H_0 &= \frac{v_F}{2} \sum_{\lambda=x,y,z} \int_{-\infty}^{\infty} dx \left\{ \Pi_\lambda^2(x) + [\partial_x \phi_\lambda(x)]^2 \right\} + \sum_{\lambda=x,y,z} K_\lambda S_\lambda^+ S_\lambda^- \\
&\quad + h_u \left[ S_+^z + \int_{-\infty}^{\infty} dx \partial_x \Phi_s(x) \right] + h_s S_+^z, \\
H_1 &= \frac{v_F}{2} \left\{ \frac{J_x^c}{\pi} \partial_x \Phi_c(0) S_+^x + \frac{J_x^s}{\pi} \partial_x \Phi_s(0) S_+^x - \frac{J_x^f}{\pi} \partial_x \Phi_f(0) S_+^x - \frac{J_x^{sf}}{\pi} \partial_x \Phi_{sf}(0) S_+^x \right\} + \sum_{\lambda=x,y,z} K_\lambda S_\lambda^+ S_\lambda^- + \frac{2J_x^c}{\pi} \sin \Phi_c(0) \sin \Phi_f(0) S_+^z + \frac{2J_x^s}{\pi} \sin \Phi_s(0) \sin \Phi_f(0) S_+^z \\
&\quad \times \cos \Phi_{sf}(0) \left[ \cos \Phi_s(0) S_+^x - \sin \Phi_s(0) S_+^y \right] - \frac{2J_x^{sf}}{\pi} \sin \Phi_f(0) \left[ \sin \Phi_s(0) S_+^x + \cos \Phi_s(0) S_+^y \right] \\
&\quad - \frac{2J_x^{sf}}{\pi} \sin \Phi_f(0) \cos \Phi_f(0) \\
H_2 &= -iV e^{i\pi \theta} \sin \Phi_{sf}(0) \cos \Phi_f(0),
\end{align*}
\]

(26)

where the phase factor is

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

(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 the \(\partial_x \Phi_c\) term inside the integral of the phase \(\theta\). The \(\cos \Phi_s(0)\) and \(\sin \Phi_s(0)\) factors in (27) can be eliminated by rotating the impurity spins around \(z\)-axis by an angle \(\Phi_s(0)\),

\[
H \rightarrow \hat{U} H \hat{U}^{-1}, \quad \text{with} \quad \hat{U} = e^{-iS_+^z \Phi_s(0)},
\]

(30)

\[
\hat{U} H_0 \hat{U}^{-1} = \frac{v_F}{2} \sum_{\lambda=x,y,z} \int_{-\infty}^{\infty} dx \left\{ \Pi_\lambda^2(x) + [\partial_x \phi_\lambda(x)]^2 \right\} + \sum_{\lambda=x,y,z} K_\lambda S_\lambda^+ S_\lambda^- + h_u S_+^z \\
&\quad + h_u \int_{-\infty}^{\infty} \frac{dx}{2\pi} \partial_x \Phi_s(x) - v_F \partial_x \Phi_s(0) S_+^z + \frac{v_F}{\alpha} (S_+^z)^2,
\]

(31)
The particle-hole symmetry breaking term becomes

\[ H = \frac{v_F}{2} \left\{ \frac{J^z_+}{\pi} \partial_x \Phi_s(0) S^z_+ + \frac{J_m^z}{\pi} \partial_x \Phi_{sf}(0) S^z_- - \frac{2iJ^z_+}{\pi \alpha} e^{i\pi \theta} \cos \Phi_{sf}(0) \sin \Phi_f(0) S^z_+ \right\}. \]  (31)

\[ \partial_x \text{in (31). The interactions in (32) only contain } \partial_x \Phi_s(0). \]  (32)

\[ \text{Again, a phase factor is included in the definition of the fermion operator } \psi_f(x). \]  (33)

\[ \psi_f(x) e^{i\pi \int_{-\infty}^{\infty} dx \psi^\dagger_{sf}(x) \psi_{sf}(x)} = \frac{1}{\sqrt{2\pi \alpha}} \psi_f(x), \]  (34)

\[ \psi_{sf}^\dagger(x) \psi_s(x) = \frac{1}{2\pi} \partial_x \Phi_s(x). \]  (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 \( \partial_x \Phi_s(0) \), we do not need to specify the phase for the fermion operator \( \psi_s(0) \). The complete Hamiltonian can be rewritten as

\[ H_0 = -i v_F \sum_{i=s, sf} \int_{-\infty}^{\infty} dx \psi_i^\dagger(x) \partial_x \psi_i(x) + K_z S^z_1 S^z_2 + K_\perp \sum_{\lambda=x,y} S^\lambda_1 S^\lambda_2 \]

\[ + h_u \int_{-\infty}^{\infty} dx \psi_s^\dagger(x) \psi_s(x) + h_s S^z_-, \]  (36)

\[ H_1 = \frac{v_F}{2} \left\{ \tilde{J}_+^z [\psi_{sf}^\dagger(0) \psi_s(0) - \psi_s(0) \psi_{sf}^\dagger(0)] S^z_1 + J_m^z [\psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0)] S^z_2 \right\} \]

\[ + J^z_- [\psi_{sf}(0) + \psi_{sf}^\dagger(0)] [\psi_f(0) - \psi_f^\dagger(0)] S^z_+ \]

\[ + i J_m^z [\psi_{sf}(0) - \psi_{sf}^\dagger(0)] S^y_+ + i J^z_+ [\psi_f(0) - \psi_f^\dagger(0)] S^y_+. \]  (37)

where

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

The particle-hole symmetry breaking term becomes
\[ H_2 = V \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] \left[ \psi_f(0) + \psi_f^\dagger(0) \right]. \] (39)

How do these 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,

Parity: \( \psi_{sf} \leftrightarrow \psi_{sf}^\dagger, \quad \psi_f \leftrightarrow -\psi_f^\dagger, \quad S_1^\lambda \leftrightarrow S_2^\lambda \) for \( \lambda = x, y, z, \)

Particle–hole: \( \psi_f \leftrightarrow -\psi_f^\dagger, \)

\( \pi \) rotation, \( x \)-axis: \( \psi_{sf} \leftrightarrow \psi_{sf}^\dagger, \quad \psi_s \leftrightarrow \psi_s^\dagger, \quad \psi_f \leftrightarrow -\psi_f, \quad S_i^y \rightarrow -S_i^y, \quad S_i^z \rightarrow -S_i^z. \)

Alternatively, one can directly verify them 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 derive an effective Hamiltonian for the finite region of the parameter space surrounding the critical point. Our identification of the critical point will make clear its physical origin.

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 \( J_z^-, J_\perp^+ \) 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 there isn’t anything containing \( \cos \Phi_s(0) \) or \( \sin \Phi_s(0). \) Thus, the \( \tilde{J}_z^\perp \) term containing the bose field \( \phi_s(x) \) can be integrated out analytically. Although \( \partial_x \Phi_s(0) \) couples to an operator \( S_+^z, \) the integration can be done formally in the path integral formalism, yielding the following two terms to the action,
\[
- \frac{v_F (\tilde{J}_z^2)}{4 \pi^2 \alpha} \int_0^\beta d\tau [S_+^z(\tau)]^2 + \frac{(\tilde{J}_z^2)^2}{8 \pi} \sum_n \nu_n |S_+^z(\nu_n)S_+^z(\nu_n)|, \text{ with } \nu_n = 2n\pi/\beta. \tag{41}
\]

The first term is a correction to the RKKY interaction, so it is absorbed into \( \tilde{K}_z \). The second term has higher dimension and is expected to be irrelevant. The point we want to make here is that the \( \tilde{J}_z^2 \) interaction does not affect the critical point and can be ignored during the search for the critical point. Thus, we see that when \( J^z = J^\perp = 0 \) the remaining Kondo interactions only involve three local spin operators, \( S^x_+, S^y_-, S^z_\perp \), which only act on three (out of four) local impurity spin states. The impurity spin state \(| \uparrow\downarrow > - | \downarrow\uparrow >)/\sqrt{2} \) decouples from the Kondo interactions when \( J^z = J^\perp = 0 \). Together with the RKKY interactions, we derive an energy level scheme for the impurity spin states in Figure 4. The critical point corresponds to the special case when the two lowest levels become degenerate. Specifically, the \(-\tilde{K}_z(S^z_\perp)^2/2\) term in (36) raises the energy of the states \(| \uparrow\downarrow > \) and \(| \downarrow\uparrow > \) by an amount \(-\tilde{K}_z/2\) (assuming \(-\tilde{K}_z > 0\)) with respect to the other two states \(| \uparrow\uparrow > \pm | \downarrow\downarrow > \). These two states, \(| \uparrow\downarrow > \) and \(| \downarrow\uparrow > \), are further split symmetrically by the transverse part of the RKKY interaction, \( K_\perp(S_1^+ S^2_\perp + S_1^- S^\perp_\perp^2)/2 \). When \(-\tilde{K}_z = K_\perp\), the two levels, \(| \uparrow\downarrow > - | \downarrow\uparrow >)/\sqrt{2} \) and \(| \uparrow\uparrow > + | \downarrow\downarrow >)/\sqrt{2} \), become degenerate, forming a doublet. Because there is almost no Kondo interaction in the state \(| \uparrow\uparrow > - | \downarrow\downarrow >)/\sqrt{2} \) when \( J^z = J^\perp = 0 \), 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 \( J^z \) and \( J^\perp \) will not change the energy level scheme as long as \( v_F J^z, v_F J^\perp < T_K \).

Now, we have identified the critical point. To describe the low energy physics, it is sufficient to project the full interacting Hamiltonian (36)+(37)+(39) onto the lowest energy doublet. For \( \tilde{J}_z^2, J^z_+, J_m^z, J^\perp, V \) all but \( J^z_m \) much smaller than one, the projection can be done accurately. Let \( \hat{Q} \) be the projection operator onto the doublet, the projected effective Hamiltonian to the second order is

\[
H_{eff} = \hat{Q} H \hat{Q} + \hat{Q} H (1 - \hat{Q}) \frac{1}{E_0 - \hat{Q} H \hat{Q} - (1 - \hat{Q}) H (1 - \hat{Q}) (1 - \hat{Q}) H \hat{Q}}, \tag{42}
\]
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 Figure 3, it is not difficult to verify $\hat{Q}S_+^y \hat{Q} = i(d - d^\dagger)$, $\hat{Q}S_+^y \hat{Q} = \hat{Q}S_+^y \hat{Q} = \hat{Q}S_+^y \hat{Q} = 0$. These relations are used for the first order projection. In the second order projection, nonvanishing terms may contain $\hat{Q}(S_z)^2 \hat{Q} = d^\dagger d$, $\hat{Q}(S_x)^2 \hat{Q} = \hat{Q}(S_z)^2 \hat{Q} = \hat{Q}(S_x)^2 \hat{Q} = d^\dagger d$, $\hat{Q}S_+^x S_+^y \hat{Q} = d$ and $\hat{Q}S_-^x S_-^y \hat{Q} = d^\dagger$. Since the extended fermions commute with the impurity spin operators, we need to 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

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

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

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

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

where $K_c$ 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 (43) 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 [24]. To the second order, the coefficients in $H_{\text{eff}}$ are given by
\[ g_0 = -\frac{J^\perp_m}{\sqrt{2\pi\alpha}} \left[ 1 + \frac{v_F J^\perp_m J^z_m}{4\pi\alpha(K^\perp + T_K)J^\perp_m} \right], \quad (48) \]

\[ g_1 = \frac{v_F^2 J^\perp_m J^z_m}{8(K^\perp + T_K)^2(2\pi\alpha)^{3/2}}, \quad (49) \]

\[ \bar{V} = \frac{v_F^2 J^\perp_m J^z_m V}{2(K^\perp + T_K)^2(2\pi\alpha)^{5/2}}, \quad (50) \]

\[ \alpha_u = \frac{v_F J^z \bar{J}^z}{8\pi T_K}, \quad (51) \]

\[ \alpha_s = -\frac{v_F J^\perp_m}{(K^\perp + T_K)\sqrt{2\pi\alpha}}. \quad (52) \]

The projection induces corrections to the RKKY interactions so the critical value \( K_c \) is not exactly \( v_F(J^z - \pi)/(\pi\alpha) \), as determined by the condition \(-\bar{K}_z = K^\perp\). The energy \( T_K \) in the above expressions can be identified as the ground state energy gain in (45) from the hybridization term \( v_F g_0 \). From the study of the two-channel Kondo problem, we know \( T_K \sim v_F g_0^2 \).

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

\[ H_s = -iv_F \int_{-\infty}^{\infty} dx \psi_s^\dagger(x)\partial_x \psi_s(x) + h_u \int_{-\infty}^{\infty} dx \psi_s^\dagger(x)\psi_s(x) + \frac{v_F(J^z)^2 h_u}{4\pi T_K} \psi_s^\dagger(0)\psi_s(0). \quad (53) \]

Since this piece of Hamiltonian does not contain any interesting physics, we shall not discuss it hereafter. For the particle-hole symmetry breaking and staggered field coupling terms, apart from the relevant operators we have included in (45) and (47), there are also marginal operators such as (39). They will be discussed below and in appendix D.

The effective Hamiltonian (44) is the central result of this paper. The rest of this section is to prove the completeness of the (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 of the projection and spoil the critical behavior? Fortunately, it turns out that all other operators up to dimension 3/2 inclusive can be eliminated by the three discrete symmetries of (10). To show this, we first determine how
the operators \( d \) and \( d^\dagger \) transform under parity and the rotation of 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: \( d^\dagger \rightarrow -d^\dagger \), \( d \rightarrow -d \). This could also be seen from \( \hat{Q} S^z S^x \hat{Q} = d^\dagger \) and \( \hat{Q} S^z S^x \hat{Q} = d \). From them, we can also see that under the \( \pi \) rotation around \( x \)-axis, \( d^\dagger \rightarrow -d^\dagger \), \( d \rightarrow -d \). Combining these results with (40), we derive all “elementary operators” 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 \( S(\psi, \psi^\dagger) = \int_0^\beta d\tau \int_\infty^{-\infty} dx \psi^\dagger(x, \tau)(\partial_\tau - iv_F \partial_x)\psi(x, \tau) \). Secondly, we have noted before that \( \psi_s \) and \( \psi^\dagger_s \) can only appear in the product \( \psi^\dagger_s \psi_s \). Therefore, the spin degrees of freedom do not bring in the dimension 1/2 operators \( \psi_s \) and \( \psi^\dagger_s \) as additional building blocks in Table II. Thirdly, usual local fermion operators have scaling dimension zero. As can be seen from the free fermion action \( S(d, d^\dagger) = \int_0^\beta d\tau d^\dagger (\partial_\tau d^\dagger)\partial_\tau d(\tau) \), 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 combination \( d + d^\dagger \) is raised to 1/2 by the hybridization term in (45) with coefficient \( v_F g_0 \). This follows immediately from the requirement of preserving scale invariance of the hybridization term under a rescaling of \( x \) and \( \tau \). Lastly, because both \( d \) and \( d^\dagger \) are odd under parity and \( \pi \) rotation around \( x \)-axis, only \( \psi_{sf}(0) - \psi^\dagger_{sf}(0) \) could hybridize with them to give rise to a term in the effective Hamiltonian even under all discrete symmetries, as can be seen from Table II. Out of two linear independent combinations from \( d \) and \( d^\dagger \), \( \psi_{sf}(0) - \psi^\dagger_{sf}(0) \) could only hybridize with one. Requiring it to be hermitian, the hybridizing combination could be either \( d + d^\dagger \) or \( d - d^\dagger \). Thus, once \( [\psi_{sf}(0) - \psi^\dagger_{sf}(0)](d + d^\dagger) \) is generated in (45), \( (d - d^\dagger)[\psi_{sf}(0) - \psi^\dagger_{sf}(0)] \) is forbidden. This guarantees that the dimension of \( d - d^\dagger \) will remain to be zero, like usual local operators.

To construct operators in the projected Hilbert space, we only need to multiply together
the building blocks of Table [I] and keep products of even number of fermionic operators. We list all dimension 1/2 operators in Table [II], 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 Hamiltonian 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 transformation but odd under $\pi$ rotation around $x$-axis. From Tables [II] and [IV], we also verify that the only allowed operator up to dimension 1 inclusive is the one appearing in (45). As to 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 $x$-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),

$$H'_{stag} = \alpha'_s h_s \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] + \frac{\alpha''_s h_s}{\sqrt{2}} \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \left( d + d^\dagger \right), \quad (54)$$

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 (54) 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 (132). Why couldn’t we make the same argument to eliminate $[\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d + d^\dagger)$ in (134), since we already have $[\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d - d^\dagger)$ in (133). The reason is the following. For an arbitrary hybridization, we can rewrite it in the following way

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

18
where \( \alpha, \beta \) are two arbitrary real constants, \( \varphi = \tan^{-1}(\beta/\alpha) \), and the \( i \) in front of \( \beta \) in the left side of the last formula is needed to make that term hermitian. 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 second phase to eliminate \( [\psi_{sf}(0) + \psi_{sf}^\dagger(0)](d + d^\dagger) \) from the stageeder field coupling terms in (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 also two dimension 1 operators breaking only particle-hole symmetry. From Table IV, they are

\[
H_{phb}' = V \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] \left[ \psi_f(0) + \psi_f^\dagger(0) \right] + i\alpha_v V \left[ \psi_f(0) + \psi_f^\dagger(0) \right] (d + d^\dagger),
\]

(55)

where \( \alpha_v \) is a dimensionless coefficient depending on the original coupling constants of (14). The first term in (55) 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 of the last paragraph.

Summarizing this section, (44)+(54)+(55) constitutes the most general effective Hamiltonian for the solution region of Figure 1, even allowing particle-hole symmetry breaking. What are omitted up to dimension 3/2 only include:

- A dimension 1 operator \( \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \left[ \psi_f(0) + \psi_f^\dagger(0) \right] \), 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 \( V \). Close to the critical point, we expect this coefficient to be significantly suppressed. This term should be even less important than those in (44).

- 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 close to the critical point.

- 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 $T \to 0$.

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 [18].

**IV. LOW ENERGY THERMODYNAMICS**

In this section, we shall calculate low energy thermodynamic properties of the effective Hamiltonian (44) for the solution region of Figure 1. The marginal operators (54) 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 (54) will be considered in appendix D and shown to be negligible. The way we shall 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

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

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

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

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

(58)
we write the total Lagrangian in (56) as
\[
\mathcal{L} = \mathcal{L}_0 + H_{eff} = \mathcal{L}_1(a_{sf}) + \mathcal{L}_2(b_{sf}) + \mathcal{L}_3(a_f) + \mathcal{L}_4(b_f) + \mathcal{L}_{loc}(a, b),
\]
where
\[
\delta K = K^e - \frac{1}{2}(K_z + K_\perp).
\]
Introducing the Fourier transformation,
\[
a_{sf}(\tau, x) = \frac{1}{\beta} \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} a_{sf}(\omega_n, k) e^{-i\omega_n \tau + ikx},
\]
and similar transformations for the other Grassmann variables, we can write the actions corresponding to the Lagrangians (62) to (66) as
\[
\begin{align*}
\mathcal{S}_1(a_{sf}) &= \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[ -\frac{1}{2} (i\omega_n - v_F k) a_{sf}(-\omega_n, -k) a_{sf}(\omega_n, k) \\
&+ 2i\alpha_s h_a a_{sf}(\omega_n, k) b(-\omega_n) \right], \\
\mathcal{S}_2(b_{sf}) &= \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[ -\frac{1}{2} (i\omega_n - v_F k) b_{sf}(-\omega_n, -k) b_{sf}(\omega_n, k) \\
&- 2i v_F [g_0 a(-\omega_n) - i g_1 k b(-\omega_n)] b_{sf}(\omega_n, k) \right], \\
\mathcal{S}_3(a_f) &= \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[ -\frac{1}{2} (i\omega_n - v_F k) a_f(-\omega_n, -k) a_f(\omega_n, k) + 2i V a_f(-\omega_n, -k) b(\omega_n) \right], \\
\mathcal{S}_4(b_f) &= \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[ -\frac{1}{2} (i\omega_n - v_F k) b_f(-\omega_n, -k) b_f(\omega_n, k) \right].
\end{align*}
\]
\begin{align}
+2i\alpha_u h_u a_{sf}(-\omega_n, -k) b_f(\omega_n, k),
\end{align}

\begin{align}
S_{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\}.
\end{align}

The uniform magnetic field term in (72) is an exactly marginal operator. This is most easily seen by setting \( h_u = 0 \) and combining (69) with (72). 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 \( h_u = 0 \), (69)+(72) is completely decoupled from the rest of the Hamiltonian responsible for the critical behavior. Moreover, the \( h_u \) term of (72) is simply a potential scattering term in terms of the fermions corresponding to \( \psi \) and \( \bar{\psi} \),

\begin{align}
S(a_{sf}) + S(b_f) &= \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{align}

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 Figure 4. From now on, we shall set \( h_u = 0 \) and drop (72) from further discussion.

We can diagonalize (69) to (71) simply by shifting the Grassmann variables corresponding to the extended degrees of freedom,

\begin{align}
\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),
\end{align}

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

\begin{align}
\tilde{a}_f(\omega_n, k) &= a_f(\omega_n, k) - \frac{2i\tilde{V}}{i\omega_n - v_F k} b(\omega_n).
\end{align}

Upon inserting the results for the following integrals,

\begin{align}
\int_{-\infty}^{\infty} \frac{dk}{2\pi \sqrt{i\omega_n - v_F k}} = -\frac{i\text{sgn}\omega_n}{2v_F},
\end{align}

\begin{align}
\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi \sqrt{i\omega_n - v_F k}} = -\frac{1}{v_F^2} \left( \frac{v_F \Lambda}{\pi} - \frac{1}{2} \left| \omega_n \right| \right),
\end{align}

\begin{align}
\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi \sqrt{i\omega_n - v_F k}} k^2 = \frac{i\omega_n}{v_F^3} \left( \frac{v_F \Lambda}{\pi} - \frac{1}{2} \left| \omega_n \right| \right),
\end{align}

\begin{align}
\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi \sqrt{i\omega_n - v_F k}} k^3 = \frac{i\omega_n}{v_F^4} \left( \frac{v_F \Lambda}{\pi} - \frac{1}{2} \left| \omega_n \right| \right),
\end{align}

\begin{align}
\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi \sqrt{i\omega_n - v_F k}} k^4 = \frac{i\omega_n}{v_F^5} \left( \frac{v_F \Lambda}{\pi} - \frac{1}{2} \left| \omega_n \right| \right).
\end{align}
where $\Lambda$ is the ultraviolet cutoff, the actions (80) to (74) become

\[ S_1(a_{sf}) = - \sum_n \int_{-\infty}^{\infty} \frac{dk}{\pi} (i\omega_n - v_F k) \tilde{a}_{sf}(-\omega_n, -k) \tilde{a}_{sf}(\omega_n, k) \]
\[ - \frac{i(\alpha s h_s)^2}{v_F} \sum_n \text{sgn} \omega_n b(-\omega_n) b(\omega_n), \] (81)

\[ S_2(b_{sf}) = - \sum_n \int_{-\infty}^{\infty} \frac{dk}{\pi} (i\omega_n - v_F k) \tilde{b}_{sf}(-\omega_n, -k) \tilde{b}_{sf}(\omega_n, k) - iv_F g_0^2 \sum_n \text{sgn} \omega_n a(-\omega_n) a(\omega_n) \]
\[ + 2ig_0 \sum_n |\omega_n| a(-\omega_n) b(\omega_n) + \frac{i g_0^2}{v_F} \sum_n \omega_n \left( |\omega_n| - \frac{2v_F \Lambda}{\pi} \right) b(-\omega_n) b(\omega_n) \]
\[ - \frac{4iv_F g_0^2 \Lambda}{\pi} \sum_n a(-\omega_n) b(\omega_n), \] (82)

\[ S_3(a_f) = - \sum_n \int_{-\infty}^{\infty} \frac{dk}{\pi} (i\omega_n - v_F k) \tilde{a}_{f}(-\omega_n, -k) \tilde{a}_{f}(\omega_n, k) - \frac{i V}{v_F} \sum_n \text{sgn} \omega_n b(-\omega_n) b(\omega_n). \] (83)

The last term in (82) is a correction to the relevant operator $\delta K$ term of (73) and can be absorbed into the critical value of the RKKY interaction $K_c$. Collecting the local terms containing Grassmann variables $a$, $b$ from (81) to (83) and combining them with (73), we obtain the effective local action,

\[ S_{\text{loc}}^{\text{eff}} = -i \sum_{n>0} \left( a(-\omega_n), b(-\omega_n) \right) \times \left( \begin{array}{c} |\omega_n| + 2v_F g_0^2 \\ \delta K + 2g_0 g_1 |\omega_n| \\ \delta K + 2g_0 g_1 |\omega_n| \\ |\omega_n|/Z_b + 2 \left( \alpha_s^2 h_s^2 + \tilde{V}^2 - g_1^2 \omega_n^2 \right) /v_F \end{array} \right) \left( \begin{array}{c} a(\omega_n) \\ - (\delta K + 2g_0 g_1 |\omega_n|) \\ - (\delta K + 2g_0 g_1 |\omega_n|) \\ |\omega_n|/Z_b + 2 \left( \alpha_s^2 h_s^2 + \tilde{V}^2 - g_1^2 \omega_n^2 \right) /v_F \end{array} \right). \] (84)

The factor $Z_b$ is defined by

\[ Z_b = \frac{1}{1 + 4g_1^2 \Lambda / \pi}, \] (85)

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 (84) can be safely neglected since it is highly irrelevant and satisfies $g_1 \omega_n^2 / v_F \ll |\omega_n|$ for the whole energy range of practical interest. All interesting thermodynamics is contained in (84). From (84) we obtain the free energy shift due to the local interactions,

\[ F(T, h_s) = -T \ln 2 - T \sum_{n>0} \ln \left\{ (\delta K + 2g_0 g_1 |\omega_n|)^2 \right\} \]
\[ + \left( |\omega_n| + 2v_F g_0^2 \right) \left[ |\omega_n| + \frac{2}{v_F} \left( \alpha_s^2 h_s^2 + \tilde{V}^2 \right) \right], \] (86)
where \(-T \ln 2\) is the entropy of two degenerate impurity spin states. Defining several convenience notations,

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

(87)

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

(88)

\[
\tilde{\alpha}_s = 2g_0 \alpha_s \sqrt{Z_b},
\]

(89)

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

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

(90)

The roles of the parameters in (90) can be read off. \(T_K\) is the fundamental energy scale of the problem and should be identified as the Kondo temperature. We note \(T_K \approx 2v_F g_0^2\), as can be seen from (87). \(T_c\) vanishes approaching the critical point, and satisfies \(T_c \ll T_K\) inside the solution region of Figure 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. 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 (90) can be dropped since it only shifts \(T_K^2\) to \(T_K^2 + \tilde{\alpha}_s^2 h_s^2\). After some rearrangement, we finally obtain

\[
F(T, h_s) = -T \ln 2 - \int_{0}^{\infty} \frac{d\omega}{2\pi} \tanh \left( \frac{\beta \omega}{2} \right) \tan^{-1} \left( \frac{\omega T_K}{\omega^2 - T_c T_K - \tilde{\alpha}_s^2 h_s^2} \right).
\]

(91)

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 (91) and performing some minor manipulation, we obtain
\[ F(T) - F(0) = -T \ln 2 + T \int_0^\infty \frac{dx}{\pi} \frac{1}{e^x + 1} \tan^{-1} \left( \frac{x \beta T_K}{x^2 - \beta^2 T_c T_K} \right). \quad (92) \]

Two limiting behaviors follow immediately. At \( T_c \ll T \ll T_K \),

\[ F(T) - F(0) = -T \ln 2 + T \int_0^\infty \frac{dx}{\pi} \frac{1}{e^x + 1} \left( \frac{\pi}{2} - \frac{x}{\beta T_K} \right) = -\frac{T}{2} \ln 2 - \frac{\pi}{12} T^2. \quad (93) \]

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

\[ F(T) - F(0) = -T \ln 2 + T \int_0^\infty \frac{dx}{\pi} \frac{1}{e^x + 1} \left( \frac{\pi}{2} - \frac{x}{\beta T_c} \right) = -\frac{\pi}{12} \frac{1}{T_c} T^2. \quad (94) \]

The limiting behaviors of the specific heat are obvious from (93) and (94),

\[ \frac{C(T, T_c)}{T} = \begin{cases} \frac{\pi}{6T_K}, & T \gg T_c, \\ \frac{\pi}{6T_c}, & T_c \gg T. \end{cases} \quad (95) \]

The general crossover function for the specific heat is obtained from (92),

\[ \frac{C(T)}{T} = 2T_k^2 \beta^4 \int_0^\infty \frac{dx}{\pi} \frac{x}{e^x + 1} \frac{x^4 T_K - T_c(x^2 - \beta^2 T_c T_K)(3x^2 + \beta^2 T_c T_K)}{[(x^2 - \beta^2 T_c T_K)^2 + (x^2 T_K)^2]^2}. \quad (96) \]

This crossover function is plotted in Figure 4. We also plot the crossover function for the entropy (92) in Figure 5, which may be more instructive.

**B. Staggered Susceptibility**

From (91), the staggered susceptibility is given by

\[ \chi_s(T, T_c) = -\left[ \frac{\partial^2}{\partial h_s^2} F(T, h_s) \right]_{h_s=0} = \tilde{\alpha}^2 \int_0^\infty \frac{d\omega}{\pi} \frac{\omega T_K}{\left( T_c T_K - \omega^2 \right)^2 + (\omega T_K)^2}. \quad (97) \]

The limiting behaviors are found to be

\[ \chi_s(T, T_c) = \begin{cases} -\frac{\tilde{\alpha}^2}{\pi T_K} \ln T, & T \gg T_c, \\ -\frac{\tilde{\alpha}^2}{\pi T_K} \ln T_c, & T \ll T_c. \end{cases} \quad (98) \]

The crossover behavior for the function (97) is plotted in Figure 6.
C. Impurity Spin Correlation $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle$

Projecting the operator $(\vec{S}_+)^2$ onto the doublet, we find
\[
\hat{Q}\vec{S}_+^2\hat{Q} = \hat{Q}(S_+^x)^2\hat{Q} + \hat{Q}(S_+^y)^2\hat{Q} + \hat{Q}(S_+^z)^2\hat{Q} = 2dd^\dagger.
\] (99)

Thus, the calculation of the impurity spin correlation is reduced to evaluating $\langle dd^\dagger \rangle$. From (84), we have
\[
\langle dd^\dagger \rangle - \frac{1}{2} = i\langle ba \rangle = T \sum_n \frac{\delta K + 2g_0g_1|\omega_n|}{(\delta K + 2g_0g_1|\omega_n|)^2 + (|\omega_n| + T_K)(|\omega_n|/Z_b + 2\bar{V}^2/v_F)}.
\] (100)

The impurity spin correlation is
\[
\langle \vec{S}_1 \cdot \vec{S}_2 \rangle = -\frac{1}{4} + \frac{Z_b}{\beta} \sum_n \frac{\delta K + 2g_0g_1|\omega_n|}{\omega_n^2 + T_cT_K + |\omega_n|T_K}.
\] (101)

At the critical point, $\delta K = T_c = 0$, and as $T \to 0$,
\[
\langle \vec{S}_1 \cdot \vec{S}_2 \rangle \simeq -\frac{1}{4} + Z_b \int_0^{\bar{v}_F\Lambda} \frac{d\omega}{\pi} \frac{2g_0g_1}{\omega + T_K} \simeq -\frac{1}{4} + \frac{2g_0g_1Z_b}{\pi} \ln \frac{\bar{v}_F\Lambda}{T_K}.
\] (102)

The leading irrelevant operator induces a small non-universal correction to the impurity spin correlation. Although the fixed point itself (the ground state) has an extra symmetry between the two states of the doublet, $d \leftrightarrow d^\dagger$, which implies $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle = -1/4$, 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 (101), we find
\[
\frac{\partial}{\partial (\delta K)} \langle \vec{S}_1 \cdot \vec{S}_2 \rangle = \frac{Z_b}{\beta} \sum_n \frac{1}{\omega_n^2 + |\omega_n|T_K + T_cT_K} = Z_b \int_0^{\infty} \frac{d\omega}{\pi} \tanh \left( \frac{\beta \omega}{2} \right) \frac{\omega T_K}{(T_cT_K - \omega^2)^2 + (\omega T_K)^2}.
\] (103)

Comparing the last expression with (97), we find
\[
\frac{\partial}{\partial (\delta K)} \langle \vec{S}_1 \cdot \vec{S}_2 \rangle = \text{const.} \times \chi_s(T, T_c).
\] (104)

In particular, they should have the same limiting behaviors as given by (88). Since
\[
\frac{\partial}{\partial (\delta K)} \langle \vec{S}_1 \cdot \vec{S}_2 \rangle \sim \int_0^\beta d\tau \langle T(\vec{S}_1 \cdot \vec{S}_2)(\tau) (\vec{S}_1 \cdot \vec{S}_2)(0) \rangle,
\] (105)
the result (104) should not be too surprising.
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). Or eventually, the possible uncertainty boils down to the two basic energy scales $T_K$ and $T_c$, which we cannot determine exactly in terms of the initial parameters of the original Hamiltonian (1).

In order to make a comparison, we first need to answer the questions that 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 [18]. 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 [18]. 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 than the doublet of Figure 2. The strongest evidence for the universality of the critical point is the exactly same operator content around the critical point we find in our approach and in the conformal field theory approach. That is 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 (43) 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 descendent 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 for the specific heat (see (95) and reference [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 [18]. Although this does not prove the irrelevance of the spin anisotropy introduced in our approach because the introduced anisotropy is not small, it does 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 [23] and overscreened cases [25,26]. Leaving aside specifics of the two-impurity Kondo model, these early experiences in related Kondo problems give us considerable confidence that the critical point of the two-impurity model that has been studied from different approaches belongs to the same universality class.

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 inside the solution region of Figure 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 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 non-conserved 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 the 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 specific heat, $\ln T$ singularity in the staggered susceptibility, constant uniform susceptibility, and $\ln T$ singularity in the correlation function of the composite operator $\vec{S}_1 \cdot \vec{S}_2$, as can be
seen from (103) and (105). 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 [11] 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 Figure 2. So is its consequence about the value of the impurity spin correlation at the critical point, $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle = -1/4$. However, this hidden symmetry is broken by the leading irrelevant operator, as we have noted before. This is similar to the well known dynamical symmetry breaking effect. 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 (95). Our result (104), 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 $\chi_s(T = 0, T_c) \sim \ln T_c$, as can be seen from (98). Noting that the other limiting behavior of (98), $\chi_s(T, T_c) \sim \ln T$ 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 $x$-axis. Since we only have one such relevant operator, as can be seen from Table [11], 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 Figure 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 and its underlying physics. As we have explained in section III, the condition for the criticality is the degeneracy between the two lowest impurity spin states, \( |\uparrow\downarrow> - |\downarrow\uparrow> \)/\(\sqrt{2}\) and \( |\uparrow\uparrow> + |\downarrow\downarrow> \)/\(\sqrt{2}\). By varying RKKY interaction across the critical point, these two levels cross each other. The non-Fermi-liquid behavior at the critical point 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. Because of the special symmetry of the doublet, i.e. one level is an even triplet and the other is an odd singlet, the local degrees of freedom of the doublet can only be compensated by the extended spin-flavor degrees of freedom of 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 species of Majorana fermions, \(\psi_{sf} - \psi_{sf}^{\dagger}\), 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. 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 numerical 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 section [V] 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 \( \vec{q} \) dependence of the spin susceptibility \( \chi''(\omega, \vec{q}) \). As a result of the competition, we should expect drastically different enhancement at different momentum transfer \( \vec{q} \). From this perspective, the picture of a periodic array of coherent Kondo scattering centers for the heavy fermion compounds is surely oversimplified. Non-perturbatively 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 \( \hat{U} \hat{H} \hat{U}^{-1} \), only two terms in \( H_0 \) are affected. They are \( h_u / (2\pi) \int_{-\infty}^{\infty} dx \partial_x \Phi_s(x) \) and

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

(A1)

As for \( H_1 \), the transformation affects the term containing \( \partial_x \Phi_s(0) S_z^s \) apart from eliminating \( \cos \Phi_s(0) \) and \( \sin \Phi_s(0) \). Using the mode expansions,
\[ \phi_s(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi \sqrt{2|p|}} \left[ \phi_s(p)e^{ipx} + \phi_s^\dagger(p)e^{-ipx} \right] e^{-\alpha|p|/2}, \quad (A2) \]

\[ \Pi_s(x) = \int_{-\infty}^{\infty} \frac{dp \sqrt{|p|}}{4\pi \sqrt{2|p|}} \left[ -i\phi_s(p)e^{ipx} + i\phi_s^\dagger(p)e^{-ipx} \right] e^{-\alpha|p|/2}, \quad (A3) \]

we can write

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

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

The commutation relation for the Fourier components is

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

Next, let’s introduce a generalized transformation operator

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

and define two \( \lambda \)-dependent functions,

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

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

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

\[ \frac{d^2}{d\lambda^2} f_1(\lambda) = \frac{2v_F}{\alpha} (S_z^+)^2, \quad (A10) \]

\[ \frac{d}{d\lambda} f_1(\lambda)|_{\lambda=0} = -v_F \partial_x \Phi_s(0)S_z^+, \quad (A11) \]

\[ \frac{d}{d\lambda} f_2(\lambda) = -2 \int_0^\infty dp e^{-\alpha p} \cos(px)S_z^+. \quad (A12) \]

From (A10) and (A11), we obtain

\[ \hat{U}H_0^{(s)}\hat{U}^{-1} = H_0^{(s)} - v_F \partial_x \Phi_s(0)S_z^+ + \frac{v_F}{\alpha} (S_z^+)^2. \quad (A13) \]

From (A12), we obtain

\[ \hat{U}\partial_x \Phi_s(x)\hat{U}^{-1} = \partial_x \Phi_s(x) - 2 \int_0^\infty dp e^{-\alpha p} \cos(px)S_z^+. \quad (A14) \]
This implies
\[ \hat{U} \partial_x \Phi_s(0) \hat{U}^{-1} = \partial_x \Phi_s(0) - \frac{2}{\alpha} S_z^+, \quad (A15) \]
\[ \hat{U} \int_{-\infty}^{\infty} dx \partial_x \Phi_s(x) \hat{U}^{-1} = \int_{-\infty}^{\infty} dx \partial_x \Phi_s(x) - 2\pi S_z^+. \quad (A16) \]

Substituting (A13), (A15) and (A16) into $\hat{U} \hat{H} \hat{U}^{-1}$, 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
\[ \hat{Q} \hat{H} \hat{Q} = -iv_F \int_{-\infty}^{\infty} dx \sum_{\lambda=s,f,sf} \psi_{\lambda}^\dagger(x) \partial_x \psi_{\lambda}(x) + i \frac{v_F J^I_m}{\sqrt{2}\pi\alpha} \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] \hat{Q} S_y^+ \hat{Q} \]
\[ + h_u \int_{-\infty}^{\infty} dx \psi_s^\dagger(x) \psi_s(x) + H_2. \quad (B1) \]

In terms of the local fermion operators $d$ and $d^\dagger$, we have $\hat{Q} S_y^+ \hat{Q} = i(d - d^\dagger)$. 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,
\[ - \frac{v_F J^I_m}{\sqrt{2}\pi\alpha} \left[ \tilde{\psi}_{sf}(0) - \tilde{\psi}_{sf}^\dagger(0) \right] (d + d^\dagger). \quad (B2) \]

In the second order of the projection (42), the local impurity spin state is virtually excited from one of the doublet to either $(|\uparrow\uparrow> - |\downarrow\downarrow>) / \sqrt{2}$ or $(|\uparrow\downarrow> + |\downarrow\uparrow>) / \sqrt{2}$, then returns back to the doublet. From Figure 3, the mixing terms between the doublet and the excited states are those in (36) + (37) which contain $S_x^+$ and $S_z^\pm$. If the local 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
\[-K_z = K_\perp + \cdots, \tag{B3}\]

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,

\[- \left( \frac{K_z + K_\perp}{2} - K_c \right) d^d d, \quad \text{with} \quad K_c = \frac{v_F}{\pi \alpha} \left( J_+^z - \pi \right) + \cdots. \tag{B4}\]

The other contributions come from the situations when the local impurity spins start from one state but return to the other state of the doublet. From Figure 3, we see that these contributions must come from the projection of the product of \( S_+^x \) and \( S_-^z \),

\[
\hat{Q} \left\{ \frac{v_F J_m^z}{2} \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] S_-^z \right\}
\]

\[
\times \left\{ \frac{v_F J_m^x}{2} \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \hat{Q} \right. + \hat{Q} \left\{ \frac{v_F J_m^x}{2} \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] S_+^z \right\}
\]

\[
\times \left[ \frac{v_F J_m^z}{2} \left[ \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] S_-^z \right\} \hat{Q}. \tag{B5}\]

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

\[
\left\{ -(K_\perp + T_K) + i v_F \int_{-\infty}^{\infty} dx \psi_{sf}^{\dagger}(x) \partial_x \psi_{sf}(x) - V \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] \left[ \psi_f(0) + \psi_f^\dagger(0) \right] \right\}^{-1}
\]

\[
\simeq -\frac{1}{K_\perp + T_K} - \frac{i v_F}{(K_\perp + T_K)^2} \int_{-\infty}^{\infty} dx \psi_{sf}^{\dagger}(x) \partial_x \psi_{sf}(x)
\]

\[
+ \frac{V}{(K_\perp + T_K)^2} \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] \left[ \psi_f(0) + \psi_f^\dagger(0) \right]. \tag{B6}\]

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

The first contribution is

\[
- \frac{v_F^2 J_m^x J_m^z}{2(K_\perp + T_K) \sqrt{2} \pi \alpha} \left\{ \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \hat{Q} S_+^x S_-^z \hat{Q}
\]

\[
+ \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \left[ \psi_{sf}^\dagger(0) + \psi_{sf}(0) \right] \hat{Q} S_+^z S_-^x \hat{Q} \right\}. \tag{B7}\]

34
Using the fact \( \hat{Q} S_x^z S^+_x \hat{Q} = d \) and \( \hat{Q} S^+_x S^z \hat{Q} = d \), and carrying out the transformation (B3), we simplify (B7) to

\[
- v_2^2 F J^\perp + J^z m^2 (K^\perp + T_K)^2 (2\pi\alpha)^{3/2} \left[ \bar{\psi}_{sf}(0) - \bar{\psi}_{sf}^\dagger(0) \right] (d + d^\dagger).
\]  
(B8)

In deriving (B8), we have used the relation

\[
\{ \psi_{sf}(0), \psi_{sf}^\dagger(0) \} = \delta(0) = \frac{1}{2\pi\alpha}.
\]  
(B9)

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

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

\[
- i v_3^2 F J^\perp + J^z m^2 (K^\perp + T_K)^2 (2\pi\alpha)^{3/2} \left[ \bar{\psi}_{sf}(0) + \bar{\psi}_{sf}^\dagger(0) \right] \int_{-\infty}^{\infty} dx \bar{\psi}_{sf}(x) \partial_x \psi_{sf}(x) \times \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \hat{Q} S_x^z S^+_x \hat{Q} + \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \hat{Q} S_x^z S^+_x \hat{Q}.
\]  
(B10)

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

\[
\frac{v_3^3 J^\perp + J^z m^2}{8(K^\perp + T_K)^2 (2\pi\alpha)^{3/2}} i \partial_x \left[ \bar{\psi}_{sf}(0) - \bar{\psi}_{sf}^\dagger(0) \right] (d - d^\dagger).
\]  
(B11)

This is the leading irrelevant operator and has dimension 3/2. Noting 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

\[
V v_4^2 J^\perp + J^z m^2 \left[ \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \left[ \psi_{sf}(0) - \psi_{sf}^\dagger(0) \right] \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \hat{Q} S_x^z S^+_x \hat{Q} + \left[ \psi_{sf}^\dagger(0) \psi_{sf}(0) - \psi_{sf}(0) \psi_{sf}^\dagger(0) \right] \hat{Q} S_x^z S^+_x \hat{Q} \right] \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \hat{Q} S_x^z S^+_x \hat{Q} \right] \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] \hat{Q} S_x^z S^+_x \hat{Q} \right].
\]  
(B12)

This contribution can be reduced to

\[
V v_4^2 J^\perp + J^z m^2 \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] (d - d^\dagger).
\]  
(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

$$\hat{Q} \{ h_s S^z_x \} \frac{1 - \hat{Q}}{-(K_\perp + T_K)} \left\{ \frac{v_F J_\perp^+}{\sqrt{2\pi\alpha}} \left[ \psi_{sf}(0) + \psi_{sf}^\dagger(0) \right] S^x_+ \right\} \hat{Q}$$

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

(B14)

This term is simplified to

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

(B15)

To obtain the uniform magnetic field coupling term, we restore the boson field $\phi_s(x)$ through $\psi_{sf}(x) = \partial_x \Phi_s(x)/(2\pi)$ 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 $\partial_x \Phi_s(x) = \sqrt{\pi} [ \partial_x \phi_s(x) - \Pi_s(x) ]$,

$$\frac{v_F}{2} \int_{-\infty}^{\infty} dx \left\{ \Pi^2_s(x) + [\partial_x \phi_s(x)]^2 + \frac{h_u}{\pi v_F} \partial_x \Phi_s(x) + \frac{J^z_\perp}{\pi} \delta(x) \partial_x \Phi_s(x) S^z_+ \right\}$$

$$= \frac{v_F}{2} \int_{-\infty}^{\infty} dx \left\{ \left[ \Pi_s(x) - \frac{h_u}{2\sqrt{\pi} v_F} \right]^2 + \left[ \partial_x \phi_s(x) + \frac{h_u}{2\sqrt{\pi} v_F} \right]^2 + \frac{J^z_\perp}{\pi} \delta(x) \partial_x \Phi_s(x) S^z_+ \right\},$$

up to an additive constant. By introducing

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

we can recast (B16) in the form

$$\frac{v_F}{2} \int_{-\infty}^{\infty} dx \left\{ \tilde{\Pi}^2_s(x) + [\partial_x \tilde{\phi}_s(x)]^2 + \frac{J^z_\perp}{\pi} \delta(x) \partial_x \tilde{\Phi}_s(x) S^z_+ - \frac{h_u J^z_\perp}{\pi v_F} S^z_+ \delta(x) \right\},$$

(B18)

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

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

(B19)

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

$$\tilde{Q} \left\{ \frac{v_FJ_z}{2} \left[ \psi_s(0) + \psi_s^\dagger(0) \right] \left[ \psi_f(0) - \psi_f^\dagger(0) \right] S_z^+ + v_F\tilde{J}_z \psi_s^\dagger(0)\psi_s(0)S_z^+ \right\}$$

$$\times \frac{1 - \hat{Q}}{-T_K} \left\{ -\frac{h_u\tilde{J}_z}{2\pi} S_z^+ \right\} \hat{Q} + \hat{Q} \left\{ -\frac{h_u\tilde{J}_z}{2\pi} S_z^+ \right\} \frac{1 - \hat{Q}}{-T_K}$$

$$\times \left\{ \frac{v_FJ_z}{2} \left[ \psi_s(0) + \psi_s^\dagger(0) \right] \left[ \psi_f(0) - \psi_f^\dagger(0) \right] S_z^+ + v_F\tilde{J}_z \psi_s^\dagger(0)\psi_s(0)S_z^+ \right\} \hat{Q}. \quad (B21)$$

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

$$\frac{h_u v_F \tilde{J}_z J_z}{8\pi T_K} \left[ \psi_s(0) + \psi_s^\dagger(0) \right] \left[ \psi_f(0) - \psi_f^\dagger(0) \right] + \frac{h_u v_F (\tilde{J}_z)^2}{4\pi T_K} \psi_s^\dagger(0)\psi_s(0). \quad (B22)$$

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). The qualitative physics does not depend on the numerical values of the coefficients $g_0, g_1, \tilde{V}, \alpha_u$ and $\alpha_s$ in the effective Hamiltonian. It should be kept in mind that the obtained expressions, (48) to (52), for the numerical coefficients of the effective Hamiltonian should not be taken too literally.

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 (55)**

In this appendix, we shall show that the only effect of including the marginal particle-hole symmetry breaking operators (55) is to slightly renormalize the two basics energy scales $T_K$ and $T_c$.

The marginal operators (55) correspond to the following terms in the action,

$$S'_{phh} = 2iV \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} a_f(\omega_n, k) \left[ \alpha_n a(-\omega_n) - \int_{-\infty}^{\infty} \frac{dk'}{2\pi} b_{sf}(-\omega_n, k') \right]. \quad (C1)$$

Our task now is to diagonalize
In terms of the shifted Grassmann variables, the action (C2) becomes

\[ S(b_{sf}, a_f) = S_2(b_{sf}) + S_3(a_f) + S'_{phb}, \]  

where \( S_2(b_{sf}) \) and \( S_3(a_f) \) are given by (70) and (71) respectively. More specifically, we need to find new linear transformations other than (76) and (77) such that the hybridizing terms in (C2) are canceled out. The desired transformations are

\[ \tilde{b}_{sf}(\omega_n, k) = b_{sf}(\omega_n, k) + \xi_1(\omega_n, k) a(\omega_n) + \xi_2(\omega_n, k) b(\omega_n), \]  

\[ \tilde{a}_f(\omega_n, k) = a_f(\omega_n, k) + \xi_3(\omega_n, k) a(\omega_n) + \xi_4(\omega_n, k) b(\omega_n), \]  

where the four transformation coefficients are given by

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

\[ \xi_2(\omega_n, k) = \frac{2v_F}{i\omega_n - v_F k} \left[ g_1 k - \frac{iV \sgn \omega_n}{v_F^2 + V^2} \left( \tilde{V} - \frac{2V g_1 \Lambda}{\pi} + \frac{V g_1}{v_F} |\omega_n| \right) \right], \]  

\[ \xi_3(\omega_n, k) = -\frac{2i V}{i\omega_n - v_F k} \frac{\alpha_v - g_0 \sgn \omega_n}{1 + V^2/v_F^2}, \]  

\[ \xi_4(\omega_n, k) = -\frac{2i V}{i\omega_n - v_F k} \frac{\tilde{V} - 2V g_1 \Lambda/\pi + V g_1 |\omega_n|/v_F}{1 + V^2/v_F^2}. \]

The ultraviolet cutoff \( \Lambda \) enters the transformation coefficients through the integrals (79) and (80). In terms of the shifted Grassmann variables, the action (C2) becomes

\[ S(b_{sf}, a_f) = -\sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left\{ \frac{1}{2} (i\omega_n - v_F k) \left[ \tilde{a}_f(-\omega_n, -k) \tilde{a}_f(\omega_n, k) + \tilde{b}_{sf}(-\omega_n, -k) \tilde{b}_{sf}(\omega_n, k) \right] \right\} + 2iV \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \tilde{a}_f(\omega_n, k) \tilde{b}_{sf}(-\omega_n, k') + S_{gen}(a, b). \]  

The generated local terms are

\[ S_{gen}(a, b) = -i \sum_n \left\{ \frac{\sgn \omega_n}{2} \left[ M_{aa}(\omega_n) a(-\omega_n) a(\omega_n) + M_{bb}(\omega_n) b(-\omega_n) b(\omega_n) \right] \right\} + M_{ab}(\omega_n) a(-\omega_n) b(\omega_n), \]  

with

\[ M_{aa}(\omega_n) = \frac{2v_F}{1 + V^2/v_F^2} \left[ g_0^2 + \left( \frac{\alpha_v V}{v_F} \right)^2 \right], \]

\[ M_{bb}(\omega_n) = \frac{2}{1 + V^2/v_F^2} \left[ \frac{1}{v_F} \left( \tilde{V} - \frac{2V g_1 \Lambda}{\pi} \right)^2 \right]. \]
\[ + |\omega_n| \left\{ \frac{2g_1^2 \Lambda}{\pi} \left( 1 - \frac{V^2}{v_F^2} \right) + \frac{2g_1 V \tilde{V}}{v_F^2} \right\} , \quad (C12) \]

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

To obtain the total effective local action, we add the generated terms (C10) to (73). Introducing a new local Grassmann variable,

\[ \tilde{b}(\omega_n) = b(\omega_n) + \frac{\alpha_v V}{V - 2V g_1 \Lambda/\pi} a(\omega_n) , \quad (C14) \]

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

\[
S_{\text{eff}}^{\text{loc}} = -i \sum_{n>0} \left( a(\omega_n), \tilde{b}(\omega_n) \right) \\
\times \left( \begin{array}{cc} \omega_n/Z_a + 2v_F \tilde{g}_0^2 & (\tilde{\delta}K + 2\tilde{g}_0 \tilde{g}_1 \omega_n) - \eta \omega_n \\
\tilde{\delta}K + 2\tilde{g}_0 \tilde{g}_1 \omega_n - \eta \omega_n & \omega_n/Z_b + 2\tilde{V}^2/v_F \end{array} \right) \left( \begin{array}{c} a(\omega_n) \\
\tilde{b}(\omega_n) \end{array} \right) . \quad (C15) \]

The renormalized parameters are,

\[
\tilde{g}_0 = \frac{g_0}{\sqrt{1 + V^2/v_F^2}} , \quad (C16) \\
\tilde{g}_1 = \frac{g_1}{\sqrt{1 + V^2/v_F^2}} , \quad (C17) \\
\tilde{V}^2 = \frac{\tilde{V} - 2V g_1 \Lambda/\pi}{\sqrt{1 + V^2/v_F^2}} , \quad (C18) \\
\tilde{\delta}K = \delta K - \frac{2v_F g_0}{1 + V^2/v_F^2} \left( \frac{V \tilde{V}}{v_F^2} + \frac{2g_1 \Lambda}{\pi} \right) , \quad (C19) \\
\frac{1}{Z_a} = 1 + \left( \frac{\alpha_v V}{V - 2V g_1 \Lambda/\pi} \right)^2 \left( 1 + \frac{4g_1^2 \Lambda}{\pi} \right) , \quad (C20) \\
\frac{1}{Z_b} = 1 + \frac{2}{1 + V^2/v_F^2} \left[ \frac{2g_1^2 \Lambda}{\pi} \left( 1 - \frac{V^2}{v_F^2} \right) + \frac{2g_1 V \tilde{V}}{v_F^2} \right] , \quad (C21) \\
\eta = \frac{\alpha_v V}{V - 2V g_1 \Lambda/\pi} \left( 1 + \frac{2(2g_1^2 \Lambda/\pi + g_1 V \tilde{V}/v_F^2)}{1 + V^2/v_F^2} \right) . \quad (C22) \]

The effective action (C13) has essentially the same form as (84) 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 \(\alpha_v V\) 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 (54) TO THE STAGGERED SUSCEPTIBILITY**

In this appendix, we show that the contributions to the staggered susceptibility from the marginal operators (54) are negligible.

The marginal operators (54) have the following corresponding terms in the action

\[
S_{stag}' = 2i h_s \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi} a_{sf}(-\omega_n, k) \left[ \alpha'_s \int_{-\infty}^{\infty} \frac{dk'}{2\pi} b_{sf}(\omega_n, k') + \alpha''_s a(\omega_n) \right].
\] (D1)

Combining the last expression with the staggered field coupling term in (69) and inserting the transformation (76), we can write the complete staggered field coupling terms in the following form

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

The staggered susceptibility is obtained by calculating the second order perturbation of \(S_{stag}\),

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

where the average is weighted by an action consisting of the free and decoupled Grassmann variables \(a_{sf}, \tilde{b}_{sf}\) and the effective local action (84). The first term in \(S_{stag}\) is a potential scattering term and does not mix with the other terms of \(S_{stag}\) 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
\[ \chi_s = \frac{2}{v_F} \left( \alpha_s + \frac{2\alpha'_s g_1 \Lambda}{\pi} \right)^2 \frac{1}{\beta} \sum_n i \text{sgn} \omega_n \langle b(-\omega_n)b(\omega_n) \rangle. \]  

(D4)

The propagator is given by, from (84),

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

(D5)

where we have taken \( 2v_F g_0^2 \sim T_K \) 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 the logarithmic singularity for the Matsubara frequency summation in (D4). From (D4), we see that the only effect of the marginal operators (54) is to shift \( \alpha_s \) to \( \alpha_s + 2\alpha'_s g_1 \Lambda/\pi \). Actually, one should be able to see this from (D3) without doing calculation.
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### TABLE I. Definition of frequently used parameters and symbols

| Symbol | Definition (Eq. No.) | Symbol | Definition (Eq. No.) |
|--------|---------------------|--------|---------------------|
| $v_F$  | Fermi velocity      | $g_1$  | (46), (48)          |
| $\rho_F$ | 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) |
| $S_{x,y,z}^\pm$ |                      | $\delta K$ | (67)               |
| $h_u, h_s$ |                      | $\Lambda$ | (79)               |
| $J_{\pm,\perp}^z, J_{m,\perp}^z$ |      | $Z_b$ | (85)               |
| $V$ |                      | $T_K$ | (87)               |
| $\tilde{J}_z, \tilde{K}_z$ |      | $T_c$ | (88)               |
| $g_0$ |                      | $\tilde{\alpha}_s$ | (89) |
TABLE II. The building blocks for constructing operators 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 | $+$ | $+$ | $+$ |
TABLE III. All dimension 1/2 operators. The first one is the relevant operator. The second one could couple to the staggered 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.

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

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 Fermi-liquid type everywhere. The shaded area is the region where our solution applies. The radius of the solution region is a fraction of $T_K$.

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 $S^z_1$ and $S^z_2$. 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 $J_m^z$.

FIG. 3. The four impurity-spin states and the impurity spin operators connecting them, $S^\lambda_\pm = S^\lambda_1 \pm S^\lambda_2$ for $\lambda = x, y, z$.

FIG. 4. The crossover function for the specific heat, Eq. (96), 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. (92), for various values of $T_c/T_K$.

FIG. 6. The crossover function for the staggered susceptibility, Eq. (97), for various values of $T_c/T_K$, normalized to its value at $T_K/2$. 
\[ \frac{|\tilde{K}_z|}{2} \]

\[ E = 0 \]

\[ |\uparrow\downarrow\rangle \]

\[ |\uparrow\downarrow\rangle \]

\[ |\uparrow\rangle + |\downarrow\rangle \]

\[ K_{\perp} \]

\[ |\uparrow\rangle - |\downarrow\rangle \]

\[ T_K \]

\[ |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \]

\[ |\uparrow\rangle + |\downarrow\rangle \]

\[ |\uparrow\rangle - |\downarrow\rangle \]
$|\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\uparrow\rangle$

$|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle$

$S_x^+ \quad S^+_z$

$S^+_y \quad S^+_z$

$S^+_x \quad S^+_z$

$|\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\downarrow\rangle$

$d^+ d = 1$

$d^+ d = 0$
$T_c/T_K = 0.0225, 0.04, 0.09, 0.16$
\[ T_c/T_K = 0.01, 0.04, 0.09, 0.16 \]
