Two-Channel Kondo Physics from Tunnelling Impurities with Triangular Symmetry.

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Tunnelling impurities in metals have been known for some time to have the potential for exhibiting Kondo-like physics. However previous models based on an impurity hopping between two equivalent positions have run into trouble due to the existence of relevant operators that drive the system away from the non-Fermi-liquid Kondo fixed point. In the case of an impurity hopping among positions with higher symmetry, such as triangular symmetry, it is shown here that the non-Fermi-liquid behavior at low temperatures can be generic. Using various bosonization techniques, the fixed point is shown to be stable. However, unlike the conventional two-channel Kondo (2CK) model, it has four leading irrelevant operators, implying that while the form of the singular temperature dependence of physical quantities is similar to the 2CK model, there will not be simple universal amplitude ratios. The phase diagram of this system is analyzed and a critical manifold is found to separate the non-Fermi-liquid from a conventional Fermi liquid fixed point. Generalization to higher symmetries, such as cubic, and the possibility of physical realizations with dynamic Jahn-Teller impurities is discussed.

I. INTRODUCTION

Following pioneering work by Nozières and Blandin, the multichannel Kondo model has attracted much attention because of the prospect of novel, low temperature behavior. Various theoretical methods have been developed to study the nature of the zero temperature Kondo fixed points for a variety of cases, in particular with an arbitrary number of channels, and with either one or two impurity Kondo impurities. Despite various intriguing predictions, no experimental realization of the multichannel Kondo effect has yet been conclusively demonstrated. The difficulty lies in the fact that the non–Fermi–liquid fixed points are unstable to various symmetry–breaking processes, such as channel anisotropy, which turn out to be present in real experimental situations. For example, Nozières and Blandin pointed out that anisotropy between the channels, caused by lattice effects, would destroy the non–Fermi–liquid ground state.

Subsequently, Vladár and Zawadowski were the first to suggest a different realization of the two-channel Kondo model, with the role of the spins and the channels of the conventional magnetic model interchanged. In this case, a non-magnetic impurity tunnelling between two sites plays the role of the magnetic spin-1/2 impurity in the original Kondo formulation with electrons coupled orbitally to the impurity, while the spin index of the electrons is a spectator, playing the role of the channel index. Therefore, since in the absence of a magnetic field in the magnetic Kondo system the spin-up and spin-down electrons are degenerate, channel anisotropy is no longer a problem. This led Vladár and Zawadowski to predict that such a system should exhibit non–Fermi–liquid behavior at low temperatures, characteristic of the two-channel Kondo (2CK) model. Recently, low temperature tunnelling data by Buhrman et al. in very small metallic contacts have been interpreted by Buhrman et al. in terms of two-channel Kondo-like physics. Their measurements are claimed to be consistent with certain exact results for the 2CK model obtained by Affleck and Ludwig, but at this point, the interpretation is controversial. Again, the problem arises from the absence of a symmetry which prevents other relevant terms from appearing; the most important of these is bare impurity tunnelling, which in the conventional Kondo model corresponds to a magnetic field on the impurity. In a previous paper, we studied this system in detail and argued that it is very unlikely that 2CK physics could be observable over a substantial temperature range in such a two-site impurity system.

A way to circumvent the problem of the appearance of relevant operators is to impose symmetry conditions on the orbital degrees of freedom so that the relevant operators which plagued the two-site impurity system are not allowed to appear by symmetry. The first question that naturally arises is what are the minimum symmetry requirements at some high (or intermediate) energy scale so that the system will flow under renormalization (RG) towards the non-Fermi liquid fixed point, without any fine tuning. Clearly, the low temperature non-Fermi liquid behavior one should be primarily aiming for, is that of the two-channel Kondo model due to its relative simplicity.

For tunnelling non-magnetic impurities, the “channel” (i.e. spin) symmetry is ensured, in the absence of a magnetic field, due to time reversal invariance. As for the symmetry of the impurity motion, an essential requirement is that at intermediate energies the impurity, dressed with high energy electrons, should behave like a degenerate doublet, just as the impurity spin-1/2 does in the conventional 2CK model. For this to be true without any parameter tuning, the symmetry group of the system has to allow for degenerate doublets to occur, i.e. it has to have a two dimensional representation. The simplest group with such a property is the triangular group $C_{3v}$, which, with six elements, is the smallest non-abelian group.
In this paper we are thus led to consider a non-magnetic impurity in a metal that can tunnel between the corners of an equilateral triangle. In this case, the left and right moving impurity states are related by symmetry and are thus degenerate. Not surprisingly, in order for the system to be in the basin of attraction of the 2CK point, we must require that at some intermediate energy, the left-right doublet of the impurity is the lowest energy orbital state of the impurity. Naively one might expect that this is impossible, since the ground state of a particle in an external potential is very generally non-degenerate. However, in a solid the impurity interacts with other electrons, including localized atomic electrons, whose state is affected by the impurity motion. By taking these interaction effects into account, we explicitly demonstrate in some simple and potentially physically relevant examples, that it is indeed possible for the ground state of the impurity-plus-high-energy-electrons complex to be degenerate.

We then analyze the weak electron-impurity interaction limit, determine the criterion for flowing under the renormalization group (RG) toward the 2CK fixed point, and find the energy scale below which the low lying impurity doublet becomes substantially separated from the excited symmetric orbital state. Below this energy scale the impurity complex can be regarded as a degenerate doublet, and the system can be mapped to a 2CK model with only irrelevant perturbations away from the intermediate coupling 2CK fixed point. As a result, the 2CK fixed point is accessible at low temperatures for generic values of the bare couplings provided that the conditions for an impurity doublet obtain.

In order to demonstrate the existence of novel 2CK-like behavior at low temperatures, one must do more than show that the RG flows at zero temperature go to the 2CK fixed point. As shown by Affleck, Ludwig and others, the singular low temperature behavior of various physical quantities in the 2CK model is controlled by the leading irrelevant operators about the 2CK fixed point: i.e. by the flow towards the fixed point. We must thus show that the structure of the irrelevant operators for the tunnelling impurity system is similar to that of the 2CK model. Indeed, we will show that the scaling dimension of the leading irrelevant operators, which characterize the form of the singularities in physical quantities at low temperatures, is the same in the two cases. However the number of leading irrelevant operators is larger for the tunnelling impurity system. Analyzing the behavior close to the 2CK fixed point, we find four leading irrelevant operators, in contrast to the pure 2CK model, which has only two, due to the fact that our problem does not have the full symmetry of the conventional 2CK problem, $U(1)_{\text{charge}} \times SU(2)_{\text{orbital}} \times SU(2)_{\text{spin}}$.

We thus conclude that since different physical quantities can have singularities controlled by different combinations of the various leading irrelevant operators, various amplitude ratios and scaling functions will be less universal than in the 2CK problem, although the form of the singular low temperature behavior will be the same.

In real systems, there will of course generally be some—hopefully small—symmetry-breaking perturbations. By studying the relevant symmetry breaking perturbations, in particular strains, we conclude that their effective strength will generally be screened by the fluctuations at the 2CK fixed point, making their effects less important than would be guessed by naively comparing energy scales. However, for the experiments by Buhrman and collaborators, simple order-of-magnitude estimates show that the strains have to be extremely small for the 2CK fixed point to be approached.

Within the space of full triangular symmetry, we find that by tuning the splitting between the impurity doublet and the singlet states, (e.g. by pressure) there will be a phase transition at zero temperature from the 2CK behavior to conventional Fermi liquid behavior. This transition is conjectured to be controlled by a fixed point with $SU(3)$ orbital symmetry.

Impurity configurations with high symmetry, such as cubic, are also discussed briefly, and found to be characterized, up to additional leading irrelevant operators, by the 2CK fixed point.

A. Outline

In the next Section we motivate and introduce the model we will be using. In Section II, we discuss the importance of the impurity degeneracy and analyze three physically relevant situations, for which the impurity ground state can indeed be two-fold degenerate. The weak coupling analysis is performed in Section III, at which the crossover from the 3-site problem to a degenerate 2-level impurity system, as well as $C_{3v}$-symmetry breaking processes are discussed. In Section IV, the intermediate coupling regime for the 2CK system is studied, while in Section V conjectures about the behavior on and near the critical manifold separating 2CK from conventional Fermi liquid behavior are made. Finally, we conclude in Section VII with the potential relevance of the model to experimental situations and, in particular, to recent experiments by Buhrman and collaborators.
II. MODEL

In this Section we introduce an effective Hamiltonian for the impurity and conduction electron system, valid at some intermediate energy scale substantially less than the conduction electron bandwidth. The effects of higher energy electronic processes have already been taken into account by introducing renormalized parameters in the effective Hamiltonian. It is crucial that at this intermediate energy scale all processes that are allowed by symmetry will be present, even if they were absent in the “bare” Hamiltonian. Therefore we have to include all processes that are relevant (in the RG sense) at either weak or intermediate coupling, since their amplitudes, albeit small initially, can grow under the RG flows. [Other processes that are irrelevant for both weak and intermediate coupling will end up yielding at worst non-universal order one corrections to the various quantities of interest.]

Since the impurity-electron interactions are predominantly local, the electronic degrees of freedom which interact most strongly with the impurity at low energies can be viewed as centered around the three minimum energy positions of the impurity. Therefore for low enough energies we only need to consider three electronic wavefunctions for each energy and each spin. These can be represented as a symmetric state \( c^\dagger_{S\sigma} \) with spin \( \sigma = \uparrow \downarrow \) and energy \( \epsilon \), transforming according to the trivial representation \( \Gamma_1 \) of \( C_{3v} \), and an orbital doublet \( \{ c^\dagger_{L\sigma \epsilon}, c^\dagger_{R\sigma \epsilon} \} \), in the two dimensional representation, \( \Gamma_3 \). Neglecting weaker interactions of the impurity with other electronic \( \Gamma_3 \)-doublets, \( \Gamma_1 \)-singlets and antisymmetric \( \Gamma_2 \)-singlets will not change the behavior of the system. In an analogous way the impurity states can be described by a \( \Gamma_3 \)-doublet \( d^\dagger_L, d^\dagger_R \) and the symmetric state \( d^\dagger_S \).

Before introducing the effective Hamiltonian \( H \), let us summarize its symmetries. Impurity and electron numbers are separately conserved, \( d \to e^{i\phi} d \) and \( c \to e^{i\theta} c \). In addition, in the absence of spin-orbit coupling or magnetic fields, our system has spin-\( SU(2) \) and time reversal symmetry. The latter acts also on the orbital degrees of freedom: \( i \to -i; \ d_L \leftrightarrow d_R; \ c_L \leftrightarrow c_R \). Finally, \( H \) has the \( C_{3v} \) symmetry, which includes exchange symmetry around an axis (\( c_L \leftrightarrow c_R; \ d_L \leftrightarrow d_R \)) and rotational symmetry by \( \pm 2\pi/3 \): \( c_L \to \exp[\pm 2\pi i/3] c_L; \ c_R \to \exp[\mp 2\pi i/3] c_R; \ c_S \leftrightarrow c_S \) and similarly for the \( d \)'s.

The Hamiltonian \( H \) includes several types of terms:

\[
H = H_{el} + H_{int} + H_{hop} + H_{mix}
\]

with \( H_{el} \) the electron kinetic energy in the absence of the impurity

\[
H_0 = \sum_{\sigma} \int \frac{d\epsilon}{2\pi} \left[ c^\dagger_{L\sigma \epsilon} c_{L\sigma \epsilon} + c^\dagger_{R\sigma \epsilon} c_{R\sigma \epsilon} + c^\dagger_{S\sigma \epsilon} c_{S\sigma \epsilon} \right],
\]

with the energy \( \epsilon \) measured from the Fermi surface. Note that for convenience we consider a linear conduction band with a cutoff of order the bandwidth \( W \). Although we will generally work in the \( S,L,R \) representation, in order to see the physical origin of various terms, it is convenient to first work in a basis of wave-functions centered around the three equivalent impurity sites, with

\[
c_n = \frac{1}{\sqrt{3}} \left( c_S + e^{-i(n-1)\frac{2\pi}{3}} c_L + e^{i(n-1)\frac{2\pi}{3}} c_R \right)
\]

for \( n = 1, 2, 3 \). If the impurity is at rest, then the only allowed one electron terms are

\[
V_1 \sum_{n\sigma} d^\dagger_{n\sigma} c_{n\sigma} c_{n\sigma} \tag{4}
\]

and

\[
V_2 \sum_{i \neq j \neq n} \sum_{\sigma} d^\dagger_{n\sigma} c_{i\sigma} c_{j\sigma}. \tag{5}
\]

The other such terms consistent with the symmetries can be rewritten, using \( \sum_n d^\dagger_{n\sigma} d_{n\sigma} = 1 \), in terms of these two and terms which mix the electronic states centered at the different sites:

\[
H_{mix} \propto \sum_{i \neq j} \sum_{\sigma} c^\dagger_{i\sigma} c_{j\sigma} = \sum_{\sigma} \left[ 2c^\dagger_{S\sigma} c_{S\sigma} - c^\dagger_{L\sigma} c_{L\sigma} - c^\dagger_{R\sigma} c_{R\sigma} \right] \tag{6}
\]

which must, in any case, be present due to the non-orthogonality of the \( c_{1,2,3} \) states [We ignore the unimportant term \( \sum_n c^\dagger_{n\sigma} c_n \)].
In the absence of impurity motion, the bare impurity hopping term can be written
\[
H_{\text{hop}}^{(0)} = \frac{\xi}{3} \sum_{i \neq j} d_i^\dagger d_j = \frac{\xi}{3} \left( 2d_S^\dagger d_S - d_L^\dagger d_R - d_L^\dagger d_L \right)
\]
where the \(d_{1,2,3}\) and \(d_{L,R,S}\) are related as in Eq. (8). The sign of \(\xi\) is of crucial importance. In particular, if all electron-impurity interaction terms are much smaller than \(\xi\), then the sign of \(\xi\) determines whether the impurity ground state is an orbital singlet (\(\xi < 0\)) or a \(\Gamma_3\) doublet (\(\xi > 0\)). At energy scales such that the renormalized electronic bandwidth is smaller than \(|\xi|\), in which case tunnelling events of the impurity from the ground state configuration to excited states will be suppressed, the low temperature behavior clearly depends crucially on the symmetry of the impurity ground state in the absence of interactions.

Of course, as was noted in the Introduction, naively the sign \(\xi\) should generally be negative to ensure a non-degenerate ground state. However, situations can exist for which the interaction of the impurity with atomic (high energy) electrons conspires to make the effective low energy impurity hopping matrix element \(\xi\) positive and hence favor the doublet impurity ground state. Some illustrative examples are discussed in the next Section.

In addition to the bare impurity hopping, various “electron assisted” impurity hopping terms \((H_{\text{hop}}^{(1)})\) can occur. These may involve either terms of the form \(d_{m,n}^\dagger c_j^\dagger c_j\) or \(d_{m,n}^\dagger c_{L,R,S}\) with \(i \neq j\). At the Fermi surface there are six independent such terms with coefficients \(A_1 \ldots A_6\). In the \(L,R,S\) basis, these give rise to several terms that are diagonal in this basis:
\[
V_{\text{diag}} = \pi Q_1 \sum_{\sigma} \left( c_{L,\sigma}^\dagger c_{L,\sigma} - c_{R,\sigma}^\dagger c_{R,\sigma} \right) (d_L^\dagger d_L - d_R^\dagger d_R)
\]
\[
+ \frac{\pi Q_2}{3} \sum_{\sigma} \left( 2c_{S,\sigma}^\dagger c_{S,\sigma} - c_{R,\sigma}^\dagger c_{R,\sigma} - c_{L,\sigma}^\dagger c_{L,\sigma} \right) (2d_S^\dagger d_S - d_R^\dagger d_R - d_L^\dagger d_L)
\]
\[
+ \pi Q_3 \left( c_{L,\sigma}^\dagger c_{L,\sigma} + c_{R,\sigma}^\dagger c_{R,\sigma} + c_{L,\sigma}^\dagger c_{L,\sigma} \right) (2d_L^\dagger d_L - d_R^\dagger d_R - d_S^\dagger d_S)
\]
where \(c_{\mu,\sigma}\), for \(\mu = L,R,S\), are the “local” electron creation operators, represented as \(c_{\mu,\sigma}^\dagger \equiv c_{\mu,\sigma}^\dagger (x = 0)\) where
\[
c_{\mu,\sigma}^\dagger (x) = \int \frac{d\epsilon}{2\pi} e^{-i\epsilon x} c_{\mu,\sigma}^\dagger
\]
are the incoming (outgoing) electronic s-wave states for \(x > 0\) (\(x < 0\)). The effect of the first two of these terms is to screen transitions between the different states \(L, R\) and \(S\) of the impurity. Their amplitudes \(Q_1, Q_2, Q_3\) correspond to linear combinations of various electron-assisted tunnelling processes \((A_1 \ldots A_6)\) and, \(Q_1\) and \(Q_2\) will be assumed to be positive. If \(Q_1 < 0\), then it will be seen later that the system behaves like a ferromagnetic Kondo model [see discussion after Eq. (20)]. In order for these important terms to be of appreciable magnitude (in Section \(\ref{impurity}\) we will allow \(Q_1\) to be of order unity), we focus on impurities with relatively fast (renormalized) tunnelling rates.

The interaction terms \(V_1\) and \(V_2\) give rise to a number of processes in the \(L,R,S\) basis which change the state of the impurity; to be consistent with \(C_{3y}\) symmetry the total orbital “angular momentum” – with \(L = -1, R = +1\) and \(S = 0\) – of each of these terms must be zero (mod 3). The electron assisted hopping terms \((A_1 \ldots A_6)\) also contribute to \(V_{\text{off-diag}}\). We have
\[
V_{\text{off-diag}} = 2\pi \Delta_1 \sum_{\sigma} \left( d_L^\dagger d_R c_{L,\sigma} + h.c. \right)
\]
\[
+ 2\pi \Delta_2 \sum_{\sigma} \left( d_L^\dagger d_S c_{S,\sigma} + d_R^\dagger d_S c_{S,\sigma} + h.c. \right)
\]
\[
+ 2\pi \Delta_3 \sum_{\sigma} \left( d_L^\dagger d_L c_{L,\sigma} + d_R^\dagger d_R c_{L,\sigma} + h.c. \right)
\]
\[
+ 2\pi \Delta_4 \sum_{\sigma} \left( d_L^\dagger d_S c_{R,\sigma} + d_R^\dagger d_S c_{R,\sigma} + h.c. \right)
\]
\[
+ 2\pi \Delta_5 \sum_{\sigma} \left( d_L^\dagger d_S c_{L,\sigma} + d_R^\dagger d_S c_{L,\sigma} + h.c. \right)
\]
In the absence of impurity motion, \(V_{\text{diag}}\) is zero, but \(V_{\text{off-diag}}\) has contributions from both electron-impurity interactions and electron-assisted hopping and is thus still non-zero.
Of all the terms we have so far, \( \Delta_3 \) and \( \Delta_5 \) are the only processes, that break the \( O(2) \)-symmetry in the \( \Gamma_3 \)-manifold (which, using different notation, was discussed in Ref. \[14\] in the context of the two-site tunnelling impurity). However, these terms are clearly \( C_{3v} \) invariant and their effects will be discussed in later Sections.

The terms we have included so far can be conveniently grouped into

\[
\mathcal{H}_0 = \mathcal{H}_{el} + \mathcal{H}_{hop}^{(0)}
\]

and the \( \mathcal{V}_{diag} \) and \( \mathcal{V}_{off-diag} \) combinations exhibited above. The electron mixing term, as it is diagonal in the \( L, R, S \) basis, will not play a substantial role (in contrast with the two-site case of Ref. \[13\]). In addition to the various impurity one-electron coupling terms, the impurity can also affect electron-electron interactions, and two-electron assisted hopping can take place. Although these terms are strongly irrelevant for weak coupling as discussed in Ref. \[13\], the latter can play an important role near the intermediate coupling 2CK fixed point; we denote them as \( \mathcal{H}_{hop}^{(2)} \). Putting all the important terms together, we primarily study the effective Hamiltonian

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{V}_{diag} + \mathcal{V}_{off-diag} + \mathcal{H}_{hop}^{(2)}.
\]

At this point, one can immediately guess which terms will play dominant roles at very low energy scales where, with \( \mathcal{E} \) positive, the higher energy symmetric impurity state \( d_S^\dagger \) will be strongly suppressed. In this limit, the most important terms will be \( Q_1 \) which is analogous to the \( J_z \) coupling in the Kondo system, and \( \Delta_1 \) which is analogous to the \( J_L \) coupling. The only other one-electron term which does not involve \( d_S \) is \( \Delta_3 \) which involves the \( c_S \) electrons and breaks the \( O(2) \) symmetry of the \( L, R \) subspace.

In general there can also be \( C_{3v} \)-symmetry breaking processes, but, by assumption, these will be small. Nonetheless we will need to investigate their role. The most important terms correspond to bare impurity transitions from state \( L \) to \( R \), such as

\[
\left(M d_L^\dagger d_R + M^* d_R^\dagger d_L\right),
\]

or from \( L \) and \( R \) to \( S \), such as \( d_S^\dagger (d_L + d_R) + (d_L^\dagger + d_R^\dagger) d_S \). [Note that \( d_L^\dagger d_L - d_R^\dagger d_R \) and \( d_S^\dagger (d_L - d_R) + (d_L^\dagger - d_R^\dagger) d_S \) cannot appear if the system is time-reversal invariant]. These will originate from various effects, including strains, other nearby static impurities etc. Of the above processes, the one corresponding to \( M \) will be the most important to our discussion, because it will persist even on very low electronic scales below which \( \mathcal{E} \) becomes larger than the renormalized bandwidth and transitions to the \( S \)-state are effectively quenched. The real part of \( M \) will be a linear combination of two independent bare impurity terms that are even under parity \( d_L^\dagger \leftrightarrow d_R^\dagger \), i.e. an energy bias term \( 2d_1^\dagger d_1 - d_2^\dagger d_2 - d_3^\dagger d_3 \) and an asymmetry in the hopping amplitudes \( d_2^\dagger d_3 + d_3^\dagger d_2 \), while in the imaginary part of \( M \) similar terms will appear which are odd under parity. Thus, two independent parameters have to be tuned for \( |M| \) to vanish. Finally, note that asymmetries in the electronic states due to other impurities etc., can generate \( M \) under renormalization.

**III. JAHN-TELLER EFFECT, BERRY’S PHASE AND EXCITED IMPURITY CONFIGURATIONS: EFFECTS ON IMPURITY DEGENERACY**

As already mentioned, the degeneracy of the lowest lying effective impurity state at intermediate energy scales is crucial to our analysis. The generic case of a non-degenerate impurity ground state, corresponding to \( \mathcal{E} < 0 \), leads to uninteresting impurity screening and hence to ordinary Fermi-liquid behavior at low temperatures. Instead, a doubly degenerate \( \Gamma_3 \) orbital impurity state will be our focus, and in this Section we will show how the necessary condition, \( \mathcal{E} > 0 \), is possible. First, we will analyze in two model cases the effects on the impurity motion of high energy atomic orbitals or valence electrons in solids, ignoring coupling to the conduction electrons. The impurity will be assumed to move slowly on the scale of the atomic electronic time scales. We can thus consider the adiabatic evolution of the electronic ground state as the impurity moves. In the second part of this Section we will demonstrate how, when we include the conduction electrons, the existence of intermediate excited impurity configurations between the low lying states \( d_1^\dagger, d_2^\dagger, d_3^\dagger \), can serve as a mechanism for changing the sign of the effective \( \mathcal{E} \) at lower energies.

**A. Effects of atomic electrons on impurity degeneracy**

We focus first on an orbital- and spin-singlet interstitial impurity, tunnelling between three equivalent positions–1, 2 and 3–on the corners of an equilateral triangle. The underlying physical reason for the desired effect on the sign of
is the appearance of degeneracies in the states of the surrounding medium (electrons and neighboring nuclei) when the impurity is located at a position of special symmetry—in our case, the center of the triangle. Even if the impurity is forbidden energetically from occupying this central symmetric position, e.g. by the presence of a host lattice atom, the effect is manifested in the behavior of the wavefunctions of the system when the impurity is away from the center.

The simplest example is an electronic state on the impurity, which, with the impurity located in the center of the triangle, is doubly degenerate, i.e. an \( L, R \) doublet. When the impurity is at, say, site 1, the degeneracy is broken. However, by adiabatically moving the impurity once around the triangle and back to site 1, the electron returns to its original state, but with its wavefunction multiplied by a factor of \(-1\). The extra phase acquired by the electronic state is just Berry’s phase; it will change the sign of the effective impurity-plus-electron tunnelling matrix elements.

With one electron in an appropriate energy level on the impurity, this effect can occur but the impurity will be magnetic. What is needed instead is an orbital (non-magnetic) electronic doublet on the impurity when it is at the center of the triangle.

This is a situation which is a classical example of the Jahn-Teller effect and was also proposed recently in this context by Gogolin. Due to the coupling of the electronic doublet of the impurity and the neighboring atoms, the triangle-center position of the impurity is unstable to displacements of the impurity from its equilibrium position: this linearly splits the electronic degeneracy, but only costs elastic energy that is quadratic in the distortion. A massive impurity will be displaced to one of three minimum energy equilibrium positions on the corners of an equilateral triangle. But, since the impurity wavefunctions at these three positions will generally have a finite overlap, the impurity can tunnel between them. The phases of the tunnelling matrix elements add up to \( \pi \) on tunnelling around the triangle, yielding an extra minus sign from the Berry’s phase. This ensures that the tunnelling \( \Gamma_S \)-doublet will be the ground state of the impurity complex. This restoration of the degeneracy via tunnelling of the impurity is a dynamic Jahn-Teller effect—the triangular symmetry is not broken in the ground state and the original electronic doublet has merely been modified into an impurity orbital doublet.

Unfortunately, orbital electronic doublet ground states at high symmetry positions of an impurity are not too common. Instead, in many cases the minimum energy configuration has magnetic character, due to Hund’s rules splittings. Nevertheless, for large enough local lattice distortions due to the impurity, the effective tunnelling impurity ground state can still be a doublet. To explicitly demonstrate this effect, we consider a simple situation with four atoms on the impurity, perturbed by the surrounding medium, with spin-orbit interactions neglected. For ground state can still be a doublet. To explicitly demonstrate this effect, we consider a simple situation with four electronic states will mix, e.g., \( S \leftrightarrow R \)

\[ \sum_{\sigma=x,y} a_{S,\sigma}^\dagger a_{R,\sigma} \]

states, corresponding to angular momentum of \( m = \pm 1, 0 \) (mod 3) respectively. We denote the creation operators for these \( a_{L, R, S}^\dagger \). If the environment is such as to make the atomic one-electron \( S \) state the lowest by energy \( \epsilon_a \), two electrons will fill this and the other two will go in the degenerate \( L, R \) states. The simplest situation is with effective electron-electron interactions smaller than the splitting \( \epsilon_a \). In this case, Hund’s rules will give rise to ferromagnetic exchange, \( J \), between the two \( L \) or \( R \) electrons, resulting in a spin triplet \( 3S \) ground state, with orbital angular momentum (mod 3), \( m=0 \), a doublet pair \( E \) of spin singlet, \( m = \pm 1 \) states (being the lowest by energy \( \epsilon_a \), two electrons will fill this and the other two will go in the degenerate \( L, R \) states. The simplest situation is with effective electron-electron interactions smaller than the splitting \( \epsilon_a \). In this case, Hund’s rules will give rise to ferromagnetic exchange, \( J \), between the two \( L \) or \( R \) electrons, resulting in a spin triplet \( 3S \) ground state, with orbital angular momentum (mod 3), \( m=0 \), a doublet pair \( E \) of spin singlet, \( m = \pm 1 \) states (being the lowest by energy \( \epsilon_a \), two electrons will fill this and the other two will go in the degenerate \( L, R \) states. The simplest situation is with effective electron-electron interactions smaller than the splitting \( \epsilon_a \). In this case, Hund’s rules will give rise to ferromagnetic exchange, \( J \), between the two \( L \) or \( R \) electrons, resulting in a spin triplet \( 3S \) ground state, with orbital angular momentum (mod 3), \( m=0 \), a doublet pair \( E \) of spin singlet, \( m = \pm 1 \) states (being the lowest by energy \( \epsilon_a \), two electrons will fill this and the other two will go in the degenerate \( L, R \) states.

motion of the impurity away from the triangle center by a displacement \((x, y)\) with \(-x\) in the direction of one of the three neighboring atoms, will give rise to mixing of the one-electron states via terms of the form

\[ \mathcal{H}_{\text{split}} = -\delta_1 \sum_{\sigma=\uparrow, \downarrow} a_{L,\sigma}^\dagger a_{R,\sigma}(x + iy) + h.c. \]

\[ -\delta_2 \sum_{\sigma=\uparrow, \downarrow} a_{R,\sigma}^\dagger a_{S,\sigma}(x + iy) + a_{L,\sigma}^\dagger a_{S,\sigma}(x - iy) + h.c. \]

These will give rise to splittings of the doublet excited state that are linear in the displacement; this is just what would be the Jahn-Teller splitting if the doublet had been the ground state. If the displacement is directly towards or...
FIG. 1. Schematic representation of the minimum energy impurity positions (1,2,3) in the environment of the neighboring atoms (open circles). The solid triangle is the boundary between the regions in which the electronic ground state is a spin-triplet (interior) and a spin-singlet (exterior). Points 0, α, β, γ represent positions of the impurity at which the two lowest lying electronic spin-singlet levels are degenerate. At point 0 these two states form an orbital $^1E$ doublet [see Fig.3 and Section III.1]. This figure corresponds to large $\epsilon_a$, with the parameters defined in Section III.1 $\epsilon_a = 33.3J = 10K = 20(1 = 1062$ and units of $x$ and $y$, such that α, β and γ are at distance approximately 0.6 from 0, see Fig.4. Depending on the choice of these parameters, the crossing points α, β and γ may lie inside or outside of the triangle. Two types of lowest action tunnelling paths “A” and “B” are shown and discussed in Section III.1.

Away from one of the triangle corner atoms, say, with $y = 0$, the states can still be categorized as even or odd under reflection through that atom. The even state will also mix with the $m = 0$ spin singlet excited state.

We are interested in distortions large enough that the ground state is no longer the spin triplet, but one of the even or odd singlet states. It can readily be seen in simple models, like the one above, that this can occur, at least in principle. There will be then, for a classical impurity, three equivalent spin-singlet ground states, with displacements $(R,0)$, $(-R/2,\pm\sqrt{3}R/2)$. In general, the lowest action tunnelling path between these positions will go around the excited state doublet degeneracy in the center of the triangle, and hence pick up a minus sign from Berry’s phase.

Unfortunately, there may also be other degeneracies in the spin singlet sector that can play a role. In particular, level repulsion between the even singlet states along the line $y = 0$ (and two equivalent lines), can result in a second crossing between the even and odd singlet states. It should be stressed that these extra level crossings α, β, γ [see Fig.3] are distinct points, occurring only when the impurity lies on one of the three lines of symmetry, so that the two low-lying singlet states have different (even-odd) symmetry and hence can cross, see Fig.4. In particular, if the modification of the effective interactions by the distortion is small, (e.g. for $\epsilon_a \gg J, K$ with no modification of the interactions that give rise to $J$ and $K$ due to the distortion), the main effect of the distortion will be the repulsion between the even singlet states; this situation is shown schematically in Fig.3. In this case the degeneracies and region of spin singlet or triplet ground states are shown in Fig.4. If the lowest action tunnelling path is like that denoted by “A” in Fig.3, four degeneracies in the spin singlet sector will be encircled as the impurity moves around the triangle, resulting in four minus signs and hence a conventional symmetric orbital ground state of the tunnelling impurity, i.e. $\mathcal{E} < 0$. On the other hand, if the impurity tunnels via a path like that shown as “B” in Fig.3, only the triangle center degeneracy will be encircled and the tunnelling ground state will be the impurity $L, R$ doublet. Either possibility can occur.

Note that spin flip effects can complicate matters somewhat, but will not change the overall conclusion.

We have shown in this Section that the existence of an electronic degeneracy in either the ground state or some particular excited state when the impurity is located in a special, albeit energetically unfavorable, point in space (the triangle center) can be responsible for the restoration of that degeneracy for the combined impurity-plus-environment system. This only occurs in some regimes of atomic electron interactions and couplings to the environment. Clearly, a complicated calculation would be required to determine the amplitudes of the various processes reasonably accurately.
in an actual physical example. Furthermore, the above analysis is valid only when the impurity moves slowly compared to the atomic electron time scales. One should note that the above assumption, although intuitively obvious in many cases (especially away from electronic level crossings) is still controversial. However the above discussion demonstrates that, at least in principle, the appearance of a Berry phase, and therefore an orbitally degenerate impurity ground state, is indeed possible.

B. Effect of an excited impurity configuration

In realistic situations, impurity tunnelling rates will probably be appreciable if the barriers between the three impurity positions are relatively small. Therefore the excited energies of intermediate impurity configurations that are comparable to these barriers, will be substantially lower than the bandwidth. As a result, a considerable fraction of conduction electron excitations will have energies large enough to allow transitions between the low lying and these excited impurity states. However, since the electronic excitation spectrum is continuous in the thermodynamic limit, the impurity motion cannot be treated adiabatically for these energies, as it was for the atomic electron states discussed above. Instead, the conduction electron assisted tunnelling of the impurity between the low lying and these excited states can be analyzed systematically by RG scaling. Here we show how the existence of an excited impurity configuration can lead to a positive effective $E$ at low energies via coupling to conduction electrons.

For simplicity, we only consider two sites, with the low lying impurity states at each site being $d_1^\dagger$, $d_2^\dagger$. Let $d_E^\dagger$ denote an intermediate excited impurity state, with extra energy $U$, that is large compared to the bare impurity tunnelling matrix element between sites 1 and 2, but small compared to the bandwidth $W$ ($U/W \ll 1$), see Fig. 3. In this regime we can perform a two-stage renormalization procedure: Initially we include the excited state, allowing electron assisted tunnelling events between states 1, 2 and $E$, these may have tunnelling amplitudes $t_1$ much greater than $E$. Then, when the renormalized bandwidth becomes of the order of $U$ or smaller, excitations of the impurity to state $E$ will become negligible, in which case we can drop the excited state from the effective Hamiltonian. Thus the effect of the impurity excited state can be described by the following terms

$$\Delta H = Ud_E^\dagger d_E + y \sum_{\sigma} \left( c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma} \right)$$

$$+ 2\pi t_1 \sum_{\sigma} \left( d_E^\dagger d_1 c_{1\sigma}^\dagger c_{E\sigma} + d_E^\dagger d_2 c_{2\sigma}^\dagger c_{E\sigma} + h.c. \right)$$

(16)
where \( c^{\dagger}_{E \sigma} \) is an extra local electronic state, which is even under the exchange of site indexes 1 and 2 and \( y \) is the average mixing amplitude of conduction electron states 1 and 2 in the presence of the impurity. Note that in the absence of the impurity, \( y \) (together with the other terms in \( \Delta \mathcal{H} \)) will vanish, restoring the orthogonality of states 1 and 2. In general, both \( t_1 \) and \( y \) are energy dependent. For simplicity, we only consider their constant part, evaluated at the Fermi energy. Energy dependent deviations will introduce corrections but will not qualitatively change the behavior described here. A crucial observation is that \( y \) can be positive or negative due to two effects. First, as it was seen in Ref. \( \text{[9]} \) since \( c^{\dagger}_{1 \sigma}, c^{\dagger}_{2 \sigma} \) involve electronic excitations in the conduction band, \( y \) is an oscillatory function of \( k_F R \), where \( k_F \) and \( R \) are the Fermi wavevector and the intersite distance, respectively. Roughly, this oscillatory behavior corresponds to the amplitude of an electron at the Fermi energy tunnelling between sites 1 and 2. Second, since it is the presence of the impurity that causes the mixing of the otherwise orthogonal states 1 and 2, \( y \) should also depend on the impurity-electron coupling. As a result, its sign should also depend on the sign of the coupling \( \mathcal{U} \).

Neglecting all other terms involving the impurity, in this regime the RG equation of \( \mathcal{E} \) normalized by the conduction bandwidth \( W \) is

\[
\frac{d\mathcal{E}}{dt} = \mathcal{E} + 6yt^2,
\]

while \( y \) and \( t_1 \) are marginal (for weak electron-impurity interaction). The second term ceases to contribute to the renormalization of \( \mathcal{E} \) once the renormalized bandwidth becomes of the order of \( U \). At that scale \( e^L = W/U \), \( \mathcal{E}(L) \approx (\mathcal{E} + 6yt^2)W/U \) so that (after reinstating the renormalized bandwidth factors) the effective renormalized \( \mathcal{E} \) that should appear in the lower energy effective Hamiltonian, Eq.(17), is

\[
\tilde{\mathcal{E}} \approx \mathcal{E} + 6yt^2W,
\]

independent of \( U \). Below the energy scale \( U \), the impurity is limited to hops between the low lying states \( d^{\dagger}_1, d^{\dagger}_2 \) (and \( d^+_3 \), with an effective hopping \( \tilde{\mathcal{E}} \). Note that since the \( d^{\dagger}_3 \) state has appreciable amplitude in both wells, \( t_3W \) may be larger than \( \mathcal{E} \). Therefore \( yt^2W \) may be comparable to \( \mathcal{E} \), and, since the sign of \( y \) may be positive or negative, whatever \( \mathcal{E} \) may have been originally. [Note that there will also be contributions to \( \tilde{\mathcal{E}} \) from hops 1 \( \rightarrow \) 2 not involving electrons, but these need not dominate over the electron-assisted process included here. The effects of an excited impurity configuration were first considered by Zarán and Zawadowski in the context of an impurity tunnelling between two sites, in order to show that the one-electron assisted tunnelling between the low-lying levels (which, for simplicity, we did not consider here) can be enhanced. However, they did not consider the equally strong enhancement of the tunnelling rate of the impurity alone, which we analyzed above.]

In summary, we have presented three situations which can result in an impurity \( L, R \) doublet ground state at low energies. The first two (Section III.1) involved the effect of localized atomic electrons with energies far from the Fermi level. In the third case (Section III.1) we saw that, closer to the Fermi level, conduction electrons in the presence of excited impurity configurations can renormalize the effective bare tunnelling element \( \mathcal{E} \), so that it can take either sign. After all these effects have been taken into account, at intermediate energy scales the coupling of the remaining conduction electron degrees of freedom to the impurity can be represented by the effective renormalized coupling terms introduced in Section III. these will now be analyzed.

![Diagram of a double well potential for an impurity with low lying states](image-url)
IV. WEAK TUNNELLING CROSSOVER

In most physical situations, it is likely that the bare impurity tunnelling $E$ and the electron assisted tunnelling processes will be small. If the impurity-position-dependent electron-impurity interactions $V_1$ and $V_2$ are also small, then there will be a simple crossover at an energy scale of order $E$. At lower energy scales, the processes that involve $d_s$ will be strongly suppressed; those remaining will be $\Delta_1$, $Q_1$ and $\Delta_3$. By this crossover scale, the various $Q_j$ and $\Delta_j$, as they are all marginal for weak coupling, will only have been modified from their original values by amounts quadratic in the various couplings; $E$ will have been renormalized similarly in addition to its simple growth under renormalization with eigenvalue one. For weak coupling, two-electron terms, like those in $\mathcal{H}^{(2)}_{\text{hop}}$, will be irrelevant with eigenvalue $-1$ and hence will be negligible at the crossover scale.

Beyond this crossover scale for weak interactions, the couplings other than $\Delta_1$, $\Delta_3$ and $Q_1$ can be ignored (at least for now), but these will renormalize each other. With all three of these small the flow equations in this regime are

$$\frac{d\Delta_1}{dl} = 2Q_1\Delta_1 \tag{19}$$

$$\frac{dQ_1}{dl} = 2\Delta_1^2 \tag{20}$$

(reflecting the approximate $SU(2)$ symmetry for $\Delta_1 = Q_1$) and

If $Q_1 < -|\Delta_1|$, then the system is like a ferromagnetic Kondo problem so that $\Delta_1$ flows to zero and the ground state will be an impurity orbital doublet. We thus restrict consideration to $Q_1 > -|\Delta_1|$. Since $Q_1$ involves impurity hopping but $\Delta_1$ does not, we expect $|Q_1| < |\Delta_1|$, although this need not be the case.

We thus see that $\Delta_3(l)$ will tend to decrease in the interesting regime, while $Q_1$ and $\Delta_1$ increase. The Kondo temperature $T_K$, below which the intermediate coupling behavior will obtain, is determined by the energy scale at which $\Delta_1(l)$ becomes of order unity, yielding

$$T_K \sim W \exp \left[ -\frac{\kappa}{|\Delta_1|} \right] \tag{21}$$

with $W$ the electron bandwidth and $\kappa$ depending on the ratio of $Q_1$ and $\Delta_1$ initially, or more precisely, at the crossover scale at which $E(l)$ is of the order the renormalized bandwidth: specifically for $|Q_1| < |\Delta_1|$, $\kappa$ is $\pi/4$ in the small $Q_1$ limit.

If the interactions of electrons with the impurity are reasonably strong, i.e $V_1$ and/or $V_2$ are not small, then the RG flow away from weak tunnelling is more complicated. In particular, the weak tunnelling eigenvalue of the impurity hopping, $\lambda_E$ is modified to

$$\lambda_E = 1 - \frac{1}{6\pi^2} \left( V_1^2 + 2V_2^2 \right) \tag{22}$$

by orthogonality catastrophe effects. This expression is valid for $V_1$ and $V_2$ of order unity if they are replaced by the associated phase shift-like quantities, see Ref.\textsuperscript{[13]} The renormalization of the various electron assisted tunnelling terms $A_1, \ldots, A_6$ will also be modified by the impurity-electron interactions, as discussed in Ref.\textsuperscript{[18]} Indeed, for sufficiently large $V_1$ and/or $V_2$ some of these can be more relevant than $E$, although in this case the feedback of these into $E$ will become important. Likewise, $E$ combined with $\mathcal{H}_{\text{mix}}$ will generate the electron-assisted hopping terms if these do not already exist.

Thus for strong interactions, the weak tunnelling crossover will be rather complicated with several processes potentially playing significant roles. But the coupling of primary importance for the Kondo-like physics, $\Delta_1$, can itself be quite large initially; in this case the Kondo temperature will essentially be when $E$ becomes of order the renormalized bandwidth i.e.
\[ T_K \sim W (E/W)^{1/\lambda_E} \]  

(24)

with \( \lambda_E \leq 1 \). Note that initially \( Q_1 \) will not be generated by the \( V_i \) terms, although they will affect its renormalization, but once the effective \( \mathcal{E} \) becomes appreciable, \( Q_1 \) will be generated by \( \Delta_1 \) as in Eq(19) and then rapidly become of order unity.

A. Symmetry Breaking Processes

The dominant \( C_{3v} \) symmetry breaking process is given by Eq(13). For weak coupling \( M \) is relevant with eigenvalue one. Beyond the crossover energy scale at which \( \mathcal{E}(l) \) becomes large, \( M \) can be renormalized non-trivially by \( Q_1 \) and \( \Delta_1 \). If \( \Delta_1 \) is large, there will not be a substantial regime in which this will occur and we can simply use the magnitude of \( M \) at this crossover as an input to the flows in the interesting intermediate coupling regime analyzed in the next Section. On the other hand if \( \Delta_1 \) (and \( Q_1 \)) is small, then there will be a regime of non-trivial renormalization of \( M \), with corrections to its eigenvalue of order \( \Delta_1^2 \) and \( Q_1^2 \). But since the logarithmic range of scales over which this will obtain is of order \( l \sim 1/\Delta_1 \), the net effect of this will be small.

Thus in both regimes, the weak tunnelling crossover will not appreciably alter the effective magnitude of the dominant symmetry breaking perturbations.

V. INTERMEDIATE COUPLING 2CK FIXED POINT

We now analyze the intermediate coupling regime and show how two-channel Kondo-like behavior arises. We work in the regime where the gap between the symmetric impurity state and the lower lying \( \Gamma_3 \)-doublet is much larger than the renormalized electronic bandwidth, i.e. at energy scales much less than the Kondo temperature \( T_K \). In this case the impurity is essentially frozen in its doublet ground state and we can therefore impose the constraint

\[ d^\dagger_L d_L + d^\dagger_R d_R = 1 \]  

(25)

and limit the analysis to processes involving only these two states. In this Section we first identify the 2CK fixed point, which is located at intermediate values of the important coupling parameters \( Q_1 \) and \( \Delta_1 \) and therefore cannot be accessed using a weak coupling analysis. We then show that it is stable when \( C_{3v} \) is an exact symmetry. Finally we find the set of leading irrelevant operators which will control the low temperature behavior of the system.

It is convenient to introduce pseudo-spin operators for the impurity doublet

\[ \sigma_z = d^\dagger_L d_L - d^\dagger_R d_R \]  

(26)

and

\[ \sigma_+ = d^\dagger_L d_R \]

\[ \sigma_- = d^\dagger_R d_L \]  

(27)

In order to proceed with our analysis we bosonize the electronic degrees of freedom by introducing bosonic fields \( \Phi_{\mu\sigma}(x) \) for \( \mu = L, R, S \) and \( \sigma = \uparrow, \downarrow \) in the following way:

\[ c_{L\uparrow}(x) = \frac{1}{\sqrt{2\pi\tau_c}} e^{i\Phi_{L\uparrow}(x)} e^{i\pi N_{S\uparrow}} \]  

(28)

\[ c_{R\uparrow}(x) = \frac{1}{\sqrt{2\pi\tau_c}} e^{i\Phi_{R\uparrow}(x)} e^{i\pi N_\uparrow} \]

\[ c_{S\uparrow}(x) = \frac{1}{\sqrt{2\pi\tau_c}} e^{i\Phi_{S\uparrow}(x)} e^{i\pi N_{S\uparrow}} \]

\[ c_{L\downarrow}(x) = \frac{1}{\sqrt{2\pi\tau_c}} e^{i\Phi_{L\downarrow}(x)} e^{i\pi N_{S\downarrow}} e^{i\pi N_\uparrow} \]

\[ c_{R\downarrow}(x) = \frac{1}{\sqrt{2\pi\tau_c}} e^{i\Phi_{R\downarrow}(x)} e^{i\pi (N_\uparrow + N_{S\downarrow})} \]

\[ c_{S\downarrow}(x) = \frac{1}{\sqrt{2\pi\tau_c}} e^{i\Phi_{S\downarrow}(x)} e^{i\pi N_{S\downarrow}} e^{i\pi N_\uparrow} \]
where the exponentials with the number operators

\[ N_{\mu\sigma} = \int dx\, c_{\mu\sigma}^\dagger(x) c_{\mu\sigma}(x) \]

\[ N_{\sigma} = \sum_{\mu} N_{\mu\sigma} \quad (29) \]

have been inserted to insure anticommutation relations between the various different fermion operators. Also, \( \tau_c^{-1} \) is a cutoff energy scale of the order the renormalized bandwidth. In the above notation the (normal ordered) local electron operators can be expressed simply in terms of the bosonic variables

\[ c_{\mu\sigma}^\dagger(x) c_{\mu\sigma}(x) = \frac{1}{2\pi} \frac{\partial \Phi_{\mu\sigma}(x)}{\partial x} \quad (30) \]

The electronic kinetic energy can also be represented in a standard manner in terms of bosonic variables \( \phi_{\mu\sigma}(\epsilon) \) which obey the canonical commutation relations

\[ [\phi_{\mu\sigma}(\epsilon), \phi_{\mu\prime\sigma'}(\epsilon')] = 2\pi \delta_{\mu\mu'} \delta_{\sigma\sigma'} \delta(\epsilon - \epsilon') \quad (31) \]

with

\[ \Phi_{\mu\sigma}(x) = \int_0^\infty d\epsilon \, \sqrt{\frac{\epsilon}{2\pi}} \left[ \phi_{\mu\sigma}(\epsilon) e^{i\epsilon x} + \phi_{\mu\sigma}^\dagger(\epsilon) e^{-i\epsilon x} \right] e^{-\frac{\epsilon}{\tau_c}} \quad (32) \]

by

\[ H_0 = \sum_{\mu\sigma} \int_0^\infty d\epsilon \, \frac{\epsilon}{2\pi} \phi_{\mu\sigma}^\dagger(\epsilon) \phi_{\mu\sigma}(\epsilon) e^{-\epsilon \tau_c} \quad (33) \]

with both integrals involving only positive energies (corresponding to the fact that the electrons \( c_{\mu\sigma}^\dagger(\epsilon) \) are only left moving) and with a cutoff energy of the order of the renormalized bandwidth \( \tau_c^{-1} \). [Note that the energy \( \delta \)-function in Eq(31) is rounded at energies \( \epsilon \approx \tau_c^{-1} \).] It is useful to define even and odd combinations of the \( L, R \) Bose fields

\[ \Phi_{e,o\sigma} = \frac{1}{\sqrt{2}} (\Phi_{L\sigma} \pm \Phi_{R\sigma}) \quad (34) \]

Then the most important parts of the effective Hamiltonian can be written as

\[ H_{\text{eff}} = H_0 + \frac{Q_1}{\sqrt{2}} \sum_{\sigma} \sigma_z \frac{\partial \Phi_{\sigma\sigma}}{\partial x} \]

\[ + \frac{\Delta_1}{\tau_c} \sum_{\sigma} \left( \sigma_+\eta_\sigma \exp \left[ i\sqrt{2}\Phi_{\sigma\sigma} \right] + h.c. \right) \quad (35) \]

where the boson fields in the last two terms are evaluated at the origin \( (x = 0) \) and we consider later the term proportional to \( \Delta_3 \), which will turn out to be irrelevant. Here we have defined the factors

\[ \eta_\sigma = e^{i\pi(N_{L\sigma} + N_{R\sigma})} \quad (36) \]

which can take values \( \pm 1 \), since the number operators \( N_{\mu\sigma} \) can only take integer values. In the case that \( \eta_\sigma \) has a definite sign, (i.e. when \( N_{L\uparrow} + N_{R\uparrow} \) and \( N_{L\downarrow} + N_{R\downarrow} \) are separately conserved) these factors can be neglected, as we shall do for the moment. Note that at this point the \( S \)-electrons are decoupled; we will later reintroduce terms that couple them to the \( L \) and \( R \) degrees of freedom.

Eq(35) is essentially equivalent to the Hamiltonian of the anisotropic 2CK model, which has an \( O(2) \) symmetry

\[ \Phi_{\sigma\sigma} \rightarrow \Phi_{\sigma\sigma} + \theta \sqrt{2}, \quad \sigma_\pm \rightarrow \sigma_\pm e^{i\theta}, \quad \Phi_{\sigma\sigma} \rightarrow -\Phi_{\sigma\sigma}, \quad \sigma_+ \rightarrow \sigma_+, \quad \sigma_- \rightarrow -\sigma_- \]; this is sufficient to make it flow to the \( SU(2) \) symmetric 2CK fixed point.

After decomposing the bosonic fields and \( \eta_\sigma \) into charge and spin components,

\[ \Phi_{e\sigma} = \frac{1}{\sqrt{2}} (\Phi_{ec} + \sigma \Phi_{es}) \quad \text{etc.} \quad (37) \]
and
\[ \eta_\sigma = e^{i\pi(N_{e\sigma} + \sigma N_{oc})}, \] (38)
with \( \sigma = \pm \) for spin \( \uparrow, \downarrow \), respectively, we follow Emery and Kivelson and perform a unitary transformation
\[ U = \exp \left[ -\frac{i}{2} \sigma_z \Phi_{oc} \right] \] (39)
which transforms \( \mathcal{H}_{eff} \) to the form
\[ \mathcal{H}'_{eff} = U \mathcal{H}_{eff} U^+ = \mathcal{H}_0 + \left( Q_1 - \frac{1}{2} \right) \sigma_z \frac{\partial \Phi_{oc}}{\partial x} + \frac{2\Delta_1}{\tau_c} \sigma_x \cos \Phi_{oc}. \] (40)

As was first pointed out by Emery and Kivelson, the above Hamiltonian can be diagonalized exactly when \( Q_1 = 1/2 \) via renormalizing the bosonic and pseudo-spin operators. This solution is analogous to the Toulouse limit of the one-channel Kondo model; here it captures the behavior of the 2CK model. Sengupta and Georges showed that \( \sigma_z \frac{\partial \Phi_{oc}}{\partial x} \) is one of the leading irrelevant operators with dimension 3/2, while a second dimension 3/2 operator was found by us in the context of the 2CK model, consistent with expectations from conformal field theory. The RG eigenvalues here are one minus the dimension of the local operators. There are no relevant operators consistent with \( O(2) \) [and spin \( SU(2) \)] symmetry. However, the underlying symmetry of our system is \( C_{3v} \), which is lower than \( O(2) \). Although no extra relevant operators exist if we lower the symmetry to \( C_{3v} \), there will turn out to be one extra irrelevant, dimension 3/2 operator allowed and a fourth, if electrons \( c^A_i \) from the antisymmetric representation \( \Gamma_2 \) are coupled to the impurity.

Unfortunately, the renormalization technique does not work for all important operators allowed by \( C_{3v} \). Thus, in order to show that the above are indeed the only allowed leading irrelevant operators, we analyze the problem with a method recently used by Fabrizio and Gogolin in the context of the four-channel Kondo model following ideas of Fisher and Zwerger and Schmidt.

### A. Analysis of effective Hamiltonian

The approach described below is based on the observation that \( \Delta_1 \) in Eq(40) formally has dimension 1/2 and therefore will flow under RG to arbitrarily large values. In this case it makes sense to “diagonalize” this term first and treat \( \mathcal{H}_0 \) as a perturbation. Without loss of generality we assume that \( \Delta_1 > 0 \). Neglecting \( \mathcal{H}_0 \), the minimum energy values of \( \Phi_{oc}(x = 0) \) are, in the impurity basis where \( \sigma_x \) is diagonal, \( \Phi_{oc}(x = 0) = (2n + 1)\pi \) when \( \sigma_x = +1 \) and \( \Phi_{oc}(x = 0) = 2n\pi \) when \( \sigma_x = -1 \). The presence of \( \mathcal{H}_0 \) has two effects. First, it includes (via Eqs 32 and 33) the conjugate momentum of \( \Phi_{oc}(0) \), \( \Pi_{oc}(0) = -\frac{1}{\tau_c} \frac{\partial \Phi_{oc}(0)}{\partial x} \). Thus, in the semi-classical approximation, which is valid for large \( \Delta_1 \), the phase \( \Phi_{oc}(0) \) will tunnel occasionally between its various minimum energy values, with an effective tunnelling rate proportional to \( e^{-S_{kink}} \), where \( S_{kink} \) is the classical action of the motion of \( \Phi_{oc}(0) \) in the inverted potential \( \Delta_1 \to -\Delta_1 \) from, say, \( -\pi \) to \( \pi \). The value of \( S_{kink} \), which is large when \( \Delta_1 \) is large, is not important and clearly non-universal, since it depends on the details near the cutoff energy.

The other effect of \( \mathcal{H}_0 \) is via the coupling of \( \Phi_{oc}(x = 0) \) to bosons located away from the impurity \( \Phi_{oc}(x \neq 0) \), which will tend to screen the “kinks” (tunnelling events) of \( \Phi_{oc}(0) \). The underlying reason is that the ground states of \( \Phi_{oc}(x \neq 0) \) with different values of \( \Phi_{oc}(0) \) are mutually orthogonal, the manifestation of Anderson’s electron orthogonality catastrophe. To analyze this effect, we integrate out the bosons \( \Phi_{oc}(x \neq 0) \), leading to the following effective imaginary time action for \( \Phi_{oc}(x = 0, \tau) \equiv \Phi_{oc}(\tau) \)
\[ S_{eff} = \frac{1}{(2\pi)^2} \int d\tau \int d\tau' \frac{(\Phi_{oc}(\tau) - \Phi_{oc}(\tau'))^2}{(\tau - \tau')^2} \] (41)
with \( \Phi_{oc}(\tau) \) typically being a series of widely separated (on the cutoff scale) kinks between different minima. This action has been studied extensively in a variety of quantum impurity problem contexts and it is straightforward to show that the operators \( O_m \), corresponding to \( \Phi_{oc}(\tau) \) hopping by \( m\pi \), have dimension \( \frac{3}{2} \). Therefore, when \( \sigma_x \) has no dynamics, the leading irrelevant operator is \( O_2 \), corresponding to hops between adjacent minima of the \( \cos \Phi_{oc} \) term.
B. Leading and other Irrelevant Operators

In the absence of relevant operators, at temperatures small compared to $T_K$ the system will flow towards the fixed point. The flow close to the fixed point, will be dominated by the leading irrelevant operators, i.e. the ones with the least negative RG eigenvalue, since other operators, being more irrelevant, will renormalize to zero faster and therefore will become negligible. At non-zero temperatures the RG flows will be terminated when the renormalized bandwidth becomes of order the temperature. At this scale the only non-negligible processes that will enter in physical quantities are the leading irrelevant ones and the temperature dependence of their renormalized amplitudes will determine the low temperature behavior of the system.

First we analyze the leading irrelevant operators with dimension 3/2. As mentioned above, the first is $\sigma_z \partial \Phi_{os}/\partial x$. Since $\Phi_{os}$ is decoupled from $\Phi_{os}$ and $\sigma_x$ when $Q_1=1/2$, the derivative term clearly has dimension 1. The effect of $\sigma_z$ (or equivalently $\sigma_y$) is non-trivial: since it anticommutes with $\sigma_x$ in the $\Delta_1$ term, it effectively reverses the sign of $\sigma_z$. As a result, the ground state value of $\Phi_{os}$ shifts by $\pi$ when $\sigma_z$ is applied, thereby giving $\sigma_z$ (and $\sigma_y$) dimension 1/2, since it forces a $\pi$ kink in $\Phi_{os}$, just like $\mathcal{O}_1$ above. As a result, the operator proportional to $(Q_1-1/2)$ has overall dimension 3/2, in agreement with other approaches.

As discussed in Refs.\cite{26} there is a second dimension 3/2 operator in the spin sector, which in the original electron operator representation is

$$d_L^R d_R \left[ c_{R1}^+ c_{L1} + c_{R1}^+ c_{R1} c_{L1} \right] + c_{R1} c_{L1} + \left[ c_{L1}^+ c_{L1} \right] + h.c.,$$

written in an explicitly spin-$\text{SU}(2)$ invariant form. Note that this operator involves two electron processes [part of $\mathcal{H}_{\text{hop}}^{(2)}$] and thus is irrelevant for weak coupling. After bosonizing and performing the unitary transformation of Eq.\cite{39}, the most relevant part in the square brackets becomes

$$\sigma_y \sin \Phi_{os} \frac{\partial \Phi_{os}}{\partial x}. \quad (43)$$

Apart from the above operators there is an extra leading irrelevant operator consistent with the $C_{3v}$ symmetry. Similar to the above, in the original fermion representation, this operator has the spin-$\text{SU}(2)$ invariant form

$$d_L^R d_R \left[ c_{S1}^+ c_{RL} + c_{RL}^+ c_{S1} c_{RL} \right] - \frac{1}{2} \left( c_{RL}^+ c_{L1} + c_{RL}^+ c_{RL} \right) \left( c_{S1}^+ c_{SL} - c_{S1}^+ c_{SL} \right) + h.c. \quad (44)$$

After bosonizing and performing the unitary transformation of Eq.\cite{39}, the last term in the square brackets becomes proportional to

$$\sigma_y \sin \Phi_{os} \frac{\partial \Phi_{os}}{\partial x}. \quad (45)$$

exactly analogous to Eq.\cite{43}. Since $\sigma_y$ flips the sign of $\sigma_x$ in the $\Delta_1$-term and $\Phi_{os}$ is essentially frozen, Eqs.\cite{43} and \cite{45} have dimension 3/2. Note that although nominally $\sin \Phi_{os} = 0$ at the minima of the cosine potential, the kink forced by the $\sigma_y$ gives $\sin \Phi_{os}$ a non-zero value at the kink.

It is important to comment that the extra dimension 3/2 operator (Eq.\cite{43}) only exists because of the presence of the symmetric electron state $c_{S1}^+$, which is invariant under $C_{3v}$. In fact, any $C_{3v}$ singlet fermion bilinear made up of electrons that can couple to the impurity through its spin, like $c_S$ here, will produce a dimension 3/2 operator. In particular the operator similar to Eq.\cite{44}, but with the $c_S$-electrons replaced by the $c_A$ electrons of the odd one-dimensional $\Gamma_2$-representation, will also have dimension 3/2. Note however, that due to their symmetry, $\Gamma_2$-electrons tend to interact more weakly with the impurity.

The first two terms in Eq.\cite{44}, transformed via Eq.\cite{39}, become proportional to

$$\sigma_x \cos \left[ \Phi_{es} - \sqrt{2} \Phi_{os} \right]. \quad (46)$$

where we have neglected the exponential factors $\exp \left[ i (N_{ec} \pm N_{es}) \right]$. Naively this operator also has dimension 3/2. However, due to the presence of $\Phi_{es}$, we need to be more careful with the $\exp \left[ i (N_{ec} \pm N_{es}) \right]$ in the $\Delta_1$ term of $\mathcal{H}_{\text{eff}}$, Eq.\cite{10}. Including these factors explicitly alters the dominant terms in $\mathcal{H}_{\text{eff}}$ to
\[ \hat{H}_{\text{eff}} = \hat{H}_0 + \frac{2\Delta_1}{\tau_c} (\sigma_x \cos \pi N_{\text{ee}} + \sigma_y \sin \pi N_{\text{ee}}) \cos [\Phi_{\text{os}} - \pi N_{\text{ee}}] \]  

(47)

Thus the presence of an \( \exp \pm i \Phi_{\text{es}} \) factor in Eq. (46) causes a sign change of the \( \Delta_1 \) term since it takes \( N_{\text{ee}} \to N_{\text{ee}} + 1 \) and therefore behaves just as \( \sigma_z \) does, increasing the dimension of the operator to 2. Similar arguments hold for subleading terms from Eq. (42).

Naively one would expect all parts of operators such as Eqs (12) and (14) to contribute to the \textit{leading} irrelevant operators since the they are orbital and spin singlets. The reason they do not is that through the bosonization scheme implemented above, in addition to the unitary transformation of Eq (59), the underlying orbital SU(2) symmetry of the Hamiltonian is broken down to an O(2) symmetry \( (\text{which is the symmetry of the XXZ anisotropic orbital Kondo model}) \). Therefore some of the various operators will mix with orbital-spin-2 operators associated with this symmetry breaking, thereby acquiring different scaling dimensions. Since the orbital-spin-2 operators have dimension 2 at the orbitally \( SU(2) \) invariant fixed point and are thus more irrelevant than the dimension 3/2 leading irrelevant operators, the breakdown of the orbital \( SU(2) \) symmetry to an \( O(2) \) symmetry will not affect the low temperature behavior, as the dimension 2 operators will become negligibly small at low temperatures. This is the underlying reason why the solvable point of the 2CK model found by Emery and Kivelson \( \text{c}\) captures correctly the singular low temperature behavior of the 2CK fixed point.

Other than \( \Delta_1 \) and \( Q_1 \), the only one-electron impurity operator that survives when \( d_S \) is suppressed, is \( \Delta_3 \). The most relevant part of this near the 2CK fixed point can be written as

\[ \sigma_x \cos \left( \frac{\Phi_{\text{eg}}}{\sqrt{2}} - \frac{\Phi_{\text{es}} + \Phi_{\text{os}}}{2} \right) \cos \left( \frac{\Phi_{\text{eg}} + 3\Phi_{\text{os}}}{2} \right). \]  

Naively this has dimension 15/8, since \( \Phi_{\text{os}} \) is frozen. However, the presence of \( \exp \pm i \Phi_{\text{es}} \) shifts \( N_{\text{ee}} \) in Eq (47) by \( \pm 1/2 \), turning the cosine into a sine. This forces a shift of \( \Phi_{\text{es}} \) by \( \pm \pi/2 \), thereby increasing the dimension of the \( \Delta_3 \) operator in Eq (48) by 1/8 to 2. This is in complete agreement with the dimension of \( \Delta_3 \) derived using conformal field theory methods. To see this, we observe that this operator combines \( c_{S\sigma} \) or \( c_{S\sigma}^\dagger \), which are free Fermi fields, uncoupled from the impurity at the fixed point, and hence having dimension 1/2, to \( d_L^\dagger d_Rc_{L\sigma}^\dagger + d_R^\dagger d_Lc_{R\sigma}^\dagger \) and \( \left( d_L^\dagger d_Rc_{R\sigma} + d_R^\dagger d_Lc_{L\sigma} \right) \), respectively. These operators by themselves would break the \( U(1) \)-charge symmetry of the model; since they involve an odd number of electron operators, they have charge 1. [In our bosonization scheme, this is manifested in them changing sign under \( \Phi_{\text{es}} \to \Phi_{\text{es}} + 2\pi \).] Furthermore, they clearly transform as a spin-doublet. The dimension of a charge-1, spin-1/2 operator at the 2CK fixed point is \( n + 1/2 \), with \( n \) a non-negative integer \( \geq 0 \). However the operators with \( n = 0 \) do not respect the \( C_{3v} \) symmetry, in particular, unlike the above operators, they are not invariant under \( c_L \to c_L \exp \left[ \frac{2\pi i}{3} \right] \) and \( c_R \to c_R \exp \left[ -\frac{2\pi i}{3} \right] \), since they transform as doublets under \( C_{3v} \). As a result, the allowed operators have \( n = 0 \) so that the scaling dimension of \( \left( d_L^\dagger d_Rc_{L\sigma}^\dagger + d_R^\dagger d_Lc_{R\sigma}^\dagger \right) \) and \( \left( d_L^\dagger d_Rc_{R\sigma} + d_R^\dagger d_Lc_{L\sigma} \right) \) is 3/2; combined with the 1/2 of \( c_{S\sigma} \) or \( c_{S\sigma}^\dagger \), this makes the dimension of \( \Delta_3 \) equal to 2, as found above.

By similar arguments, it can be shown that the dimensions of all physical operators are integers or half integers. This should be expected from the conformal field theory point of view, since the 2CK fixed point only has boundary operators with half-integer dimension. \( \text{Combining these with free fermions, such as } c_{S\sigma} \text{, that couple only through their spin (which plays the role of the “flavor” in the spin 2CK model), does not alter this result, as we saw explicitly in the case of } \Delta_3. \)

### C. Physical consequences

The low temperature behavior of the impurity and the electrons that couple to it will be governed by the 2CK fixed point discussed above and the flow towards the fixed point. In the absence of the irrelevant operators, the effective Hamiltonian of Eq (41) with \( Q_1 = 1/2 \), i.e. Eq (15), couples only the \( \Phi_{\text{es}} \) Bose fields to the impurity. [Although strictly speaking this is not the fixed point Hamiltonian, as discussed in Ref (13) it has the same essential structure, differing from the fixed point primarily in \( \Delta_1 \) being finite.]

This means that quantities like the spin susceptibility, \( \chi \), which involve only other linear combinations of the Bose fields—this case correlations of the spin operators from electrons in different representations, e.g. \( \frac{\partial \Phi_{\text{es}}}{\partial \delta \Phi_{\text{es}}} \)—will decouple from the impurity and be non-singular. However the leading irrelevant operator in the spin sector Eq (43) can combine with \( \frac{\partial \Phi_{\text{os}}}{\partial \delta \Phi_{\text{es}}} \) to yield \( \sigma_y \sin \Phi_{\text{os}} \), which has dimension 1/2 as discussed above. Similarly, the other two leading irrelevant operators involving \( S \)-electrons and \( A \)-electrons can also yield \( \sigma_y \sin \Phi_{\text{os}} \). As shown by Sengupta and Georges, this effect gives rise to a contribution to the susceptibility.
\[ \Delta \chi \sim \ln \left( \frac{T_K}{T} \right) \] (49)

at low temperatures, with the coefficient being proportional to the sum of the squares of the coefficients of these three leading irrelevant operators in the effective low energy Hamiltonian.

On the other hand, all dimension 3/2 operators, including the one proportional to \((Q_1 - 1/2)\), will contribute to the specific heat \(C_V\), giving a singular correction

\[ \Delta C_V \sim T \ln \left( \frac{T_K}{T} \right) \] (50)

with the coefficient being proportional to the sum of squares of all four leading irrelevant operators. As a result, the normalized ratio of \(T\Delta \chi\) to \(\Delta C_V\)–the Wilson ratio–will not be universal. However, due to the similarity in their form, the three operators entering the susceptibility, \(\frac{\partial}{\partial x} \sigma_y \sin \Phi_{es}, \Phi_{Ss}\), and \(\Phi_{As}\), will enter the specific heat in exactly the same combination. Thus for \(Q_1 = 1/2\) the normalized ratio of the specific heat over the susceptibility will be universal. As a consequence, to find a general universal ratio, one extra independent measurable quantity is required, that involves, e.g. only \((Q_1 - 1/2)^2\). It should be noted that the contribution to the resistivity which scales as

\[ \Delta \rho \sim \sqrt{T} \] (51)

is not suitable, because it involves a sum over the amplitudes of all the leading irrelevant operators.

**D. Symmetry breaking perturbations**

The most important symmetry breaking perturbation is a strain or other anisotropy that favors one of the three impurity positions. This most simply appears in the Hamiltonian as in Eq(13) where the phase of \(M\) determines the preferred direction for the impurity relative to the center of symmetry. This corresponds to \(\sigma_x \Re M + \sigma_y \Im M\) in the effective Hamiltonian, operators which have dimension 1/2 and are hence relevant, albeit less so than from naive power counting. At energy scales above \(T_K\), \(M\) just grows linearly with energy [as described in Section IV.1], but on scales below \(T_K\), it grows more slowly with eigenvalue 1/2. The perturbation thus becomes important and destroys the non-Fermi-liquid behavior below the energy scale

\[ T_M \sim \frac{|M|^2}{T_K} \] (52)

the \(|M|^2\) reflecting the eigenvalue of 1/2. Thus the novel 2CK behavior is more stable than might be expected. Note that similar crossovers are found in the presence of spin and electron-orbitally-coupled magnetic fields since these break the spin symmetry or the \(L, R\) symmetry, respectively.

It should be noted that the operator \(M\) in Eq(13) can also be generated through electronic processes that break the triangular symmetry caused, e.g., by the presence of static impurities in the vicinity of the tunnelling impurity. These give rise to mixing between the electronic wavefunctions interacting with the tunnelling impurity or between these and other wavefunctions. This mixing breaks the \(C_{3v}\) symmetry. In the presence of electron-assisted-tunnelling processes, such as \(A_1, \ldots, A_6\) discussed before Eq(8), these \(C_{3v}\) symmetry breaking electronic terms, such as

\[ \sum_\sigma \left( P c_{L\sigma}^\dagger c_{R\sigma} + P^* c_{R\sigma}^\dagger c_{L\sigma} \right) \] (53)

will generate under RG the operator \(M\).

**E. Effects of higher symmetries**

Impurities with a \(\Gamma_3\)-doublet ground state tunnelling around a point in the lattice with higher symmetry, such as octahedral symmetry in a cubic lattice, will clearly not have any relevant operators at the 2CK fixed point. The reason is that since these relevant operators are not allowed by \(C_{3v}\), a subgroup of the octahedral group \(O\), they will not be allowed by \(O\) either. However, there will be extra irrelevant operators, which turn out also to have dimension 3/2, therefore not essentially changing the low temperature physics of the 2CK fixed point. Electrons from representations \(\Gamma\) such that \(\Gamma \otimes \Gamma\) contains the trivial representation, will also have an associated dimension 3/2 operator of the form of Eq(14). Furthermore, since \(\Gamma_4 \otimes \Gamma_4\) and \(\Gamma_5 \otimes \Gamma_5\) contain, apart from \(\Gamma_1\), also the doublet \(\Gamma_3\),
electrons in these representations can couple orbitally with the impurity, in the form $d_i^\dagger d_R \sum_\sigma c_{l_\sigma}^\dagger c_{l_\sigma}$, for $i = 4, 5$, giving two additional dimension $3/2$ operators. As a result, in the case of octahedral symmetry $O$, where there are two 3-dimensional representations of electrons, $\Gamma_4$ and $\Gamma_5$, there will be four extra dimension $3/2$ operators, leading to a total of eight leading irrelevant operators.

If the impurity is in a triplet ground state ($\Gamma_4$ or $\Gamma_5$ in the octahedral, or $T$ in the tetrahedral case), due to arguments similar to those in this paper, it is anticipated that there will be a stable non-Fermi-liquid fixed point, analogous to, but different from, the 2CK fixed point for an impurity $\Gamma_3$-doublet ground state. In this case the situation is similar to the critical point of the doublet case at which $E$ changes sign, corresponding roughly to a triplet impurity ground state: this is briefly discussed in the next Section.

VI. CRITICAL MANIFOLD SEPARATING THE 2CK FROM THE FERMI LIQUID FIXED POINTS

For all of the physics discussed so far, the sign of $\mathcal{E}$ is crucial. Here we consider what happens if $\mathcal{E}$ can be made to change sign by a change in the system, for example by applying pressure. From the analysis of Section IV, it should be clear that it is really the sign of the effective hopping, $\tilde{\mathcal{E}}$, which includes renormalizations due to the effects of the electron assisted tunnelling, etc., that is important. Generally there will be a critical manifold separating the novel 2CK low temperature behavior from a conventional Fermi liquid regime in which the impurity is in its non-degenerate symmetric state with simply potential scattering of the electrons. This is schematically shown in Fig. 4. Since both the fixed points are stable at zero temperature, the critical manifold separating their domains of attraction can generically be crossed by a one parameter change in the system.

When the system lies on the critical manifold, which corresponds to $\mathcal{E} = 0$ at small coupling, it will presumably flow to a new unstable fixed point. We conjecture that, apart from the charge-$U(1)$ and spin-$SU(2)$ symmetries, this has an additional orbital-$SU(3)$ symmetry, where the $L, R, S$ triplet is identified with the fundamental representation of $SU(3)$. The behavior of the system on the critical manifold and close to this fixed point will be analyzed elsewhere, but below we quote some of the important results.

Within the critical manifold this fixed point is stable and the RG flows close to the fixed point are determined from the dimension of the leading irrelevant operator, which in this case is $7/5$. Therefore the impurity corrections to the specific heat, resistivity and susceptibility at low temperatures are $\Delta C_V \sim T^{4/5}$, $\Delta \rho \sim T^{2/5}$ and $\Delta \chi \sim T^{-1/5}$, respectively. Note that although the leading irrelevant operator and the symmetry of this fixed point are the same as those of the three-channel Kondo model, the fixed point itself and the operator content are not the same. This can easily be seen by noting that while in the three-channel Kondo model an impurity $SU(2)$-doublet couples to 3 channels of electrons through their spin, in this case the impurity is an $SU(3)$-triplet coupling to 2 channels of electrons through their orbital $SU(3)$ index.

Deviations away from the critical manifold are relevant dimension $3/5$. In a $C_{3v}$ symmetric situation only one such operator exists, which can be represented by $(2d^\dagger_d - d^\dagger_L - d^\dagger_R)/3$. This is therefore analogous to $\mathcal{E}$ and it governs the RG flows away from the critical fixed point toward the Fermi-liquid and the 2CK stable fixed points. Therefore, tuning only one parameter (such as external pressure) the novel non-Fermi-liquid fixed point associated with this higher orbital symmetry might be observed. In particular, close to the critical pressure, there will be a low temperature regime with the critical behavior crossing over below a temperature

$$T_X \sim |p - p_c|^{5/2}$$

(54)

to one of the two possible low temperature behaviors.

It should be noted that the above behavior also holds for the case of spinless impurities with a triplet degenerate ground state in tetrahedral or octahedral sites in a cubic crystal. In that case there will be no unstable directions close to the fixed point in the absence of symmetry breaking terms, just as for the 2CK fixed point in the case of $C_{3v}$, and the low temperature physics would be governed by the critical fixed point and its corresponding non-Fermi-liquid behavior.

VII. CONCLUSIONS AND RELEVANCE TO EXPERIMENTS

We finally discuss briefly the possible relevance of impurity tunnelling to the nanoconstriction experiments of Ralph and Buhrman, as well as potential future experiments.

In Ref. 14 we showed that the interpretation of the observed non-Fermi-liquid-like behavior of these experiments as a defect tunnelling between two site runs into trouble due to the existence of two relevant operators, that drive the...
FIG. 4. Schematic of renormalization group flows for the three site problem at zero temperature. There are two stable fixed points, namely the non-Fermi-liquid 2CK fixed point and the conventional Fermi-liquid fixed point, at which the impurity ground state is a $\Gamma_1$-singlet which is completely screened at low temperatures. The critical manifold separating the basins of attraction of the two stable fixed points is also shown. The flow on this manifold goes to a critical fixed point, which has higher orbital symmetry. The critical fixed point has one unstable direction that respects $C_3$; the dashed lines show the universal crossover flows in this unstable direction from the unstable to the stable fixed points.

system away from the 2CK fixed point and therefore make it highly improbable that a typical impurity could lie close enough to the critical manifold for the non-Fermi-liquid behavior to be observable. Another possible interpretation is in terms of an interstitial, vacancy or other impurity in the copper lattice structure which has a $\Gamma_3$-degeneracy. In such a situation, the relevant perturbations would only be induced by strains or other such effects; these tend to split the doublet, as discussed above.

In the copper nanoconstriction experiments the apparent Kondo temperatures are quite large, approximately $T_K \approx 10-15K$. This suggests that the impurity-electron interactions are appreciable and thus the Kondo temperature, within our model, would be the energy scale at which $\xi$ becomes large. [As seen in Section V, the RG eigenvalue of $\xi$ should be less than one. However, for not too large $V_1$ and $V_2$ a lower bound for $\xi$ is $T_K$.] Such a fast tunnelling rate suggests that a hopping process might involve either the slight rearrangement of several atoms, as this can have a lower effective mass, or a small displacement of an impurity (or impurity complex) from its central symmetric position.

In the copper nanoconstriction devices no significant deviation from the $\sqrt{T}$ temperature dependence of the impurity conductance signal has been seen down to $50mK$, the lowest temperature studied. From Eq(52) one can therefore estimate that the splitting energy scale $|M|$ would have to be less than $0.7K$, i.e. less than $0.05\xi$. In more recent experiments in $Pd$ and $V$ a larger crossover temperature of about $1.5K$ was observed, which would correspond to $M \sim 5K$, which is about $0.3T_K$. The stronger splitting in these materials might be attributed to the fact that the nanoconstrictions are more stressed than the corresponding copper devices.

In order to see whether a scenario involving impurities with triangular symmetry might be reasonable, we need a rough estimate of the magnitude of the effects of strain. To be concrete, we assume a Jahn-Teller potential, which in polar coordinates about the center of the triangle has the form

$$V_{JT}(r) = \frac{A}{2} r^2 - Br^3 \cos 3\theta + Cr^4$$

$$- \Delta r - \Delta' r^2 \cos 3\theta - e \cdot D \cdot r$$

with $e$ the strain tensor and $\Delta$ and $\Delta'$ respectively the linear and quadratic splittings due to the Jahn-Teller effect. [Note that the potential for a Jahn-Teller impurity with cubic symmetry that has a doubly degenerate ground state would have a similar form to Eq(55). In this case $r$ would be a tensor quantity, even under inversion, that parameterizes the deviations of atoms close to the impurity from their equilibrium positions.] If $r$ is measured in units of the lattice constant, $a$, then $A$, $B$, $C$ and the third rank tensor $D$ are all of order elastic energies $10^5K$. In the absence of strain, there will be three minimum energy positions of the impurity with, for $\Delta$ and $\Delta' \approx \Delta/a$ small, $r \approx r_0 \approx \Delta/A$. These will be separated by barriers of order $(r_0/a)^3 10^5K$, with comparable contributions arising from both the second and fifth terms in Eq(55). The tunnelling rate will be
\[ \mathcal{E} \sim \omega_D \sqrt{\frac{r_0}{a}} e^{-S} \]  

(56)

with \( \omega_D \) the Debye frequency and \( S \) the tunnelling action. Thus for \( \mathcal{E} \) to be about 10K, the action \( S \) cannot be very large.

The dominant effects of strain arise in two ways: first, the tunnelling rates between the three sites can become asymmetric. Since some of the barriers will be changed by of order \( eD r_0 \) from Eq (55), we see that the effective \( M \) resulting from this will be

\[ M_{\text{tunnelling}} \sim \delta \mathcal{E} \sim \mathcal{E} \frac{eD r_0}{B r_0^2} \sim \mathcal{E} \left( \frac{a}{r_0} \right)^2 \]  

(57)

which decreases with \( r_0 \). In contrast, the direct splitting from the change in energy of the minima is

\[ M_{\text{split}} \sim eD r_0 \sim e \left( \frac{r_0}{a} \right) 10^5 K, \]  

(58)

which grows with \( r_0 \). For both of these to be less than 1K, one would need \( r_0 \approx 0.1 \text{Å} \) and \( e \sim 10^{-4} \). So small a strain appears implausible in a nanoconstriction. Thus, unless an impurity configuration with anomalously weak coupling to strain or with other special properties were to exist, this explanation for the experiments of Ralph et al. \(^{14,15}\) seems unlikely.

Other possible interpretations exist, in particular, a possible explanation of the data was proposed by Wingreen et al. \(^{16}\) that involves the existence of static randomness in the neighborhood of the constriction. But overall, the interpretation of these experiments is controversial at this time.

But impurity tunnelling about symmetric positions in metals might occur in other situations. For example, it has been known for some time \(^{35,36}\) that undersized impurities often form rather stable complexes with interstitials. These complexes, in \( fcc \) lattices, form octahedral configurations. Thermally activated hopping between equivalent configurations of these complexes has been experimentally demonstrated at low temperatures in the case of dilute \( Co_x Al_{1-x} \) alloys \(^{37}\), which suggests that low barriers might exist, even though in this system the tunnelling rates are probably very low. \(^{37}\)

In conclusion, we have shown that an impurity in a metal tunnelling between positions with high symmetry—in particular, triangular symmetry—can lead to generic non-Fermi-liquid behavior, which can be characterized by the two-channel Kondo model. Symmetry breaking perturbations were shown to be partially screened, thereby reducing their effects and widening the potential temperature range for observation of the novel 2CK behavior. In addition, we have shown that by tuning a single parameter, such as pressure, the impurity behavior can change to that of a conventional Fermi liquid, but at the critical pressure the behavior would be controlled by a fixed point that is conjectured to have a higher \( SU(3) \) orbital symmetry. A detailed analysis of the behavior on and close to this critical manifold will be discussed in a future publication. \(^{33}\)

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