Instability of the marginal commutative model of tunneling centers interacting with metallic environment: Role of the electron-hole symmetry breaking

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The role of the electron-hole symmetry breaking is investigated for a symmetrical commutative two-level system in a metal using the multiplicative renormalization group in a straightforward way. The role of the symmetries of the model and the path integral technique are also discussed in detail. It is shown that the electron-hole symmetry breaking may make the model non-commutative and generate the assisted tunneling process which is, however, too small itself to drive the system into the vicinity of the two-channel Kondo fixed point. While these results are in qualitative agreement with those of Moustakas and Fisher (Phys. Rev. B 51, 6908 (1995), *ibid* 53, 4300 (1996)) the scaling equations turn out to be essentially different. We show that the main reason for this difference is that the procedure for the elimination of the high energy degrees of freedom used by Moustakas and Fisher leaves only the free energy invariant, however, the couplings generated are not connected to the dynamical properties in a straightforward way and should be interpreted with care. These latter results might have important consequences in other cases where the path integral technique is used to produce the scaling equations and calculate physical quantities.

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I. INTRODUCTION

The two-channel Kondo model originally introduced for magnetic ions with crystalline splitting and tunneling two-level systems (TLS) in metals has recently attracted broad interest. In some of those problems the orbital variables play the role of the spins of the impurity and the conduction electrons while the real spins of the conduction electrons are not dynamical variables but instead represent an extra twofold degeneracy for the conduction electrons interacting with the impurity. A TLS can be considered as a good realization of the two-channel orbital Kondo problem. Besides the fast TLS’s and the impurity ions with orbital dynamical variables mentioned before the two-channel Kondo problem can also be related to the two-impurity Kondo problem. Due to the double degeneracy of the real conduction electron spins the fixed point of these models is in the intermediate strong coupling region.

It became obvious in recent years that the breaking of the electron-hole (e-h) symmetry may result in the instability of the fixed points found in the e-h symmetric case and new fixed points might become relevant as in the two-impurity Kondo problem.

The present paper is devoted to a special class of the TLS problem, called the dissipative or commutative TLS model, where there is only one dynamical coupling to describe the electron-TLS interaction in contrary to the orbital Kondo problem (non-commutative TLS problem), where there must be at least two non-commuting interaction terms. Usually, when dealing with such impurity models an e-h symmetrical conduction electron band is assumed. Then the dissipative two-state model provides an example of marginal models in the renormalization group sense, i.e., its dynamical couplings remain unrenormalized under scaling. The main goal of the present paper is to show that the commutative model becomes unstable due to the presence of e-h symmetry breaking of a specific form, and serves as a toy model to examine the role of e-h symmetry breaking occurring in a realistic model of a TLS. As we shall see, in the presence of e-h symmetry the model has an additional symmetry which ensures the stability of the line of marginal fixed points. This problem has its own interest even if it does not play a major physical role in most of the cases of realistic systems. By developing numerical estimates, we will argue that for realistic parameters of a TLS, this effect is extremely small for metals, and can be safely neglected for practical purposes. Therefore, in case the screening interaction is not anomalously strong, the dominant mechanism making the commutative TLS model unstable will be the intrinsic assisted tunneling considered in Refs. and .

The essential effect of the e-h symmetry breaking can be demonstrated by considering the two time-ordered diagrams in Fig. . If the conduction electron is scattered by a simple potential scatterer and both diagrams provide a diverging term , but these contributions cancel each other due to e-h symmetry. That is one of the most important ingredients of the X-ray absorption problem. In case of e-h symmetry breaking the cancellation is not exact, and a non-diverging contribution remains. Such contribution may change the mathematical structure and the universality class of the theory.

To be specific, we imagine a TLS, where a heavy particle (HP) can jump between two positions in a double potential well. In general the HP can dynamically interact with the conduction electrons in two different ways (see Fig. ):

(i) The electrons try to form a screening cloud around the heavy particle. If only this interaction is taken into account then, using the logarithmic approximation, the usual e-h symmetrical model (called the dissipative or commutative TLS model mentioned above) results in a marginal theory, where the screening interaction is unrenormalized but the hopping rate of the HP is essentially reduced, because the overlap matrix element of the electronic screening clouds at neighboring positions of the HP vanishes.

(ii) The conduction electrons also assist the hopping of the HP (assisted hopping) both in the case of tunneling and virtual transitions through the excited states. If the second process (ii) is also taken into account then the couplings are not commuting in the momentum space, and the non-commutative model belonging to the class of two-channel Kondo models is recovered.

In the present paper we concentrate on case (i), where the assisted tunneling (ii) is absent in the bare hamiltonian. As mentioned above, in the original treatment of the problem one usually assumes that the local density of states is the same for each orbital channel of the conduction electrons and that it is e-h symmetrical. In a realistic case, however, these assumptions are not a priori justified.

Recently, using a path integral approach Moustakas and Fisher argued that in the commutative problem (i) the above mentioned potential scattering at the HP is relevant and changes the scaling behavior of the TLS. The possibility has been pointed out that such a potential may generate an electron assisted hopping. Such a potential is usually neglected which is certainly not justified for the case when the heavy particle is different from the atoms of the host material. (The problem of this static potential scattering has been investigated earlier by Kagan and Prokof’ev by applying the adiabatic renormalization technique.)

As we shall see both scattering on a local static potential and a realistic dispersion relation for the conduction electrons validate the previous assumptions for the local density of states, and generate process (ii). Therefore, in the
present paper we shall drop them and treat a general local density of states incorporating both mechanisms.

To investigate the relevance of the static potential and the generation of assisted tunneling two different methods will be developed. First, applying a straightforward multiplicative renormalization group method in the leading and next to leading logarithmic approximation, appropriate in the small coupling limit, we show that while the energy dependence of the local electronic spectral functions really generates the assisted tunneling term, it can be neglected in most of the cases and the commutative behavior is recovered. We also investigate the problem with a path integral technique. In the concluding section of this paper and Appendix B we discuss the ambiguity in the construction of the scaling equations derived by Moustakas and Fisher. We point out that in the path integral approach the elimination of the events with small time difference is not uniquely defined, and two procedures are possible: (i) Any events being closer to each other than a certain time difference must be replaced by a generated interaction. (ii) Only those processes must be eliminated, where electrons are involved. While both procedures leave the free energy of the HP unchanged, the couplings generated and the electronic sector behave essentially differently. We will argue that the physical argument behind the second procedure is more sound.

It is interesting to note that the first method applied by Moustakas and Fisher generates the electron-TLS coupling even in that trivial case where there is no dynamical coupling between the TLS and the conduction electrons. (This important point has also been mentioned in footnote 20 of Ref. 22). We show that the meaning and the application of these couplings to calculate real physical quantities is not straightforward, as the scaled couplings are usually plugged into formulas obtained by conventional diagram technique not directly related to the path integral method. In this way different sets of the scaled couplings lead to different measurable quantities. Thus in the path integral formalism no more than one if any scaling procedure can be appropriate to provide the correct scaled couplings to calculate physical quantities. Since the path integral technique should be also correct in the weak coupling region where the multiplicative renormalization group technique is adequate, we can decide which procedure is correct by comparing the scaling equations in this limit. We show that the second scaling procedure is the one which reproduces the dynamical behavior obtained in the next to leading logarithmic approximation. With the elimination procedure (ii) the assisted hopping is not generated by the combination of spontaneous tunneling and simple potential scattering if all the dynamical couplings are switched off.

We also show using the multiplicative renormalization group method that in the presence of e-h symmetry and without assisted tunneling the TLS-conduction electron dynamical couplings remain unrenormalized up to the next to leading logarithmic order. This also contradicts to the elimination scheme used in Refs. 21,22.

The relevance of different terms in the Hamiltonian has been discussed by Moustakas and Fisher in terms of symmetry breaking. In order to clarify the problem special emphasis will be put on these symmetries. We show that the conventional commutative TLS model without potential scattering and with an e-h symmetrical band has an additional symmetry reflecting the role of e-h symmetry. This symmetry is a combination of reflection to the middle of the TLS for the conduction electrons (but not for the tunneling HP), and the e-h symmetry, and it can be broken in different ways, e.g. by potential scattering, an asymmetrical conduction electron band, or an energy dependent coupling between the HP and the conduction electrons. (This latter, analyzed in Appendix B of Ref. 21 is closely related to the energy dependence of the local density of states, studied in the present paper.) in the Hamiltonian which do not conserve the number of right (left) electrons in the sense introduced by Moustakas and Fisher. The breaking of e-h symmetry can also be the consequence of an energy dependent coupling in agreement with the suggestion of Moustakas and Fisher. The new symmetry found guarantees that the low energy fixed point is marginal (the Hamiltonian is invariant under the scaling procedure) and no Kondo effect occurs. On the other hand if it is violated then in general the assisted tunneling is generated and the system starts to flow in the direction of the two-channel Kondo fixed point until the energy scale becomes smaller than the renormalized splitting between the two lowest states of the TLS, and the TLS dynamics is frozen out.

However, we shall see that the assisted tunneling generated in this way is very weak and usually unobservable. In fact, the numerical renormalization group study of the same problem by Libero and Oliveira in the absence of e-h symmetry does not indicate the scaling toward the intermediate coupling fixed point. This is due to the fact that
since the generated assisted tunneling is always very weak the splitting of the TLS stops the scaling before the system could approach the neighborhood of the two-channel Kondo fixed point. It will be speculated, that it can result in an observable effect only in the case of very asymmetrical band (degenerate semiconductors).

In general the question can be raised whether a spontaneous hopping process renormalized by the screening interaction between the TLS and the electrons can induce an effective assisted hopping or not. A straightforward calculation of the diagrams in Fig. 3 shows that electron assisted hopping is generated but only if the local electronic propagator breaks e-h symmetry. The simplest realization of such symmetry breaking is an asymmetric electron band or a static potential scattering at the tunneling centers. The diagram in Fig. 3 is logarithmic, but it contains an extra small factor $\Delta_0/\epsilon_F \sim 10^{-4}$, $\Delta_0$ being the amplitude of spontaneous tunneling of the TLS and $\epsilon_F$ the Fermi energy. Such processes are usually dropped in the next to leading logarithmic calculations because of the appearance of the small term $\Delta_0/D$ in these equations. The appearance of this instability can be traced back in the path integral technique and supports the legitimacy of the the second elimination scheme discussed above.

The paper is organized as follows. In Sec. II the model is introduced and the time-ordered perturbation theory is applied to demonstrate the importance of the e-h symmetry breaking and how the assisted tunneling is generated. In Sec. III the additional symmetry is introduced in the presence of e-h symmetry and it is shown how that insures the stability of the marginal fixed point. In Sec. IV the strength of the assisted tunneling generated by the breaking of the e-h and the additional symmetry is estimated. In Sec. V the results and the ambiguity in the path integral method are discussed. In Appendices A and B we calculate the amplitude of the different e-h symmetry breaking parameters and $e$ show how the scaling equations obtained in the different path integral techniques may be related by a formal transformation. Finally, in Appendix C and D we investigate the mixing of the high- and low-energy conduction electron degrees of freedom due to a simple potential scatterer and the e-h symmetry in the case of a cubic tight binding model.

II. THE MODEL AND APPLICATION OF THE TIME ORDERED DIAGRAM TECHNIQUE

First we introduce the model and the notations used closely following Ref. 22. Since the results of this Section are independent of the real spin indices of the electrons, for the sake of simplicity we drop them throughout this Section. The creation operators of the HP at site 1 and 2 are denoted by $d_1^+$ and $d_2^+$. The conduction electron annihilation operators at positions $\pm R/2$, $c_{\pm}$, can be expressed in terms of the annihilation operators for spherical waves (s-waves) with momentum $k$ at the positions $\mathbf{r} = \pm R/2$ denoted by $c_{\pm,k}$ and $c_{-k}$:

$$c_{\pm} = \int \frac{dk}{2\pi} c_{\pm,k} = \int \frac{dk}{2\pi} \int \frac{d\Omega_k}{(2\pi)^2} \exp(\pm i\mathbf{kR}/2)c_k , \quad (2.1)$$

where the $c_k$'s denote plane wave annihilation operators. Furthermore for convenience the following even and odd operators are defined:

$$c_{e,k}^+ = \frac{1}{\sqrt{N_e(k)}} (c_{+k}^+ + c_{-k}^+) ,$$ $$c_{o,k}^+ = \frac{1}{\sqrt{N_o(k)}} (c_{+k}^+ - c_{-k}^+) , \quad (2.2)$$

where the normalization constants are given by

$$N_{e,o}(k) = \frac{2k^2}{\pi} \left( 1 \pm \frac{\sin kR}{kR} \right) , \quad (2.3)$$
and the operators in Eq. (2.2) satisfy the anticommutation relations: \( \{c_{\alpha k}, c_{\beta k'}^+\} = 2\pi\delta(k - k')\delta_{\alpha\beta} \) with \( \alpha, \beta = e, o \).

The spin variables are not indicated in the above formulae. Then the Hamiltonian can be written in a concise form in terms of the operators

\[
c_{e(o)} = \int \frac{dk}{2\pi} c_{e(o),k}.
\]

Assuming a local HP-electron interaction, the Hamiltonian considered by Moustakas and Fisher can be written as

\[
H = H_0 + H_d + U,
\]

where

\[
H_0 = \int \frac{dk}{2\pi} \epsilon_k(c_{ek}^+ c_{ek} + c_{ok}^+ c_{ok}),
\]

\[
H_d = \Delta_0 (d_{1d}^+ d_2 + d_{2d}^+ d_1),
\]

\[
U = V_1 (c_e^+ c_e + c_o^+ c_o) + V_2 (c_e^+ c_o - c_o^+ c_e) + V_3 (d_1^+ d_1 - d_2^+ d_2)(c_o^+ c_o + c_e^+ c_e).
\]

Here \( \epsilon_k \) is the energy of the conduction electrons, \( \Delta_0 \) is the spontaneous tunneling rate of the HP, and the different momentum dependent couplings have been approximated by their values at the Fermi energy. The terms proportional to \( V_1 \) and \( V_2 \) describe potential scatterings while \( V_3 \) denotes the amplitude of the screening interaction. Note that in the interaction part \( U \) the constraint \( d_{1d}^+ d_1 + d_{2d}^+ d_2 = 1 \) has already been taken into account. In the case of an asymmetric double potential well there is an additional asymmetry term for the HP

\[
H_d' = \Delta^z (d_{1d}^+ d_1 - d_{2d}^+ d_2).
\]

The couplings \( V_1 \) and \( V_2 \) can be incorporated to the one-particle properties of the conduction electrons. The unperturbed one particle Green’s functions are usually defined as

\[
G_{e,k}^{(0)}(\omega_n) = G_{o,k}^{(0)}(\omega_n) = \frac{1}{i\omega_n - \epsilon_k},
\]

where the \( \omega_n \)’s denote Matsubara frequencies. Then the electronic local Green’s functions modified by the potential scattering

\[
\delta_{\alpha\beta} G_{\alpha}(\omega_n) = -\langle T\{c_\alpha^+ c_\beta\}\rangle_{\omega_n}
\]

with \( \alpha = e, o \) can be calculated easily and one obtains

\[
G_{e,o}(\omega_n) = \frac{G_{e,o}^{(0)}(\omega_n)}{1 - (V_1 \pm V_2)G_{e,o}^{(0)}(\omega_n)},
\]

where \( G_{e,o}^{(0)}(i\omega) = \int dk (i\omega - \epsilon(k))^{-1}/2\pi \). The corresponding spectral functions are given by

\[
\varrho_{e,o} = \frac{1}{\pi} \frac{\text{Im} G_{e,o}^{(0)}(\omega - i\delta)}{\left[1 - (V_1 \pm V_2)\text{Re} G_{e,o}^{(0)}(\omega - i\delta)\right]^2 + \left[(V_1 \pm V_2)\text{Im} G_{e,o}^{(0)}(\omega - i\delta)\right]^2}.
\]
Since to the lowest order in \( \omega \) the imaginary and real parts of the Green’s functions can be approximated as \( \text{Im} G_{e,o}^{(0)}(\omega - i\delta) \sim \text{const} \) and \( \text{Re} G_{e,o}^{(0)}(\omega - i\delta) \sim \omega \), from Eq. (2.13) immediately follows that in the presence of \( V_1 \) or \( V_2 \) the e-h symmetry can not hold even if the original band is symmetrical.

Now it is useful to introduce the Pauli operators

\[
\begin{align*}
  d_2^+ d_2 - d_1^+ d_1 &= \tau_z, \\
  d_2^+ d_1 + d_1^+ d_2 &= \tau_x
\end{align*}
\]  

(2.14) (2.15)

to describe the motion of the TLS, then the remaining terms to be treated are

\[
V_3 (c_e^+ c_o + c_o^+ c_e) \tilde{\tau}_z + \Delta_0 \tilde{\tau}_x .
\]  

(2.16)

To make the analogy with the two-channel Kondo model more transparent a new rotated representation of spin symmetry can not hold even if the original band is symmetrical.

That interaction has resemblance to the anisotropical Kondo Hamiltonian in an external field \( \Delta_0 \) with a single coupling \( J_z \), but with \( \varrho_e(\omega) \neq \varrho_o(\omega) \).

As we have shown above the effect of the the scattering processes \( V_1 \) and \( V_2 \) can be incorporated into the spectral functions \( \varrho_{e,o}(\omega) \), so in the following we formulate everything in terms of these quantities and drop the terms \( V_1 \) and \( V_2 \). Since these are slowly varying functions, as a first step, they can be approximated by their values at the Fermi energy. Then treating \( V_3 \) perturbatively one can notice that in the different diagrams only the combination \( (\varrho_e(0)\varrho_o(0))^{1/2} \) occurs and therefore the corresponding dimensionless coupling is given by

\[
g = (\varrho_e(0)\varrho_o(0))^{1/2} V_3 .
\]  

(2.18)

Apart from the present modification in this approximation the calculation is identical to the one in Ref. [14] Calculating the leading and the next to leading logarithmic diagrams no corrections to the invariant couplings occur as the second order vertex corrections cancel the self-energy correction part. The only relevant renormalization is due to the HP wave function renormalization which generates the renormalization of the spontaneous splitting: \( \Delta_0(\omega) = \Delta_0(\omega/D)^{N_s g^2/2} \), where \( D \) is a high energy cutoff of the order of the Fermi energy, \( \epsilon_F \), and \( N_s = 2 \) denotes the spin degeneracy of the conduction electrons.

The next question is whether the \( \omega \) dependence of \( \varrho_{e,o}(\omega) \) due to the breaking of e-h symmetry is crucial in these considerations or not. As it can be seen from Fig. the diagrams for first order vertex corrections are diagonal both in the even-odd electron channels and the TLS indices, and therefore they only renormalize \( V_1 \) and \( V_2 \). Their contribution can be estimated by approximating

\[
\varrho_{e,o}(\omega) = \varrho_{e,o}(0)(1 + \alpha_{e,o} \omega) ,
\]  

(2.19)

where \( \alpha_e \neq \alpha_o \approx 0.1 \epsilon_F^{-1} - 0.3 \epsilon_F^{-1} \). Then the logarithmic part of the diagrams in Fig. is exactly canceled and they give only a constant renormalization of the potential scattering, which can be taken into account by the redefinition of the \( \alpha_{e,o}'s \). The order of magnitude of this renormalization can be estimated as

\[
\delta(\varrho(0)V_{1,2}) \propto \varrho^2 g D \ll 1 .
\]  

(2.20)

It is important to note that the constants \( \alpha_{e,o} \) characterize the spectrum of the local low energy excitations coupled to the TLS, and they should remain unscaled under the elimination of the high energy states \( D \to D' \). This subtility
turns out to be non-trivial if one tries to simulate the e-h symmetry breaking with a potential scattering term as in Refs. 21,22 since then $\alpha \sim 1/D$ (see Appendix C). The main difficulty arises from the fact that the potential scattering strongly mixes the original low- and high-energy excitations. One could, in principle, proceed in two different ways: (a) One tries to treat the potential scattering similarly to the dynamical interaction terms and eliminates the high-energy degrees of the model without potential scattering ($D \to D'$). This procedure has been used in Refs. 21,22. Since $\alpha \sim 1/D$ this procedure obviously changes the local low-energy excitation spectrum coupled to the TLS. (b) One first diagonalizes the exactly solvable potential scattering part of the Hamiltonian to find the real low- and high-energy excitations coupled to the TLS and then eliminates the latter ones. This is the one followed throughout this paper. Some insight to the difference between these two procedures is given in Appendix C. As shown in Appendix C, due to the strong mixing of the original low-energy and high-energy degrees of freedom, procedure (a) also eliminates a fraction of the real low energy excitations (in the presence of potential scattering) coupled to the TLS, and therefore the correct procedure is the second one. The essential difference between the two elimination procedures is closely related to the fact that the mass terms (i.e. the potential scattering in our case) can never be treated at equal footing with the interaction terms in a renormalizable field theory. We also mention that elimination scheme (a) results in scaling equations which do not reproduce the perturbative results.

Let us now observe that the diagrams in Fig. 3 generate a new assisted tunneling process (ii) originally absent from the starting Hamiltonian Eq. (2.1):

$$H_{\text{assst.}} = \frac{1}{2} \Delta_1 \tau^x (c_e^+ c_e - c_o^+ c_o) = \frac{1}{2} \Delta_1 \tau^x (c_1^+ c_2 + c_2^+ c_1), \quad (2.21)$$

where the annihilation operators for the orthogonal left and right electron states $c_{1,2}$ have been defined following Ref. 22 as

$$c_{1,2} = (c_e \pm c_o)/\sqrt{2}. \quad (2.22)$$

The contributions of the diagrams in Fig. 3 to the scaling equations depend on whether the intermediate electron line is even or odd and can be calculated by rescaling the cutoff $D \to D - dD$ (see Ref. 3)

$$\Delta_0 V_3^2 \left[ \int_{D - dD}^D - \int_{-D}^{-D+dD} \right] \frac{1}{e^2} \psi_{e,o}(0)(1 + \alpha_{e,o,e}) d\epsilon, \quad (2.23)$$

and generate the following terms

$$\sim \Delta_0 V_3^2 \frac{dD}{D} \left\{ \frac{\alpha_e \alpha_e + \alpha_o \alpha_o}{2} (c_e^+ c_e + c_o^+ c_o) + \frac{\alpha_e \alpha_e - \alpha_o \alpha_o}{2} (c_1^+ c_e - c_2^+ c_o) \right\}. \quad (2.24)$$

Here the first term is a dynamical renormalization of the tunneling amplitude which commutes with the screening term $V_3$, but the second term is a generated assisted tunneling. Thus if $\alpha_e \neq \alpha_o$ then the two diagrams in Fig. 3 generate the assisted tunneling process. For $\alpha_e = \alpha_o$ the condition $\alpha_e \neq \alpha_o$ is equivalent with the one that in the site representation $c_{1,2}$ the Green’s function for the conduction electrons has also off-diagonal matrix elements. This result is in accordance with the suggestion of Moustakas and Fisher who related the appearance of the assisted tunneling to cross scattering between the electron channels ‘1’ and ‘2’ and in this way to the non zero value of the coupling $V_2$ (see Eq. (2.13)). However, as one can see from Eq. (2.24) one has a logarithmic contribution only if the electron-hole symmetry is broken in the even and odd channels in different ways, which means that this is a combination of $1 \to 2$ scattering with the e-h symmetry breaking which generates the assisted tunneling. (In the simple model of Ref. 21 the term $V_2$ generated both cross scattering between channels 1 and 2 and the e-h symmetry breaking.) Another important difference is that the term generated is proportional to
$g^2$ in contrast to the scaling equations of Refs. 21,22, where such a coupling is also generated in the $g = 0$ case, where the conduction electron sector and the HP is dynamically completely decoupled. This indicates that, although the scaling equations of Ref. 21 leave the free energy of the system invariant, the scaled couplings there have nothing to do with physically measurable quantities like the scattering amplitudes directly connected to the vertex function, and must be interpreted with care.

Thus for $\alpha_e \neq \alpha_o$, the assisted tunneling term is really generated and it makes the marginal fixed point unstable. However, its coefficient is very small as $g \sim 0.1$ and $\Delta_0/D_0 \sim 10^{-4}$, and therefore it has always been dropped in the previous calculations, even if it gives a logarithmic contribution (see Refs. 14,6). It will be shown later that this amplitude is too small to generate an assisted tunneling which brings the TLS into the vicinity of the two-channel Kondo fixed point described in the introduction when the hopping rate $\Delta_0$ is also taken into account as a lower cutoff for the scaling.

It is worth mentioning that the e-h symmetry can also be broken in the case of a constant density of states but by using different upper and lower cutoffs $D_{\text{upp}}$ and $-D_{\text{low}}$. In this case, however, the contribution is not logarithmic.

III. ANALYSIS OF THE ADDITIONAL SYMMETRY VALID FOR ELECTRON-HOLE SYMMETRY IN THE ABSENCE OF THE ELECTRON ASSISTED HOPPING $\Delta_1$

In the present section we analyze the symmetry properties of the commutative TLS problem and show that the model has an additional very restrictive symmetry related to the generation of the assisted tunneling. This symmetry is closely related to the conservation of the number of the conduction electrons in channels '1' and '2' introduced by Moustakas and Fisher.

The formulation of the e-h symmetry needs special care. In the general case the e-h symmetry does not hold exactly. There is, however, an approximate transformation nearby the Fermi surface which connects electron and hole states at the same part of the Fermi surface. In this approximate transformation the density of states is assumed to be independent of the energy and the momentum dependence of the different phase factors and wave functions is neglected, therefore it holds only in a very restrictive sense. The transformation is illustrated in Fig. 4, where a small section of the Fermi surface at the Fermi wave vector is considered.

The deviations in the normal directions at that small section are neglected and the dispersion is linearized along the normal direction. Thus the electron state with momentum $k$ and energy $E(k)$ can be characterized by a wave vector at the Fermi surface, $k_F$ and the energy $\epsilon = E(k) - E_F$:

$$k = k_F + \frac{v_F(k_F)}{|v_F(k_F)|^2} \epsilon,$$

(3.1)

where $v_F(k_F)$ is the Fermi velocity at point $k_F$. Then the e-h transformation can be written as

$$\alpha_{k_F,\epsilon} \rightarrow \alpha_{k_F,-\epsilon}^+.$$

(3.2)

In that approximation the energy independent density of states can be written as

$$\varrho_0 = \frac{1}{(2\pi)^3} \int dS_{k_F} |v_F(k_F)|^2,$$

(3.3)

where $dS_{k_F}$ is the Fermi surface element. That approximation becomes more accurate as the Fermi surface is approached. Thus a systematic expansion around the Fermi surface can be developed, where the zero order contribution is given above and the further terms can be given in terms of $\epsilon$. Such expansion has been used in the previous Section for the local density of states by introducing the $\alpha_{e,o}$ factors.
As an illustration the electron annihilation operators at ±R/2 are considered for |Rk_F| ≪ 1, thus the phase factors are slowly varying functions of ϵ. Now c_± is defined similarly to Eq. (2.1):

\[ c_± = \int \frac{dϵ}{2\pi} \int \frac{dS_{k_F}}{(2\pi)^2} \frac{1}{v(k_F)} e^{±(k_F+ω(k_F)/v^2(k_F))R/2} c_{k_F,ϵ} . \]  

(3.4)

Ignoring the ϵ-dependence of the exponent the e-h stransformation takes the simple form c_± → (c_±)^+, which combined with Eqs. (2.2) and (2.22) gives the simple form

\[ c_1 → c_2^+ . \]  

(3.5)

In the calculation of the infrared divergencies in the leading order the approximate e-h symmetry can be applied. The corrections in the sense discussed above are less divergent or even convergent due to the occurring extra powers of ϵ. Thus the above approach provides a systematic expansion in breaking of the e-h symmetry for an arbitrary Fermi surface. There are, however, special cases, where exact e-h transformations exist, e.g., for a half filled cubic tight binding model discussed in Appendix D. These transformations differ essentially from the above-discussed one as different

regions of the Brillouin zone are connected by them. In order to study the interaction first its structure must be discussed. The following combinations of the creation and annihilation operators of the HP span a complete Hilbert space, and thus are conveniently described by Pauli matrices

\[ d_1^d_1 + d_2^d_2 \leftrightarrow I = \tau^0 , \]  

(3.6)

\[ d_1^d_1 - d_2^d_2 \leftrightarrow \tau^z , \]  

(3.7)

\[ d_1^a_2 + d_2^a_1 \leftrightarrow \tau^x , \]  

(3.8)

\[ d_1^d_2 - d_2^d_1 \leftrightarrow i\tau^y , \]  

(3.9)

where I is the unit matrix. A suitable choice of a basis for the electron operator products c_1^d c_j^e (i, j = 1, 2) is:

\[ O_1 = c_1^d c_1 - c_2^d c_2 = c_1^d c_o + c_2^d c_e , \]  

\[ O_2 = \frac{1}{2} (c_1^d c_1 - c_2^d c_2) = \frac{1}{2} (c_1^d c_o - c_2^d c_e) , \]  

\[ E_1 = c_1^d c_1 + c_2^d c_2 = c_1^d c_e + c_2^d c_o , \]  

\[ E_2 = c_1^d c_2 + c_2^d c_1 = c_1^d c_e - c_2^d c_o , \]  

(3.10)

where E_i are symmetric and O_i antisymmetric under the transformation 1 ↔ 2.

Now the following assumptions are made:

(i) the interaction between the atom and the electrons is invariant under the parity transformation between left and right.

The energy of the atom at left and right positions may be different thus the tunneling atom may sit in an asymmetric potential well. The assumption (i) is obvious for the screening interaction (see the term proportional to \( V_3 \) in Eq. (2.3)) and the assisted tunneling exhibits the same invariance (see Eq. (2.22)). This symmetry poses a constraint on the possible combinations of operators in the Hamiltonian:

\[ H^x = \tau^x (V_1^x O_1 + V_2^x O_2) , \]  

(3.11)

\[ H^y = \tau^y (V_1^y E_1 + V_2^y E_2) , \]  

(3.12)

\[ H^y = \tau^y (V_1^y O_1 + V_2^y O_2) , \]  

(3.13)
and the last combination, proportional to $x^0$ is not given since it can be incorporated into the potential scattering. The $V_i^\alpha$’s ($i=1,2$, $\alpha=x,y$) are the appropriate couplings for assisted tunneling. The simplest form of the screening interaction is described by $V_i^z$, where the scattering on the atom is s-type.

We note at this point that the most general form of the Hamiltonian may contain operators which can not be expressed simply by means of the operators in Eq. (3.10) because the operators $c_1$ and $c_2$ have simple specific structure in the momentum space (see Eqs. (2.4) and (2.22)), and interactions containing more elaborate momentum dependence can not be described in terms of these operators.

A specific commutative model can be defined by adding to the general assumption (i) the followings

(ii) The electron hole symmetry holds for the kinetic energy part of the Hamiltonian: $q_1(\epsilon) = q_2(-\epsilon) = q_0(\epsilon) = q_0(-\epsilon)$.

(iii) Additional symmetry: The interaction is also symmetric under the transformation: $c_1 \leftrightarrow c_1^\dagger$, $c_2 \leftrightarrow c_2^\dagger$. As discussed above this symmetry transformation is connected to the approximate local e-h symmetry of the Fermi surface.

(iv) Time reversal symmetry, which connects the creation operators of the time reversal states $\lambda$ and $\lambda^T$, $a_{\lambda}^\dagger \rightarrow a_{\lambda^T}^\dagger$, and replaces any C-number by its complex conjugate as $c \rightarrow c^\ast$.

Assuming that the wave functions of the tunneling atom are real ($\lambda^T = \lambda$)

$$d_1^T = d_1, \quad d_2^T = d_2.$$  \hspace{1cm} (3.14)

Using the definition of time reversal symmetry for the free electron operators $(c_k)^T = c_{-k}$ and Eq. (2.1) we find that $(c_{\pm k})^T = c_{\pm k}$, and similarly $c_1^T = c_1$ and $c_2^T = c_2$.

(v) Moustakas and Fisher pointed out, that in the present case the transformation $c_1 \rightarrow e^{i\phi_1} c_1$ and $c_2 \rightarrow e^{i\phi_2} c_2$ also leaves the Hamiltonian invariant. This symmetry is connected to the conservation of the number of electrons in channels 1 and 2. It actually follows from the previously mentioned assumptions (i – iv).

For completeness we mention that in assumption (iii) the left-right transformation for the electron could be replaced by performing it in the atomic variable ($d_1 \leftrightarrow d_2$) instead of $c_1 \leftrightarrow c_2$. In that case, however, the potential well must be symmetric, thus the atomic energies must be degenerate ($\Delta^T = 0$). For symmetry (iii) only the exchange of the relative positions of the HP and the electrons are important.

As a consequence of the time reversal symmetry (iv) $V_i^z = 0$, $V_i^y = 0$ and $V_i^x = 0$. The additional symmetry (iii) rules out all the terms except those proportional to $O_1$, thus that excludes the assisted tunneling. In that way the symmetries (iii) and (iv) allow only the interaction term of coupling $V_i^z$, thus they ensure the commutativity of the model even for an asymmetric TLS Hamiltonian ($\Delta^z \neq 0$).

All the above consideration hold only for the initial Hamiltonian, but for all the renormalized vertices. Thus the commutative model remains commutative during the scaling as a consequence of symmetries (ii)–(iv), and no terms can be generated which are different from $V_i^z$, and $\Delta_0$. As also mentioned in the Introduction the elimination scheme of Moustakas and Fisher also violates this symmetry property of the Hamiltonian and generates terms even for the commutative TLS with the maximum symmetry (i)-(iv), which are not allowed.

**IV. INSTABILITY OF THE MARGINAL LINE DUE TO ELECTRON-HOLE SYMMETRY BREAKING**

It has been argued in Sec. II that the marginal line of fixed points is unstable due to breaking of the e-h symmetry. There is, however, an infrared cutoff appearing as the energy splitting $\Delta_0$ between the symmetric and antisymmetric heavy particle states as a consequence of the direct, spontaneous hopping between the left and right states. The asymmetry of the potential well $\Delta_z$ further increases that cutoff to $\Delta = (\Delta_0^2 + \Delta_z^2)^{1/2}$. Thus the same direct hopping $\Delta_0$ is responsible for the instability of the fixed point and for blocking the scaling at lower energies. It will be shown, that for a TLS with realistic parameters in metals the scaling is restricted to the neighborhood of the marginal line which is far from the two channel fixed point. In order to demonstrate this statement in this section the notation
of the TLS literature is used, which results in much more symmetrical scaling equations. With these notations the interaction part of the Hamiltonian is

\[ H_{\text{int}} = \sum_{i=0,x,y,z} \sum_{\alpha,\beta} V_i c_i^{\dagger} \sigma_{\alpha \beta}^{\dagger} c_{\beta \sigma}^{\dagger}, \]  

(4.1)

where \( \alpha, \beta = 1, 2 \) label the orbital degrees of freedom and the spin index \( \sigma \) has been restored. (Note that the matrix \( \sigma_i \) is acting in the orbital indices of the conduction electrons.) The \( V_i \)'s denote the TLS-electron couplings, and \( \sigma^0 \) denotes the unit matrix. Note that now \( V^0 \) is initially set to zero, since its effect is incorporated in the local electronic propagators. Assuming \( \rho_e(0) = \rho_o(0) = \rho_0 \) for the sake of simplicity, the dimensionless values of the couplings are defined as \( v_i = \rho_0 V_i \). This approximation is not essential, but makes the equations more transparent. These couplings of Ref. 6 can be expressed with the notations of the previous sections as \( V_z \rightarrow V_3 \), \( V_x \rightarrow \Delta_1 \) and \( V_0 \rightarrow V_1, V_2 = 0 \).

In the e-h symmetric case \( \alpha_e,\alpha_o = 0 \) the scaling equations of the next to leading logarithmic order are

\[ \frac{dv_0^0}{dx} = 0, \]  

(4.2)

\[ \frac{dv_x^0}{dx} = 4v_y v_z - 8v^z ((v^y)^2 + (v^z)^2), \]  

(4.3)

\[ \frac{dv_y^0}{dx} = 4v_z v_x - 8v^y ((v^z)^2 + (v^y)^2), \]  

(4.4)

\[ \frac{dv_y^z}{dx} = 4v_x v_y - 8v^z ((v^x)^2 + (v^y)^2), \]  

(4.5)

where \( x = \log D_0/D \) with the scaled band width \( D \), and the scaling of the splitting is described by

\[ \frac{d\Delta_0}{dx} = -8\Delta_0 ((v^y)^2 + (v^z)^2). \]  

(4.6)

(In Ref. 8 instead of notation \( \Delta_0 \) the parameter \( \Delta x = \Delta_0 \) is used.) Typical starting values of these parameters can be estimated as \( v^z \sim 0.2, v^x < 10^{-3} - 10^{-4}, v^y = 0, \Delta_0 \sim 1 - 10 K, D \sim 10^5 K \sim 10 eV \).

The breaking of e-h symmetry can be taken into account in two different ways: (i) a slope in the density of states and (ii) different lower and upper cutoff, \( D_{\text{up}} \) and \( D_{\text{down}} \). (One can also imagine a combination of the previous two cases.)

First we consider the simplest case (i). In this case the general scaling equations are quite complicated, however, in the limit \( |v^x| \gg |v^y|, |v^z| \), they can be linearized in the 'small couplings', \( \Delta_0, v^x \) and \( v^y \), and one can convince himself easily that the discussed diagrams only modify the linearized version of Eq. (4.3). Then using the result given by Eq. (2.23) and combining that with Eqs. (4.2–4.4) one gets

\[ \frac{d\Delta_0}{dx} = -8(v^z)^2 \Delta_0, \]  

(4.7)

\[ \frac{dv_x^0}{dx} = 4v_y v_z - 8v^z ((v^y)^2 + \delta \alpha \Delta_0 v^z)^2, \]  

(4.8)

\[ \frac{dv_y^0}{dx} = 4v_x v_y - 8v^z ((v^x)^2 + (v^y)^2), \]  

(4.9)

where \( \delta \alpha = \alpha_e - \alpha_o \) and \( v^z \approx \text{const} \). These linear differential equations can be easily solved and one obtains for not too large \( v^z \)'s:
\[ \Delta_0(x) = \Delta_0 \left( \frac{D_0}{D} \right)^{-8(v^*)^2} , \]  
(4.10) 

\[ v_x(x) \approx \delta \alpha \frac{v^z}{4} \Delta_0 \left( \frac{D_0}{D} \right)^{4v^z-8(v^*)^2} . \]  
(4.11)

The scaling stops when \((\Delta_0/D)(x) \sim 1\). Using the typical values given above and \(\alpha \sim 1\) (See App. A) the value of the generated coupling \(v^z\) at the freezing out of the TLS can be estimated as

\[ v_{\text{final}}^z \sim 10^{-3} - 10^{-4} , \]  
(4.12)

which is too small to give an observable effect. This situation is sketched in Fig. 5.

In the last part of this section we briefly discuss case (ii) with \(\alpha_{e,o} = 0\), \(\bar{\rho}_e(0) = \bar{\rho}_o(0)\) but with \(D_{\text{up}} \gg D_{\text{low}}\) for both the even and odd channels, which means a very asymmetrical band. In this case a two-cutoff scaling can be used. The derivation of the scaling equations can easily generalized for the case of this asymmetrical cutoff. Assuming \(D_{\text{up}} > D_{\text{low}}\) the integration now has to be carried out first for the energy range \(D_{\text{low}} < |\omega| < D_{\text{up}}\) and the couplings obtained by scaling must be then used for a symmetric model with \(D = D_{\text{low}}\) as starting values. Now the results of Sec. II can be generalized by keeping only the first part of integral (2.23). Thus the coupling \(v^z\) at \(D = D_{\text{low}}\) \((D_{\text{up}} > D_{\text{low}})\) is

\[ V^z(D = D_{\text{low}}) \sim \Delta_0(0)(V^z(0))^2 \left( \frac{1}{D_{\text{low}}} - \frac{1}{D_{\text{up}}} \right) (\rho_e(0) - \rho_o(0)) . \]  
(4.13)

As for a realistic metallic case \(D_{\text{up}} \sim D_{\text{low}} \sim 10\ \text{eV}\) and \(\rho_e(0) \sim \rho_o(0) \sim 1/D\) the corresponding dimensionless assisted tunneling can be estimated as \(v^z(D = D_{\text{low}}) \sim 10^{-6}\). That initial value is too small to be increased essentially by scaling to obtain a value at the lower cutoff the scaling \(D = \Delta_0\) which is comparable with the two channel fixed point \(v^z \approx 0.25\). Indeed using Eq. (2.17b) of Ref. 6 one obtains

\[ v^z(D = \Delta_0) = v^z(D_{\text{low}}) \cosh(4v^z x) , \]  
(4.14)

where \(x = \log(D_{\text{low}}/\Delta_0) \sim 10\), thus

\[ v^z(D = \Delta_0) \sim 6 \cdot 10^{-4} , \]  
(4.15)

which is still smaller by a factor \(\sim 10^{-3}\) then the fixed point value \(v^z \sim 0.25\). Finally it should be mentioned that the spontaneous tunneling rate \(\Delta_0\) also renormalizes downward, but not more then 1–2 orders of magnitude, and since the typical renormalized value of \(\Delta_0\) is \(\sim 1\)K the estimation (4.15) is not essentially modified by the renormalization of \(\Delta_0\).

In the discussion above it was assumed that \(D_{\text{up}}/D_{\text{low}}\) can not be very large. That is not the case of a degenerate semiconductor, as a Pb\(_{1-x}\)Ge\(_x\)Te crystal with \(x \ll 1\), where orbital Kondo effect has been observed\(^{24}\) in such a case even \(D_{\text{up}}/D_{\text{low}} \sim 100\) can be realistic and also \(\alpha\) can be present. In that case an essential strength of the assisted tunneling can be developed by scaling, even if it is negligible in the unrenormalized Hamiltonian. That problem deserves further studies.

V. CONCLUSIONS AND DISCUSSION OF THE PATH INTEGRAL TECHNIQUE

In the previous sections the instability of the commutative TLS model against the breaking of the e-h symmetry has been studied using the multiplicative renormalization group. We found that without this symmetry breaking the line \(V_x = V_y = 0\) is marginally stable.
The instability of this marginal line has been shown by Moustakas and Fisher who pointed out that the original commutative TLS model has an artificial internal symmetry, connected to the conservation of the electron numbers in the left and right channels defined in Eq. (2.22). In the present paper we have shown that the model possesses an even more restrictive additional symmetry reflecting the role of e-h symmetry. This symmetry ensures the stability of the previously mentioned marginal line in the presence of e-h symmetry and in the absence of assisted tunneling. The breaking of the e-h symmetry combined with the screening $V_z$ and the spontaneous tunneling $\Delta_0$ leads to the generation of assisted tunneling which drives the system in the direction of the two-channel Kondo fixed point where the two channels are due to the double degeneracy of the conduction electrons because of their real spin. However, as it has been shown in Sec. III, this fixed point can never be reached by the present mechanism as the driving force for the instability and the energy scale stopping the scaling are both provided by the spontaneous tunneling, $\Delta_0$.

It has also been pointed out that there is an ambiguity in the definition of the e-h symmetry transformation. Our symmetry (iii) is valid for the kinetic part of the Hamiltonian in an arbitrary system nearby the Fermi surface if the curvature of the Fermi surface and the momentum dependence of the conduction electrons’ energy are neglected, i.e., a local e-h symmetry is assumed at the Fermi surface, and the two minima of the TLS are close to each other: $Rk f \ll 1$. As pointed out, this kind of transformation can also be realized by an exact e-h symmetry transformation of a half-filled tight binding model.

We have also estimated how far the system can get from the marginal line. For a conventional metal the dimensionless measure of the e-h symmetry breaking term can be estimated to be of the order of one, $\alpha \sim 1$. Then the generated assisted tunneling at the freezing out of the TLS motion is of the order of $v_x \sim v_y \sim 10^{-3} - 10^{-4}$, which are too small to produce an observable effect and the system is still not displaying the two-channel Kondo behavior.

On the other hand, for degenerate semiconductors the high asymmetry in the lower and upper cutoffs may generate a much larger $v_x$ via $\Delta_0$, which might be responsible for the Kondo effect occurring in such materials.

The above discussion leads to the conclusion that for a TLS in an ordinary metal a strong enough initial assisted tunneling is required in addition to the Hamiltonian (2.5) to get a scaling into the intermediate vicinity of the two-channel Kondo fixed point and to have logarithmic minima in the electric resistivity. The required assisted tunneling can also be generated via virtual excitations to the excited states of the HP. The latter mechanism seems to be very promising, however, further studies are needed to check that these virtual hoppings do not generate a too large splitting $\Delta_0$ which might block the formation of the resistivity minimum.

We stress at this point that the role of $\Delta_0$ is completely different in the commutative model and the non-commutative model with $V_{\alpha}=V_{\beta} \neq 0$. In the latter case $\Delta_0$ plays basically the role of an infrared cutoff parameter in the scaling and it drives the system from a non-fermi-liquid to a fermi-liquid transition. This crossover has also been observed in recent point contact measurements, where it has also been possible to tune the crossover parameter $\sim \Delta_0$ by electron migration. This cross-over, of course, is only observable if $\Delta_0$ is not too large to stop the evolution of the non-Fermi liquid properties. We also mention that in the very strong coupling region $\Delta_0$ might become irrelevant, thereby playing again a qualitatively different role. This situation, however, is very unlikely to occur for realistic model parameters.

The present calculations support the general considerations of Moustakas and Fisher concerning the instability of the marginal line, there are, however, essential differences. The source of these differences can be due to the ambiguities in the scaling procedures based on the path integral method. Since this technique is well established in the literature, we only briefly sketch the procedure used.

In the path integral method the partition function of the system is written in an imaginary time path integral form, and is factorized as $Z = Z_1 Z_2$, where $Z_1$ involves only the screening operator $V^2$, while all the hopping terms are pushed into the second term, $Z_2$, which is calculated perturbatively in the hoppings. Following the same lines as Nozières and de Dominicis in the solution of the X-ray absorption edge problem one can integrate over the electronic degrees of freedom and obtain an effective functional for the TLS path, containing logarithmic interactions between the (spontaneous and assisted) flips of the TLS. Finally, one can generate scaling equations for the ‘fugacities’ (corresponding to the different couplings and hopping amplitudes) by reducing the high energy cutoff interoccurring in
the conduction electrons Green’s function.

The ambiguity of the path integral technique lies in the last step of the procedure, i.e. in the elimination of the high energy degrees of freedom, which corresponds to the change of a small time scale \( \tau_0 \sim 1/\epsilon_F \) in the path integral scheme.

In general two different elimination procedures can be applied:

(i) One eliminates events of any kind which are closer in the imaginary time than the cutoff \( \tau_0 \).

(ii) One eliminates only those events which are closer to each other than \( \tau_0 \) and in which electrons are involved.

Method (i) is followed by Moustakas and Fisher and in many other applications. It has been applied, e.g., for the problem of 1D disordered metals where a special scheme had to be applied to avoid artificial generation of interactions. The aforementioned case of Ref. 21 is somewhat similar. On the other hand method (ii) rather corresponds to Anderson’s poor man scaling, where the electronic heat bath is eliminated step by step via the reduction of the bandwidth cutoff \( \Delta \).

To show that method (i) delivers unphysical results let us consider the path of the TLS in Fig. 6 where a potential scattering occurs immediately after a spontaneous tunneling. Using method (i) Moustakas and Fisher replaced the event inside the box by a generated assisted tunneling interaction (see also Fig. 2 in Ref. 21). The artificial nature of this assisted tunneling is obvious since it is generated even if the dynamics of the TLS and the electrons are completely decoupled (\( v_x = v_y = v_z = 0 \)). This generated interaction, of course, can not be related to any measurable dynamical process.

The path integral method and the diagrammatic renormalization group are essentially different with respect to dynamical quantities. In the path integral approach, in principle, both methods (i) and (ii) can be followed, to calculate thermodynamical quantities even if method (i) is more frequently used. As a matter of fact in Appendix B we show that the scaling equations for the two-electron scattering obtained by methods (i) and (ii) are related by a formal transformation in the small coupling limit. The relationship between the different dynamical quantities is, however, much more complicated. To see this it is enough to consider the HP Green’s function \( D(\tau) = \langle d_1^\dagger(\tau) d_2(\tau) d_2^\dagger(0) d_1(0) \rangle \).

While this Green function is invariant under the transformation (ii), using method (i) it acquires corrections of the type \( \delta D \sim \langle d_1^\dagger(\tau) d_2(\tau) c_j^\dagger(\tau) d_2^\dagger(0) d_1(0) \rangle \) and \( \sim \langle d_1^\dagger(\tau) d_2(\tau) c_j(0) d_2^\dagger(0) d_1(0) \rangle \) already in the first step of the renormalization group \((i, j = 1, 2)\), and under the subsequent steps it becomes a very complicated object composed from different many particle propagators.

The multiplicative renormalization group, on the other hand, guarantees the invariance of the different Green’s functions. Thus the best way to choose the correct elimination procedure in the path integral technique is to compare it to the perturbative results. This comparison gives also the result that the it is method (ii) which gives the correct dynamical quantities. Therefore the scaling equations derived in Refs. 21 and 22 must be interpreted with care.

This conclusion may serve as a hint for other models where the strength of dynamical processes must be determined.

Finally, we shortly discuss the case of two-electron scattering \( \Delta_2 \). It has been raised in Refs. 21,22 that this process becomes relevant at the two-channel Kondo fixed point. While this statement seems to be correct in the highly anisotropic limit it is questionable in the strong coupling limit, where both the Bosonization approach (used in these works) and the Anderson-Yuval type scaling analysis loose their validity. On the other hand, this process has a small amplitude initially and is highly irrelevant in the weak coupling limit. This should be contrasted to the splitting of the TLS which is relevant in both the strong and weak coupling limits. Therefore, even if the two-electron scattering would be a relevant process at the Kondo fixed point, the dominant process driving away the TLS from the non-Fermi liquid fixed point will be the splitting for a realistic TLS, usually discussed in the literature.

The generation of the \( \Delta_2 \) interaction term by the e-h symmetry breaking can be analysed very similarly to that of the assisted tunneling process. Our investigations show that the generated \( \Delta_2 \) is of the order of \( v_0^2 \alpha^2 \Delta_0 \) and in the region \( v_z \leq 0.4 \) the two-electron scattering is frozen out before it acquires an observable amplitude. On the other hand the role of \( \Delta_2 \) in the strong screening case is still not completely clear and deserves further studies.

To summarize, the general conclusion of the present study is, that the breaking of the e-h symmetry may have important consequences in cases, where the e-h symmetry ensures the cancellation of some diagrams (validity of
Ward identities) and thus the stability of some fixed points. In this way, the e-h symmetry breaking may change the universality class of the problem, as it actually does in case of the two-impurity Kondo problem and in some other realizations of the two-channel Kondo problem.

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APPENDIX A: CALCULATION OF THE PARAMETERS $\alpha_{E,O}$

In the present Appendix we show that the e-h asymmetry parameters $\alpha_e$ and $\alpha_o$ are generated even in the absence of potential scattering due to band structure effects. A simple free-electron like parabolic band with mass $m$ is assumed for the electrons. The $V_3$-term of the Hamiltonian can be derived by assuming a local electron-TLS interaction and it can be written as

$$H_3 = V \left( \varrho(r/2) - \varrho(-r/2) \right) \tau^z, \tag{A1}$$

where $\varrho(r) = \psi^+(r)\psi(r)$ denotes the density of the conduction electrons and we assumed that the average potential set by the TLS for the conduction electrons has already been taken into account in the calculation of the parabolic electronic dispersion. As the field operators are taken at the atomic sites a point-like $s$-wave TLS-electron interaction is assumed. In the conventional way an upper cutoff can be introduced by using a form factor in the momentum representation which also makes the interaction non-local. The interaction part (A1) can be rewritten by using the notations $\psi_{e(o)} = \frac{1}{2} (\psi (R/2) \pm \psi (-R/2))$ as

$$H_3 = 2V (\psi_e^{\dagger}\psi_o + \psi_o^{\dagger}\psi_e), \tag{A2}$$

where the field operators can be written in a momentum representation as

$$\psi_{e(o)} = \frac{1}{(2\pi)^3} \int d^3k \left( e^{ikR/2} \pm e^{-ikR/2} \right) c_k. \tag{A3}$$

Note that these operators are different from the $c_{e,o}$ operators defined in Eq. (2.4). Then the spectral function for the Green’s function $G_{ab} = -\langle T\{\psi_a^{\dagger}\psi_b\} \rangle = \delta_{a,b}G_a$, ($a, b = e, o$) can be expressed as

$$\varrho_{e,o}(\omega) = \frac{1}{(2\pi)^3} \int d^3k \delta(\omega - \frac{k^2}{2m}) \left\{ \cos^2(\frac{kR}{2}) \right\}, \tag{A4}$$

These integrals can be easily evaluated by taking the $z$-axis parallel to $R$, and one finally obtains

$$\varrho_{e(o)}(\omega) = \frac{\varrho(\omega)}{2} \left[ 1 \pm \frac{\sin R(2m\omega)^{1/2}}{R(2m\omega)^{1/2}} \right], \tag{A5}$$
where \( g(\omega) = m^{3/2}2^{-1/2}(2\pi)^{-2}\omega^{1/2} \) is the density of states for the free electrons for one spin direction, and the factor in the bracket is related to the normalization factor \( N_{\alpha,\sigma}(k) \) given by Eq. (2.3). In Ref. 21 these factors taken at the Fermi surface are incorporated in the definition of the coupling \( V_3 \) as \( (\rho_e(\epsilon_F)\rho_o(\epsilon_F))^{1/2} \sim (1 - (\sin k_FR/k_FR)^2) )^{1/2}. \) There complete k-dependence can only be taken into account by a k-dependent coupling breaking the e-h symmetry.

Finally, from expression (A5) the \( \alpha \) parameters at the Fermi energy can easily be calculated as

\[
\alpha_{e,o} = \left( \frac{d \ln \rho_{e,o}}{d\omega} \right)_{\epsilon_F} = \frac{1}{2} \frac{1 - \cos k_FR}{1 + \sin k_FR} \epsilon_F^{-1},
\]

with \( k_F = (2m\epsilon_F)^{1/2} \). The parameters \( \alpha_{e,o} \) are of the order of \( \epsilon_F^{-1} \) and, e.g., for \( k_FR \ll 1 \) one obtains \( \alpha_e = \alpha_o/3 = 1/2 \epsilon_F^{-1} \).

APPENDIX B: CONNECTION BETWEEN THE TWO SCALING EQUATIONS OBTAINED BY THE TWO DIFFERENT PATH INTEGRAL METHODS

In this Appendix we show that there exists a simple formal correspondence between the small coupling limit of the scaling equations of Refs. 21 and 22 and those obtained by Vladár, Zimányi and Zawadowski 28. This connection is based on the artificial mixing of the TLS and conduction electron degrees of freedom.

Throughout this Appendix, for the sake of compactness, following Ref. 6 we write the Hamiltonian in the following form:

\[
H_{\text{int}} = \sum_{\mu,\sigma,\alpha,\beta} c_{\alpha\sigma}^+ V_{\alpha\beta}^{\mu} c_{\beta\sigma} \tau^\mu, \\
H_{\text{TLS}} = \sum_{i=x,y,z} \Delta^i \tau^i,
\]

(B1)

(B2)

where \( \mu = 0, x, y, z \) and the indices \( \alpha, \beta = 1, 2 \) refer to the orbital degrees of freedom of the conduction electrons. In the special case considered in Sec. IV the couplings take the simple form \( V_{\alpha\beta}^{\mu} = V^{\mu} \cdot \sigma_{\alpha\beta} \). For the conduction electrons a constant density of states \( \rho_0 \) is used for both channels \( \alpha = 1, 2 \).

Introducing the matrix notations \( \rho_0 V_{\alpha\beta}^{\mu} \rightarrow \tilde{v}_\mu \) the leading logarithmic scaling equations obtained by the multiplicative renormalization group are

\[
\frac{dv}{dx} = 0, \\
\frac{dv_i}{dx} = 2i \epsilon^{ijk} \sum_j v_j v_k, \tag{B3}
\]

with \( \epsilon^{ijk} \) denoting the Levi-Civita symbol. These equations coincide with the small coupling limit of the scaling equations of Ref. 28 obtained by using elimination scheme (ii) in Sec. V.

The new couplings corresponding to Refs. 21 and 22 can be expressed as

\[
\tilde{\tau}^\mu \tau^\mu = \left( 1 - \frac{\Delta^i}{D \tau^i} \right)^{-1/2} \rho^\mu \tau^\mu \left( 1 - \frac{\Delta^i}{D \tau^i} \right)^{-1/2}, \tag{B4}
\]

where a summation must be carried out over repeated indices. This transformation can be motivated as follows. In the high-energy region \( \omega \approx D \) the unperturbed 'dimensionless' TLS propagator \( g^{(0)}(\omega) = \omega G^{(0)}(\omega) \) can be written
as \( g(0)(D) \approx (1 - \Delta^i \tau^i / D)^{-1} \) Transformation (B4) corresponds to mixing this factor (which is part of the TLS Green’s function) into the vertex in an artificial way.

Writing out Eq. (B4) explicitly and plugging into Eq. (B3) we obtain the following scaling equations for the \( \tilde{v}^j \)’s

\[
\begin{align*}
\frac{d\tilde{v}_0}{dx} &= \frac{\tilde{v}_j \Delta^i}{D}, \\
\frac{d\tilde{v}_i}{dx} &= 2i\epsilon^{ijk} \tilde{v}_j \tilde{v}_k + \tilde{v}_0 \frac{\Delta^i}{D}. \tag{B5}
\end{align*}
\]

Replacing the simple couplings of Sec. IV into these equations and putting \( \Delta^y = \Delta^z = 0 \) one obtains exactly the expanded version of the scaling equations in Ref. 22. We note at this point as well that terms proportional to \( \sim \Delta^j / D \) give no contribution to the universal properties of the the model and can not be taken into account by a simple renormalization group procedure since they vanish in the scaling limit \( D \to \infty \), \( \varphi^j(D_{\text{ref}}), \Delta^j(D_{\text{ref}}) = \text{cst} \), \( D_{\text{ref}} \) being a reference energy scale kept constant (it can be chosen to be the Kondo temperature, e.g., in the non-commutative model). One can also show easily that the solution of the scaling equations derived from terms like \( \sim \frac{1}{D} \ln \frac{D}{\omega} \) does not reproduce the perturbative results and is inconsistent with the scaling hypothesis. Therefore the terms generated in Eq. (B5) by the transformation should vanish in the scaling limit.

**APPENDIX C: MIXING OF THE HIGH- END LOW-ENERGY STATES IN A SIMPLE POTENTIAL SCATTERING MODEL**

In this appendix we show how the original low- and high-energy degrees of freedom are mixed up by a simple potential scattering and how the elimination procedure during the renormalization group procedure should be carried out. For this purpose we investigate the simplest model possible: the scattering of spinless Fermions by a Dirac delta scatterer. In this case only s-wave scattering must be considered and the Hamiltonian can be written as

\[
H = H_0 + H_U, \tag{C1}
\]

where we assume for the sake of simplicity that the spectrum of the unperturbed Hamiltonian \( H_0 \) is given by \( \epsilon_n = \frac{2\pi}{L}(n + 1/2), \{n = -N, ..., N\}, L \) being the linear size of the system, and \( c_n^+ \) denotes the creation operator of a conduction electron with label \( n \). This assumption corresponds to a constant density of states (DOS) between the high- and low-energy cutoffs \( \pm D = \pm 2\pi N/L \).

Eq. (C1) can be diagonalized easily via the unitary transformation

\[
c_\epsilon = \sum_n \gamma(\epsilon, n) c_n, \tag{C2}
\]

where the operator \( c_\epsilon \) annihilates an electron with energy \( \epsilon \) and \( \sum_n \gamma(\epsilon, n) \gamma(\epsilon', n) = \delta_{\epsilon, \epsilon'} \). The energy spectrum is determined by the self-consistent equation

\[
1 = \frac{U}{L} \sum_n \frac{1}{\epsilon - \epsilon_n}, \tag{C3}
\]

17
Then the factors $\gamma$ can be expressed as
\[
\gamma(\epsilon, n) = \frac{U \cdot S(\epsilon)}{L} \cdot \epsilon - \epsilon_n ,
\] (C4)
where the constant $S(\epsilon)$ is determined by the unitarity condition
\[
1 = \sum_n \gamma^2(\epsilon, n) = \frac{U^2 S^2(\epsilon)}{L^2} \sum_n \frac{1}{(\epsilon - \epsilon_n)^2} .
\] (C5)
Eqs. (C3), (C4), and (C5) constitute the complete solution of the problem.

Our main purpose is to determine the exact eigenstates and the local density of states (LDOS) for the Hamiltonian above, which is given by the spectral function of the Green’s function
\[
G(\tau) = -(Tc(0, \tau)c^+(0, 0)) ,
\] (C6)
where $c(0) = (\sum_n c_n)/\sqrt{L}$. This can be easily expressed in terms of the parameters $\gamma(\epsilon, n)$ as
\[
g(\omega) = \sum_\epsilon \delta(\omega - \epsilon) \left( \sum_n \frac{1}{\sqrt{L}} \gamma(\epsilon, n) \right)^2 .
\] (C7)
The last factor in this expression is nothing but the squared of the wave function amplitude $A_\epsilon = |\psi_\epsilon(0)|^2$ of the state with energy $\epsilon$.

As one can convince himself easily from the investigation of Eq. (C3) the spectrum of the total Hamiltonian consists of $2N$ nearly equally spaced states forming a continuum with energies $-D < \epsilon < D$ and a single bound state with energy
\[
\epsilon_B = \pm D \pm \frac{2D}{e^{\pm 1/\sqrt{\rho_U}} - 1} ,
\] (C8)
where $\rho_0 = 1/2\pi$ and the ‘±’ sign refers to attractive and repulsive interactions, respectively. This bound state gives a finite contribution to $g(\omega)$ with a weight
\[
|\psi_B(0)|^2 = \frac{\pi D}{U^2} \frac{1}{\operatorname{sh}^2(\pi/U)} .
\] (C9)
While the energy spectrum of the continuum is hardly affected by the potential scattering (see Eq. (C4)), the wave function of the states at the impurity site is, and therefore the continuous part of the LDOS becomes strongly energy-dependent. The selfconsistency equations for the states in the continuum can also be solved exactly by using the identity
\[
\sum_{n=-\infty}^{\infty} \frac{1}{\epsilon - \epsilon_n} = -\frac{L}{2} \log \left( \frac{\epsilon L}{2} \right) .
\] (C10)
Then the self-consistency equation (C3) simplifies to
\[
1 = \frac{U}{2\pi} \left\{ \ln \left( \frac{D + \epsilon}{D - \epsilon} \right) - \pi \tan \left( \frac{\epsilon L}{2} \right) \right\} .
\] (C11)
In the limit \( L, N \to \infty, D = \text{cst} \) the continuous part of the spectrum is given by

\[
\varepsilon = \frac{2\pi}{L} (n + 1/2) + \frac{2}{L} \delta_n, \\
\text{ctg}\delta_n = \frac{2}{U} - \frac{1}{\pi} \ln \frac{D + \varepsilon}{D - \varepsilon},
\]

and the coefficients \( \gamma(\varepsilon, n) \) can also be determined exactly:

\[
\gamma(\varepsilon, n) = \frac{2}{L f(\varepsilon)} \frac{1}{\varepsilon - \varepsilon_n},
\]

with

\[
f(\varepsilon) = \left( \frac{1}{\pi} \ln \frac{D + \varepsilon}{D - \varepsilon} - \frac{2}{U} \right)^2 + 1 \right)^{1/2}.
\]

The wave function amplitude of the state with energy \( \varepsilon \) can also be determined in this limit:

\[
A_\varepsilon = |\psi_\varepsilon(0)|^2 = \frac{1}{L} \left[ \left( \frac{U}{2\pi} \ln \frac{D + \varepsilon}{D - \varepsilon} - 1 \right)^2 + \frac{U^2}{4} \right]^{-1}.
\]

Replacing these amplitudes into Eq. (C7) we reproduce the results of the Green’s function calculations Eq. (2.13) and one can easily calculate the parameter \( \alpha \) as well:

\[
\alpha = \frac{2U}{\pi(1 + U^2/4)} \frac{1}{D}.
\]

The calculation above reveals the origin of the e-h symmetry breaking in the local properties. Eqs. (C4) and (C16) tell us that the original high-energy states of \( H_0 \) are mixed into the true low-energy excitations of the model with potential scattering. If one tries to do the renormalization group transformation by eliminate the high-energy states of \( H_0 \) \( (D \to D') \) one immediately deforms the wave function of the true low-energy excitations and changes their coupling to the TLS drastically. This manifests in the change of their amplitude at the origin (C16) and the cutoff dependence of the parameter \( \alpha \) (C17). Therefore the correct procedure is first to diagonalize the total Hamiltonian \( H_0 + H_U \) and then eliminate the high-energy states of the model.

**APPENDIX D: THE E-H SYMMETRY ON A CUBIC TIGHT BINDING MODEL**

The half-filled cubic tight binding band shows the e-h symmetry \( c_k = -c_{-k+K} \) with \( K = (\pi/a, \pi/a, \pi/a) \). In this cubic case the lattice can be divided into two sublattices \( A \) and \( B \). The e-h transformation can be given in the site representation of the electrons’ creation and annihilation operators as \( a_i \to a_i^+ \) and \( b_j \to -b_j^+ \) \((i\epsilon A, j\epsilon B)\). If one confines artificially the positions of the TLS onto the lattice sites even the non-commutative model is invariant under the above e-h transformation combined with a left-right exchange of the electronic onsite operators similarly to Ref. [21]. This situation is similar to that of the two-impurity Kondo model.[22]

The situation is drastically changed if the tunneling atomic sites are not at the lattice points. For the sake of simplicity we assume that the the TLS sites \( \pm R/2 \) are between two neighboring lattice points labeled by \( (\pm a/2, 0, 0) \).
and the corresponding operators are denoted by $a^+$ and $b^+$, respectively. In this case the electronic field at $\pm R/2$ is a combination of the atomic orbitals at sites corresponding to $\pm a/2$. Assuming that the atomic orbitals $\psi$ are s-tyme the field operators at sites $\pm R/2$ are

$$\Psi^+(\pm R/r) = A \left[ \psi \left( \frac{|a \mp R|}{2} \right) a^+ + \psi \left( \frac{|-a \mp R|}{2} \right) b^+ \right], \quad (D1)$$

$A$ being a normalization constant. The interaction operators Eq. (2.8) and (2.21) can now be expressed in terms of $\Psi(\pm R/2)$ instead of $c_{1,2}$. If the overlap of the wave function $\psi \left( \frac{|a \mp R|}{2} \right) \psi \left( \frac{|-a \mp R|}{2} \right)$ is not neglected then the assisted tunneling part of the Hamiltonian Eq. (2.21) is not invariant under the e-h transformation but it is invariant under the left-right exchange. Thus if the positions of the tunneling atom are not on the lattice sites then only the commutative model shows the combined e-i invariance. This transformation is, however, defined differently from the one used in Sec. [II] and the difference is in the different momentum dependence of the transformation. We mention at this point that the cubic tight-binding model has a very large symmetry. Instead of the e-h transformation discussed in this Appendix one can also use an e-h transformation which connects electron and hole states at the same part of the Fermi surface, the exact analog of the symmetry transformation in Fig. [II].
FIG. 1. The two first order vertex corrections for the heavy particle (dashed line) and conduction electron (solid line) interaction. In diagrams (i) and (ii) the intermediate state contains an electron and a hole, respectively.

FIG. 2. Schematic representation of the interaction processes between the conduction electron and the HP. In the screening process (i) the atom sitting in one of the wells scatters the electron while in the assisted tunneling process (ii) the electron scattering induces the jump of the atom between the two wells.

FIG. 3. Time ordered diagrams generating the assisted tunneling process in the presence of appropriate e-h symmetry breaking. The notations are identical to those of Fig. 1. The cross indicates a spontaneous tunneling between the two positions of the HP. The labels on the electron lines refer to the even and odd parity electron channels with respect to reflection through the center of the system.

FIG. 4. (a) The electron and hole states (filled and open circles, respectively) connected by the approximate e-h transformation through the Fermi surface element $dS$. (b) Schematic of the additional symmetry of the standard TLS model consisting of an e-h transformation and a reflection through the center of the TLS in the electronic degrees of freedom.
FIG. 5. Sketch of the scaling trajectories of the TLS. The appropriate e-h symmetry breaking drives the TLS away from the marginally stable fixed line $V_x = 0$ ($\Delta_1 = 0$) towards the two-channel Kondo fixed point. The scaling is stopped by the renormalized splitting, and the final ground state is a Fermi liquid. The freezing out of the TLS is indicated by a light continuous line.

FIG. 6. The diagram resulting in the generation of artificial interaction terms in the elimination scheme (i). The heavy line represents the motion of the heavy fermion. The artificial interaction is generated by the elimination of a spontaneous tunneling event ($\Delta_0$) and a potential scattering close to it ($V_{1,2}$). The lines with arrows represent the conduction electrons.
FIG. 1. A. Zawadowski et al., "Instability of the marginal commutative model of tunneling centers..."

FIG. 2. A. Zawadowski et al., "Instability of the marginal commutative model of tunneling centers..."
FIG. 3. A. Zawadowski et al., "Instability of the marginal commutative model of tunneling centers..." 

FIG. 4. A. Zawadowski et al., "Instability of the marginal commutative model of tunneling centers..."
FIG. 5. A. Zawadowski et al., "Instability of the marginal commutative model of tunneling centers..."

FIG. 6. A. Zawadowski et al., "Instability of the marginal commutative model of tunneling centers..."