Effective low-energy description of the two impurity Anderson model: RKKY interaction and quantum criticality

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We show that the RKKY interaction in the two-impurity Anderson model comprise two contributions: a ferromagnetic part stemming from the symmetrized hybridization functions and an anti-ferromagnetic part. We demonstrate that this anti-ferromagnetic contribution can also be generated by an effective local tunneling term between the two impurities. This tunneling can be analytically calculated for particle-hole symmetric impurities. Replacing the full hybridization functions by the symmetric part and this tunneling term leads to the identical low-temperature fixed point spectrum in the numerical renormalization group. Compensating this tunneling term is used to restore the Varma-Jones quantum critical point between a strong coupling phase and a local singlet phase even in the absence of particle-hole symmetry in the hybridization functions. We analytically investigate the spatial frequencies of the effective tunneling term based on the combination of the band dispersion and the shape of the Fermi surface. Numerical renormalization group calculations provide a comparison of the distance dependent tunneling term and the local spin-spin correlation function. Derivations between the spatial dependency of the full spin-spin correlation function and the textbook RKKY interaction are reported.

I. INTRODUCTION

Using technology based on quantum-mechanical phenomena for efficient computations, requires the realization of quantum bits, which might be implemented via quantum impurity systems [1–5]. Magnetic adatoms and molecules on surfaces as well as nano-structured gate controlled devices could serve as smallest building blocks for such systems [6–19], which allows to combine the traditional electronics with novel spintronics and have been intensively studied in the last decades.

The two impurity Anderson model (TIAM) provides one of the simplest systems of two independent local moments that indirectly couple through the conduction band of the host or substrate material. It is particular interesting since it accounts for the competition of two mechanisms [20–35] that influences the magnetic properties of the ground state. For a ferromagnetic Ruderman-Kittel-Kasuya-Yosida (RKKY) [36–38] interaction $J_{RKKY}$, both impurity spins align parallel and are screened by the itinerant conduction electrons, while for strong antiferromagnetic interactions, both spins form an inter-impurity singlet which decouples from the conduction band.

This observation triggered intensive research in the 1970s and 1980 in the context of Heavy Fermions [39] since it has been suggested that this competition provides a basic understanding of this class of materials: depending on the interaction strength either a heavy Fermi liquid or an antiferromagnetically ordered ground state is found driven by the local singlet formation [40]. There is an ongoing discussion [41, 42] whether the change of ground states in a lattice system is connected to a quantum phase transition [22, 43, 44] in a two-impurity system.

The transition between these two singlet phases in the TIAM is driven by the ratio between the Kondo temperature $T_K$ and $J_{RKKY}$ [40, 44–50]. While a quantum critical point (QCP) separates both ground states in the presence of a special kind of particle-hole (P-H) symmetry [22, 43, 49], the quantum phase transition is replaced by a crossover if that symmetry is broken [51]. Including the energy dependence in the impurity coupling function generally leads to a P-H asymmetric model and, consequently, to a crossover behavior. Therefore, the QCP found by Varma and Jones [22, 43, 44] is a consequence of an oversimplification of the problem [52]. Recently, however, it has been shown [53] that for certain dispersions and distances between the impurities the TIAM exhibits a QCP, separating two orthogonal ground states with different degeneracy. This QCP is of different nature and has been experimentally observed in PTCDA-Au complexes on an Au surface [12] and is driven by the additional direct tunneling term between the two neighboring molecular orbitals [12, 53].

In this paper, we present an analytical, non-perturbative formula, based on a symmetry analysis of the parity dependent and distance dependent hybridization function, which allows to map the emerging scattering terms onto an effective tunneling $t_{eff}(\vec{R})$ between the impurities. We present a full numerical renormalization group (NRG) calculation [54–57] to prove the equivalence of the effective and the original two impurity problem.

The construction of the effective tunneling term provides a new insight to the nature of the AF contribution to the RKKY interaction. For the wide band limit we find that the AF contribution to $J_{RKKY}$ is determined by $(t_{eff})^2/U$, where $U$ denotes the Coulomb interaction. This result is contrary to a separate two step transformation: (i) a Schrieffer Wolff transformation [58] onto the two impurity Kondo model and (ii) the perturbative calculation of $J_{RKKY}$ using this two impurity Kondo
model, which would predict a $1/U^2$ dependency. The distance dependence of the effective tunneling term can explain our numerical findings, that the impurity spin-spin correlation function decays remarkably slower than the textbook expression of the RKKY interaction, even for a finite bandwidth of the conduction band. We study the spatial anisotropy of this tunneling term on a simple cubic lattice and find a surprising direct connection between slow (fast) spatial oscillations and particle (hole) doping, that is beyond the standard $2k_F$ oscillations.

The understanding of the effective tunneling term enables us to engineer the recovery of the Varma and Jones quantum critical point in the TIAM for arbitrary distances, even for a particle-hole symmetry broken model that generically only shows a continuous change of the conduction electron scattering phase. Such additional local tunneling term can also naturally occur in neighboring molecular orbitals as shown by density functional theory [12].

This paper is structured as follows. We start by defining the model, its mapping onto the parity eigenbasis and the fixed point (FP) structure of the NRG level flow in Sec. II. In Sec. III, we review the different types of P-H symmetries and derive the effective low-temperature description of the model, based on an additional spatial-dependent local tunneling term $t_{\text{eff}}(R)$. This approach is applied in Sec. IV to restore the QCP of Varma and Jones by investigating the impurity spectral functions, the scattering phase of the Green function and the NRG level flow. We also cover the finite distance and finite bandwidth corrections to the impurity spin-spin correlation function. Section V is devoted to the analytical analysis of the spatial frequencies governing the spatial anisotropy of the spin-spin correlation function in a simple cubic lattice as function of the chemical potential, and, therefore, the shape of the Fermi surface. We close with a summary in Sec. VI.

II. THEORY

A. Two Impurity Anderson Model

The Hamiltonian of the TIAM can be divided into three parts

$$H_{\text{TIAM}} = H_{\text{imp}} + H_{\text{host}} + H_{\text{hyb}}. \quad (1)$$

The impurity part is given by

$$H_{\text{imp}} = \sum_{l \in \{1,2\}, \sigma} \epsilon_l f_{l,\sigma}^\dagger f_{l,\sigma} + \frac{t}{2} \sum_{l, \sigma} f_{l,\sigma}^\dagger f_{l,\sigma}^\dagger f_{l,\sigma} + \frac{1}{2} \sum_{l \in \{1,2\}, \sigma} U_l f_{l,\sigma}^\dagger f_{l,\sigma}^\dagger f_{l,\sigma} f_{l,\sigma}. \quad (2)$$

The operator $f_{l,\sigma}^\dagger$ destroys (creates) an electron with spin $\sigma = \pm$ on impurity $l$, whose onsite energy is labeled by $\epsilon_l$. $U$ denotes the onsite Coulomb repulsion. Furthermore, we also allow for a tunneling term $t$ between both impurities. Such an hopping term is realized in a system where the local orbitals are given by the lowest unoccupied molecular orbitals of two neighboring molecule complexes that start to overlap at short distance and form dimers [12].

The metallic host is described by a free conduction band

$$H_{\text{host}} = \sum_{k, \sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma},$$

where $c_{k,\sigma}^\dagger$ is the annihilation (creation) operator of an electron in the conduction band with dispersion $\epsilon_k$. The interaction between the impurities and the host is accounted for by

$$H_{\text{hyb}} = \sum_{l \in \{1,2\}, \bar{k}, \sigma} \left( V_{lk} c_{\bar{k},\sigma}^\dagger e^{i\bar{k}R_l} f_{l,\sigma} + \text{h.c.} \right). \quad (4)$$

Here $V_{lk}$ denotes the hybridization of the impurity located at position $R_l$ with the conduction band state $\bar{k}$.

In the following, we consider the parity symmetric case, $V_{1\bar{k}} = V_{2\bar{k}} = V_{\bar{k}}, \epsilon_0^l = \epsilon_1^l = \epsilon_2^l; U_1 = U_2$, unless stated otherwise. Close to integer valence of one electron per impurity, a local moment is formed at intermediate temperatures [58] that is screened for $T \to 0$ [20, 21, 55]. This is the case for $\epsilon_0^l \approx -U/2 < 0$ and will be the main focus of this paper.

The hybridization induces an effective Heisenberg exchange interaction, the RKKY interaction, between the two impurities that alters in sign with the characteristic spatial dependency of $\cos(2k_F R)/R^d$ for $R k_F \gg 1$ with $d$ being the spatial dimension of the host, assuming a simplified energy dispersion of the conduction band.

We can also artificially add an additional direct Heisenberg exchange interaction $J_{12}\tilde{S}_1^z\tilde{S}_2^z$ to the full two impurity Hamiltonian

$$H'_{\text{TIAM}}(J_{12}) = H_{\text{TIAM}} + J_{12}\tilde{S}_1^z\tilde{S}_2^z$$

as an external control parameter for the investigation of the QCP of the Varma-Jones (VJ) type.

B. Energy representation of the TIAM Hamiltonian

It is convenient to convert to a site-dependent and energy-dependent operator [51, 54], defining

$$c_{l,\sigma}(\epsilon) = \sqrt{\frac{\pi}{\Gamma(\epsilon)}} \sum_{k} V_{k} \delta(\epsilon - \epsilon_k^l) e^{i\bar{k}R_l} c_{k,\sigma},$$

where the hybridization function $\Gamma(\epsilon)$,

$$\Gamma(\epsilon) = \pi \sum_{k} |V_k|^2 \delta(\epsilon - \epsilon_k^l)$$

(6)
is determined from the equal site anti-commutator \( \{ c_{\mu,\sigma}(\epsilon), c_{\mu,\sigma}'(\epsilon') \} = \delta_{\mu,\mu'} \delta(\epsilon - \epsilon') \).

The hybridization takes the form
\[
H_{\text{hyb}} = \sum_{\mu \in \{e,o\}, \sigma} \int_{-D}^{D} d\epsilon \sqrt{\frac{\Gamma(\epsilon)}{\pi}} f_{\mu,\sigma} c_{\mu,\sigma}(\epsilon) + h.c. \tag{8}
\]
in the continuum limit, with the bandwidth \( 2D \) of the host.

Using the effective hybridization matrix element \( V \) given by
\[
\int_{-D}^{D} d\epsilon \Gamma(\epsilon) = V^2 \pi \tag{9}
\]
we can define an effective conduction band density of states \( \rho(\epsilon) = \Gamma(\epsilon)/(\pi V^2) \).

The operators \( c_{\mu,\sigma}(\epsilon) \) are connected to the same single conduction band and are not linear independent. Therefore, they are combined to parity eigenstates [12, 20, 22, 43, 51, 59, 60] with even \( (e) \) and odd \( (o) \) parity that anti-commute by symmetry. The spatial dependence in this even-odd parity basis is included into the new orthogonal energy-dependent field operators
\[
c_{\mu,\sigma}(\epsilon) = \sqrt{\frac{\pi}{\Gamma(\epsilon)}} \sum_{k} V_k \delta(\epsilon - \epsilon_k^c) \left( e^{\frac{i\epsilon_k}{\epsilon_k}} + s_{\mu} e^{-i\frac{\epsilon_k}{\epsilon_k}} \right) c_{k,\sigma}, \tag{10}
\]
with \( \mu \in \{e,o\} \), \( \vec{R} = \vec{R}_1 - \vec{R}_2 \) and \( s_e = 1 \), \( s_o = -1 \).

The effective hybridization functions,
\[
\Gamma_e(\epsilon, \vec{R}) = \pi \sum_{k} |V_k|^2 \delta(\epsilon - \epsilon_k^c) \cos^2(\vec{k} \vec{R}/2),
\]
\[
\Gamma_o(\epsilon, \vec{R}) = \pi \sum_{k} |V_k|^2 \delta(\epsilon - \epsilon_k^c) \sin^2(\vec{k} \vec{R}/2), \tag{11}
\]
are defined such that the standard anti-commutation relation \( \{ c_{\mu,\sigma}(\epsilon), c_{\mu',\sigma'}'(\epsilon') \} = \delta(\epsilon - \epsilon') \delta_{\mu,\mu'} \delta_{\sigma,\sigma'} \) is fulfilled. They determine the effective coupling of the two different flavors even and odd to the impurity and obey
\[
\Gamma(\epsilon) = \Gamma_e(\epsilon, \vec{R}) + \Gamma_o(\epsilon, \vec{R}). \tag{12}
\]

Introducing an even/odd parity basis also for the impurity operators,
\[
f_{\mu,\sigma} = \frac{1}{\sqrt{2}} \left( f_{1,\sigma} + s_{\mu} f_{2,\sigma} \right), \tag{13}
\]
yields a flavor diagonal hybridization between the impurities and these even/odd conduction bands
\[
H_{\text{hyb}} = \sum_{\mu \in \{e,o\}, \sigma} \int_{-D}^{D} d\epsilon \sqrt{\frac{\Gamma(\epsilon, \vec{R})}{2\pi}} c_{\mu,\sigma}'(\epsilon) f_{\mu,\sigma} + h.c., \tag{14}
\]
By extracting the effective flavor coupling constant \( V_\mu \),
\[
V_\mu^2(\vec{R}) \pi = \int_{-D}^{D} d\epsilon \Gamma_\mu(\epsilon, \vec{R}) \tag{15}
\]
we define the effective density of states of the flavor bands by normalization [57, 61]
\[
\bar{\rho}_\mu(\epsilon, \vec{R}) = \frac{1}{V_\mu^2(\vec{R}) \pi} \Gamma_\mu(\epsilon, \vec{R}). \tag{16}
\]
One can always find a proper normalized \( \bar{\rho}_\mu(\epsilon, \vec{R}) \) in the limit \( \vec{R} \to 0 \): The decoupling of the odd conduction band is accounted for by \( V_o \to 0 \). To this end, the hybridization can be expressed as
\[
H_{\text{hyb}} = \sum_{\mu,\sigma} V_\mu(\vec{R}) \int_{-D}^{D} d\epsilon \sqrt{\bar{\rho}_\mu(\epsilon, \vec{R})} c_{\mu,\sigma}'(\epsilon) f_{\mu,\sigma} + h.c.,
\]
separating the coupling strength to the impurity from the energy dependency of a normalized conduction band used to construct the semi-infinite Wilson chains [20, 22, 43, 51, 59, 60]. Note that the energy dependence of \( \bar{\rho}_\mu(\epsilon) \) generally destroys P-H symmetry.

1. Low temperature fixed points

In this section we briefly review the known low-temperature FP structure of the TIAM model [20, 22, 43, 51, 57]. Since we are interested in the competition between the Kondo effect and the singlet formation due to the RKKY interaction, we focus on the regime of singly occupancy of each impurity orbital.

Starting from a single impurity Anderson model in a parameter regime where the Schrieffer-Wolff transformation [58] is applicable, the low-temperature FP is given by a strong-coupling (SC) FP describing the Kondo effect. The crossover to this FP is governed by a non-analytic energy scale \( T_K \) that is exponentially small in terms of the bar coupling constants. The local spin of the magnetic impurity is dynamically screened by the conduction electrons and the remaining conduction electron degrees of freedom decouple from the impurity. Thus the SC FP agrees with that of a free electron gas (FEG) with one electron removed that forms the Kondo singlet. The conduction electrons close to the Fermi energy acquire a phase shift of \( \delta \) in accordance with Friedel’s sum rule [62, 63].

While P-H symmetry pins the phase shift to \( \delta = \pi/2 \), P-H asymmetry leads to potential scattering in the conduction band which changes the phase shift continuously.

The SC FP is given [55, 56] by a P-H symmetric term \( H_{PH}^{SC} \)
\[
H_{PH}^{SC}(K) = H_{PH}^{SC} + K \sum_{\sigma} \left( \bar{c}_{0\sigma} \bar{c}_{0\sigma} - 1 \right) \tag{17}
\]
and a marginal operator breaking P-H symmetry that is parameterized by the constant \( K \). The operators \( \bar{c}_{n\sigma} \) annihilate an electron with spin \( \sigma \) on site \( n = 0, 1, \ldots \) of the semi-infinite Wilson chain. All other scattering terms are irrelevant. Below, we will make use of the fact that the FP is fully characterized by a single constant \( K \).
III. DERIVATION OF THE EFFECTIVE TUNNELING TERM

Now we derive an analytical counter term to the bare Hamiltonian that allows to restore the Varma-Jones QCP for arbitrary impurity distances. The naive strategy would be to add a suitable potential scattering term to the conduction electrons to restore P-H symmetry at the FP [64]. The parameter, however $K_{\mu}$ is subject to an RG flow, and it is very cumbersome to iteratively determine $K_{\mu}$. In addition, the physical insight gained from such a term is limited.

It turns out that modifying the tunneling term in $H_{\text{imp}}$ defined in Eq. (2) has the identical effect and the required $\Gamma_{\mu}^{\text{eff}}$ can be analytically derived from the coupling functions $\Gamma_{\mu}(\epsilon, \vec{R})$.

There are essential two scenarios. (i) If the impurities are P-H symmetric ($\epsilon_{\ell} = -U/2$), there is a strong symmetry restriction of the type of potential scattering counter term. In this case the low-temperature FP becomes P-H symmetric and $\delta_{\mu} = \delta_{\sigma} = \pi/2$. (ii) Local P-H asymmetry on the impurities generates potential scattering in at least one of the channels. Although we can modify these scattering terms to achieve $\delta_{\mu} = \delta_{\sigma}$, which is sufficient to restore the Varma-Jones QCP [51, 65], the scattering phases differ from $\pi/2$.

Since the parameters necessary to restore the QCP can be analytical derived only for first scenario, we start with $\epsilon_{\ell} = -U/2$ and come back to the second case latter.

A. Particle-Hole symmetry and potential scattering

We now review the connection between P-H symmetry and the arising potential scattering terms discussed by Affleck et al. [51].

The TIAM with a P-H symmetric impurity can exhibit two different types of particle-hole symmetries. The first type of P-H transformation requires a flavor diagonal transformation

$$c_{\mu,\sigma}(\epsilon) \to c_{\mu,\sigma}^{\dagger}(-\epsilon),$$

and is a symmetry of the Hamiltonian if the effective conduction bands are compatible with

$$\bar{\rho}_{\mu}(\epsilon, \vec{R}) = \bar{\rho}_{\mu}(-\epsilon, \vec{R}).$$

However, the system can also be invariant under the second, flavor exchanging P-H transformation

$$c_{\sigma/e,\sigma}(\epsilon) \to c_{\sigma/o,\sigma}^{\dagger}(-\epsilon)$$

if $V_{\mu}^{2}(\vec{R})\bar{\rho}_{\mu}(\epsilon, \vec{R})$ satisfy the relations

$$V_{\mu}^{2}(\vec{R})\bar{\rho}_{\mu}(\epsilon, \vec{R}) = V_{\sigma}^{2}(\vec{R})\bar{\rho}_{\sigma}(\epsilon, \vec{R}).$$

In general the potential scattering terms generated in higher order of perturbation theory take the form

$$H_{s} = \sum_{\mu \in \{e, o\}} \int_{-D}^{D} d\epsilon d\epsilon' \left[ S_{\mu}(\epsilon, \epsilon') c_{\mu}^{\dagger}(\epsilon) c_{\mu}(\epsilon') \right].$$

If the original problem is P-H symmetric, the effective potential scattering term must also satisfy the special type of symmetry transformation. Depending on the type of P-H symmetry, we require

- first type $\rightarrow S_{e/o}(\epsilon, \epsilon') = -S_{e/o}(-\epsilon, -\epsilon')$,
- second type $\rightarrow S_{e/o}(\epsilon, \epsilon') = -S_{o/e}(\epsilon, -\epsilon')$,

thus the scattering function must vanish at zero-energy in the presence of the first type of symmetry, whereas the second type only requires a connection between the even and odd channels:

- first type $\rightarrow S_{e/o}(0, 0) = 0$,
- second type $\rightarrow S_{e/o}(0, 0) = -S_{o/e}(0, 0)$.

Since the zero-energy scattering terms in the even and odd channels in general lead to different phase shifts $\delta_{e/o}$ and hence destroy the QCP, only the first type of P-H symmetry ensures the existence of a QCP in the TIAM automatically.
B. Low energy description and effective tunneling

Even for a P-H symmetric dispersion $\epsilon_k^c$ of the original problem, the effective densities of states $\bar{\rho}_\mu(\epsilon, \vec{R})$ defined in Eq. (16) will generally not comply with any of the two types of P-H symmetries. However, one can divide $\bar{\rho}_\mu(\epsilon, \vec{R})$ into the two contributions

$$
\bar{\rho}_\mu^{(\pm)}(\epsilon, \vec{R}) = \frac{1}{2} \left[ \bar{\rho}_\mu(\epsilon, \vec{R}) \pm \bar{\rho}_\mu(-\epsilon, \vec{R}) \right],
$$

(25)

While $\bar{\rho}_\mu^{(+)}(\epsilon, \vec{R})$ satisfies Eq. (19) and is normalized, $\bar{\rho}_\mu^{(-)}(\epsilon, \vec{R})$ has a vanishing integral spectral weight and, therefore, cannot be interpreted as an effective bath. This term breaks the P-H symmetry of first type and contributes to the scattering terms.

Consequently, the Hamiltonian of each conduction band flavor $\mu$ can be decomposed into

$$
H_{\text{host},\mu} = H^+_{\text{host},\mu} + \Delta H_{\text{host},\mu},
$$

(26)

where $H^+_{\text{host},\mu}$ describes a fictitious bath with P-H symmetry of the first type, while $\Delta H_{\text{host},\mu}$ stems from redistribution of spectral weight due to $\bar{\rho}^{(-)}_\mu(\epsilon, \vec{R})$ that can be accounted for by an appropriately chosen scattering function $S_\mu(\epsilon, \epsilon')$ in Eq. (22).

We make use of the fact [55, 56, 64] that the P-H symmetry breaking leads to a modification of the fixed point Hamiltonian controlled by a single scattering parameter $K_\mu$ in each band, such that we alternatively can approximate the host by

$$
H_{\text{host},\mu} \approx H^+_{\text{host},\mu} + K_\mu \sum_\sigma \left( \epsilon_{0,\mu,\sigma} \delta_{\mu,\sigma} - 1 \right). 
$$

(27)

If $\rho(\epsilon)$ as defined below Eq. (9) is invariant under energy inversion, i.e. $\rho(\epsilon) = \rho(-\epsilon)$, one can show that $V^2(\vec{R})\bar{\rho}^{(-)}_\mu(\epsilon, \vec{R}) = -V_d^2(\vec{R})\bar{\rho}^{(-)}_\mu(\epsilon, \vec{R})$. As a consequence $K_e = -K_\sigma$ or $K_\mu = s_\mu K_e$ and the problem is reduced to a single parameter that determines the low-temperature effect of $\bar{\rho}^{(-)}_e(\epsilon, \vec{R})$.

Now we turn to the full Hamiltonian of the TIAM that also contains the local impurity degrees of freedom and the coupling between both subsystems. An impurity interaction that is invariant under the transformation

$$
f_{e/o,\sigma} \rightarrow f_{e/o,\sigma}^\dagger \\
\Leftrightarrow \ f_{1,\sigma} \rightarrow f_{1,\sigma}^\dagger; \ f_{2,\sigma} \rightarrow -f_{2,\sigma}^\dagger,
$$

(28)

but not under the transformation

$$
f_{e/o,\sigma} \rightarrow f_{e/o,\sigma}^\dagger \\
\Leftrightarrow \ f_{1/2,\sigma} \rightarrow f_{1/2,\sigma}^\dagger,
$$

(29)

is only compatible with the second type of P-H transformation and hence inevitably generates potential scattering terms in the form of $K_e = -K_\sigma \neq 0$ in the low-energy FP that is compatible to Eq. (24). Therefore we can replace the scattering terms in Eq. (27) by an effective impurity interaction $H_{\text{eff}}^\text{imp}$ that leads to the same low-energy FP. Note that the invariance of $H_{\text{eff}}^\text{imp}$ under the transformations of Eqs. (29) ensures that the full Hamiltonian in Eq. (27) remains P-H symmetric.

The only parity-conserving single particle term involving only impurity degrees of freedoms that is invariant under local P-H transformation of the second type, Eq. (28), but not under (29) is given by

$$
H_{\text{eff}}^\text{imp} = \frac{t_{\text{eff}}}{2} \sum_\sigma \left( f_{e,\sigma}^\dagger f_{e,\sigma} - f_{o,\sigma}^\dagger f_{o,\sigma} \right)
$$

$$
\Leftrightarrow \ \frac{t_{\text{eff}}}{2} \sum_\sigma \left( f_{1,\sigma}^\dagger f_{2,\sigma} + f_{2,\sigma}^\dagger f_{1,\sigma} \right). 
$$

(30)

This term is parameterized by a single parameter $t_{\text{eff}}$ that has a simple physical interpretation: It describes an additional electron tunneling term between the two impurities and is fully compatible with $H_{\text{imp}}$. Mahmoud et al. already mentioned the existence of such an effective charge exchange in the non-interacting two impurity Anderson model on a lattice [66].

C. Estimate of effective tunneling

One of the key messages of this paper is that one can subtract an appropriately chosen local impurity counter term $H^\text{imp}_{\text{eff}}$ in order to restore the Varma-Jones QCP. It is well established [45, 51] that the QCP is destroyed only by scattering terms compatible with the P-H symmetry of the second kind, leading to different scattering phases in the even and the odd channel. The goal of the counter term is to produce identical scattering phase $\delta_e = \delta_o$ for $T, \omega \rightarrow 0$.

In order to gain some insight and actually calculate $t_{\text{eff}}$ in a certain limit, we demand that the low-temperature FP of the full model $H_{\text{TIAM}}$ augmented with a counter term $H^\text{eff}_{\text{imp}}$

$$
H_{\text{eff}}^\text{TIAM} = H_{\text{TIAM}} - H^\text{eff}_{\text{imp}}
$$

(31)

is identical to those of the effective model $H^\uparrow_{\text{TIAM}} \equiv H^\uparrow_{\text{TIAM}}$ where the full DOS $\bar{\rho}_\mu(\epsilon, \vec{R})$ has been replaced by $\bar{\rho}^{(+)}_\mu(\epsilon, \vec{R})$ of Eq. (17). If the parameters of the impurities are P-H symmetric, i.e. $\epsilon_0^f + U/2 = 0$, the scattering phases of $H^\uparrow_{\text{TIAM}}$ is distance independent and equal $\delta_e = \delta_o = \pi/2$ and likewise in $H^\text{eff}_{\text{TIAM}}$.

The phase shifts at the Fermi energy can be extracted from the local single-particle Green functions. For the full problem including the counter term, the Green function takes the form

$$
G_\mu(z, \vec{R}) = \left( z - \epsilon_0^f - \Delta_\mu(z, \vec{R}) - \Sigma_\mu^U(z) + s_\mu t_{\text{eff}} \right)^{-1}
$$

(32)
where $\Sigma^U(\varepsilon) = \Sigma^U(G)$ denotes the correlation self-energy that is given by a functional of the Green function [67], and

$$
\Delta^+(\varepsilon, \hat{R}) = V^2(\hat{R}) \int_{-D}^D d\omega \frac{\rho^{(\pm)}(\omega, \hat{R})}{\varepsilon - \omega} \quad (33)
$$

$$
\Delta(\varepsilon, \hat{R}) = \int_{-D}^D d\omega \frac{\Gamma^U(\omega, \hat{R})}{\varepsilon - \omega} = \Delta(\varepsilon, \hat{R}) = \Delta^+(\varepsilon, \hat{R}) + \Delta^-(\varepsilon, \hat{R}). \quad (34)
$$

For $T \to 0$, the spectral function always takes the form [62, 63]

$$
\rho^f(\varepsilon, \hat{R}) = \lim_{\delta \to 0^+} \frac{1}{\pi} \Im \Sigma^U(\varepsilon - i\delta, \hat{R}) = \frac{1}{\pi \Gamma(0)} \sin^2 \delta
$$

relating the scattering phase $\delta$,

$$
\cot(\delta) = \varepsilon_0^f + \Re \Delta(0) + \Re \Sigma^{U}(0) - s \Gamma^{\text{eff}}(0) \quad (35)
$$

to the ratio of the real and imaginary part of the inverse Green function [62, 63]. Note that the Fermi-liquid property $\Im \Sigma^U(0 + i\delta) = 0$ at $T = 0$ has entered as well as a coupling $|\Gamma(0)| > 0$.

In general, this a complicated problem determining $t^{\text{eff}}$ by the condition $\delta = \text{const}$. Therefore, we restrict ourselves to a locally P-H symmetric impurity $\varepsilon_0^f + U/2 = 0$ that implies a Hartree term $\Re \Sigma^U(0) = U/2$. Since $\delta = \pi/2$ independent of $\Gamma(0)$, the nominator must vanish which leads to the condition

$$
t^{\text{eff}}(\hat{R}) = 2s \rho \int_{-D}^D d\omega \frac{\tilde{\rho}(\omega, \hat{R})}{\omega}
$$

$$
= 2s \rho \Re \left( \Delta(0, \hat{R}) \right) = 2s \rho \Re \left( \Delta^-(0, \hat{R}) \right). \quad (37)
$$

In order to set the stage for the full NRG calculations below, we assume a constant DOS $\rho(\varepsilon) = \rho_0 = 1/2D$ and an isotropic linear dispersion $\varepsilon_{\hat{k}} = v_F (|\hat{k}| - k_F)$, where $v_F$ is the Fermi velocity and $k_F$ the Fermi wave-vector. The evaluation of Eq. (11) can be performed analytically [22, 43, 59, 60] for different spatial dimensions

$$
1d : V^2(\hat{R}) \rho(\varepsilon, \hat{R}) = 2 \rho_0 \left\{ 1 + s \cos \left[ \frac{Rk_F (1 + \frac{\varepsilon}{D})}{2} \right] \right\}, \quad (38)
$$

$$
2d : V^2(\hat{R}) \rho(\varepsilon, \hat{R}) = 2 \rho_0 \left\{ 1 + s J_0 \frac{Rk_F (1 + \frac{\varepsilon}{D})}{2} \right\}, \quad (39)
$$

$$
3d : V^2(\hat{R}) \rho(\varepsilon, \hat{R}) = 2 \rho_0 \left\{ 1 + s \frac{\sin \left[ \frac{Rk_F (1 + \frac{\varepsilon}{D})}{2} \right]}{Rk_F (1 + \frac{\varepsilon}{D})} \right\}, \quad (40)
$$

where $R = |\hat{R}|$ is the absolute distance between the impurities and $J_0(x)$ denotes the zeroth Bessel function of the first kind.

We defined $\Gamma_0 = V^2 \rho_0$ and plot the effective hopping parameter $t^{\text{eff}}(\hat{R})$ as function of the dimensionless distance $x/Rk_F/\pi$ for different spatial dimensions in Fig. 1.
IV. APPLICATION OF THE EFFECTIVE TUNNELING TERM

A. Study of the low temperature fixed point

The effective scattering terms generated by the P-H asymmetric densities of states \( \tilde{\rho}_a(\epsilon, \vec{R}) \) influence the fixed point spectrum of the full Hamiltonian \( H_{\text{TIA}} \) in Eq. (1). For the analysis the distance dependence of these scattering terms, we examine the fixed point properties of the full Hamiltonian \( H_{\text{TIA}} \) in Eq. (1), the P-H symmetric fraction \( H_{\text{TIA}}^+ \) in Eq. (31) and the FEG \( H_{\text{host}} \) in Eq. (3) by means of NRG [54–57] in the P-H symmetric case \( \epsilon_f + |U|/2 = 0 \).

Fig. 3 shows the low-temperature NRG FP spectrum of the full Hamiltonian as function of the dimensionless distance \( x = R k_F / \pi \) and at odd iteration for the interacting Hamiltonians and even iteration of the FEG. Since the odd conduction band decouples for \( R \to 0 \) [12, 25, 47], the level flow of \( H_{\text{TIA}} \) matches those of \( H_{\text{TIA}}^+ \) that is very different to the flow of the FEG. This FP is well understood: only one half of the local triplet state can be screened by the conduction electrons and the system remains in an underscreened Kondo fixed point [12, 25, 47, 53].

In this paper, however, we will focus on finite distances. The low temperature FP spectrum of \( H_{\text{TIA}}^+ \) at odd iterations coincides with those of the free electron gas at even iterations in contrast to those of the full Hamiltonian where the influence of the effective potential scattering terms lifts the degeneracies caused by the P-H symmetry of \( H_{\text{TIA}} \). The periodic structure of the fixed point spectrum of the full Hamiltonian as function of distance traces the oscillation of \( t_{\text{eff}}(\vec{R}) \) defined by Eq. (37) which is also added to Fig. 2 as red solid curve. Note that those distances where \( t_{\text{eff}}(\vec{R}) \) vanished, the FP spectra of \( H_{\text{TIA}} \) matches the one for the P-H symmetric free electron gas.

In order to check the accuracy of the predicted effective hopping element we need to prove that \( t_{\text{eff}}(\vec{R}) \) is able to compensate the scattering terms due to P-H asymmetry in \( \tilde{\rho}_a(\epsilon, \vec{R}) \) so that the FP spectra of \( H_{\text{TIA}} - H_{\text{imp}} \) and \( H_{\text{TIA}}^+ \) become identical. These two FP spectra are depicted in Fig. 3. The oscillations of the energy levels disappear in \( H_{\text{TIA}} - H_{\text{imp}}^{\text{eff}} \) as a consequence of the counter term \( H_{\text{imp}}^{\text{eff}} \) and both fixed point spectra coincide up to NRG discretization errors that would require a small correction of analytically calculated \( t_{\text{eff}} \) in order to obtain a perfect cancelation.

The single-particle spectral function of the impurities depicted in Fig. 4 proves the restoring of the P-H symmetry around the Fermi energy by adding the additional counter term. In the absence of the counter term, the spectral function (black line) is asymmetric and the Kondo peak is split [23, 47, 68] as can be seen in the inset of Fig. 4. By compensating the intrinsic, effective tunneling, the splitting of the Kondo resonance vanishes (light blue line).

![Figure 3](image1.png)

**FIG. 3.** Low temperature fixed point spectrum for an odd number of NRG-iterations in dependence of the dimensionless distance \( x = R k_F / \pi \) for an isotropic linear dispersion \( \epsilon_f \) in two dimensions. Comparison between the full Hamiltonian minus the effective tunneling (red line) and the symmetric fraction (blue line). NRG parameters: as in Fig. 2.

![Figure 4](image2.png)

**FIG. 4.** One particle spectral function of the impurities for different tunneling parameters and a spatial separation of \( R k_F / \pi = 0.7 \) on a two dimensional surface. The effective tunneling \( t_{\text{eff}}(R k_F / \pi = 0.7) = -1.295 t_0 \) leads to an P-H asymmetric gap formation around \( \omega = 0 \) that can be effaced with an additional hopping element \( t = -t_{\text{eff}} \). NRG parameters: as in Fig. 2 but with \( \Lambda = 2 \) and \( D/\Gamma_0 = 30 \).
B. Resorting the Varma and Jones quantum critical point

1. Local P-H symmetry on the impurities

The Varma and Jones (VJ) QCP is inevitably stable in the presence of the P-H symmetry of the first type, as becomes apparent by describing the Fermi-liquid phase in terms of the phase shifts in the even and odd channels at zero energy [51]. Making use of the symmetry transformation (18) in combination with the boundary conditions for incoming and outgoing conduction electrons

\[ e^{(t)}_{e/o} (\epsilon) = e^{(-2i\delta_{e/o})} (-\epsilon), \]  

pins the possible phase shift to \( \delta_{e/o} = 0 \) or \( \pi/2 \). As a result there is a QCP separating the Kondo-screening phase \( (\delta_{e/o} = \pi/2) \) and the inter-impurity singlet phase \( (\delta_{e/o} = 0) \), whereas absence of the P-H symmetry of the first type allows a general phase shift \( \delta_{e/o} \in [0, \pi/2] \) with a smooth crossover from 0 to \( \pi/2 \).

In the preceding section IV A we established the restoration of the P-H symmetry of the first kind in the Kondo regime \( (J_{12} \rightarrow -\infty) \) to the inter-impurity singlet regime \( (J_{12} \rightarrow \infty) \) is continuous for a generic distance such as \( R_{K} = 1.2 \) (blue lines in Fig. 5(a)) without an additional counter term.

As demonstrated by the FP spectra, the Varma-Jones QCP can be restored by adding a direct tunneling \( t^* = -t^{\text{eff}}(R) \). The level flow jumps discontinuously from one to another FP spectrum at a critical coupling \( J_{12} \) revealing clearly the QCP. Evaluating Eq. (37) for this distance yields \( t^* (R_{K}/\pi = 1.2) / \Gamma_0 \approx -0.2915 \).

Alternatively, the distance can be varied to values \( R^* \) such that \( t^{\text{eff}}(R^*) \) vanished and hence \( \cot \delta_e = \cot \delta_o = 0 \). Fig. 5(b) shows the distance dependency of the scattering phase using the model parameters of Fig. 2. We determined the shortest finite distance for which this condition is fulfilled as \( R_{K}/\pi \approx 1.30925 \). For this distance \( R^* \), we scan the FP level flow as function of \( J_{12} \) and add the results to Fig. 5(a) as solid black line. Clearly, we also find a QCP at almost the same critical value for \( J_{12} \). The inset in Fig. 5(a) resolves the very small distance dependent shift of the critical value compared to the case of the generic distance \( R_{K}/\pi = 1.2 \) with the additional counter term.

![FIG. 5. (a) Development of the low temperature fixed point spectrum with increasing antiferromagnetic inter-impurity spin exchange \( J_{12}/T_0 \) in two dimensions. A smooth crossover appears for a general P-H asymmetric Hamiltonian with \( t = 0 \) and \( t^{\text{eff}}(R) \neq 0 \) (blue lines) by contrast with a quantum phase transition for the special case \( t^* = t^{\text{eff}}(R) = 0 \) (red lines) as well as \( t = 0 \) and \( t^{\text{eff}}(R^*) = 0 \) (black lines). The inset depicts a zoom around the critical value \( J_{12}/T_0 \). (b) Scattering phase in the even and odd channels for a P-H symmetric impurity, plotted against the impurity distance. The QCP exists for \( \delta_e = \delta_o = \pi/2 \) at \( R \approx 1.30925 \). NRG parameters: as in Fig. 2 but with \( \Lambda = 2 \).](image)

2. Local P-H asymmetry on the impurities

Now we proceed to the generic case where also the local P-H symmetry on the impurities is broken but the parity remains conserved. For a fixed \( U \), the single particle energy is given by the onsite energy \( \epsilon^f = -U/2 + \Delta \epsilon \) where \( \Delta \epsilon \) parameterizes its deviation from the P-H symmetric point. Leaving \( \epsilon^f_0 = -U/2 \), the addition term

\[ H_{\Delta \epsilon} = \Delta \epsilon \sum_{\sigma} (f_{e,\sigma}^+ f_{e,\sigma} + f_{o,\sigma}^+ f_{o,\sigma}) \]  

accounts for the local P-H asymmetry on the impurities. It leads to potential scattering parameter in the form of \( K_e \neq K_o \). Since the absolute value of the scattering terms in the even and in the odd channel does not coincide, it is not possible to cancel both terms simultaneously by introducing a direct tunneling term or varying the spatial separation.

We will demonstrate that the VJ QCP can be restored by changing the low energy scattering terms such that...
they generate identical scattering phases in the even and odd channel, i.e. \( \delta_e = \delta_o \). Zhu and Varma [65] pointed out that the scattering phase acquires an additional contribution \( \Delta \delta \) in the SC FP caused by a P-H asymmetry.

Since neither \( \Delta \delta_e \) nor \( \Delta \delta_o \) is directly accessible in the NRG, we use a different strategy that is directly based on the NRG FP spectra. Close to the P-H symmetric point, the difference between the lowest single-particle excitation relative to the NRG ground state, \( E_{\mu}^1 \), with an even parity (\( \mu = e \)) and an odd parity (\( \mu = o \)),

\[
\Delta \omega_0 = E_{e}^1 - E_{o}^1,
\]

is proportional to the difference of the phase shifts.

Tuning the inter-impurity spin exchange \( J_{12} \) generically drives the system continuously from a SC to a local singlet FP and \( \Delta \omega_0 \) changes continuously. For a sharp transition, \( \Delta \omega_0 \) must vanish at the critical coupling \( J_{12}^c \)

\[
J_{12}^c = \lim_{\delta \to 0} (J_{12}^c + \delta).
\]

Note that the phase shifts at \( J_{12} = J_{12}^c \) are not defined. Since the critical value \( J_{12}^c \) is unknown apriori, it leads to the self-consistency condition:

\[
\Delta \omega_0 (\Delta \epsilon, R^*, t^*, U, J_{12}^c) = 0.
\]}

This equation is solved iteratively.

As starting point, we choose the critical value \( J_{12}^c \) for the local P-H symmetric case, i.e. \( \Delta \epsilon = 0 \). Then we compute \( \Delta \omega_0 \) as function of \( R \) (\( t \) respectively) and determine the roots for \( R_{12}^* (t) \) for constant \( t \) (\( R \) respectively). In the next step, we determine the \( J_{12}^c \) at the midpoint of the crossover regime. Inserting \( J_{12}^c \) into Eq. (46) results in new \( R_{12}^* (t) \). This steps are iterated until convergence is achieved.

Starting at the critical distance \( R_{12}^* = 1.30925 \pi/k_F \), obtained for \( \Delta \epsilon = 0, U/T_0 = 10 \), \( t/T_0 = 0 \) in Sec. IV B1, this procedure converged after four iterations to \( R_{12}^* k_F = 1.24049 \pi \) to a precision of 5 digits.

Fig. 6(a) displays the even and odd scattering phases in the last iteration, i.e. for the critical spin exchange \( J_{12}^c \), as function of the distance. This convincingly demonstrates the consistency of our approach: Fixing the last value of \( J_{12}^c \), the point of coincidence of the two scattering phases agrees perfectly with the critical \( R^* (\Delta \epsilon/T_0 = -2) k_F = 1.24049 \pi \) obtained by the iteration procedure.

In order to prove that the VJ QCP is really restored for this set of parameters, we present the FP level flow as function of the coupling \( J_{12} \) in Fig. 6(b) for the starting distance starting distance \( R_{12}^* k_F = 1.30925 \pi \) (blue lines) and the final distance \( R^* \) (black lines). While only a crossover is observed for \( R_{12}^* \), clearly the VP QCP is restored at the final distance \( R^* \) even for \( \Delta \epsilon/T_0 = -2 \). The additional term \( t_{\text{eff}} \) is not needed. Note the FP level flow in both phases: the different magnitude of the P-H symmetry breaking scattering term in both phases is clearly visible.

C. Splitting of the RKKY interaction in two contributions

The RKKY interaction between two local moments with a distance \( R \) apart is mediated by the metallic host. This effective coupling constant \( J_{\text{RKKY}} \) is distance dependent and shows the characteristic alternating signs with \( 2k_F \) oscillations – at least for a simplified dispersion of the conduction electrons.

Consequently, we can divide the RKKY interaction into two contributions with opposite signs. Extending the argument for a constant DOS [21, 59] one can show that a P-H symmetric effective DOS \( \rho^{(+)}(\epsilon) \) can only generate a ferromagnetic RKKY interaction \( J_{\text{RKKY}} \) at arbitrary distances. Hence, the antiferromagnetic contribution results from the breaking of the P-H symmetry of the first type that can be parameterized by a local \( t_{\text{eff}} \).

Decoupling of the impurities from the effective conduction electrons allows for an exact solution of this effective two impurity problem. For \( t_{\text{eff}} = 0 \), the local triplet state involving both even and odd orbital is degenerate with the singlet state given by the linear combination of both electrons in the even or both electrons in the odd state [12]. A finite \( t_{\text{eff}} \) induces an imbalance between the mixing of these singlet states and an energy gain
To illustrate that the full energy dependent TIAM can be mapped to an effective model at low energies comprising an P-H symmetric conduction band, generating the FM RKKY interaction, as well as a local hopping term, which induces the AF part $J_{RKKY}^{AF}$, the impurity spin-spin correlation function of both models, calculated by means of NRG, is shown in Fig. 7. The correlation function $\langle \vec{S}_1 \vec{S}_2 \rangle$ for $H_{\text{TIAM}}^+$ is purely positive demonstrating that the RKKY interaction $J_{RKKY}^{FM}$ for a P-H symmetric DOS can only be FM [21]. The correlation function of the effective model $H_{\text{TIAM}}^+ + H_{\text{imp}}^\text{eff}$ agrees excellently with those of the full model in the short distance regime. We discuss the corrections, which occur for larger distances due to a finite bandwidth, in the next section.

Note that there are infinitely many distances $R_n$ at which $t_{\text{eff}} = 0$, so that $J_{RKKY} = J_{RKKY}^{FM}$ holds. At these distances, the spin-spin correlation function of all models coincided, and the full energy dependent model with an additional direct spin-spin interaction $J_{12}$ exhibits the VJ QCP.

Note that the effective tunneling $t_{\text{eff}}$ which restores the P-H symmetric FP $H_{\text{TIAM}}^+ = H_{\text{TIAM}} - H(t_{\text{eff}})$, and the one that restores the FP of the full Hamiltonian out of the P-H symmetric fraction $H_{\text{TIAM}} = H_{\text{TIAM}}^+ + H(t_{\text{eff}})$, in general are not fully identical. While for a P-H symmetric FP, only the value at zero-frequency is relevant, and, consequently, Eq. (37) is exact, corrections stemming from the derivative $d\rho_{\mu}(\varepsilon)/dz$ need to be taken into account to recover the FP of the full Hamiltonian.

1. Finite bandwidth corrections

Focusing on a 1d conduction band with a linear dispersion for a moment, we noticed that the amplitude of the correlation function of the effective model $H_{\text{TIAM}}^+ + H_{\text{imp}}^\text{eff}$ will not decay for $t_{\text{eff}}$ given by Eq. (37). At the distances $R_n k_F = (2n + 1)\pi/2$, the Hamiltonian is P-H symmetric of the second type: The symmetric fraction of the effective DOS $\rho_{\mu}(R_n, \varepsilon)$ is constant and distance independent. Furthermore, the effective tunneling is given by the analytical expression

$$t_{\text{eff}}(R_n) \propto \int_{-1}^{1} \frac{\sin(R_n k_F x)}{x} dx = 2\text{Si}(R_n k_F),$$

where $\text{Si}(R_n k_F)$ is the sine integral, which is constant for large distances $\text{Si}(\infty) = \pi/2$. Apparently, the effective model cannot capture the decay of the impurity spin-spin correlation function for large distances and corrections to the effective model need to be taken into account.

To estimate the magnitude of the corrections, we analyze the resonant level model ($U = 0$), where we can derive an analytic expression for the correlation function. One can show that the correlation function is proportional to the difference of the distance dependent occupation of the even impurity orbital $n_e(R)$ and the odd

![Graph showing impurity spin-spin correlation function as function of the distance for the full TIAM Hamiltonian, for the effective model and the symmetric part $H_{\text{TIAM}}^+$. A featureless symmetric conduction band with a 2d linear dispersion has been used for the locally P-H symmetric regime for $T \to 0$. Parameters: $U/\Gamma_0 = 10$, $D/\Gamma_0 = 100$, $N_0 = 4000$, $\Lambda = 2$.](graph.png)
impurity orbital \( n_o(\vec{R}) \),
\[
\langle \langle \vec{S}_1 \vec{S}_2 \rangle \rangle^{U=0} = -\frac{3}{8} \left[ n_o(R) - n_e(\vec{R}) \right]^2 .
\tag{49}
\]
At zero temperature these occupation numbers are given by the integral of the analytically obtained spectral functions
\[
n_{\mu}(\vec{R}) = \int_{-\infty}^{0} \frac{d\omega}{\pi \pi_0} \frac{\Gamma_{\mu}(\omega, \vec{R})}{\left( \omega - \Re(\Delta_{\mu}(\omega, \vec{R})) \right)^2 + \Gamma_{\mu}^2(\omega, \vec{R})} ,
\tag{50}
\]
where the real and imaginary part of the hybridization function can be decomposed into the contributions from both symmetry types: \( \Gamma_{\mu}(\omega) = \Gamma_{\mu}^+(\omega) + \Gamma_{\mu}^-(\omega) \) and \( \Delta_{\mu}(\omega) = \Delta_{\mu}^+(\omega) + \Delta_{\mu}^-(\omega) \).

In order to derive corrections, we turn to the wide band limit. We can always find the lowest \( D \) such that \( \varepsilon_x = \varepsilon_x/D \in [-1, 1] \) defines a dimensionless band structure. From Eq. (11), it is clear that the energy dependence of \( \Gamma_{\mu}(\omega) \) and \( \Re(\Delta_{\mu}(\omega)) \) can be expressed through the dimensionless functions \( f_{\mu}(\omega/D) \) and \( F_{\mu}(\omega/D) \): \( \Gamma_{\mu}(\omega) = \Gamma_{0} f_{\mu}(\omega/D) \), \( \Re(\Delta_{\mu}(\omega)) = \Gamma_{0} F_{\mu}(\omega/D) \) and the occupation number can be written as
\[
n_{\mu}(\vec{R}) = \int_{-\infty}^{0} \frac{d\omega}{\pi \pi_0} \frac{f_{\mu}(\omega/D, \vec{R})}{\left[ f_{\mu}(\omega/D, \vec{R}) + F_{\mu}(\omega/D) \right]^2} ,
\tag{51}
\]
For fixed hybridization strength \( \Gamma_0 \), and \( \Gamma_0/D \to 0 \), the total spectral weight is located around
\[
\omega_{0,\mu} \approx \Gamma_0 F_{\mu}(0) + O \left( \frac{\Gamma_0}{D} \right) ,
\tag{52}
\]
where we can neglect the correction in the wide band limit \( D \to \infty \).

In the effective Hamiltonian, we include the contributions \( \Gamma_{\mu}^+(\omega) \) and \( \Re(\Delta_{\mu}^+(\omega)) \), and the \( \Re(\Delta_{\mu}^-(\omega)) \) only up to zero-order. In a Taylor series, the leading corrections are generated by the derivatives of these functions. Since
\[
\frac{d}{d \omega} \Re(\Delta_{\mu}^-(z)) \bigg|_{\omega=0} \propto P \int_{-1}^{1} \frac{\Gamma_{-}(x)}{x^2} dx = 0 ,
\tag{53}
\]
where \( x = \omega/D \), the leading corrections are proportional to \( \frac{d}{d \omega} \Gamma_{\mu}(\omega) \bigg|_{\omega=0} \), at least for small coupling strengths \( U/\Gamma_0 \). The distance dependence enters in \( \frac{d}{d \omega} \Gamma_{\mu}(\omega) \bigg|_{\omega=0} \) differently for different spatial dimensions, but is always proportional to \( \Gamma_0/D \). For a linear dispersion we obtain analytically
\[
1d : \quad \frac{d}{d \omega} \Gamma^{+}_{\mu}(\omega) \bigg|_{\omega=0} \propto \frac{R_{k_F} \Gamma_0}{D} ,
\tag{54}
\]
\[
2d : \quad \frac{d}{d \omega} \Gamma^{-}_{\mu}(\omega) \bigg|_{\omega=0} \propto \frac{\sqrt{R_{k_F} \Gamma_0}}{D} ,
\tag{55}
\]
\[
3d : \quad \frac{d}{d \omega} \Gamma^{-}_{\mu}(\omega) \bigg|_{\omega=0} \propto \frac{\Gamma_0}{D} .
\tag{56}
\]
In the limit case of an infinite bandwidth \( \Gamma_0/D \to 0 \), the effective tunneling determines the AFM part of the RKKY interaction on all length scales in any dimension.

These theoretical considerations are backed by a comparison of analytical calculations for the two-impurity resonant level model \( (U = 0) \) in Fig. 8 (a) and a full NRG study of the spin-spin correlation function for a finite \( U/\Gamma_0 = 10 \) in Fig. 8 (b) in 1d. Fig. 8 shows the correlation as function of \( x = (R_{k_F} \Gamma_0)/(\pi D) \) \( \propto d\Gamma_{1d,\mu}/d\omega(\omega = 0) \). In order to extract the power-law of the universal corrections, we logarithmically plot the antiferromagnetic correlation function normalized to its maximum value of \(-0.75\). Panel (a) depicts the evaluation of Eq. (49) for the resonant level model, whereas panel (b) shows the results for the TIAM with \( U/\Gamma_0 = 10, \epsilon/\Gamma_0 = -5 \) calculated using the NRG with \( N_s = 4000 \) and \( \Lambda = 3 \).
neling is nearly constant, the universality with respect to
the scaling variable \( x \) is clearly demonstrated. For \( x \to 0 \),
the correlation function approaches a finite value above
its theoretical minimum. While the correlation function
is constant for small \( x \) the corrections become clearly
visible for \( 0.1 < x \). Phenomenologically, we found that
a powerlaw fit \( \propto x^{1/4} \) agrees remarkably with the data.
Since the effective tunneling is nearly constant, only the
corrections lead to a decay, wherefore the correlation is
a universal function of the parameter that characterizes
the strength of these corrections.

2. \( U \)-dependency of the RKKY interaction

For \( \frac{d}{dw} \Gamma_i^{-}(\omega)|_{\omega=0} \ll 1 \), the corrections at large
distances are small, and \( H_{\text{TIA}} = H_{\text{TIAM}} + H_{\text{imp}}^{\text{eff}} \) is a
good approximation. Our analysis, \( J_{\text{RKKY}} \propto \frac{t_{\text{eff}}^2}{U} \),
demonstrates that the RKKY interaction should be propor-
tional to \( 1/U \) instead of the \( 1/U^2 \) dependency expected
by a separate two step transformation: (i) a Schrief-
fer Wolff transformation onto the two impurity Kondo
model and (ii) the perturbative calculation of \( J_{\text{RKKY}} \) us-
ing this two impurity Kondo model.

Fig. 9(a) depicts the local entropy of the impurities for
a 1d linear dispersion, plotted against the dimensionless
temperature \( t = T \cdot U/(t_{\text{eff}})^2 \) for the distances \( R_n \)
as defined above but a fixed ratio \( R_n k_F \Gamma_0 / D \) so that always
an AF RKKY interaction is generated. The different lines
represent different coupling strengths \( U/T_0 \) in a range of
1 < \( U/T_0 < 60 \). The FP spectra of the NRG level flow
discerns the three regimes \( J_{\text{RKKY}} > T_K \) (black line)
and \( J_{\text{RKKY}} < T_K \) (blue lines). In the upper panel of
Fig. 9(a) the corrections can be neglected, \( R_n k_F \Gamma_0 / D \pi =
0.0075 \), and the universal crossover of the entropy proves
that \( J_{\text{RKKY}} \propto \frac{(t_{\text{eff}})^2}{U} \).

This simple scaling does not hold for a larger
\( R_n k_F \Gamma_0 / D \pi = 0.05 \) as demonstrated in the lower panel
of Fig. 9(a). Since the crossover to a local singlet should still
occur at a temperature scale \( J_{\text{RKKY}} \) the energy curves
suggest a modification from the \( 1/U \) behavior.

In order to shed some light on the \( U \) dependency of
\( J_{\text{RKKY}} \), we calculated the crossover temperature \( T_{\text{RKKY}} \)
as a function of \( U/T_0 \). \( T_{\text{RKKY}} \) is defined as the tem-
perature where the Entropy \( S_{\text{imp}} \) has reached the value
\( S_{\text{imp}}(T_{\text{RKKY}}) = \frac{1}{2} \ln(4) = \ln(2) \). Fig. 9(b) shows
\( T_{\text{RKKY}} \cdot (U/T_0)^{\frac{1}{2}} \) as function of the coupling strength \( U/T_0 \)
for different values of \( \frac{R_n k_F \Gamma_0}{\pi D} \).

The linear increase of the curves for small \( U \) proves the \( 1/U \) dependency.
For very large \( U \), the curves approach a constant. In this
regime, \( J_{\text{RKKY}} \propto 1/U^2 \) in accordance with the Schrief-
fer Wolff transformation onto the TIKM. The crossover
from a charge fluctuation driven \( J_{\text{Kondo}} \propto 1/U \) to a
Kondo interaction driven \( J_{\text{RKKY}} \propto J^2 \propto 1/U^2 \) does not
only depend on \( U \) but is also strongly influenced by ra-
tio \( R_n k_F \Gamma_0 / D \pi \). Consequently, the replacement of
the TIAM by the TIKM is distance dependent and requires
more care than just investigating the local regimes.

In case of a linear dispersion in 3d, the corrections
(56) are \( R \)-independent and the amplitude of \( t_{\text{eff}} \) always
decays as function of \( R \). Fig. 10 (a) shows a comparison
of \( J_{\text{RKKY}} \) calculated by the textbook expression which
can be found in the appendix A of Ref. [59] as black line
with \( (t_{\text{eff}})^2 \) as light blue line. While the envelope function
of \( J_{\text{RKKY}} \) decays as \( R^{-3} \) as expected from the analytical
formula, \( (t_{\text{eff}})^2 \cdot R^3 \) is increasing with distance for small
\( R \). Consequently, \( J_{\text{Kondo}} \propto (t_{\text{eff}})^2 \) decays as \( R^{-2} \) in
the wide band limit for \( U/D \ll 1 \) in contrary to the expected
\( R \) dependency of \( J_{\text{RKKY}} \).

While \( J_{\text{RKKY}} \) describes an effective spin-spin interac-

\[
\mathbf{\Gamma_{\text{0}}^{\text{AF}}} = \frac{\pi D}{R_{\text{kF}}} \Gamma_{\text{0}}^{\text{AF}} \quad \frac{\pi D}{R_{\text{kF}}} \Gamma_{\text{0}}^{\text{AF}} \quad \frac{\pi D}{R_{\text{kF}}} \Gamma_{\text{0}}^{\text{AF}} \quad \frac{\pi D}{R_{\text{kF}}} \Gamma_{\text{0}}^{\text{AF}} \]

\[
\ln(4) = \ln(2) \quad \ln(4) \quad \ln(4) \quad \ln(4) \]

\[
J_{\text{RKKY}} < T_K \quad J_{\text{RKKY}} < T_K \quad J_{\text{RKKY}} > T_K \quad J_{\text{RKKY}} > T_K
\]

\[
U/T_0 \in [1, 60] \quad U/T_0 \in [1, 60] \quad U/T_0 \in [1, 60] \quad U/T_0 \in [1, 60]
\]
tion in an effective local moment Hamiltonian, the $R$-dependence of the spin-spin correlation function is a different property that is governed by the competition between the Kondo screening and the RKKY interaction. Fig. 10(b) depicts $(\vec{S}_1 \cdot \vec{S}_2) R^3$ in the TAIM for moderate values of $U/\Gamma_0$ (blue and grey curve with points). For a better comparison of the decay of the envelope function, we normalized $(\vec{S}_1 \cdot \vec{S}_2) (R)$ at $R_{K} = \pi$, where the correlations are AF, thus positive values belong to AF correlations.

The $R$ dependence of $\epsilon^*_{\text{eff}}$ governs the physics in the wide-band limit and for small $U/\Gamma_0$ (dashed bline in Fig. 10(b)). For $U \rightarrow 0$ the analytic equation (49) proves that the spin-spin correlation function is purely AF, whereas the sign of $J_{\text{RKKY}}$ always oscillates with the distance. With increasing $U/\Gamma_0$, the FM correlations emerge continuously from the purely AF function and the power-law decay of the correlation function seems to cross from those of $(\epsilon^*_{\text{eff}})^2$ over to those of $J_{\text{RKKY}}$ for $U/\Gamma_0 \rightarrow \infty$. Note that we can not resolve this weak coupling regime using the NRG, since the numerical noise is rapidly amplified by the $R^3$ scaling for $U/\Gamma_0 > 15$. We added $(\vec{S}_1 \cdot \vec{S}_2)$ calculated for the two-impurity Kondo model with a Kondo coupling $\rho_{JK} = 0.25$ as a solid black line in Fig. 10(b). Just like small $U/\Gamma_0$ in the Anderson model, large Kondo couplings such as $\rho_{JK} = 0.25$ lead to a supression of the FM correlations due to the Kondo effect [70] and a slower decay as $J_{\text{RKKY}}$, at least in the small distance regime.

V. SIMPLE CUBIC LATTICE

The RKKY interaction has been investigated for more than 60 years and it is well established, that the anisotropy caused by the lattice of the host has a strong influence on the RKKY interaction [71–76]. However, for a large Kondo-coupling $J_K$ and small $U/\Gamma_0$ respectively, the Kondo effect has a strong influence on the spin-spin correlation function and the textbook expression for the RKKY interaction is not sufficient to describe the magnetic order [70]. Therefore, the effective tunneling for an non spherical band dispersion $\epsilon_{\vec{k}}$ provides additional insight to established knowledge on the RKKY interaction.

In this section, we exemplify this by focusing on the well studied simple cubic lattice with lattice spacing $a$ at half band filling. The dispersion $\epsilon_{\vec{k}}$ in $d$ dimensions takes the form

$$\epsilon_{\vec{k}} = -\frac{D}{d} \sum_{\alpha=1}^{d} \cos(k_{\alpha} a).$$

(57)

Defining a nesting wave vector $\vec{Q}$ and the reciprocal lattice vectors $\vec{G}_{\alpha}$

$$\vec{Q} = \frac{\pi}{a} \sum_{\alpha=1}^{d} \epsilon_{\alpha}, \quad \vec{G}_{\alpha} = \frac{2\pi}{a} \epsilon_{\alpha},$$

(58)

which satisfy the relations $\epsilon_{\vec{k}+\vec{Q}} = -\epsilon_{\vec{k}}$ and $\epsilon_{\vec{k}+\vec{G}_{\alpha}} = \epsilon_{\vec{k}}$, we can always find a bijection $f : 1.Bz. \rightarrow 1.Bz., \vec{k} \rightarrow \vec{k}'$, for which $\epsilon_{\vec{k}'} = -\epsilon_{\vec{k}}$

$$f(\vec{k}) = \vec{k}' = \vec{k} + \vec{Q} + \sum_{\alpha=1}^{d} z_{\vec{k},\alpha} \vec{G}_{\alpha}, \quad z_{\vec{k},\alpha} \in \{\pm 1, 0\}.$$  

(59)

Using this mapping, we analyze the effective densities of states with respect to inversion symmetry in energy space as well as P-H symmetry:

$$\Gamma_{\epsilon}(\epsilon, \vec{R}) = \pi V^2 \sum_{\vec{k}'} \delta(\epsilon - \epsilon_{\vec{k}'}) \cos^2 \left(\vec{k}' \cdot \vec{R}/2 - \Phi/2\right),$$

$$\Gamma_{\epsilon}(\epsilon, \vec{R}) = \pi V^2 \sum_{\vec{k}'} \delta(\epsilon - \epsilon_{\vec{k}'}) \sin^2 \left(\vec{k}' \cdot \vec{R}/2 - \Phi/2\right).$$

(60)

Due to the additional phase $\Phi/2$,

$$\Phi = (\vec{Q} + \sum_{\alpha=1}^{d} z_{\vec{k},\alpha} \vec{G}_{\alpha}) \vec{R}.$$
the hybridization function is P-H symmetric ($\phi = n\pi$) for $R_\alpha/a \in \mathbb{Z}$ only. We can distinguish between the two different types of symmetries in the following way [51]:

\[
\begin{align*}
\sum_{\alpha=1}^{d} R_\alpha &= 2na & \rightarrow & \text{first type} \quad (62) \\
\sum_{\alpha=1}^{d} R_\alpha &= (2n+1)a & \rightarrow & \text{second type} \quad (63)
\end{align*}
\]

Since the two types of P-H symmetry generate a contribution to the RKKY interaction with opposite sign, this result is equivalent to the general RKKY oscillations on a bipartite lattice at half filling [77]. Moreover, the effective tunneling vanishes for impurities placed on the same sub-lattice.

### A. Two-dimensional lattice at half filling

Fig. 11(a) shows the square of the effective hopping element in two dimensions, color-coded as function of the impurity distance $\vec{R} = (R_x, R_y)$. The periodic structure in the two-dimensional plane indicate the importance of well-defined momenta in k-space that govern the RKKY interaction in real space.

In order to gain an analytical insight of the anisotropic structure, we rewrite the effective tunneling of Eq. (37) as a sum over the Brillouin zone

\[
t^{\text{eff}}(\vec{R}) = \gamma \cdot s_\mu \sum_{\vec{k} \not\in \text{FS}} \frac{1 + s_\mu \cos(\vec{k} \cdot \vec{R})}{\epsilon_\vec{k}} ,
\]

excluding the Fermi surface (FS) which does not contribute to the principle value integral. All distance independent constants are merged into the constant $\gamma$.

In a second step, we perform a Fourier transformation into k-space

\[
t^{\text{eff}}(\vec{q}) = \gamma \int d^2R \sum_{\vec{k} \not\in \text{FS}} e^{i\vec{q} \cdot \vec{R}} \cos(\vec{k} \cdot \vec{R}) \epsilon_\vec{k} = \begin{cases} \frac{\gamma}{\pi}, & \vec{q} \not\in \text{FS} \\ 0, & \vec{q} \in \text{FS} \end{cases}
\]

(65)

exploiting the fact that the distance independent part vanishes by symmetry for a P-H symmetric conduction band. For inversion symmetric dispersion, $\epsilon_\vec{k} = \epsilon_{-\vec{k}}$, $t^{\text{eff}}(\vec{q})$ obeys the relation

\[
t^{\text{eff}}(\vec{q}) = t^{\text{eff}}(-\vec{q}) \quad (66)
\]

and for P-H symmetry of the conduction band, the condition

\[
t^{\text{eff}}(\vec{R} = 0) = \int_{-\infty}^{\infty} t^{\text{eff}}(\vec{q})d\vec{q} = 0 \quad (67)
\]

must hold.

The largest contribution to the $k$-summation in Eq. (65) is generated at the anti-nodal points of the dispersion $\epsilon_\vec{k}$, located at $\vec{p}_{1/2} = \pm(0, \pi/a)$ and $\vec{l}_{1/2} = \pm(\pi/a, 0)$, and we can approximate the Fourier transformation $t^{\text{eff}}(\vec{q})$ by a sum of $\delta$-functions

\[
t^{\text{eff}}_{\text{anti-nodal}}(\vec{q}) \propto \sum_{i=1,2} \left[ \delta(\vec{q} + \vec{p}_i) - \delta(\vec{q} + \vec{l}_i) \right] \quad (68)
\]

with an appropriate prefactor that is independent of $\vec{q}$.

This simplified expression can be transformed back into real space. Along the direction $\vec{n} = \vec{R}/R = |\vec{R}|$, $t^{\text{eff}}_{\text{anti-nodal}}(\vec{R})$ is given by a product of modulations,

\[
t^{\text{eff}}_{\text{anti-nodal}}(\vec{R}) \propto \sin(Rk_{F,+}^x) \sin(Rk_{F,-}^x) .
\]

(69)

govern by the two characteristic spatial frequencies

\[
k_{F,\pm}^x = \frac{\pi}{2a} |n_x \pm n_y|.
\]

(70)

Along the basis vector direction $\vec{n} = \vec{\epsilon}_\alpha$, the frequencies are identical and the sign of the effective tunneling remains positive.
Within this anti-nodal point approximation, the amplitude of the oscillating effective hopping remains constant. This provides a better understanding why full $t^{\text{eff}}(\vec{R})$ plotted in Fig. 11(b) does not decay as function of the distance $\vec{R}$ and explains the different oscillation frequency in the different spatial directions.

To illustrate the quality of the approximation, a comparison between the full $t^{\text{eff}}(\vec{R})$ and the approximative quantity $t^{\text{eff}}_\text{anti-nodal}(\vec{R})$ obtained from Eq. (69), is shown for a more generic direction $\vec{n} = \frac{1}{\sqrt{65}}(\vec{e}_1 + 8\vec{e}_2)$ in Fig. 12. The plot demonstrates that the oscillations of the AF contribution to the RKKY interaction are determined by $k_{\text{FS}}^{\pm}$. We also added the spatial dependency of the impurity spin-spin correlation function along the same direction as grey dotted curve to Fig. 12 illustrating that the sin changes and the oscillatory behavior tracks the spatial dependency of $t^{\text{eff}}$.

Since $k_{\text{F}}^{\pm}$, and with that Eq. (69), vanishes along the diagonal $r_x = r_y$, the AF contributions cannot originate from the anti-nodal points $\vec{l}_{1/2}$ and $\vec{r}_{1/2}$ in that case. Therefore, we reexamine the original expression. The main contributions to the sum in Eq. (64) stem from $k$-points around the Fermi surface

$$\vec{k}_{\pm}^{\text{FS}} = \lim_{\delta \rightarrow 0} \vec{k}_{\text{FS}} \pm \delta \vec{n}^{\text{FS}}_k$$

(71)

where $\vec{n}^{\text{FS}}_k$ denotes the local normal vector of the FS. If the oscillations of the numerator $\cos(k_{\text{FS}}\vec{R})$ in the vicinity of the FS are small, in general for short distances, the generic spatial structure should be reproduced by focusing on the summation of a very small $k$-shell around the FS and we obtain the approximation

$$t^{\text{eff}}(\vec{R}) \approx \tilde{t}^{\text{eff}}(\vec{R}) \propto \sum_{k_{\pm}} \cos(k_{\pm}^{\text{FS}}\vec{R}) \propto \sum_{k_{\pm}} \cos(k_{\pm}^{\text{FS}}\vec{R})$$

(72)

substituting $\epsilon_{k_{\pm}} = \pm \delta \nabla_{\vec{k}^{\text{FS}} \epsilon_\vec{k}}$ into this expression, we can restrict Eq. (72) to a summation over the Fermi surface and a directional derivation along $\vec{n}^{\text{FS}}_\vec{k}$:

$$\tilde{t}^{\text{eff}}(\vec{R}) \propto \sum_{\vec{k} \in \text{FS}} \lim_{\delta \rightarrow 0} \frac{\cos((\vec{k} + \delta \vec{n}^{\text{FS}}_\vec{k})\vec{R}) - \cos((\vec{k} - \delta \vec{n}^{\text{FS}}_\vec{k})\vec{R})}{\delta \nabla_{\vec{k}^{\text{FS}} \epsilon_\vec{k}}}$$

$$= \sum_{\vec{k} \in \text{FS}} \frac{\nabla_{\vec{k}^{\text{FS}}} \cos(\vec{k}\vec{R})}{\nabla_{\vec{k}^{\text{FS}} \epsilon_\vec{k}}}.$$  

(73)

The 2d Fermi surface of a simple cubic lattice is given by a square in the first Brillouin zone that is parametrized by the four conditions $k_x \pm k_y = \pm \pi/a$ and the corners are given by the four anti-nodal points introduced before. We have shown above that these corners, at which the nominator and denominator in Eq. (73) vanishes, does not contribute to $t^{\text{eff}}(\vec{R})$ along the diagonal in real space. Therefore we focus on the four nodal points between the corners given by $(\pm \pi/2a, \pm \pi/2a)$ on the 2d FS. The dispersion is linear around these points close to the FS and $\nabla_{\vec{k}^{\text{FS}} \epsilon_\vec{k}} \approx 2$ in appropriate units. Therefore, we replace the denominator in (73) by a constant and integrate over some part of the FS around these nodal points, which can be easily parameterized by a 1d integral,

$$\tilde{t}^{\text{eff}}_{\text{nodal}}(\vec{R}) \propto \left( \int_{\frac{\pi}{2a}}^{\frac{\pi}{2a} + \tau} dk_x + \int_{\frac{\pi}{2a} - \tau}^{-\frac{\pi}{2a} + \tau} dk_x \right)$$

$$\left( \langle \vec{n}^{\text{FS}}_k \vec{R} \rangle \sin \left( (R_x k_x - R_y |k_x|) + R_y \frac{\pi}{a} \right) \right).$$  

(74)

The distance from the nodal points include here is parametrized by $\tau$, and the explicit shape of the FS, $|k_y| = \pi/a - |k_x|$, was inserted.

For a general direction, this leads to small contributions due to the oscillations of the integrand. Only along the diagonal direction, these oscillations cancel. In addition $R_y \pi/a = R k_{\text{FS}}^{\pm}$, holds and we find a linear increase with the distance $\vec{R}$

$$\tilde{t}^{\text{eff}}_{\text{nodal}} \left( \frac{\vec{R}}{\sqrt{2}} \left( \frac{1}{1} \right) \right) \propto R \sin \left( R k_{\text{FS}}^{\pm} \right).$$  

(75)

This provides the deeper understanding of the surprising increase of the amplitude of the full $t^{\text{eff}}(\vec{R})$ shown in Fig. 11(b). Our analytical calculation links this observation to the properties of the dispersion at the nodal points of the FS for the P-H symmetric band. Note that for large values of $R$, the oscillations around the FS in the nominator of Eq. (72) lead to a damping of the linear increase: The simplification entering Eq. (73) are not valid for large $\vec{R}$.
For larger distances $R$, the amplitude of the tunneling stays constant in all directions as a consequence of the perfect FS-nesting for a 2d simple-cubic dispersion at half-filling. The linear increase of the effective tunneling along the diagonal direction strongly depends on the structure of the FS, but is not a consequence of FS-nesting and the divergency of the Lindhard function in momentum space respectively.

The spatial and band width corrections to the spin correlation function discussed in Sec. IV C predict a decay of the correlation function even for constant $t_{\text{eff}}$ that contains the exact AFM RKKY interaction in the limit $\Gamma_0/D \to 0$. Fig. 13 depicts the impurity spin-spin correlation function of the perfect FS-nesting for a 2d simple-cubic dispersion at half-filling. The linear increase of the effective tunneling along the diagonal direction strongly depends on the structure of the FS, but is not a consequence of FS-nesting and the divergency of the Lindhard function in momentum space respectively.

To understand this change in the frequency in the direction of the basis vectors, we focus on $t_{\text{eff}}^0(R) = t_{\text{eff}}^0(R \hat{e}_x)$ and perform a one-dimensional Fourier transformation of (64)

$$t_{\text{eff}}^0(q) = \gamma \int_{-\infty}^{\infty} dR \sum_{\vec{k} \in \text{FS}} \frac{e^{iR \cos(k_x R)}}{\epsilon_{\vec{k}}} = \frac{\pi \gamma}{t} \sum_{\vec{k} \in \text{FS}} \frac{\delta(q - k_x) + \delta(q + k_x)}{\cos(k_x a) + \cos(k_y a) + \mu/t} \quad (78)$$

where we substituted $\epsilon_{\vec{k}}$ defined with respect to the chemical potential.

We have to perform a $k_y$ summation for every $q$ while $k_x$ is fixed by $\delta$-functions. $t_{\text{eff}}^0(q)$ has the largest contribution for those $q$ values for which many $k$-vectors $(xq, ky)$ are very close to the FS.

We recall that upon hole doping the Fermi-surface shrinks and become more spherical. While the nodal points remain almost unaltered, the major change occurs in the vicinity of the anti-nodal points which are shifted to smaller $k_x$ ($k_y$) values for $k_y = 0$ ($k_x = 0$). For negative $\mu$, the major contribution arises from the intersection of the FS with the $k_x$ axis since the FS is perpendicular to the axis at these shifted anti-nodal points. Solving $\epsilon_{k_x=0} = 0$ for $k_x^* (\mu)$ yields

$$k_x^* (\mu) = \arccos(|\mu| - 1) \quad (79)$$

and therefore, the major contributions stem from large $k_x^* (\mu)$ that develop adiabatically from $k_x = \pi$. Simultaneously, the contributions from the second pair of anti-nodal points, $(0, \pm \pi/a)$ rapidly vanishes with increasing hole doping. At the end, we are left with

$$t_{\text{eff}}^0(q, \mu) \approx \delta(q + k_x^* (\mu)) + \delta(q - k_x^* (\mu)) \quad (80)$$

$$\Leftrightarrow t_{\text{eff}}^0(R, \mu) \propto \cos[R k_x^* (\mu)]. \quad (81)$$

The missing contribution for $k_x = 0$ leads to a doubling of the spatial frequency away from half filling as can be
The situation is qualitatively different for electron doping ($\mu > 0$), where the FS is formed by the four hole pockets. This is illustrated for the two different cases in Fig. 14(b), the general characteristics of the slow oscillations along the basis vector direction, for positive and negative values of the chemical potential.

For a negative chemical potential and a spherical FS, the antiferromagnetic part of the correlation function almost shows the same oscillations as the square of the effective tunneling as can be seen in the upper panel of Fig. 14(b). The small deviations of the correlation function from the behavior of the effective tunneling can be ascribed to the FM part of the RKKY interacting which is not captured by the effective tunneling and evolves for finite $U/T_0$.

In the presence of hole pockets, lower panel of Fig. 14(b), the general characteristics of the slow oscillations can be identified in the impurity spin-spin correlation function, too. In the vicinity of a vanishing effective tunneling, only ferromagnetic correlations are observed. The sign of the correlation function oscillates only in the presence of an antiferromagnetic contribution to the RKKY interaction, generated by $t^{\text{eff}}(\vec{R})$.

Fig. 15 shows the spin-spin correlation function (blue curve) as well as the $|t^{\text{eff}}|^2$ (black curve) as function of $\mu$ for a constant impurity distance $\vec{R}$ in order to illustrate the non-linear dependence of the frequency of the spin-spin correlation function on the chemical potential.

\[ k^*_x(\mu) = \arccos(1 - \mu). \]  

seen in Fig. 14(a) along the $x$ ($y$)-axis compared to Fig. 11(a).

The situation is qualitatively different for electron doping ($\mu > 0$), where the FS is formed by the four hole pockets. The FS does not intersect with either $k_y$-axis. However, the FS becomes parallel to the $k_x$ axis close to the Brillouin zone boundary for a small value $k^*_x(\mu)$.

As a consequence the spatial oscillation of $t^{\text{eff}}(\vec{R})$ along the $x$ or $y$ axis are very slow as shown in Fig. 14(a) for

\[ k^*_x(\mu) \approx 2 \cdot k^{\text{eff}}_{xy}, \]

in contrast to slow oscillations in the presence of hole pockets. This is illustrated for the two different cases in Fig. 14(b) where the full $t^{\text{eff}}(\vec{R})$ (black solid curve) is compared to the main contribution stemming from the spatial frequency $k^*_x(\mu)$ (dashed line).

We augment this analysis for $t^{\text{eff}}(\vec{R})$ with the NRG calculation of the impurity spin-spin correlation function along the basis vector direction, for positive and negative values of the chemical potential.

The Brillouin zone boundary for a small value $k^*_x(\mu)$,

\[ k^*_x(\mu) = \arccos(1 - \mu). \]  

\[ |t^{\text{eff}}|^2 \]

\[ \mu = -0.01D \]

\[ \mu = 0.01D \]

\[ \mu = 0.01D \]
C. Three-dimensional lattice at half filling

In the previous sections, we demonstrated that the richer spatial dependency of the spin-spin correlation function as well as the effective tunneling, beyond the simplified isotropic $2k_F$ oscillations, originates from the generically non-spherical FS and can be analysed by the investigation of the analytical properties of the integrals.

We now extend our study to the 3d simple cubic dispersion. The effective tunneling term along the three symmetry directions is depicted in Fig. 16. Just like in two dimensions, the superposition of different frequencies account for complex oscillations. The symmetry properties on the lattice places, defined by Eq. (62) and (63), are fulfilled.

1. AFM RKKY coupling - The Doniach scenario

In section III we discussed the transition from the Kondo singlet to an inter-impurity singlet groundstate as function of an external applied magnetic exchange-interaction $J_{12}$. In principle, the transition can also be realized by changing the ratio between the antiferromagnetic RKKY interaction and the Kondo temperature. The transition is typically discussed in terms of the Kondo coupling $J_K$ in the context of the TIKM. In lattice systems this is referred to as the Doniach scenario [40]: the heavy fermi liquid [39] is replaced at the QCP by an AF ordered state generated by the inter-impurity singlets in a lattice.

Decreasing $J_K$ causes an exponential decay of $T_K$, whereas the RKKY interaction only falls off as $J_K^2$ leading to a increase of the ratio $J_{RKKY}/T_K$. In the TIAM, the Kondo coupling $J_K$ is related to the ratio of the Coulomb interaction $U$ and the coupling strength $\Gamma_0$.

Linneweber et al. investigated the TIAM on the three-dimensional simple cubic lattice via a Gutzwiller variational approach and found such a QCP at a critical $U_c$ provided the impurities are placed on the lattice sites [78]. The authors indicated that their QCP is probably an artifact of the Gutzwiller variational approach: the Gutzwiller trial wave function only includes local correlations on the impurity site while the NRG reveals already for the Kondo problem the extended nature of the correlated singlet [59, 60].

If the impurities are placed on different sublattices, e.g. if they are separated by an odd number of the lattice spacing along the basis vector direction $\vec{R} = R^{\text{odd}} < 1,0,0>$, the RKKY interaction is always antiferromagnetic. The NRG level flow of the stable FP as function of $U/\Gamma_0$ is shown in Fig. 17. Clearly, the FP changes continuously from the SC fixed point with P-H symmetry breaking scattering term to the inter-impurity singlet FP with the absence of a phase shift of the conduction electron states. The crossover occurs in the vicinity of $U/\Gamma_0 \approx 14$. The inset of Fig. 17 depicts the corresponding impurity spin-spin correlation and illustrated the formation of a local inter-impurity singlet in the limit of $U/\Gamma_0 \rightarrow \infty$. Non indication of a QCP is found by the NRG when increasing $U$.

The absence of the QCP originates from the fact, that the RKKY interaction cannot only be reduced to an spin exchange interaction. The RKKY driven charge exchange between the impurities, which is responsible for the antiferromagnetic interaction, generates marginal relevant operators in the renormalization flow, driving the system away from the QCP.
FIG. 18. The impurity entropy vs $T$ for different values of $U$ for an impurity distance $\vec{R} = <2a, 0, 0>$. Inset: impurity spin-spin correlation function. NRG parameters: $N_s = 3000$, $\Lambda = 4$.

In order to restore the QCP as function of $U/\Gamma_0$, a compensating effective tunneling $-t^{\text{eff}}(\vec{R})$ has to be added as well as an additional, antiferromagnetic spin exchange $J_{12}$ that would control the distance to the Varma-Jones type QCP.

2. **FM RKKY coupling**

If the impurities are placed on the same sublattice, the RKKY interaction is ferromagnetic according to Eq. (62). After the local moments are formed, they align with increasing RKKY interaction, and the resulting triplet state is screened in a two-stage Kondo effect [21]. This is clearly visible by tracking the impurity entropy as function of temperature [27] for different values of $U$ as depicted in Fig. 18. The local moment formation occurs on a scale of $U/\Gamma_0$ leading to a $\ln(4)$ impurity entropy contribution at intermediate temperatures. By lowering $T$ further, we observe the crossover to a local triplet on the scale defined by $J_{RKKY}$: The larger $U$ is, the more pronounced the consecutive two stage Kondo screening is visible revealing the different unstable FP of the RG flow.

The inset of Fig. 18 shows the impurity spin-spin correlation as function of $U/\Gamma_0$ and displays the formation of a local inter-impurity triplet. Since the Kondo temperature is suppressed with increasing $U$, the RKKY interaction dominates at higher temperature and favors a correlated triplet that is collectively screened in a two stage process for $T \to 0$.

We do not find a breakdown of the Kondo effect in the presence of FM RKKY interaction found in a recent perturbative RG treatment of the TIKM [42]. While this RG approach focuses on the renormalization of the effective Kondo coupling at one of the impurity sites, the NRG includes all couplings for both impurities on equal footing.

VI. SUMMARY AND CONCLUSION

Mapping the TIAM onto degrees of freedom with even and odd parity symmetry generates two, in general P-H asymmetric, hybridization functions. Both hybridization functions can be decomposed into a symmetric part with respect to the frequency and an asymmetric correction. Neglecting the asymmetric part generates always a FM RKKY interaction. A QCP as observed by Varma and Jones is found after adding an direct antiferromagnetic exchange interaction. The asymmetric part, however, is responsible for an additional relevant scattering term at zero energy and hence destroys the Varma and Jones QCP.

We have shown that the effect of the asymmetric part is equivalent to an effective tunneling term between the two impurities: Replacing the full hybridization function by the symmetrized contribution and this local tunneling term leads to the identical low-temperature FP spectrum in the NRG.

This opened the door for restoring the QCP by adding a suitable tunneling term to the full Hamiltonian at a fixed distance $R$ or by adjusting the distance between the impurities. While the counter term can be analytically calculated for P-H symmetric impurities, the term is determined by an numerical iteration procedure for P-H asymmetric impurities. Using the estimates from the case of P-H symmetric impurities as the initial value, the parameter $t^{\text{eff}}$ or $R$ are iteratively adjusted such that the lowest single-particle excitation in the even and the odd channel are equal. We checked the consistence with the scattering phases of both single-particle Green functions and found that both phases are also identical at the QCP.

Using the replacement of the full model by a symmetric hybridization function and a local tunneling term, provides an better understanding of the antiferromagnetic contribution to the RKKY interaction. In contrary to the RKKY interaction of a two-impurity Kondo model resulting from a Schrieffer Wolff transformation, we find $J_{RKKY}^{AF} \propto (t^{\text{eff}})^2/U$. Only for very large $U$, a crossover to $J_{RKKY}^{AF} \propto 1/U^2$ is observed. Furthermore, the value of $J_{RKKY}^{FM}$ decays much more rapidly than $J_{RKKY}^{AF}$. The distance dependency of the corresponding spin-spin correlations, however, tracks the distance dependency of $(t^{\text{eff}})^2$ indicating a significant derivation for small and intermediate $U$.

For a constant tunneling $t^{\text{eff}}$, the impurity spin-spin correlation function is governed by a dimensionless variable that accounts for the distance-dependent correction and the correction to the wide-band limit.

We analyzed the spatial anisotropy of the RKKY interaction as well as the impurity spin-spin correlation function for square lattices in different dimensions. We
identified the major spatial frequencies that governs the oscillation in real space for different chemical potentials close to half-filling and link them to the single-particle dispersion as well as the shape of the Fermi surface.

No QPT is found upon increasing the local Coulomb repulsion for a distance at which the RKKY interaction effect only becomes more pronounce with increasing $U$. Therefore, the Doniach scenario for Heavy Fermion QCP requires lattice effects that are included in the particle-hole Bethe saltpetter equation that enters the lattice spin susceptibility.

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