We test the method of infinitesimal unitary transformations recently introduced by Wegner on the Anderson single impurity model. It is demonstrated that infinitesimal unitary transformations in contrast to the Schrieffer–Wolff transformation allow the construction of an effective Kondo Hamiltonian consistent with the established results in this well understood model. The main reason for this is the intrinsic energy scale separation of Wegner's approach with respect to arbitrary energy differences coupled by matrix elements. This allows the construction of an effective Hamiltonian without facing a vanishing energy denominator problem. Similar energy denominator problems are troublesome in many models. Infinitesimal unitary transformations have the potential to provide a general framework for the systematic derivation of effective Hamiltonians without such problems.

1. INTRODUCTION

The construction of effective Hamiltonians is an important step for many problems in theoretical physics. Recently a new technique termed “flow equations” has been introduced by Wegner for such problems. In Ref. [1] Wegner applied infinitesimal unitary transformations on a many-particle Hamiltonian to find a unitarily equivalent Hamiltonian that is block-diagonal, i.e., that conserves the number of quasiparticles. The conceptual advantage of his approach is that matrix elements connecting states with large energy differences are treated first and smaller energy differences are treated only after these large energy differences are already effectively decoupled.

Wegner's approach is reminiscent of ideas underlying renormalization theory. The separation of energy scales in the flow equations is similar to the sequence of subsequent diagonalizations in Wilson's numerical renormalization method [2]. Analogously, analytical renormalization schemes start integrating out the modes at the UV-cutoff. Wegner's flow equations might provide an analytic framework for energy scale separation with respect to arbitrary energy differences, not only between ground state and UV-cutoff. In this sense it incorporates some key features...
of both numerical and perturbative renormalization methods, though the language of infinitesimal unitary transformations is less familiar than the usual notions of renormalization theory.

Independent of Wegner [1], Glazek and Wilson [3, 4] also have recently proposed using continuous unitary transformations to construct renormalization group equations for effective Hamiltonians in quantum field theory. Wilson et al. [5] applied this “similarity renormalization scheme” to light-front quantum chromodynamics. Their goal is to eliminate “far-off-diagonal” matrix elements in a given Hamiltonian, which means off-diagonal matrix elements connecting states that have a larger energy difference than some given value. This means that the final Hamiltonian has a banded structure. In contrast Wegner’s goal is to eliminate matrix elements so that the final Hamiltonian is diagonalized approximately or is block-diagonal. Still the energy scale separation with respect to all energy differences is common to both approaches. In particular small energy denominators are avoided [3, 4].

This paper aims at testing Wegner’s method on the interesting and well-understood Anderson impurity model [6] of solid state physics. The Hamiltonian contains the electron band, the energy of the impurity orbital $\varepsilon_d$ together with a repulsive interaction $U$ on the impurity site and a hybridization interaction $V_h$ between the band states and the impurity state,

$$H = \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{\sigma} \varepsilon_d d_{\sigma}^\dagger d_{\sigma} + \sum_{k,\alpha} V_h (c_{k,\alpha}^\dagger d_{\alpha} + d_{\alpha}^\dagger c_{k,\alpha}) + Ud_{\uparrow}^\dagger d_{\downarrow}^\dagger d_{\downarrow} - \downarrow d_{\downarrow}. \quad (1.1)$$

This Hamiltonian has been introduced to serve as a microscopic model for systems exhibiting the Kondo effect, that is, the behavior of a single magnetic impurity coupled antiferromagnetically to a conduction band of electrons. After eliminating the charge fluctuations introduced by the hybridization term one expects to find an effective Kondo Hamiltonian

$$H_K = \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} - \vec{S} \cdot \sum_{k,\alpha,\beta} V_{k,\alpha,\beta}^{(2)} c_{k,\alpha}^\dagger \vec{\sigma}_{\alpha,\beta} c_{k,\beta} \quad (1.2)$$

describing the low energy properties of the system for appropriate initial parameters in Equation (1.1). The matrix elements $V_{k,\alpha,\beta}^{(2)}$ have to be derived from (1.1).

Our motivation for studying this particular model is to test Wegner’s method on this well-understood model with its rich physical behaviour. Different energy scales appear in the Hamiltonian (1.1) set by the conduction band width $D$, the impurity orbital energy $\varepsilon_d$, and the on-site interaction $U$. Since the hybridization is the small perturbation of a non-quadratic Hamiltonian, the usual perturbation techniques based on Wick’s theorem cannot be applied.

The Anderson impurity model has been investigated by many different methods of theoretical physics. In the case of a linear dispersion relation for the conduction band and $V_k = V = \text{const.}$ it was solved using a Bethe ansatz [7]. In a more general
situation renormalization techniques are available for studying its universal properties. Haldane has already obtained the various crossovers in Refs. [8, 9]. Wilson's numerical renormalization group [2] has been applied to the Anderson impurity model by Krishna-murthy et al. [10]. For a recent review of these and other approaches see Ref. [11]. In the past few years there has been renewed interest in the properties of the Anderson impurity model in connection with the limit of infinite dimensionality [12, 13] where many of these traditional techniques cannot be applied.

In this paper we demonstrate that Wegner's flow equations provide a tool to find an effective Kondo Hamiltonian consistent with the established results of other methods. Usually this construction is sidestepped by direct application of e.g. renormalization theory on the Anderson impurity Hamiltonian. Hence we add some new perspective to an old problem of solid state physics.

Let us already emphasize that the construction of the effective Kondo Hamiltonian with the well known Schrieffer–Wolff unitary transformation [14] generally does not give a satisfactory treatment of this problem. The main reason will turn out to be the missing separation of energy scales. This gives rise to vanishing energy denominators if the impurity orbital energies lie in the continuum of conduction band states. The transformation is in fact ill-defined then and yields an UV-cutoff of the Kondo Hamiltonian that is inconsistent with known results from renormalization theory or the Bethe ansatz.

Similar problems with vanishing energy denominators in induced interactions also occur in other problems of solid state physics. One important example is the Fröhlich transformation [15] used for eliminating the electron–phonon coupling to derive the effective electron–electron coupling responsible for BCS superconductivity. A region of phase space where this interaction is attractive is separated from a repulsive region by a pole in the Fröhlich result. The application of flow equations by Lenz and Wegner [16] gives a different picture where the induced interaction for BCS pairs is always attractive. For this problem the other techniques available for the Anderson impurity model cannot be applied and it is not immediately clear which expansion should be trusted.

However, judging from the results for the Anderson impurity model in this work it seems possible to argue that the flow equation approach is a systematic way of constructing an effective Hamiltonian in contrast to a single unitary transformation of the Schrieffer–Wolff or Fröhlich type. Due to the intrinsic energy scale separation we obtain a controllable expansion where small energy denominators are avoided. This background serves as the main motivation for this work where we can compare our approach with established results. For other applications of flow equations see also Refs. [16–18].

This paper is organized as follows. In the following section we derive the general flow equations for the coupling constants of the Anderson impurity model. In Section 3 we illustrate the method in the case of a vanishing interaction of the electrons on the impurity. It is shown that in this case the flow equations yield the exact solution. Furthermore we introduce an approximation that still gives the exact result.
for the case of vanishing interaction and which is applied in Section 4 to the case of a non-vanishing interaction $U$. We calculate implicit equations for the renormalized interaction and the renormalized impurity energy. These equations can in principle be solved for any given density of states and hybridization. In the key section, 5, the induced antiferromagnetic spin–spin interaction is calculated. This defines the effective Kondo Hamiltonian (1.2). Our result is compared with the result obtained by Schrieffer and Wolff [14]. In Section 6 we generally discuss the method of continuous unitary transformations as compared to a single unitary transformation. Finally, in Section 7 our method is compared with traditional scaling approaches. The last section contains the conclusions.

2. THE FLOW EQUATIONS FOR THE ANDERSON IMPURITY MODEL

Our starting point is the Anderson impurity Hamiltonian

$$H = \sum_{k, \sigma} \epsilon_k c_{k, \sigma}^\dagger c_{k, \sigma} + \sum_{\alpha} \sum_{k, \sigma} V_{\alpha} c_{k, \sigma}^\dagger d_{\alpha} + \sum_{k, \sigma} U d_{\sigma}^\dagger c_{k, \sigma} c_{k, \sigma}^\dagger d_{\sigma} + E_0.$$ (2.1)

Here we introduced a normal ordering prescription for the conduction band electron operators $c_{k, \sigma}^\dagger$ and $c_{k, \sigma}$. It is defined by: $c_{k, \sigma}^\dagger c_{k, \sigma} := c_{k, \sigma}^\dagger c_{k, \sigma} - n_k$ where $n_k = (\exp(\beta \epsilon_k) + 1)^{-1}$ is the occupation number of the band state with wave vector $k$. We set the Fermi energy equal to zero. The reason for the normal ordering is that additional interactions, which will be generated by our procedure and which we neglect, should be written down in a normal ordered form as well since otherwise the ground state expectation value of such additional contributions does not vanish. A detailed discussion has been given in a previous work [19]. In contrast to Ref. [19] we do not introduce normal ordering for the impurity electron operators $d_{\sigma}^\dagger$ and $d_{\sigma}$. The reason is that in our approximation contributions containing such operators are not neglected if they have a non-vanishing expectation value in the ground state. It is possible to introduce a normal ordering on the impurity site as well, but the results are not changed. Due to the normal ordering a constant $E_0 = 2 \sum_{k} \epsilon_k n_k$ has been introduced in the Hamiltonian.

We now want to apply a general continuous unitary transformation to the Hamiltonian. Such a transformation is defined by a generator $\eta$ that depends on a continuous variable, which we call $l$. The continuous unitary transformation is defined by

$$\frac{dH}{dl} = [\eta(l), H(l)].$$ (2.2)
with the initial condition

$$H(l = 0) = H$$  \hspace{1cm} (2.3) $$

from Equation (2.1). In order to simplify notation we denote the initial values of $\varepsilon_d$ and $U$ by

$$\varepsilon_d^0 \overset{\text{def}}{=} \varepsilon_d(l = 0), \quad U^0 \overset{\text{def}}{=} U(l = 0) \hspace{1cm} (2.4)$$

and the asymptotic (“renormalized”) values for $l \to \infty$ by

$$\varepsilon_d^\infty \overset{\text{def}}{=} \varepsilon_d(l = \infty), \quad U^\infty \overset{\text{def}}{=} U(l = \infty). \hspace{1cm} (2.5)$$

If these parameters appear without an argument this will imply that they are to be considered as functions of $l$.

We choose $\eta$ to be of the form

$$\eta = \sum_{k, \sigma} \eta_k (c^+_{k, \sigma} d_{\sigma} - d^+_\sigma c_{k, \sigma}) + \sum_{k, q, \sigma} \eta_{k, q} (c^+_{k, \sigma} c_{q, \sigma} - c^+_{q, \sigma} c_{k, \sigma})$$

$$+ \sum_{k, \sigma} \eta_k^{(2)} (c^+_{k, \sigma} d^+_\sigma d_{-\sigma} d_{-\sigma} - d^+_\sigma d^+_{-\sigma} d_{-\sigma} c_{k, \sigma}) \hspace{1cm} (2.6)$$

The commutator of $\eta$ and $H$ is easily calculated, we obtain

$$[\eta, H] = \sum_{k, \sigma} \eta_k (\varepsilon_d - \varepsilon_k) (c^+_{k, \sigma} d_{\sigma} + d^+_\sigma c_{k, \sigma})$$

$$+ \sum_{k, q, \sigma} \eta_{k, q} V_q (c^+_{k, \sigma} c_{q, \sigma} + c^+_{q, \sigma} c_{k, \sigma})$$

$$- 2 \sum_{k, \sigma} \eta_k V_k d^+_\sigma d_{\sigma} + 2 \sum_{k, \sigma} \eta_k V_k n_k$$

$$+ U \sum_{k, \sigma} \eta_k (d^+_\sigma d^+_{-\sigma} d_{-\sigma} c_{k, \sigma} + c^+_{k, \sigma} d^+_{-\sigma} d_{-\sigma} d_{-\sigma})$$

$$- \sum_{k, q, \sigma} \eta_{k, q} (\varepsilon_k - \varepsilon_q) (c^+_{k, \sigma} c_{q, \sigma} + c^+_{q, \sigma} c_{k, \sigma})$$

$$+ 2 \sum_{k, q, \sigma} \eta_{k, q} V_q (c^+_{k, \sigma} c_{q, \sigma} + c^+_{q, \sigma} d_{\sigma})$$

$$- \sum_{k, \sigma} \eta_k V_k d^+_{-\sigma} d_{-\sigma} c_{k, \sigma} + c^+_{k, \sigma} d^+_{-\sigma} d_{-\sigma} d_{-\sigma})$$

$$- 2 \sum_{k, \sigma} \eta_k^{(2)} V_k d^+_{\sigma} d^+_{-\sigma} d_{-\sigma} d_{-\sigma}. \hspace{1cm} (2.6)$$
Many additional couplings are generated which did not occur in the original Hamiltonian in (2.1). But some of these terms can be eliminated by a suitable choice of $\eta$. Let us first consider terms containing $: c_{k,\sigma} c_{q,\sigma} + c_{q,\sigma} c_{k,\sigma} :$. Such terms do not occur if we choose

$$\eta_{k,q}(e_k - e_q) = \frac{1}{2}(\eta_k V_q + \eta_q V_k).$$  

(2.8)

Similarly, terms containing operators of the type $d_{\sigma}^\dagger d_{-\sigma} c_{k,\sigma} + c_{k,\sigma} d_{-\sigma} d_{-\sigma}$ do not occur if we choose

$$U\eta_k + (e_d - e_k) \eta_{k}^{(2)} + U\eta_k^{(2)} = 0$$  

(2.9)

These equations may be used to determine $\eta_{k,q}$ and $\eta_k^{(2)}$. The only contribution that does occur additionally is the term

$$\sum_{k, q, \sigma} \eta_k^{(2)} V_q c_{k,\sigma}^\dagger d_{-\sigma} c_{q,\sigma} + c_{q,\sigma} c_{k,\sigma} d_{-\sigma} d_{-\sigma}.$$  

(2.10)

Notice that the interaction term in (2.10) is marginal in some of the fixed points of the Anderson impurity model. In principle it has to be included in the Hamiltonian in (2.1). But the commutator of this term with $\eta$ does not yield contributions to the other terms in the Hamiltonian. Therefore we do not take it into account in our first analysis of the problem. But it is clear that this additional term is important. A part of it yields the antiferromagnetic interaction between the impurity spin and the spins of the band electrons that is responsible for the Kondo effect. We will come back to the induced interactions in Section 5 and first of all calculate the flow equations for the parameters in the Hamiltonian (2.1). From (2.7) we obtain

$$\frac{dV_k}{dt} = \eta_k (e_d - e_k) + 2 \sum_{\rho} \eta_{k,\rho} V_{\rho}$$  

(2.11)

$$\frac{de_k}{dt} = 2\eta_k V_k$$  

(2.12)
\[ \frac{d\epsilon_d}{dt} = -2 \sum_k \eta_k V_k + 2 \sum_k \eta_k^{(2)} V_k n_k \]  
\[ \frac{dU}{dt} = -4 \sum_k \eta_k^{(2)} V_k \]  
\[ \frac{dE_0}{dt} = 4 \sum_k \eta_k V_k n_k \]

The last equation yields directly \(E_0 = 2 \sum \epsilon_k n_k\), which is the energy of the filled Fermi sea. In the following we are interested in the thermodynamic limit. For large \(N\), the number of states in the band, one has \(V_k \propto N^{-1/2}\). Thus, \(\eta_k\) must as well be of the order \(N^{-1/2}\), and the derivative of \(\epsilon_k\) with respect to \(l\) is of order \(N^{-1}\). For large values of \(N\) the band energies do not depend on \(l\) as should have been expected.

### 3. VANISHING INTERACTION \(U = 0\)

We first study the case \(U = 0\) to illustrate our method. Then we have a quadratic Hamiltonian that can be solved exactly, see for example Ref. [20]. Our method also yields the exact solution in this case. For \(U = 0\) the flow equations simplify to

\[ \frac{dV_k}{dt} = \eta_k (\epsilon_d - \epsilon_k) + 2 \sum_p \eta_{k,p} V_p \]  
\[ \frac{d\epsilon_d}{dt} = -2 \sum_k \eta_k V_k \]

The flow equations are exact in the case \(U = 0\) since the neglected terms in (2.7) vanish in this limit. We let

\[ \eta_k = V_k f(\epsilon_k, l) \]

and introduce

\[ J(\epsilon, l) = \sum_k V_k^2 \delta(\epsilon - \epsilon_k). \]

One often introduces the parameter

\[ \Gamma = \pi \rho(\epsilon_p) V_{k_p}(0)^2 = \pi J(\epsilon_p, 0), \]
where $\rho(\varepsilon_F)$ is the density of states at the Fermi surface. The flow equations for $\varepsilon_d$ and $J(\varepsilon, l)$ are

$$\frac{d\varepsilon_d}{dl} = -2 \int d\varepsilon f(\varepsilon, l) J(\varepsilon, l)$$

(3.6)

$$\frac{\partial J(\varepsilon, l)}{\partial l} = 2J(\varepsilon, l) f(\varepsilon, l)(\varepsilon_d - \varepsilon) + 2 \int d\varepsilon' J(\varepsilon, l) J(\varepsilon', l)(f(\varepsilon, l) + f(\varepsilon', l)) \frac{J(\varepsilon, l)}{\varepsilon - \varepsilon'}$$

(3.7)

For the integral in the last equation one has to take its principal value. The set of flow equations may be solved if one introduces a function

$$G(\varepsilon, l) = \int d\varepsilon' \frac{J(\varepsilon', l)}{\varepsilon - \varepsilon' + G(\varepsilon, l)}.$$

(3.8)

Taking the derivative with respect to $l$, we obtain an implicit equation for this derivative, which can be solved. The final result is

$$\frac{\partial G(\varepsilon, l)}{\partial l} = 2 \left[ 1 + \int d\varepsilon' \frac{J(\varepsilon', l)}{\varepsilon - \varepsilon' + G(\varepsilon, l)} \right]^{-1} \times \int d\varepsilon' f(\varepsilon', l) J(\varepsilon', l) \frac{\varepsilon_d - \varepsilon' + G(\varepsilon, l)}{\varepsilon - \varepsilon' + G(\varepsilon, l)}.$$

(3.9)

Calculating the derivative of $G(\varepsilon, l)$ with respect to $\varepsilon$ we obtain similarly

$$1 + \frac{\partial G(\varepsilon, l)}{\partial \varepsilon} = \left[ 1 + \int d\varepsilon' \frac{J(\varepsilon', l)}{\varepsilon - \varepsilon' + G(\varepsilon, l)} \right]^{-1}.$$

(3.10)

This yields

$$\frac{\partial G(\varepsilon, l)}{\partial l} = 2 \int d\varepsilon' f(\varepsilon', l) J(\varepsilon', l) \frac{\varepsilon_d - \varepsilon' + G(\varepsilon, l)}{\varepsilon - \varepsilon' + G(\varepsilon, l)}.$$

(3.11)

Comparing the right hand side with the derivative of $\varepsilon_d$ with respect to $l$, we obtain

$$\frac{d\varepsilon_d}{dl} = -\frac{\partial G(\varepsilon, l)}{\partial l} \bigg|_{\varepsilon = \varepsilon_d(l)}.$$

(3.12)

This equation can be integrated and the final result is

$$\varepsilon_d(l) + G(\varepsilon_d(l), l) = \varepsilon_d^R.$$

(3.13)
In the last step we used \( G(\varepsilon, \infty) = 0 \), which follows directly from \( J(\varepsilon, \infty) = 0 \) and holds for an appropriate choice of \( f(\varepsilon, l) \). Solving for \( \varepsilon_d(l) \), we obtain

\[
\varepsilon_d(l) = \varepsilon_d^R - \int_0^l \frac{J(\varepsilon, l)}{\varepsilon_d^R - \varepsilon} \, dl
\]

Again, for the integral on the right hand side we have to take its principal value. This means that we have to choose \( J(\varepsilon, l) \) and therefore \( f(\varepsilon, l) \) such that the principal value exists for all \( l \). We obtain the value of \( \varepsilon_d^R \), if we let \( l = 0 \) and solve for \( \varepsilon_d^R \).

As a simple example we take a semi-circle

\[
J(\varepsilon, 0) = \frac{2V}{\pi D^2} \sqrt{D^2 - \varepsilon^2}
\]

where \( 2D \) is the band width and \( V = \sqrt{\sum_k V_k^2} \). Here we have \( \Gamma = 2V^2/D \). The main reason for this choice of the hybridization is that all the integrals can be worked out in closed form in the sequel. But it should be noted that it is a main advantage of our approach that it can be used for arbitrary functions \( J(\varepsilon, 0) \), in particular for any distribution of the density of states in the conduction band. However, if one chooses a linear dispersion relation and constant hybridization \( V_k \), that is \( J(\varepsilon, 0) = V^2/2D \Theta(D - |\varepsilon|) \) as usually done in renormalization group treatment of the Anderson impurity model, one must be careful due to the discontinuous behaviour close to the band edge. The self-consistency equations in the flow equations approach will then generally have more than one solution, however, the actual solution of the differential equations chooses the correct one. Close to the band edge one expects unphysical behaviour anyway due to the unphysical choice of \( J(\varepsilon, 0) \) and neither approach should be trusted. Therefore it is natural in our approach to choose a function \( J(\varepsilon, 0) \) that is continuous at the band edge as should be expected on physical grounds anyway.

Let us come back to our example introduced in Equation (3.15). We have to distinguish between the case where \( \varepsilon_d^R \) lies in the band and the case where it lies outside the band. We first consider the latter case. The integral can be calculated and we obtain

\[
\varepsilon_d^R - \varepsilon_d^R + \frac{\Gamma}{D} \left( \text{sign}(\varepsilon_d^R) \sqrt{(\varepsilon_d^R)^2 - D^2} - \varepsilon_d^R \right) = 0
\]

if \( |\varepsilon_d^R| > D \). This equation yields a simple quadratic equation for \( \varepsilon_d^R \), which has always two solutions. If \( \Gamma < D \) at most one of these solutions lies outside the band. If \( \Gamma > D \) and \( |\varepsilon_d^R| > F - D \), there is a single solution for \( \varepsilon_d^R \) outside the band, but if \( |\varepsilon_d^R| < F - D \) we obtain two solutions outside the conduction band.
The situation is much simpler when $\varepsilon_d^R$ lies inside the band. The integral in (3.14) has to be interpreted as its principal value and we obtain

$$\varepsilon_d^R - \varepsilon_d^f - \frac{\Gamma}{D} \varepsilon_d^R = 0. \quad (3.17)$$

The only solution is

$$\varepsilon_d^R = \frac{\varepsilon_d^f}{1 - (\Gamma/D)} \quad (3.18)$$

$\varepsilon_d^R$ lies inside the band if $\Gamma < D - |\varepsilon_d^f|$. The various cases are shown in Fig. 1.

The fact that for a sufficiently large value of $V$ ($\Gamma > D$ in our example) two solutions for $\varepsilon_d^R$ exist, is generic. It holds for any $J(\varepsilon, 0)$ with a connected support of length $2D$. It is clear that with the present approach of flow equations only a single solution can be obtained. Nevertheless, the second solution is of physical importance. It is possible that a localized state develops from the original band states that has an energy which lies outside the band. Such a state cannot be obtained within the present formulation of the flow equations. In the case $U = 0$ one can introduce a different representation of the Hamiltonian and of $\eta$ that includes a localized band state explicitly. Since we are at present not able to deal with similar problems in the case $U > 0$, we restrict ourselves to the parameter regime $\Gamma < D$ (in fact later we will need $\Gamma < D/2$). This is reasonable since we do not expect that the hybridization is the largest parameter in the system but rather the smallest.

Equation (3.14) is obtained as well if one uses two simple approximations to the flow equation. The first approximation neglects the terms proportional to $\varepsilon_d^e - \varepsilon_d^f$, in the Hamiltonian that are generated by the transformation and consequently one neglects such terms in $\eta$ as well. This is an approximation that can be justified from

![Fig. 1. Various regimes for the solution of the $U=0$ Anderson impurity model.](image)
a physical point of view since these terms are one-body potentials that are irrelevant in all fixed points. Then the second term in (2.11) vanishes and the equation for $V_k$ is linear in $V_k$. Similarly, the second term in (3.7) vanishes, whereas (3.6) remains unchanged. Both equations together yield

$$\frac{d\epsilon_d}{dl} = -\int d\epsilon \frac{\partial J(\epsilon, l)}{\partial l} \frac{1}{\epsilon_d - \epsilon}. \quad (3.19)$$

Furthermore we assume that $\epsilon_d(l)$ converges rapidly to $\epsilon_d^p$, so that we can replace $\epsilon_d(l)$ with $\epsilon_d^p$ on the right hand side (3.19). This yields (3.14). We will use similar approximations for $U > 0$ as well. Although it is possible to choose $\eta$ in such a way that only very few new terms are generated, the flow equations become very complicated. One has to truncate the scheme at some stage in order to be able to analyse the flow equations.

Depending on the problem, there can be various justifications for this truncation:

- The higher normal ordered interactions are in some sense “irrelevant” for the properties that one is interested in.
- The generator of the infinitesimal unitary transformation $\eta(l)$ is proportional to some small parameter and one expands in this parameter. Notice that this procedure is not equivalent to perturbation theory in the small parameter due to the infinitesimal nature of the flow equation approach as will become clear later.

In the sequel one can have the second reasoning in mind as the hybridization $V_k$ is the natural small parameter of the Anderson impurity model. All the following equations can thus be interpreted as correct in $O(V^2)$. But we will see that the results are in fact even better than this since only irrelevant interactions in the renormalization sense are neglected.

Finally one can analyse why the self-consistency condition obtained by replacing $\epsilon_d$ by $\epsilon_d^p$ on the right hand side of (3.19) yields a good approximation to the exact solution of (3.19). To discuss this point let us introduce a special choice of $f(\epsilon, l)$. Since we want $J(\epsilon, l)$ to vanish in the limit $l \rightarrow \infty$, a natural choice would be $f(\epsilon, l) = - (\epsilon_d - \epsilon)_+$. But for finite $U$ we will have to make a different choice for $f(\epsilon, l)$ in the next section. For consistency we therefore take $f(\epsilon, l) = -(\epsilon_d - \epsilon)^p/(4\epsilon_d^p)$. This obviously works as well and it is easy to see that in the present case both choices are essentially equivalent. The following argument then holds: Unless $\epsilon = \epsilon_d$, $J(\epsilon, l)$ decays exponentially on a scale set by $l \propto \epsilon_d^p/(\epsilon_d - \epsilon)^4$. If $\epsilon_d$ lies outside the band it will tend to $\epsilon_d^p$ exponentially and the approximation $\epsilon_d \approx \epsilon_d^p$ on the right hand side of (3.19) is justified. On the other hand, if $\epsilon_d$ lies inside the band, we can estimate the relevant $l$-scale on which $\epsilon_d$ changes by calculating the ratio of the total change of $\epsilon_d$ to its derivative with respect to $l$ for small $l$. This shows that $\epsilon_d$ changes on a scale set by $l \propto \epsilon_d^p/D^4$, i.e. much faster than $J(\epsilon, l)$ for values of $\epsilon$ near the Fermi energy. Therefore $\epsilon_d$ can be replaced by its renormalized value on the right hand side of (3.19). We will use the same approximation in the next section to discuss the case $U > 0$, it can be justified in the same manner.
4. NON-VANISHING INTERACTION $U>0$

With the approximations introduced at the end of the last section, the flow equations for $U>0$ may be written in the form

$$\frac{dV_k}{dl} = \eta_k(e_d - \epsilon_k),$$  \hspace{1cm} (4.1)

$$\frac{de_d}{dl} = -2 \sum_k \eta_k V_k + 2 \sum_k \eta_k^{(2)} V_k n_k,$$ \hspace{1cm} (4.2)

$$\frac{dU}{dl} = -4 \sum_k \eta_k^{(2)} V_k,$$ \hspace{1cm} (4.3)

According to (2.9) we take $\eta_k^{(2)} = -U \eta_k(e_d - \epsilon_k + U)^{-1}$ and as above $\eta_k = V_k f(\epsilon_k, l)$. We assume that $\sum_k V_k^2 < D^2$ so that the renormalized $e_d^R$ is unique for $U=0$. We expect that it is unique for $U>0$ as well. With these assumptions we proceed as in the previous section. We introduce $J(\epsilon, l)$ as in (3.4) and obtain the flow equations

$$\frac{\partial J(\epsilon, l)}{\partial l} = 2f(\epsilon, l) J(\epsilon, l)(e_d - \epsilon),$$  \hspace{1cm} (4.4)

$$\frac{de_d}{dl} = - \int \frac{d\epsilon}{\partial l} \frac{\partial J(\epsilon, l)}{\partial \epsilon} \frac{(e_d - \epsilon + (1 + n(\epsilon)) U)}{(e_d - \epsilon)(e_d - \epsilon + U)},$$  \hspace{1cm} (4.5)

$$\frac{dU}{dl} = 2 \int \frac{d\epsilon}{\partial l} \frac{U}{(e_d - \epsilon)(e_d - \epsilon + U)}$$  \hspace{1cm} (4.6)

with the Fermi distribution $n(\epsilon)$.

One observes that equations (4.5) and (4.6) have a straightforward interpretation similar to renormalization theory: $\partial J(\epsilon, l)/\partial l$ are the modes that are just being decoupled from the impurity and this gives rise to a flow of the parameters. In renormalization theory one would start integrating out at the band edge of the conduction band. However, here we still have the freedom to choose the function $J(\epsilon, l)$ in Equation (4.4). This is equivalent to choosing some parametrization for $J(\epsilon, l)$. A suitable choice is

$$J(\epsilon, l) = J(\epsilon, 0) \exp \left( - \int_0^l \frac{(e_d - \epsilon)^2 (e_d - \epsilon + U)^2}{e_d^2 + (e_d + U)^2} \, dl' \right).$$ \hspace{1cm} (4.7)

This amounts to integrating out the modes with a large energy difference from the impurity orbital energies for small $l$ and small energy differences later for larger values of the flow parameter $l$. We will come back to the comparison with scaling approaches in more detail in Section 7.
With this choice the hybridization flows to zero for all $\epsilon$, in particular also for $\epsilon = \epsilon_d + U$. The reason is that $\epsilon_d - \epsilon_d^R$ decays like $l^{-1/2}$ as will be shown below. $J(\epsilon_d^R, l)$ decays algebraically to zero. Equation (4.7) corresponds to the following function $f(\epsilon, l)$

$$f(\epsilon, l) = \frac{(\epsilon_d - \epsilon)(\epsilon_d - \epsilon + U)^2}{2\epsilon_d^2 + 2(\epsilon_d + U)^2}. \quad (4.8)$$

Another reason for this choice of $f(\epsilon, l)$ or $J(\epsilon, l)$ is that now no pole terms appear in the integrals on the right hand sides of (4.5) and (4.6). The denominator in (4.8) is just introduced for convenience so that limits like $\lim_{U \to \infty}$ can be performed in all the equations without difficulties. Apart from trivial reparametrizations the function $f(\epsilon, l)$ and hence the sequence of decoupling is fixed by these requirements.

Let us consider for a moment the simplified case $\lim_{U \to \infty}$. The equation for $\epsilon_d$ takes the form

$$\frac{d\epsilon_d}{dl} = \int d\epsilon J(\epsilon, 0)(1 + n(\epsilon))(\epsilon_d - \epsilon) \exp\left(-\int_0^l (\epsilon_d - \epsilon)^2 dl'\right). \quad (4.9)$$

This equation is very similar to the flow equation for the renormalized tunneling frequency in the spin-boson problem [17]. The asymptotic behaviour can be obtained as in [17], one finds $\epsilon_d^R - \epsilon_d(\alpha) \propto l^{-1/2}$ for large $l$ if $\epsilon_d^R$ lies inside the band. Otherwise it decays exponentially. Equation (4.9) shows that $1/\sqrt{l}$ plays the role of an effective band width if $1/\sqrt{l}$ becomes smaller than the original band width of $J(\epsilon, 0)$.

For finite $U$ the situation is somewhat more complicated, but the results are similar. The effective band width is $1/\sqrt{l}$ and leads to an asymptotic behaviour $U^R - U(l) = C_1 l^{-1/2}$ and $\epsilon_d^R - \epsilon_d(l) = -C_2 l^{-1/2}$ for large $l$ with some constants $C_1$ and $C_2$. This again holds if $\epsilon_d^R$ and $\epsilon_d + U$ lie inside the band. $C_1$ and $C_2$ are positive if $\epsilon_d^R$ lies below and $\epsilon_d + U$ lies above the Fermi energy. One possibility to obtain these expressions in the flow equations one shows easily that $x = y = \frac{1}{2}$ is the only possible solution. We now replace $U$ and $\epsilon_d$ by their asymptotic values on the right hand side of (4.5) and (4.6). Both equations can be integrated and we obtain

$$\epsilon_d(l) = \epsilon_d^R - \int d\epsilon J(\epsilon, l) \frac{\epsilon_d^R - \epsilon + (1 + n(\epsilon)) U}{(\epsilon_d^R - \epsilon)(\epsilon_d^R - \epsilon + U^R)}, \quad (4.10)$$

$$U(l) = U^R + 2 \int d\epsilon J(\epsilon, l) \frac{U}{(\epsilon_d^R - \epsilon)(\epsilon_d^R - \epsilon + U^R)}. \quad (4.11)$$

These equations are good approximations to the solution of the flow equations (4.5) and (4.6). They give the correct asymptotic behaviour and a numerical
integration of the flow equations shows that the true solution differs only slightly from the approximate value given by inserting \( l = 0 \) in (4.10) and (4.11)

\[
\begin{align*}
\varepsilon_d^I &= \varepsilon_d^R - \int \frac{d \varepsilon}{2 \pi} \frac{\varepsilon d - \varepsilon + (1 + n(\varepsilon)) \, U_R^{\varepsilon}}{(\varepsilon d - \varepsilon)(\varepsilon d - \varepsilon + U_R^\varepsilon)}, \\
U^I &= U_R^\varepsilon + 2 \int \frac{d \varepsilon}{2 \pi} \frac{U_R^\varepsilon}{(\varepsilon d - \varepsilon)(\varepsilon d - \varepsilon + U_R^\varepsilon)}.
\end{align*}
\]

These two self-consistency equations are a key result of this section.

For \( U = 0 \) we showed that (4.12) yields the exact result. For \( U = \infty \), (4.10) is correct up to terms quadratic in \( J(\varepsilon, l) \). This can be seen if one notices that (4.10) is the exact solution of a set of equations similar to (3.6) and (3.7) but with \( J(\varepsilon, l) \) replaced by \( J(\varepsilon, l)(1 + n(\varepsilon)) \). An additional argument to justify this approach is similar to the one given at the end of the previous section. The relevant \( l \)-scale for changes of \( \varepsilon_d \) and \( U \) is smaller than the scale on which \( J(\varepsilon, l) \) varies. The crossover to the asymptotic behaviour occurs for \( l > D^{-\frac{1}{2}} \), whereas \( J(\varepsilon, l) \) does not change too much on this scale.

Let us mention that the results for \( \varepsilon_d^R \) and \( U_R^\varepsilon \) obtained from (4.10) and (4.11) do not depend on the special choice of \( f(\varepsilon, l) \) in (4.8). Nevertheless (4.10) and (4.11) are only good approximations to the flow equations (4.5) and (4.6) for special choices of \( f(\varepsilon, l) \) like the one in (4.8). The important point is that \( J(\varepsilon, l) \) has to be chosen so that the principal value of the integrals in (4.10) and (4.11) is well-defined for all values of \( l \). This is clearly true for \( J(\varepsilon, l) \) given in (4.7). Our results here do not depend on the details of the continuous unitary transformation. But the transformation has to be chosen such that the flow for all the parameters in the Hamiltonian is well-defined.

Let us again consider the case \( J(\varepsilon, 0) = 2V^2/\pi D^2 \sqrt{D^2 - \varepsilon^2} \). The equation for \( U_R^\varepsilon \) does not contain a factor \( n(\varepsilon) \) and the integral is easily evaluated. The result is

\[
U^I = U_R^\varepsilon - \frac{2\Gamma}{D} \left[ U_R^\varepsilon - \theta(|\varepsilon_d^R + U_R^\varepsilon| - D) \, \text{sgn}(\varepsilon_d^R + U_R^\varepsilon) \sqrt{(|\varepsilon_d^R + U_R^\varepsilon|^2 - D^2)} 
\right.
\]

\[
\left. + \theta(|\varepsilon_d^R| - D) \, \text{sgn}(\varepsilon_d^R) \sqrt{(|\varepsilon_d^R|^2 - D^2)} \right].
\]

This equation shows that if \( \varepsilon_d^R \) lies below the Fermi energy and \( \varepsilon_d^R + U_R^\varepsilon \) lies above the Fermi energy, then \( U_R^\varepsilon \) is larger than the initial value \( U^I \). This is also true if both, \( \varepsilon_d^R \) and \( \varepsilon_d^R + U_R^\varepsilon \) lie in the band. In this case we simply obtain

\[
U_R^\varepsilon = \frac{U^I}{1 - \frac{U^I}{2\Gamma/D}}.
\]

On the other hand, if \( \varepsilon_d^R \) and \( \varepsilon_d^R + U_R^\varepsilon \) lie above the energy band, \( U_R^\varepsilon \) is smaller than \( U^I \).
Symmetric Anderson Model

In the symmetric case \( U = -2 \varepsilon \), the flow equations yield \( U(l) = -2 \varepsilon \) and the above conditions give \( \varepsilon^R = -2 \varepsilon \) as it should be. Therefore we have

\[
\varepsilon'_d \equiv \frac{2 \Gamma}{D} \left[ \theta(|\varepsilon^R_d| - D) \right. \\
\left. \cdot \left( |\varepsilon^R_d| - D \right) \sgn(\varepsilon^R_d) \sqrt{|\varepsilon^R_d|^2 - D^2} - \varepsilon^R_d \right].
\]  

(4.16)

This equation is very similar to the one obtained for \( U = 0 \). If \( |\varepsilon'_d| < D - 2 \Gamma \) the renormalized value is \( \varepsilon^R = \varepsilon'_d / (1 - 2 \Gamma / D) \) and lies inside the band. If \( |\varepsilon'_d| > D - 2 \Gamma \) we obtain a quadratic equation for \( \varepsilon^R_d \). For \( 2 \Gamma < D \) this equation has a single solution outside the band, whereas for \( 2 \Gamma > D \) we can obtain two solutions of the self-consistency equations outside the conduction band similar to the case \( U = 0 \).

Asymmetric Anderson Model

In the general case \( U \neq -2 \varepsilon \), we have to calculate the integral in (4.12). It contains a factor \( \eta(\varepsilon) \) due to the normal ordering we introduced in the Hamiltonian. Therefore the renormalized impurity energy \( \varepsilon^R_d \) depends on the temperature and the chemical potential. We let \( T = 0 \) and \( \varepsilon_x = 0 \), so that \( \eta(\varepsilon) = 1 - \theta(\varepsilon) \). In this case the integrals can easily be evaluated explicitly. We have to distinguish various cases of whether the impurity orbital energies lie inside the conduction band or outside.

- \( |\varepsilon^R_d|, |\varepsilon^R_d + U_R| > D \): We obtain

\[
\varepsilon'_d = \varepsilon^R_d - \frac{\Gamma}{2D} \left[ 2 \varepsilon^R_d - U_R + \sgn(\varepsilon^R_d + U_R) \right. \\
\left. \times \sqrt{|\varepsilon^R_d + U_R|^2 - D^2} \left( 1 - \frac{2}{\pi} \text{arcsin} \frac{D}{\varepsilon^R_d + U_R} \right) \\
\left. - \sgn(\varepsilon^R_d) \sqrt{|\varepsilon^R_d|^2 - D^2} \left( 3 - \frac{2}{\pi} \text{arcsin} \frac{D}{\varepsilon^R_d} \right) \right].
\]  

(4.17)

In the limit \( U = 0 \) we have \( U_R = 0 \) and the condition for \( \varepsilon^R \) is the same as in the previous section. In the limit \( U = \infty \), we obtain a single equation for \( \varepsilon^R_d \),

\[
\varepsilon'_d = \varepsilon^R_d + \frac{\Gamma}{2D} \left[ \sgn(\varepsilon^R_d) \sqrt{|\varepsilon^R_d|^2 - D^2} \left( 3 - \frac{2}{\pi} \text{arcsin} \frac{D}{\varepsilon^R_d} \right) + \frac{2}{\pi} D - 3 \varepsilon^R_d \right].
\]  

(4.18)

In both expressions, \( |\varepsilon^R_d| > |\varepsilon'_d| \). The impurity orbital energy is pushed away from the band as it should have been expected.

- \( |\varepsilon^R_d| < D, |\varepsilon^R_d + U_R| > D \): We obtain

\[
\varepsilon'_d = \varepsilon^R_d + \frac{\Gamma}{2D} \left[ 2 \varepsilon^R_d - U_R + \frac{2}{\pi} \sqrt{D^2 - (\varepsilon^R_d)^2} \ln \left( \frac{\sqrt{D^2 - (\varepsilon^R_d)^2} + D}{|\varepsilon^R_d|} \right) \right. \\
\left. + \sgn(\varepsilon^R_d + U_R) \sqrt{|\varepsilon^R_d + U_R|^2 - D^2} \left( 1 - \frac{2}{\pi} \text{arcsin} \frac{D}{\varepsilon^R_d + U_R} \right) \right].
\]  

(4.19)
If we let \( U = \infty \) in this case, this expression simplifies to

\[
e_{d}' = e_{d}^{R} - \frac{\Gamma}{2D} \left[ 3e_{d}^{R} - \frac{2}{\pi} D + \frac{2}{\pi} \sqrt{D^2 - (e_{d}^{R})^2} \ln \left( \frac{\sqrt{D^2 - (e_{d}^{R})^2} + D}{|e_{d}^{R}|} \right) \right]. \tag{4.20}
\]

Finally for \( |e_{d}^{R}| \ll D \ll U \)

\[
e_{d}^{R} = e_{d}' + \frac{\Gamma}{\pi} \ln \left( \frac{2D}{|e_{d}|} \right) + \Gamma \left( \frac{D}{UR} \right). \tag{4.21}
\]

This is shown in Fig. 2. Equation (4.21) contains a logarithmic singularity on the right hand side for \( e_{d}^{R} = 0 \). If \( e_{d}' \) is negative and sufficiently far away from the Fermi energy, \( e_{d}^{R} \) is negative as well and increases with increasing \( e_{d}' \). At some (still negative) value of \( e_{d}' \) the renormalized impurity energy jumps discontinuously from a given value below the Fermi energy to a value above the Fermi energy and then increases further with increasing \( e_{d}' \). This behavior can be deduced from the numerical solution of the differential equations and is depicted by the full line in Fig. 2. However, it is difficult to obtain reliable numerical results in this regime. \( e_{d}^{R} \) never reaches the Fermi level except for the trivial case where \( V = 0 \) and \( e_{d}' = 0 \).

- \( |e_{d}^{R}|, |e_{d}^{R} + UR| < D \): We obtain

\[
e_{d}^{R} = e_{d}' - \frac{\Gamma}{2D} \left[ 2e_{d}' - UR + \frac{2}{\pi} D \ln \left( \frac{\sqrt{D^2 - (e_{d}' + UR)^2} + D}{|e_{d}' + UR|} \right) \right]. \tag{4.22}
\]

This expression contains two logarithmic singularities, it diverges if either \( e_{d}' \to 0 \) or \( e_{d}' + UR \to 0 \). As a consequence, both \( e_{d}^{R} \) and \( e_{d}' + UR \) cannot approach the Fermi energy as long as \( V \neq 0 \). For \( |e_{d}^{R}| \ll UR \ll D \) one finds in particular

\[
e_{d}^{R} = e_{d}' + \frac{\Gamma}{\pi} \ln \left( \frac{UR}{|e_{d}'|} \right) + \Gamma \left( \frac{UR}{D} \right). \tag{4.23}
\]

Again the solution of Equation (4.23) is non-unique for some range of the initial parameter \( e_{d}' \). In fact Equation (4.23) is well-known from renormalization theory \([10, 9, 8]\): In the valence fluctuation regime of the asymmetric Anderson model one has to replace \( e_{d}' \) by an effective impurity orbital energy \( E_{d}^{*} \) (we use the notation from \([10]\)). \( E_{d}^{*} \) can be obtained as the solution of the following equation

\[
T_{d}^{*} = -E_{d}(T_{d}^{*}) \overset{\text{def}}{=} -E_{d}^{*} \tag{4.24}
\]

with

\[
-E_{d}(T) = -e_{d}' - \frac{\Gamma}{\pi} \ln \left( \frac{U}{T} \right). \tag{4.25}
\]
One easily checks $E_d^R = e_d^R$ with $e_d^R$ from the flow equations approach. This result for $e_d^R$ is essential for the derivation of the correct effective Kondo Hamiltonian in this regime in Section 5.

Finally it should be emphasized that the flow equations immediately give the correct high-energy cutoff in Eqs. (4.21) and (4.23). Naturally the smaller of the two parameters $U$ and $D$ appears in the logarithm.

One of the main results that we have obtained for $J(\varepsilon, 0) = 2V^2/\pi D^3 \sqrt{D^2 - \varepsilon^2}$ was that the renormalized values $e_d^R$ and $e_d^R + U^R$ behave discontinuously at the Fermi energy as a function of the initial values $e_d^I$ and $e_d^I + U^I$. This is a consequence of the fact that due to the normal ordering a factor $n(\varepsilon)$ appears in (4.12). This
result is generic and holds for a general function $J(\epsilon, 0)$. A similar effect occurs at the band edge if $J(\epsilon, 0)$ is not a continuous function at the band edge. Then we obtain singularities in the integral in (4.12) if $\epsilon_0^R$ or $\epsilon_0^R + U^R$ approach the band edge. Consequently these quantities behave discontinuously at the band edge as a function of the initial values.

There is a last point that we would like to mention. In the symmetric case $U = -2\epsilon_0$, the renormalized value of $U$ does not depend on the temperature. If the system deviates only a bit from the symmetric case, (4.12) and (4.13) show that the system is pushed in the direction of the symmetric case. This can be seen if one takes $\epsilon_0 = -U/2 + \delta$ and expands the right hand side of (4.12). The renormalized value of $\delta$ is smaller than the initial value of $\delta$. In this sense the symmetric situation is stable. Near the symmetric point the temperature dependence of the renormalized values will be weak. But in the general case the renormalized values of the impurity energy and the interaction will depend on the temperature. For small enough temperature the integral in (4.12) can be evaluated using the usual Sommerfeld expansion. This yields

$$
\epsilon_0^R = \epsilon_0^I + \int d\epsilon J(\epsilon, 0) \frac{\epsilon_0^R - \epsilon + (1 + \Theta(-\epsilon)) U^R}{(\epsilon_0^R - \epsilon)(\epsilon_0^R - \epsilon + U^R)}
$$

$$
+ \frac{\pi}{6} T (k_B T)^2 ((\epsilon_0^R)^{-2} - (\epsilon_0^R + U^R)^{-2}) + O(T^4)
$$

This shows that for $|\epsilon_0^R + U^R| > |\epsilon_0^R|$ we obtain $\epsilon_0^R(T) > \epsilon_0^R(T = 0)$, whereas for $|\epsilon_0^R + U^R| < |\epsilon_0^R|$ we obtain $\epsilon_0^R(T) < \epsilon_0^R(T = 0)$. Generally Equation (4.26) is a good approximation only for $T < |\epsilon_0^R|$. When $T$ becomes larger one can show that $\epsilon_0^R(T)$ will decrease as a function of $T$ for $|\epsilon_0^R + U^R| > |\epsilon_0^R|$. The temperature dependence of $\epsilon_0^R$ leads to a weak temperature dependence of $U^R$. In the special case $J(\epsilon, 0) \propto \sqrt{D^2 - \epsilon^2}$ we obtain a temperature dependence of $U^R$ only if $\epsilon_0^R$ or $\epsilon_0^R + U^R$ lie outside the band. If $|\epsilon_0^R|, |\epsilon_0^R + U^R| < D$, (4.14) shows that $U^R$ does not depend on the temperature.

### 5. THE INDUCED SPIN–SPIN INTERACTION

So far the contribution (2.10), which is generated by the unitary transformation, and which therefore has to be included in the Hamiltonian, was not taken into account. This interaction gives rise to a spin–spin coupling term

$$
-2 \sum_{k, q} V_{k, q}^{(2)} (\psi_k^\dagger \frac{1}{2} \sigma \psi_q) \cdot (\psi_q^\dagger \frac{1}{2} \sigma \psi_k)
$$

with

$$
\psi_k = \begin{pmatrix} c_{k, +} \\ c_{k, -} \end{pmatrix}, \quad \psi_q = \begin{pmatrix} d_+ \\ d_- \end{pmatrix},
$$
the so called potential scattering term
\[
\frac{1}{2} \sum_{k, q} V^{(2)}_{k, q} \langle \psi^\dagger_k \psi_q \rangle (\psi^\dagger_q \psi_k)
\]
(5.3)
and a term
\[
\frac{1}{2} \sum_{k, q} V^{(2)}_{k, q} c^\dagger_{k, \sigma} (c^\dagger_{q, -\sigma} d^\dagger_{-\sigma} + d^\dagger_{\sigma} c^\dagger_{-\sigma} + c^\dagger_{-\sigma} d^\dagger_{\sigma} c_{k, \sigma})
\]
(5.4)

The final Hamiltonian contains no couplings between states that have a singly occupied impurity orbital and states for which the impurity orbital is either empty or doubly occupied. Whereas the spin–spin coupling (5.1) acts only on the part of the Hilbert space of states with a singly occupied impurity orbital, the term (5.4) vanishes on this part of the Hilbert space. It is important if the impurity orbital is either empty or doubly occupied. In this sense, these two terms are conjugate to each other. In fact one has a simple interpretation for these couplings in the symmetric Anderson model. Whereas the asymmetric Anderson model has only the usual SU(2)–spin symmetry, the symmetric Anderson model has an additional SU(2)–pseudo-spin symmetry. Introducing the wave vector \( \pi \), which has all components equal to \( \pi \), the symmetric energy band has the symmetry \( \epsilon_k = -\epsilon_{\pi-k} \), \( V_k = V_{\pi-k} \). For \( \epsilon_d = -U/2 \) the Hamiltonian also commutes with the operators

\[
\begin{align*}
\hat{S}_z &= \frac{1}{2} \left( 1 - d^\dagger_+ d_+ - d^\dagger_- d_- + \sum_k (1 - c^\dagger_{k, -} c_{k, +} - c^\dagger_{k, +} c_{k, -}) \right) \\
\hat{S}_+ &= d^\dagger_+ d_+ + \sum_k \epsilon_{\pi-k, +} c_{k, +} \\
\hat{S}_- &= d^\dagger_- d_- + \sum_k c^\dagger_{k, -} \epsilon_{\pi-k, -}
\end{align*}
\]
(5.5)

These operators form the second SU(2) symmetry mentioned above. The potential scattering term (5.3) and the term (5.4) together can be written as a pseudo-spin interaction. It is clear that if the original Hamiltonian has these symmetries, the transformed Hamiltonian has these symmetries too. Therefore the term (5.4) is present if the corresponding spin–spin interaction is present. Although in the asymmetric case the Hamiltonian does not have the additional symmetry, the two terms (5.3) and (5.4) have the same interpretation. The only difference is that now the coupling constant \( V^{(2)}_{k, q} \) is not symmetric with respect to a transformation \( k \rightarrow \pi-k \).

Let us come back to the construction of the effective Kondo Hamiltonian in the regime \( \epsilon^R_d < \epsilon_F \) and \( \epsilon^L_d + U^R > \epsilon_F \), where the ground state contains a localized magnetic moment. Since \( \psi^\dagger \psi = 1 \) in this regime, the pseudo-spin interaction reduces to a scattering of band electrons. Such a term has already been neglected since it is irrelevant for the low-temperature properties and its contribution is not taken into account.
Next the spin–spin coupling term (5.1) reduces to a coupling of a quantum mechanical spin-1/2 to the conduction band electron spin. Hence the effective Hamiltonian in this regime is just of the Kondo type (1.2) with matrix element $V_{k,q}^{(2)}$, that can be deduced from the infinitesimal unitary transformations.

As is well-known, an antiferromagnetic spin–spin coupling at the Fermi surface $V_{k_F,k_F}^{(2)}<0$ gives rise to the Kondo effect for low temperatures. In the Kondo model the Kondo temperature can be defined as $T_K=(2\pi Z_{imp}(T=0))^{-1}$ [7] where $Z_{imp}(T=0)$ is the impurity contribution to the susceptibility at zero temperature. Let us remark that other definitions of the Kondo temperature can be found in the literature, the definition by Wilson [2] is somewhat different. For a detailed discussion see e.g. [7]. Based on a Bethe–ansatz solution, Tsvelick and Wiegmann argue that the Kondo temperature $T_K$ is given by

$$k_B T_K = \frac{2}{\pi} D \exp \left[ -\Phi(2\rho(k_F) V_{k_F,k_F}^{(2)}) \right]$$

(5.6)

with the universal function [2]

$$\Phi(y) = \frac{1}{\ln |y|} + \frac{1}{2} \ln |y| + O(y).$$

(5.7)

In this solution a linear dispersion relation for the conduction band is used and $V_{k_F,k_F}^{(2)}$ is assumed to be constant. $D$ is the conduction band width.

In the Anderson impurity model one knows that $D$ in (5.6) has to be replaced by an effective band width $D_{\text{eff}}$ that cannot be larger than $U_R$ [9]. If one follows the perturbative calculation of e.g. the susceptibility in the Kondo problem, one notices that the breakdown of the perturbation expansion is due to the matrix elements $V_{k_F,q}^{(2)}$. These describe the scattering of an electron from the Fermi surface with the impurity to some wave vector $q$ and then back to the Fermi surface. For this reason one is not only interested in the coupling at the Fermi surface $V_{k_F,k_F}^{(2)}$, but also in $V_{k_F,q}^{(2)}$ since this determines the effective band width of the associated Kondo problem.

Let us now calculate the matrix elements $V_{k_F,q}^{(2)}$ in the flow equations approach. We already mentioned that the additional couplings (2.10) do not lead to a contribution in the equations for $\varphi_d$ and $U$. Therefore we calculate the coupling constant simply by integrating the coefficient in front of the interaction term in (5.1)

$$V_{k_F,q}^{(2)} = \int_0^\infty \frac{d\ell}{2\pi} (\eta^{(2)}_{k} V_{q} + \eta^{(2)}_{q} V_{k}).$$

(5.8)

Using (2.9) and (3.3) to replace $\eta^{(2)}_{k}$ and furthermore (4.4), we obtain

$$V_{k_F,q}^{(2)} = -\frac{1}{2} \int_0^\infty d\ell V_{k} V_{q} U \left( \frac{\partial \ln J(e_d,1)}{\partial \ell} \frac{\partial \ln J(e_q,1)}{\partial \ell} \right).$$

(5.9)
The \( \lambda \)-dependence of \( V_k \) is obtained from (4.1). Using again (3.3) and (4.4) we obtain

\[
V_k(\lambda) = V_k(0) \frac{\mathcal{J}(\epsilon_k, \lambda)}{\mathcal{J}(\epsilon_k, 0)}.
\] (5.10)

This yields

\[
V_{k,q}^{(2)} = \frac{1}{2} V_k(0) V_q(0) \int_0^\infty dl \frac{\mathcal{J}(\epsilon_k, \lambda) \mathcal{J}(\epsilon_q, \lambda) \mathcal{J}(\epsilon_q, 0) \mathcal{J}(\epsilon_q, 0) \mathcal{J}(\epsilon_q, 0)}{\mathcal{J}(\epsilon_k, 0) \mathcal{J}(\epsilon_q, 0)} \left( \frac{\partial \mathcal{J}(\epsilon_k, \lambda)}{\partial \lambda} \mathcal{J}(\epsilon_q, \lambda) + \frac{\partial \mathcal{J}(\epsilon_q, \lambda)}{\partial \lambda} \mathcal{J}(\epsilon_k, \lambda) \right)
\] (5.11)

Using the parametrization for \( \mathcal{J}(\epsilon, \lambda) \) introduced in (4.7), this expression simplifies to

\[
V_{k,q}^{(2)} = \frac{1}{2} V_k(0) V_q(0) \int_0^\infty dl \left( \frac{\epsilon_d - \epsilon_k (\epsilon_d - \epsilon_k + U)}{\epsilon_d^2 + (\epsilon_d + U)^2} \right)^{1/2}
\]

\[
\times \exp\left( -\frac{1}{2} \int_0^\infty \left( \frac{\epsilon_d - \epsilon_k}{\epsilon_d + (\epsilon_d + U)^2} \right)^2 \right)
\] (5.12)

Let us replace \( \epsilon_d \) and \( U \) on the right hand side by their renormalized values. The same reasoning applies with respect to this approximation as at the end of Section 3, in particular for the important matrix elements at the Fermi surface. One finds

\[
V_{k,q}^{(2)} = V_k(0) V_q(0) U_R^R
\]

\[
\times \left( \frac{\epsilon_d^R - \epsilon_k (\epsilon_d^R - \epsilon_k + U^R)}{(\epsilon_d^R - \epsilon_k)^2} + \frac{\epsilon_d^R - \epsilon_q (\epsilon_d^R - \epsilon_q + U^R)}{(\epsilon_d^R - \epsilon_q)^2} \right) \] (5.13)

This formula is a very good approximation to (5.12) if \( \epsilon_k \) or \( \epsilon_q \) are not too close to \( \epsilon_d^R \) or \( \epsilon_d^R + U^R \). If both band energies become equal to \( \epsilon_d^R \) or \( \epsilon_d^R + U^R \), the approximate result diverges. In this special case the asymptotic behaviour of \( \epsilon_d \) and \( U \) becomes important. One can show that the integral in (5.12) has a logarithmic divergence, which yields a logarithmic divergence of \( V_{k,q}^{(2)} \) if \( \epsilon_k \) and \( \epsilon_q \) approach \( \epsilon_d^R \) or \( \epsilon_d^R + U^R \). Such a divergence causes no problems since it is integrable as a function of the energy \( \epsilon_k \); also higher powers of \( V_{k,q}^{(2)} \) remain integrable.

When calculating the Kondo temperature, we only need \( V_{k,q}^{(2)} \) for the case where at least one of the band energies is equal (or at least very close) to the Fermi
energy. Since $\epsilon_d^R$ or $\epsilon_k^R + U^R$ can only be equal to the Fermi energy if the hybridization vanishes, we can use (5.13) in the following. At the Fermi surface this yields

$$V^{(2)}_{k_x, k_y} = V_{k_x} (0) \frac{U^R}{\epsilon_d^R (\epsilon_d^R + U^R)}, \quad (5.14)$$

and with only one wave vector at the Fermi surface

$$V^{(2)}_{k_x, q} = V_{k_x} (0) \frac{U^R}{\epsilon_d^R (\epsilon_d^R + U^R)} \left( \frac{\epsilon_k - \epsilon_q}{\epsilon_d^R + U^R} \right) \left( \frac{\epsilon_k^R - \epsilon_q^R}{\epsilon_d^R + U^R} \right) + \left( \frac{\epsilon_k^R}{\epsilon_d^R + U^R} \right) \left( \frac{\epsilon_k + U^R}{\epsilon_d^R + U^R} \right). \quad (5.15)$$

Before proceeding with the calculation of the Kondo temperature in various cases, it is interesting to compare this result with the coupling obtained by the Schrieffer–Wolff unitary transformation in Ref. [14]. There one finds

$$V^{(2)}_{k_x, q} = \frac{1}{2} V_{k_x} (0) V_q (0) U^I \left( \frac{1}{(\epsilon_d^R - \epsilon_k^R)(\epsilon_d^R + U^I)} + \frac{1}{(\epsilon_d^R - \epsilon_q^R)(\epsilon_d^R + U^I)} \right), \quad (5.16)$$

in particular at the Fermi surface

$$V^{(2)}_{k_x, k_y} = \frac{1}{2} V_{k_x} (0) V_{k_y} \frac{U^I}{\epsilon_d^R (\epsilon_d^R + U^I)}. \quad (5.17)$$

As a first remark we mention that for $\epsilon_k = \epsilon_q$ both results are identical if one replaces the initial values of $\epsilon_d^R$ and $U^I$ in the result by Schrieffer and Wolff with the renormalized values $\epsilon_d^R$ and $U^R$. For $\epsilon_k \neq \epsilon_q$ our result differs from the Schrieffer–Wolff result in $O(V^2)$ though both calculations only neglect terms in $O(V^3)$. This is very surprising at first sight and we come back to it in the next section.

Let us analyse the Schrieffer–Wolff result in more detail. The first problem with the induced spin-spin interaction in their formalism are the pole terms in $V^{(2)}_{k_x, q}$ if $\epsilon_k^R$ or $\epsilon_k^R + U^I$ lie in the conduction band. A second problem is apparent in the following limit

$$V^{(2)}_{k_x, q} \xrightarrow{\epsilon_k \to \infty} \frac{1}{2} V_{k_x} (0) V_q (0) \frac{U^I}{\epsilon_d^R (\epsilon_d^R + U^I)} \neq 0. \quad (5.18)$$

This immediately implies that the effective band width in the corresponding Kondo problem is of order the conduction band width

$$D_{\text{eff}} \propto D, \quad (5.19)$$

which is known to be wrong. It is obvious from Equation (5.15) that both these problems do not show up in the flow equations approach.

In order to obtain some more quantitative results, let us now discuss two particular regimes of the Anderson model.
Symmetric Anderson Model with $|\epsilon^R_q| < D$

In the symmetric case one has $\epsilon^R_q = -U^R/2$ and the relevant matrix elements of the spin-spin coupling are

$$V^{(2)}_{kq} = V_{kq}(0) \frac{\epsilon_q^2 - (U^R)^2/2}{(\epsilon_q^2 - (U^R)^2/4)^2 + ((U^R)^2/4)^2}$$

This is depicted in Fig. 3 where it can be compared with the Schrieffer-Wolff result. For simplicity we have assumed $V_q(0) = V_{kq}(0)$ for all wave vectors $q$ in the diagram. Furthermore, we have replaced $U^I$ by $U^R$ in the Schrieffer-Wolff result,
see also our discussion in Section 6 for this point. The Kondo temperature depends mainly on the coupling at the Fermi surface (compare Equation (5.6))

\[ 2p(\varepsilon_F) V_{kF,kF}^{(2)} = -\frac{8I}{\pi U} \left( 1 - \frac{2I}{D} \right). \]  

(5.21)

This is consistent with the Schrieffer–Wolff result except that we find an additional (usually small) correction term \( 2I/D \).

The main difference to the Schrieffer–Wolff result shows up in the effective band width of the associated Kondo problem. In the flow equations approach the effective band width is obviously proportional to the on-site interaction

\[ D_{\text{eff}} \propto U^R \]  

(5.22)

since the spin–spin coupling becomes ferromagnetic for \( |\varepsilon_q| > U^R/\sqrt{2} \) and decays to zero even further away from the Fermi surface. Since the spin–spin coupling induced by our unitary transformation is not constant (there is no physical reason why it should be), it is difficult to say quantitatively what the proportionality factor in Equation (5.22) is: The Kondo problem is usually only treated for a constant spin–spin coupling with the conduction band electrons. Nevertheless, we would like to estimate the proportionality constant in (5.22) for the special case of a constant density of states and constant \( V_q(0) \). This value can be compared with known results. To get some rather approximate estimate one can e.g. replace \( V_{kF,kF}^{(2)} \) regarded as a function of \( \varepsilon_q \) by its value at the Fermi surface in an interval around the Fermi surface that has the same area as the original curve. This should give a lower bound on \( D_{\text{eff}} \). We obtain

\[ D_{\text{eff}} \gtrsim 0.36 \ U^R. \]  

(5.23)

This result can be compared with the result from the Bethe–ansatz solution. There one obtains

\[ k_B T_K = \frac{U}{\sqrt{4\pi}} \exp(-\Phi(2p(\varepsilon_F) V_{kF,kF}^{(2)})). \]  

(5.24)

We identify the prefactor with the one in (5.6) and obtain

\[ D_{\text{eff}} = \frac{\sqrt{\pi}}{4} U = 0.443 \ U. \]  

(5.25)

This is in good agreement with (5.23). Estimates similar to (5.23) can be obtained for an arbitrary density of states and arbitrary \( V_q(0) \).
Valence Fluctuation Regime $0 < -\varepsilon_R^d \ll U^R \ll D$

This regime shows characteristic new features of the asymmetric Anderson model. The spin–spin coupling is given by

$$V^{(2)}_{k_F, q} = V_{k_F}^{(0)} V_q^{(0)} \frac{2\varepsilon_R^d - \varepsilon_q}{(\varepsilon_R^d - \varepsilon_q)^2 + (\varepsilon_q^2)^2}$$

(5.26)

with the value at the Fermi surface

$$2\rho(\varepsilon_F) V^{(2)}_{k_F, k_F} = \frac{2\Gamma}{\pi\varepsilon_d^2}$$

(5.27)

Essentially the same remarks apply as in the previous section. The coupling is depicted in Fig. 4 where it can be compared with the Schrieffer–Wolff result (again

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**Fig. 4.** Induced spin–spin interaction in the $U \to \infty$ limit.
with \( V_\alpha(0) = V_\gamma(0) \) and with \( e_d, U \) replaced by \( e_d^\theta, U^\theta \). As before the flow equations approach yields the correct scaling behaviour of the effective band width

\[
D_{\text{eff}} \propto |e_d^\theta|.
\]

It is important that the “renormalized” value of the impurity orbital energy enters in Eqs. (5.26) and (5.27). This behaviour is known from perturbative renormalization [9, 8] or numerical renormalization [10] which give the same value of the renormalized impurity orbital energy that we have calculated in Equation (4.23). In this regime the Schrieffer–Wolff unitary transformation not only gives the wrong scaling behaviour of the effective band width \( D_{\text{eff}} \propto D \), but also the wrong coupling at the Fermi surface since the initial value of the impurity orbital energy enters.

At this point one can wonder about the temperature dependence of \( e_d^\theta \) that has been found in Equation (4.26). This effect seems to be unobserved in renormalization treatments. However, the maximum effect of non-zero temperature is to increase \( e_d^\theta (T = 0) \) by a value of order \( T \). According to Fig. 2 the smallest value of \( |e_d^\theta| \) with \( e_d^\theta < 0 \) is \( e_d^\theta = -\Gamma/\pi \), that is of order \( T \). Thus one might expect to see some influence of the temperature dependence of \( e_d^\theta \) in this regime with \( |e_d^\theta| \leq \Gamma \). But this is just the mixed valence regime (for \( k_B T \leq \Gamma \)) where scaling breaks down anyway [8].

6. COMPARISON WITH OTHER METHODS, I
(SCHRIEFFER–WOLFF UNITARY TRANSFORMATION)

At this point we would like to explain in more detail why the Schrieffer–Wolff transformation and our continuous unitary transformation yield different results. At a first glance these two transformations are very similar. Our \( \eta \) has exactly the same structure as the generator \( S \) in the Schrieffer–Wolff transformation \( H \rightarrow e^\eta H e^{-\eta} \) [14] with

\[
S = \sum_{k, \alpha} V_k(0) \left( \frac{U'}{(e_d - \epsilon_k)(e_d - \epsilon_k + U)} \right) d^\dagger \sigma \rho^\dagger \sigma d \sigma + \frac{1}{e_k - e_d} \epsilon_k \sigma d^\dagger \sigma - h.c.
\]

In both approaches the same more complicated interactions in order \( V_2 \) generated due to higher commutators are neglected. But as we have seen the two transformations still show remarkable differences for the induced interactions in order \( V_1 \).

First of all, let us mention that it is possible to construct a continuous unitary transformation that reproduces the Schrieffer–Wolff result (5.16) for the coupling \( V_1 \) with the initial values of \( e_d \) and \( U \) replaced by their renormalized values. In fact one can achieve this by choosing the parametrization

\[
f(\epsilon, l) = \frac{1}{2} \frac{1}{e_d - \epsilon}
\]

(6.2)
instead of Equation (4.8). Then the hybridization $J(\epsilon, l)$ shows a very simple flow

$$J(\epsilon, l) = J(\epsilon, 0) \exp(-l).$$

(6.3)

This is depicted in Fig. 5 where it can be compared with the behaviour for our choice of $f(\epsilon, l)$ from Equation (4.8). As compared to the original Schrieffer–Wolff transformation this is an improvement since now the renormalized parameters

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**Fig. 5.** Sketch of $J(\epsilon, l)$ for the symmetric Anderson impurity model for different values of $l$, $l_2 > l_1 > l_0 = 0$ or $D_2 < D_1 < D_0 = D^0$. $J(\epsilon, 0)$ is the semi-circle. In (a) $J(\epsilon, l)$ is shown for the improved Schrieffer–Wolff transformation introduced in (6.3), (b) corresponds to the poor man’s scaling approach in the context of the flow equations, compare Section 7. In (c) the parametrization of $J(\epsilon, l)$ as chosen in this paper is depicted. The flow of $U(l)$ has been neglected in the diagram, in fact this would lead to an algebraic decay of $J(\epsilon, l)$ also for $\epsilon = \pm U^0/2$. 

enter into the expressions for the induced spin-spin interaction at the Fermi surface $V_{k_F, k_F}^{(2)}$. In the valence fluctuation regime this is of importance as discussed in the previous section.

Still the main differences between the Schrieffer–Wolff result and the flow equations are not resolved so easily. That is in the Schrieffer–Wolff approach the couplings $V_{k, q}^{(2)}$ show the wrong high-energy cutoff and contain pole terms. This is due to the fact that our transformation differs in order $V_2$ from the Schrieffer–Wolff transformation. It is of course possible to write our transformation in the form $\exp(S)$ too. Due to the infinitesimal nature of the transformation, $S$ has to be calculated from the expansion

$$S = \int_0^\infty dl \eta(l) + \frac{1}{2} \int_0^\infty dl \int_0^l dl'[\eta(l), \eta(l')] + \ldots$$ (6.4)

The term containing the commutator of $\eta$ at two different values of the flow parameter contributes in order $V_2$. It is of the form

$$\sum_{k, q, \sigma} S_{k, q, \sigma}^{(2)} c_{k, \sigma}^\dagger d_{-\sigma} c_{q, -\sigma}^{\dagger} + c_{q, -\sigma}^{\dagger} d_{-\sigma} c_{k, \sigma}^{\dagger}$$ (6.5)

and it is naturally generated by the separation of energy scales due to the flow parameter $l$.

Hence it is possible but not very enlightening to work in terms of the global unitary transformation generated by $S$. The advantage of the flow equation approach is just that its generator $S$ has a natural interpretation as being generated from infinitesimal transformations and that thereby singular interactions are avoided. Separation of energy scales and a different structure of $S$ are in this manner always intermingled. The importance of the parametrization of $f(U, l)$ in (4.8) is to generate the correct separation of energy scales as depicted in Fig. 5c.

7. COMPARISON WITH OTHER METHODS, II
(SCALING APPROACHES)

Some remarks have already been made about similarities between the flow equation approach and traditional scaling procedures. In this section we sum up some of these remarks and make them more explicit.

Let us first of all compare our method to scaling theory in the spirit of Anderson’s “poor man’s” scaling approach [21]. We will briefly review the main features of this approach as applied to the Anderson impurity model by Haldane [8]. For simplicity we assume $U \gg D \gg |e_d|$. The band width $D$ is reduced to $D - dD$ by perturbatively integrating out states with energies $D - dD < |e| < D$. This results in the following scaling equations [8]
\[
\frac{d\varepsilon_d}{d\ln D} = -\int_0^\infty \frac{e^{\varepsilon_d}}{\varepsilon_d} \left( \frac{2\varepsilon_d}{\varepsilon_d^2 - \varepsilon^2} J'(\varepsilon) + \frac{\varepsilon}{\varepsilon_d - \varepsilon} J'(\varepsilon) \right) d\varepsilon
\]
(7.1)

\[
\frac{dI}{d\ln D} = O(I^2(D)/D).
\]
(7.2)

In order to avoid confusion with the flow equations approach we have introduced the notation \( J'(\varepsilon) \triangleq J(\varepsilon, l=0) \). The second equation leads to no nontrivial scaling behaviour. In the first equation the main contributions come from \(|\varepsilon| \approx D\) and Haldane finds

\[
\frac{d\varepsilon_d}{d\ln D} = \frac{\Gamma}{\pi} + O(\varepsilon_d J'(D)/D).
\]
(7.3)

By scaling down to \( D \approx k_B T \) one obtains the effective impurity orbital energy \( E^*_d \) that is equal to our \( \varepsilon^*_d \) in (4.21). In the limit \( D \gg U \gg |\varepsilon^*_d| \) one argues that nontrivial scaling occurs only when \( D \) has been reduced to order \( U \). In this case one obtains (4.24) for the effective impurity energy that enters into the induced spin–spin interaction.

Now the scaling equation (7.1) can also be obtained in the flow equations formalism. One has to choose

\[
J(\varepsilon, l) \triangleq J(\varepsilon, l),
\]
(7.4)

where \( D' \) is the initial band width, \( D(l) \) is a parameter (effective band width) that approaches zero monotonously as \( l \to \infty \). Instead of using the unfamiliar parameter \( l \) we can then try to work with the more familiar parameter \( D \). Obviously (7.4) amounts to decoupling the high-energy modes by means of a unitary transformation as depicted in Fig. 5. It should come as no surprise that this yields flow equations in \( D \) reminiscent of the familiar scaling equations. Decoupling modes by means of a unitary transformation or integrating them out in a path integral approach leads to the same answer. Let us remark that Equation (7.4) corresponds to a certain choice of \( f(\varepsilon, l) \), but this will be of no importance for our discussion.

The flow equation (4.5) for \( \varepsilon_d \) in the limit \( U \to \infty \) expressed as a function of \( D = D(l) \) takes the following form after a short calculation

\[
\frac{d\varepsilon_d}{d\ln D} = \int d\varepsilon (1 + n(\varepsilon)) \frac{\varepsilon}{\varepsilon_d - \varepsilon} \frac{\partial}{\partial \varepsilon} J'(\varepsilon) \left( \varepsilon \frac{D'}{D} \right)
\]
(7.5)

to be integrated from \( D = D'(l) \) to \( D = 0 \). For \( T = 0 \) this obviously just reproduces Haldane’s scaling equation (7.1).

Now first of all this might make some approximations more plausible that we have used in the flow equations approach. In particular the restriction to a certain
set of interactions is standard in a renormalization framework. It is well-known that the procedure of integrating out high-energy modes leads to additional interactions in the “poor man’s” approach [8]. This will also include e.g. the induced spin–spin interaction. However, even these terms are not taken into account in the “poor man’s” approach.\(^1\) Instead one argues that on a low-energy scale the physical behaviour is determined by the scaling invariants like \(E_+\).

Though intuitively quite appealing, the parametrization (7.4) leads to immediate problems in the flow equations formalism since we do not use similar approximations. The first problem is already apparent from (7.2): Why should the infinitesimal unitary transformations stop when \(D\) is of order \(k_B T\)? Such a cutoff is necessary, otherwise Equation (7.2) leads to divergent behaviour as \(D \to 0\).

An even worse problem shows up when comparing the self-consistency equations (4.12) and (4.13) with the actual solution of the differential equations in \(D\). Let us for simplicity consider the symmetric Anderson model with (compare Equation (4.15))

\[
U_R = \frac{U}{1 - 2I/D} < D/2. \tag{7.6}
\]

However, the solution of the differential equation in \(D\) leads to \(U(l=\infty) = 0\) as can be shown rigorously for the semi-circle case. Intuitively what happens is that the modes with energies larger than \(U/2\) that are being integrated out push \(U\) closer to the Fermi surface. Before the low-lying modes can push \(U\) away again, one has reached \(U = 0\). Just this behaviour is avoided by the parametrization (4.7), compare also Fig. 5. This is the reason why the decoupling in our case can be performed all the way down to \(l = \infty\) without introducing a condition like \(D \approx k_B T\). The self-consistency conditions (4.12) and (4.13) have been obtained from (4.10) and (4.11) by taking \(l = 0\). Thus the self-consistency conditions fail if the principal value integrals in (4.10) and (4.11) are not well-defined for some value of \(l\). This happens with the parametrization (7.4). For \(l\) such that \(D(l) = \varepsilon_d^R\) or \(D(l) = \varepsilon_d^R + U_R\) the integrals diverge, a familiar band-edge problem.

The reason why this phenomenon is unobserved in the scaling approach is that it is due to neglected terms like on the right hand side of Eq. (7.2). But if one attempts to study the behaviour when \(U\) becomes of order \(D\), these terms cannot be neglected. The parametrization of \(f(c,l)\) in (4.8) is also in this manner singled out by yielding solutions of the original differential equations that are in agreement with the solution of the (decoupling procedure independent) self-consistency equations.

Finally we would like to remark that more sophisticated scaling approaches like perturbative renormalization with identification of leading log’s or Anderson–Yuval scaling can overcome the deficiencies of the “poor man’s” approach. This has been demonstrated by Haldane in Ref. [9] who already obtained all the important cross-over behaviour in the Anderson impurity model. Still the main emphasis of these

\(^1\) In this sense our approximations are clearly better although less familiar.
techniques is not on the explicit derivation of an effective Hamiltonian and its induced interactions that we were interested in here.

8. CONCLUSIONS

We have used infinitesimal unitary transformations to map the Anderson impurity Hamiltonian onto an effective Kondo Hamiltonian describing the low-energy properties in the Kondo regime. In contrast to the Schrieffer–Wolff unitary transformation our approach generates the correct parameters of this effective Kondo Hamiltonian. In particular no problematic pole terms due to vanishing energy denominators appear in the spin–spin coupling and the correct high-energy cutoff enters in all the expressions for the induced interactions. One should expect that such a unitary transformation exists since after all the Anderson impurity model has been introduced to serve as a microscopic model for dilute magnetic alloys which exhibit the Kondo effect. In this manner we have added some new perspective to an old and important model of solid state physics.

However, the main purpose of this work was to demonstrate that Wegner’s approach of infinitesimal unitary transformations with its intrinsic energy scale separation allows a systematic derivation of effective Hamiltonians. By comparison with the Schrieffer–Wolff transformation it is apparent that in both approaches terms of the same order in the small parameter $V_k$ are neglected, still the induced interactions (5.13) and (5.16) are different. The key to understanding this apparent discrepancy is simple but with far-reaching consequences: The construction of an effective Hamiltonian even in terms of a small parameter is non-unique, there are an infinite number of different unitary transformations to choose from. But an effective Hamiltonian is only useful if it does not contain singular interactions, otherwise it cannot even be treated in perturbation theory.

In this sense Wegner’s flow equations seem to be singled out (though we have no rigorous proof for this property) by avoiding singular interactions due to the infinitesimal nature of the transformation that naturally produces “counter-terms” (6.4) for the induced interactions. Dealing with large energy differences first before proceeding to smaller energy differences is also intuitively the safe order of things and at the heart of the success of scaling approaches.

Let us emphasize again that of course for finite systems with discrete spectra it should not play any role which unitary transformation to choose. But here a thermodynamic limit intervenes and close to the Schrieffer–Wolff pole terms large induced interactions are produced due to a denominator that is given by the vanishing energy difference of two discrete eigenvalues. Remarkably, “smearing” out the poles does not repair this problem since one still ends up with the wrong high-energy cutoff for the induced interactions.

A very similar problem to ours in this work is the well-known Fröhlich transformation [15]. By decoupling the electrons and phonons in a solid one finds the effective electron-electron interaction responsible for BCS-superconductivity.
A region of phase space where this interaction is attractive is separated from a repulsive region by a pole in the Fröhlich result. In contrast, the application of flow equations by Lenz and Wegner [16] yielded an induced interaction for BCS-pairs that is always attractive without any singularities.

Let us finally remark that in field theory, conceptually similar ideas where small energy denominators are systematically avoided have recently also been independently put forward by Glazek and Wilson [3, 4].

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