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Flow equations for the Anderson Hamiltonian

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Abstract. Using a continuous unitary transformation recently proposed by Wegner [1] together with an approximation that neglects irrelevant contributions, we obtain flow equations for Hamiltonians. These flow equations yield a diagonal or almost diagonal Hamiltonian. As an example we investigate the Anderson Hamiltonian for dilute magnetic alloys. We study the different fixed points of the flow equations and the corresponding relevant, marginal or irrelevant contributions. Our results are consistent with results obtained by a numerical renormalization-group method, but our approach is considerably simpler.

1. Introduction

Recently Wegner [1] developed a method to obtain flow equations for Hamiltonians. These equations result from a continuous unitary transformation that brings the Hamiltonian closer to diagonalization. The continuous unitary transformation generates a Hamiltonian $H(\ell)$ from an initial Hamiltonian $H(0)$. It may be written in the form

$$\frac{\mathrm{d}H(\ell)}{\mathrm{d}\ell} = [\eta(\ell), H(\ell)] \tag{1.1}$$

where $\eta(\ell)$ is an anti-Hermitian operator depending on ℓ as well. Assume that H is written in the form $H = H^{\mathrm{d}} + H^{\mathrm{r}}$. H^{d} is a Hamiltonian that can be diagonalized whereas H^{r} contains further terms which are not simple. We now try to choose η such that $H^{\mathrm{r}}(\ell)$ tends to zero as ℓ goes to ∞. Wegner proposed

$$\eta = [H, H^{\mathrm{r}}]\,. \tag{1.2}$$

With this choice of η, H^{r} does not necessarily vanish for $\ell \to \infty$, but η vanishes in this limit so that H can be diagonalized up to degeneracies of eigenvalues of H^{d}. Notice that of course the method of unitary transformations of a Hamiltonian is perfectly well known in solid-state theory, in particular to study non-perturbative effets. However, it is usually non-trivial to find these unitary transformation. With Wegner's choice of η in (1.2) one has a general framework to construct such unitary transformations that make Hamiltonians 'simpler'. One seems to recover a lot of standard unitary transformations in this way. A well known example is the Schrieffer–Wolff transformation [2]. The connection between the unitary transformation induced by the flow equations and the Schrieffer–Wolff transformation will be discussed in section 4.

It is clear that it is in general impossible to solve the full flow equations for a given initial Hamiltonian. The situation is even worse. If we consider for example an initial Hamiltonian

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describing electrons on a lattice with a given two-particle interaction, the flow equations generate additional interactions among three and more particles. Wegner showed that in the case of an n-orbital model in the limit $n \to \infty$, the equations for the two-particle interaction are closed. This fact allowed him to solve the flow equations for a one-dimensional model in the limit $n \to \infty$. Then it is possible to perform a $1/n$-expansion.

In the present paper we introduce an approximation to the flow equations which allows one to treat a large class of models. The approximation consists of neglecting those contributions on the right-hand side of (1.1) which are of a form different from the terms in the initial Hamiltonian $H(0)$, e.g. the terms generating three-particle interactions mentioned above are neglected. Then one obtains a set of differential equations which can be analysed. In a second step one can now add different contributions to the Hamiltonian in order to study the effect of the terms neglected before. If such a contribution changes the Hamiltonian for large ℓ significantly, it is relevant and must be included. If it does not change the Hamiltonian for large ℓ it is irrelevant. As we will see, it is also possible that such an additional contribution does not change the original terms in the Hamiltonian, but that it does not vanish either for large ℓ. In this case the contribution is called marginal. After having solved the flow equations, the goal is to find all the relevant and marginal contributions to the Hamiltonian.

In order to show how this method works, we investigate the Anderson model for dilute magnetic alloys [3]. It describes electrons on a lattice with a single defect state. The Hamiltonian contains the kinetic energy of the electrons moving on the lattice, the energy of the defect state, a hybridization of the states in the band with the defect state, and a (usually repulsive) interaction of electrons in the defect state. For an excellent overview on this model and the results obtainable by different methods see [4]. In a certain limit this model is solvable using a Bethe ansatz. Furthermore, it has been investigated by Krishnamurty *et al* [5] using a numerical renormalization technique. We compare our results with some of the results in [5]. Especially we will see that the flow equations yield 'fixed points' similar to the fixed points found in [5] and that the operators which are relevant (marginal, irrelevant) in our approach are relevant (marginal, irrelevant) in the renormalization-group approach as well. We will come back to the connection to renormalization techniques implied by our suggestive use of language later.

Our paper is organized as follows. In the next section we give a more detailed description of the method. After that we derive the flow equations for the Anderson model and we discuss the explicit structure of these equations in detail. The fixed points of the equations are described. We also present numerical solutions of the equations. In section 4 we discuss possible relevant and irrelevant contributions to the original Hamiltonian, and in section 5 we compare our results for the Anderson model with the results of [5]. Finally we summarize our results and briefly discuss possible further investigations.

2. The method

The main part of the method is already described by (1.1) and (1.2). It has been explained in detail by Wegner [1]. But since it is not yet well known and since we introduce a new approximation not used in [1], we want to point out some useful properties of the flow equations. To do this, let $H = (h_{k,q})$ be a real, symmetric $N \times N$-matrix and H^{d} be its diagonal part. H^{r} contains the off-diagonal matrix elements. Then the flow equations for $H(\ell)$ can be written in the form

$$\frac{\mathrm{d}h_{k,q}(\ell)}{\mathrm{d}\ell} = \sum_p (\eta_{k,p}(\ell)h_{p,q}(\ell) - h_{k,p}(\ell)\eta_{p,q}(\ell)) \tag{2.1}$$

and

$$\eta_{k,q}(\ell) = (h_{k,k}(\ell) - h_{q,q}(\ell))h_{k,q}(\ell) \tag{2.2}$$

so that we obtain

$$\frac{\mathrm{d}h_{k,q}(\ell)}{\mathrm{d}\ell} = \sum_p (h_{k,k}(\ell) + h_{q,q}(\ell) - 2h_{p,p}(\ell))h_{k,p}(\ell)h_{p,q}(\ell)\,. \tag{2.3}$$

In the sequel we will not explicitly write down the ℓ-dependence of the matrix elements of H and η. Since $\eta_{k,q} = -\eta_{q,k}$, (2.1) describes a continuous unitary transformation of H. The quantities $\mathrm{Tr}(H^n)$ do not depend on ℓ. To study other properties of the flow equations (2.3), let us calculate the derivative of $\sum_{k\neq q} h_{k,q}^2$:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\ell}\sum_{k\neq q} h_{k,q}^2 &= -\frac{\mathrm{d}}{\mathrm{d}\ell}\sum_k h_{k,k}^2 \\ &= -2\sum_{k,q}(h_{k,k} - h_{q,q})^2 h_{k,q}^2 \\ &= -2\sum_{k,q}\eta_{k,q}^2\,. \end{aligned} \tag{2.4}$$

$\sum_{k\neq q} h_{k,q}^2$ is a monotonously decaying function of ℓ. Since it is bounded from below, its derivative with respect to ℓ vanishes if ℓ tends to infinity. This shows that, as already mentioned in the introduction, $\eta_{k,q}$ vanishes in the limit $\ell \to \infty$. Therefore, in the limit $\ell \to \infty$, we obtain a matrix H that commutes with its diagonal part H^{d}. This means that up to degeneracies in H^{d} the matrix H has been diagonalized. Clearly it is unfortunately not possible to solve the flow equations (2.3) analytically.

In this paper we introduce an approximation to the flow equations (2.1) and (2.2). In the first step in this approximation we assume that a class of matrix elements may be neglected if these matrix elements are zero initally. Suppose that the matrix elements of H are divided into two classes, $C^{(1)}$ and $C^{(2)}$, such that the matrix elements in $C^{(2)}$ vanish for $\ell = 0$. The approximate flow equations are obtained from (2.3) if we put $h_{k,q} = 0$ if $h_{k,q} \in C^{(2)}$. In the case of an arbitrary matrix H such an approximation is perhaps not very useful, since it is difficult to estimate the error. But if we study the problem of, for example, interacting electrons on lattice, we usually start with an idealized Hamiltonian that contains a kinetic energy and a simple interaction. Multi-particle interactions or slight modifications of the kinetic energy are usually not expected to play an important role, and if they do so the model has to be modified. Therefore we expect that the physical behaviour of the model does not change too much if we neglect matrix elements corresponding to contributions to the Hamiltonian not included initially. Nevertheless, it would be desirable to have more general statements about the validity of this approximation.

Let us for a moment assume that initially the off-diagonal matrix elements are small, such that a usual perturbational treatment of H^{r} is justified. In this case it is possible to solve the flow equations (2.3) iteratively. As a first approximative solution we take

$$h_{k,q}^{(1)} = h_{k,q}(0)\exp(-(h_{k,k}(0) - h_{q,q}(0))^2\ell)\,. \tag{2.5}$$

The $(n+1)$th approximation is now obtained from the nth approximation if we put

$$\frac{\mathrm{d}h_{k,q}^{(n+1)}}{\mathrm{d}\ell} = \sum_p (h_{k,k}^{(n)} + h_{q,q}^{(n)} - 2h_{p,p}^{(n)})h_{k,p}^{(n)}h_{p,q}^{(n)}\,. \tag{2.6}$$

In the case $n = 1$ the right-hand side is easily integrated and we obtain

$$h^{(2)}_{k,q} = \sum_p \frac{h_{k,k}(0) + h_{q,q}(0) - 2h_{p,p}(0)}{(h_{k,k}(0) - h_{p,p}(0))^2 + (h_{q,q}(0) - h_{p,p}(0))^2} h_{k,p}(0)h_{p,q}(0)$$
$$\times \left[1 - \exp\left(-\left((h_{k,k}(0) - h_{p,p}(0))^2 + (h_{q,q}(0) - h_{p,p}(0))^2\right)\ell\right)\right]. \tag{2.7}$$

In the limit $\ell \to \infty$, and if no degeneracy occurs, this yields

$$h^{(2)}_{k,k}(\infty) = \sum_p \frac{h_{k,p}(0)h_{p,k}(0)}{h_{k,k}(0) - h_{p,p}(0)} \tag{2.8}$$

which is equivalent to the result obtained from ordinary perturbation theory.

In our approximation we neglected matrix elements $h_{k,q} \in C^{(2)}$ for which $h_{k,q}(0) = 0$. Since they do not contribute to the right-hand side of (2.8), our approximation agrees with a perturbational treatment up to second order in H^{r}. But it is not necessarily restricted to the regime where perturbation theory is valid.

The choice of $C^{(2)}$ above is completely arbitrary, and in the following we will choose $C^{(2)}$ almost as large as possible. The question is then whether or not the terms neglected are relevant in the sense that they alter the solution significantly. In the second step in our method we then investigate this problem by simply moving some of the elements of $C^{(2)}$ to $C^{(1)}$ and trying to analyse the new flow equations. In this way different new contributions to the Hamiltonian will be treated and for each of them we try to find out whether it is relevant or not.

3. Flow equations for the Anderson model

3.1. The model

The Hamiltonian of the Anderson model in a normal-ordered form is given by [3]

$$H = \sum_{k,\sigma} \epsilon_k : c^\dagger_{k,\sigma} c_{k,\sigma} : + \sum_\sigma \tilde{\epsilon}_{\mathrm{d}} : d^\dagger_\sigma d_\sigma : + \sum_{k,\sigma} V_k (: c^\dagger_{k,\sigma} \mathrm{d}_\sigma : + : d^\dagger_\sigma c_{k,\sigma} :) + U : d^\dagger_+ d^\dagger_- d_- d_+ : . \tag{3.1}$$

The first term represents the kinetic energy of the band electrons. In addition there is a defect state. It hybridizes with the conduction electrons. Since the phase of $c_{k,\sigma}$ is arbitrary, we choose $V_k \geqslant 0$. In a more general model, there will be many defects in the lattice and the defect states will be degenerate. Here we treat only the simplest case, a single, non-degenerate defect state. Electrons in the defect state interact due to the on-site Coulomb repulsion. This is described by the fourth term in (3.1). Normal order is defined by substracting the ground-state expectation values of the Hamiltonian with $V_k = 0$:

$$: c^\dagger_{k,\sigma} c_{k,\sigma} := c^\dagger_{k,\sigma} c_{k,\sigma} - n_k \tag{3.2}$$

$$: d^\dagger_\sigma d_\sigma := d^\dagger_\sigma d_\sigma - n_{\mathrm{d}} \tag{3.3}$$

where

$$n_k = \theta(\epsilon_{\mathrm{F}} - \epsilon_k) \tag{3.4}$$

and

$$n_{\mathrm{d}} = \tfrac{1}{2}(\theta(\epsilon_{\mathrm{F}} - \epsilon_{\mathrm{d}}) + \theta(\epsilon_{\mathrm{F}} - \epsilon_{\mathrm{d}} - U)). \tag{3.5}$$

$\tilde{\epsilon}_{\mathrm{d}}$ is given by

$$\tilde{\epsilon}_{\mathrm{d}} = \epsilon_{\mathrm{d}} + n_{\mathrm{d}} U \tag{3.6}$$

where ϵ_{d} is the energy of the single occupied defect state.

3.2. The flow equations

We now set

$$H^r = \sum_{k,\sigma} V_k^r (: c_{k,\sigma}^\dagger d_\sigma : + : d_\sigma^\dagger c_{k,\sigma} :) . \tag{3.7}$$

In the spirit of our approach it would of course be desirable to set $V_k^r = V_k$. But we will later see that this is too restrictive in some cases. Still one can always think of $V_k^r = V_k$ for nearly all values of k. η may be written as

$$\begin{aligned}\eta = [H, H^r] = &\sum_{k,\sigma} \eta_k (: c_{k,\sigma}^\dagger d_\sigma : - : d_\sigma^\dagger c_{k,\sigma} :) + \sum_{k,q,\sigma} \eta_{k,q} (: c_{k,\sigma}^\dagger c_{q,\sigma} : - : c_{q,\sigma}^\dagger c_{k,\sigma} :) \\ &+ \sum_{k,\sigma} \eta_k^{(2)} (: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : - : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :)\end{aligned} \tag{3.8}$$

where

$$\eta_k = (\epsilon_k - \tilde{\epsilon}_d) V_k^r \tag{3.9}$$

$$\eta_{k,q} = \tfrac{1}{2}(V_k V_q^r - V_q V_k^r) \tag{3.10}$$

$$\eta_k^{(2)} = -U V_k^r . \tag{3.11}$$

The commutator of η and H can be calculated easily,

$$\begin{aligned}[\eta, H] = &\sum_{k,\sigma} \eta_k (\tilde{\epsilon}_d - \epsilon_k) (: c_{k,\sigma}^\dagger d_\sigma : + : d_\sigma^\dagger c_{k,\sigma} :) + \sum_{k,q,\sigma} \eta_k V_q (: c_{k,\sigma}^\dagger c_{q,\sigma} : + : c_{q,\sigma}^\dagger c_{k,\sigma} :) \\ &-2 \sum_{k,\sigma} \eta_k V_k : d_\sigma^\dagger d_\sigma : + 2 \sum_{k,\sigma} \eta_k V_k (n_k - n_d) \\ &+U \sum_{k,\sigma} \eta_k (: d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} : + : c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma :) \\ &- \sum_{k,q,\sigma} \eta_{k,q} (\epsilon_k - \epsilon_q) (: c_{k,\sigma}^\dagger c_{q,\sigma} : + : c_{q,\sigma}^\dagger c_{k,\sigma} :) \\ &+2 \sum_{k,q,\sigma} \eta_{k,q} V_q (: d_\sigma^\dagger c_{k,\sigma} : + : c_{k,\sigma}^\dagger d_\sigma :) \\ &- \sum_{k,\sigma} \eta_k^{(2)} (\epsilon_k - \tilde{\epsilon}_d) (: d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} : + : c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma :) \\ &- \sum_{k,\sigma} \eta_k^{(2)} V_k : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : \\ &+ \sum_{k,q,\sigma} \eta_k^{(2)} V_q (: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{q,\sigma} : + : c_{q,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} : - : c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_\sigma c_{q,-\sigma} : \\ &- : c_{q,\sigma}^\dagger d_{-\sigma}^\dagger d_\sigma c_{k,-\sigma} : - : c_{k,\sigma}^\dagger c_{q,-\sigma}^\dagger d_{-\sigma} d_\sigma : - : d_\sigma^\dagger d_{-\sigma}^\dagger c_{q,-\sigma} c_{k,\sigma} :) \\ &+2 \sum_{k,\sigma} \eta_k^{(2)} V_k (n_k - n_d) : d_{-\sigma}^\dagger d_{-\sigma} : \\ &+U \sum_{k,\sigma} \eta_k^{(2)} (1 - 2n_d) (: d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} : + : c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma :) \\ &+U \sum_{k,\sigma} \eta_k^{(2)} n_d (1 - n_d) (: d_\sigma^\dagger c_{k,\sigma} : + : c_{k,\sigma}^\dagger d_\sigma :) .\end{aligned} \tag{3.12}$$

To obtain the flow equations for the matrix elements of H one has to compare the different terms on the right-hand side of (3.12) with H. For instance, the second term in (3.12) is the only term that contributes to the derivative of ϵ_k with respect to ℓ,

$$\frac{\mathrm{d}\epsilon_k}{\mathrm{d}\ell} = 2\eta_k V_k = 2(\epsilon_k - \tilde{\epsilon}_\mathrm{d}) V_k V_k^r . \tag{3.13}$$

All the terms containing $: d_\sigma^\dagger d_\sigma :$ contribute to the derivative of $\tilde{\epsilon}_\mathrm{d}$ with respect to ℓ. But, since $\tilde{\epsilon}_\mathrm{d} = \epsilon_\mathrm{d} + n_\mathrm{d} U$ and n_d eventually changes with ℓ, there is an extra contribution $U \mathrm{d}n_\mathrm{d}/\mathrm{d}\ell$. Therefore

$$\begin{aligned} \frac{\mathrm{d}\tilde{\epsilon}_\mathrm{d}}{\mathrm{d}\ell} &= -2\sum_k \eta_k V_k + 2\sum_k \eta_k^{(2)} V_k (n_k - n_\mathrm{d}) + U\frac{\mathrm{d}n_\mathrm{d}}{\mathrm{d}\ell} \\ &= 2\sum_k (\tilde{\epsilon}_\mathrm{d} - \epsilon_k) V_k V_k^r + 2U\sum_k V_k V_k^r (n_\mathrm{d} - n_k) + U\frac{\mathrm{d}n_\mathrm{d}}{\mathrm{d}\ell} . \end{aligned} \tag{3.14}$$

Similarly we obtain

$$\begin{aligned} \frac{\mathrm{d}V_k}{\mathrm{d}\ell} &= -\eta_k(\epsilon_k - \tilde{\epsilon}_\mathrm{d}) + 2\sum_p \eta_{k,p} V_p + U n_\mathrm{d}(1 - n_\mathrm{d})\eta_k^{(2)} \\ &= -V_k^r(\epsilon_k - \tilde{\epsilon}_\mathrm{d})^2 + V_k \sum_p V_p V_p^r - V_k^r \sum_p V_p V_p - U^2 n_\mathrm{d}(1 - n_\mathrm{d}) V_k^r \end{aligned} \tag{3.15}$$

and

$$\frac{\mathrm{d}U}{\mathrm{d}\ell} = -4\sum_k \eta_k^{(2)} V_k = 4U\sum_k V_k V_k^r . \tag{3.16}$$

We will now analyse these equations.

3.3. The symmetric case

If $\epsilon_{\pi-k} = -\epsilon_k$, $V_{\pi-k} = V_k$, $\tilde{\epsilon}_\mathrm{d} = 0$, $\epsilon_\mathrm{F} = 0$, $n_\mathrm{d} = \frac{1}{2}$, the Hamiltonian is invariant under particle–hole transformations

$$c_{k,\sigma}^\dagger \to -c_{\pi-k,\sigma} \qquad c_{k,\sigma} \to -c_{\pi-k,\sigma}^\dagger \qquad d_\sigma^\dagger \to d_\sigma \qquad d_\sigma \to d_\sigma^\dagger . \tag{3.17}$$

We choose $V_k = V_k^r$ and obtain

$$\frac{\mathrm{d}\epsilon_k}{\mathrm{d}\ell} = 2\epsilon_k V_k^2 \qquad \frac{\mathrm{d}V_k}{\mathrm{d}\ell} = -\left(\epsilon_k^2 + \tfrac{1}{4}U^2\right) V_k \qquad \frac{\mathrm{d}U}{\mathrm{d}\ell} = 4U\sum_k V_k^2 . \tag{3.18}$$

Due to the particle–hole symmetry $\tilde{\epsilon}_\mathrm{d}$ remains zero. The equations (3.18) show that V_k tends to zero for all k, whereas $|U|$ and $|\epsilon_k|$ increase. For the density of states at the Fermi level $\epsilon_\mathrm{F} = 0$,

$$\rho(0, l) = \frac{1}{(2\pi)^d} \int \mathrm{d}^d k\, \delta(\epsilon_k) \tag{3.19}$$

we obtain

$$\frac{\mathrm{d}\rho(0, l)}{\mathrm{d}\ell} = -2V^2 \exp\left(-\tfrac{1}{2}\int_0^\ell U^2\, \mathrm{d}\ell\right) \rho(0, l) . \tag{3.20}$$

Here V is the initial value of V_k for those k with $\epsilon_k = 0$. The density of states in the middle of the band decreases, but it does not vanish unless $U = 0$.

The case $U = 0$ must be treated seperately. In this case we obtain

$$\epsilon_k(\infty) = \mathrm{sign}(\epsilon_k(0))\sqrt{\epsilon_k^2(0) + 2V_k^2(0)} \tag{3.21}$$

and $V_k(\infty) = 0$ if $\epsilon_k(\infty) \neq 0$. If $V_k \neq 0$ for such k with ϵ_k near the Fermi energy, we obtain a finite gap in the energy band with some states in the middle of the gap. A gap does not show up for a single impurity in the thermodynamic limit, since $V_k \sim N_s^{-1/2}$ where N_s is the number of lattice sites. On the other hand, a system with a small but finite density of defects behaves like a system with a single defect in a finite volume, the volume per defect. The gap would be of the order of the density of defects. This result is presumably an artefact of our approximation, since for $U = 0$ the equations (3.18) decouple. If ϵ_k is near the Fermi energy, V_k tends to zero quite slowly and therefore other matrix elements neglected so far are important. Furthermore, the result for $U = 0$ is not stable with respect to small changes of the Hamiltonian. If one introduces, for example, a non-vanishing interaction U, the system has no gap, as expected.

3.4. The asymmetric case

In general the system has no particle–hole symmetry. The flow equations are given by

$$\frac{d\epsilon_k}{d\ell} = 2(\epsilon_k - \epsilon_d - n_d U) V_k V_k^r \tag{3.22}$$

$$\frac{d\epsilon_d}{d\ell} = 2\sum_k (\epsilon_d - \epsilon_k - n_k U) V_k V_k^r \tag{3.23}$$

$$\frac{dV_k}{d\ell} = -(\epsilon_k - \epsilon_d - n_d U)^2 V_k^r + V_k \sum_p V_p V_p^r - V_k^r \sum_p V_p V_p - U^2 n_d (1 - n_d) V_k^r \tag{3.24}$$

$$\frac{dU}{d\ell} = 4U \sum_k V_k V_k^r . \tag{3.25}$$

Now V_k does not necessarily vanish for all k and we have to choose

$$V_k^r = g_k^r V_k \tag{3.26}$$

where

$$\begin{aligned} g_k^r &= 0 \qquad \text{if} \quad (\epsilon_k - \epsilon_d - n_d U)^2 + n_d(1 - n_d)U^2 \to 0 \quad \text{for} \quad \ell \to \infty \\ g_k^r &= 1 \qquad \text{otherwise}. \end{aligned} \tag{3.27}$$

With this choice of V_k^r we ensure that the right-hand side of (3.25) vanishes for $\ell \to \infty$. Otherwise U becomes infinite for $\ell \to \infty$. Such a divergence is typical for approximate flow equations. A similar divergence also occured in the paper of Wegner [1]. It is clear that the original equation (1.1) contains no such divergences since it describes a continous unitary transformation of the Hamiltonian. But it is always possible to choose H^r such that it vanishes for $\ell \to \infty$, and with such a choice no divergences occur.

We have to distinguish four possible cases.

(1) $n_d = \frac{1}{2}$ for $\ell \to \infty$. This case is similar to the symmetric case discussed above. All V_k vanish, $|U|$ increases and the energies ϵ_k and ϵ_d are renormalized. The defect state is occupied with a single electron, it has a magnetic moment. This case is therefore called the local-moment fixed point.

(2) $n_d = 0$ or $n_d = 1$ for $\ell \to \infty$ and $g_k^r = 0$ for some k. In this case the corresponding V_k do not vanish. There is a non-vanishing coupling of the defect state to the states in the band for which $\epsilon_k = \epsilon_d + n_d U$. Since the corresponding V_k^r is zero, only the second term in (3.24) contributes and $|V_k|$ increases. This case is called the strong-coupling fixed point.

(3) $n_d = 0$ or $n_d = 1$ for $\ell \to \infty$ and $g_k^r \neq 0$ for all k. In this case ϵ_d and $\epsilon_d + U$ are both above (for $n_d = 0$) or below (for $n_d = 1$) the band. The defect state is decoupled from the band and the electrons in the band behave like free electrons. This case is called the free-electron fixed point.

(4) The non-interacting case with $n_d = 0$, $n_d = \frac{1}{2}$, or $n_d = 1$. In this case $U = 0$ and V_k vanishes if $\epsilon_k \neq \tilde{\epsilon}_d$.

The above-mentioned fixed points are not fixed points in the sense that all the parameter of the model are fixed. They merely describe classes of parameters which show a similar physical behaviour. The main question is into which of the four classes the system falls, depending on the initial Hamiltonian. The last case is simple since it describes an instable fixed point of the flow equations. Only if $U = 0$ initially it remains zero for all ℓ. The other fixed points are more interesting, we will discuss them in detail.

The first case is the local-moment fixed point, where $n_d = \frac{1}{2}$, e.g. $\epsilon_d < \epsilon_F$ and $\epsilon_d + U > \epsilon_F$ (the case $\epsilon_d > \epsilon_F$ and $\epsilon_d + U < \epsilon_F$ is similar). We shall assume that U is not too small initially. Now the last term in (3.24) is the most important term. Using $U \geqslant U(0)$ it already yields the estimate

$$V_k \leqslant V_k(0) \exp\left(-\tfrac{1}{4}U^2(0)\ell\right). \tag{3.28}$$

Inserting this in (3.25) we obtain

$$U \leqslant U(0) \exp\left(8 \sum_k \frac{V_k^2(0)}{U^2(0)}\left[1 - \exp\left(-\tfrac{1}{2}U^2(0)\ell\right)\right]\right). \tag{3.29}$$

In a typical situation, $\sum_k V_k^2(0)/U^2(0)$ is of order 1 or smaller. Now, if $|\epsilon_k - \epsilon_d - \frac{1}{2}U| \leqslant c_k$ we obtain

$$|\epsilon_k - \epsilon_k(0)| \leqslant \frac{8c_k V_k^2(0)}{U^2(0)}\left[1 - \exp\left(-\tfrac{1}{4}U^2(0)\ell\right)\right]. \tag{3.30}$$

This shows that ϵ_k does not change very much. Therefore if we start with a symmetric conduction band, it remains essentially symmetric and $\sum_k \epsilon_k V_k^2 \approx 0$. Consequently the right-hand side of (3.23) is negative and ϵ_d remains below ϵ_F. Only if the conduction band is strongly asymmetric, may the system behave differently. The derivative of $\epsilon_d + U$ is approximately given by $\sum_k (\epsilon_d + (1 - n_k)U)V_k^2$. Thus if ϵ_d becomes of the order $-(1 - \rho/2)U$, where ρ is the density of electrons, $\epsilon_d + U$ decreases and the system may change to a state where $n_d = 1$. Otherwise it remains in a state with $n_d = \frac{1}{2}$. The precise values of the parameters where the transition occurs cannot be determined using the rough estimates above.

The situation becomes more complicated if initially $n_d = 0$, i.e. $\epsilon_d > \epsilon_F$ and $\epsilon_d + U > \epsilon_F$. If ϵ_d is only slightly above ϵ_F, the right-hand side of (3.23) will still be negative so that ϵ_d decreases below ϵ_F. Then $n_d = \frac{1}{2}$ and the system rests in the local-moment fixed point. On the other hand, if $\epsilon_d > U$ and if we start with a symmetric conduction band, the right-hand side of (3.23) is positive and ϵ_d increases. Somewhere between these two possibilities there must be a transition where the system, depending on the inital values of the parameters, switches from the local-moment fixed point to a fixed point with $n_d = 0$. The question, whether this fixed point is the free-electron fixed point or the strong-coupling fixed point, cannot be decided easily.

Numerical solutions of the equations are presented below; they confirm this qualitative discussion.

3.5. Numerical results

We have implemented an adaptive stepsize fifth-order Runge–Kutta algorithm to solve the flow equations (3.22)–(3.25) numerically. All calculations were performed for a symmetric band $\epsilon_k = -1 + 2|k|$, $k \in [-1, 1]$, $\epsilon_F = 0$, one impurity site and $N_s = 50$ sites in the conduction band. The choice of the discrete N_s values of k in the conduction band does not affect the results very much. We took them equidistant in the interval $[-1, 1]$. In the thermodynamic limit these parameters correspond to a 2% density of impurities and a constant density of states in the conduction band. The hybridization energies scale as $V_k = V(0)/\sqrt{N_s}$ in this limit. We have set $V(0) = 2$.

Figures 1 to 4 show numerical solutions of the flow equations for a starting value $U(0) = 5$. Corresponding to the initial value of ϵ_d, one finds, e.g., the local-moment fixed point (figures 1 and 2) or the free-electron fixed point (figures 3 and 4). In either case the off-diagonal elements V_k vanish in the limit $l \to \infty$, as intended by the continuous unitary transformations. One notices in figure 2 that this convergence of the V_k gets much faster once ϵ_d is below the Fermi level. This is due to the last term in (3.24).

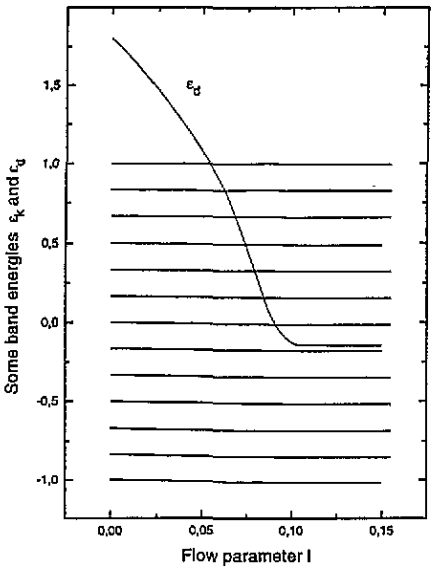

Figure 1. Local-moment fixed point. Flow of the conduction-band energies and of the impurity-site energy.

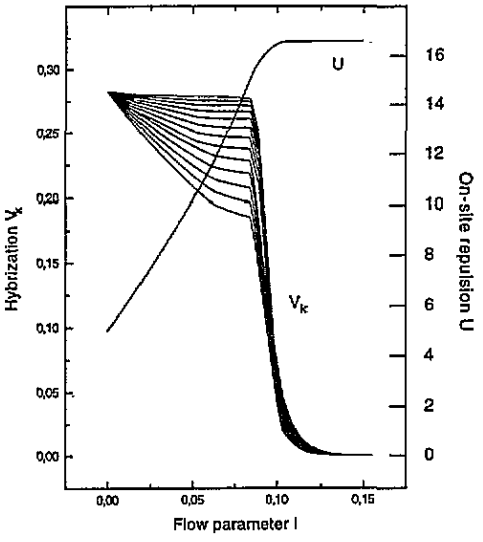

Figure 2. Local-moment fixed point. Flow of the on-site repulsion U and of the hybridization V_k.

In the free-electron case the convergence of some V_k is much slower since we are coming close to the crossover to the strong-coupling fixed point. For the same reason U gets very large. But this could only be noticed if the impurity site were twice occupied, which is a very high-lying excitation for this fixed point anyway which we cannot hope to describe by the model. The case shown in figures 3 and 4 lies near the crossover to the strong-coupling fixed point. If $\epsilon_d(0)$ is larger, the convergence is faster and the final value of U is smaller. If $\epsilon_d(0)$ is smaller, $\epsilon_d(\ell)$ intersects the curve of the first band energy and $\epsilon_d(\infty)$ lies in the band.

Finally, one can wonder about the attraction regions belonging to the different fixed points. There are four parameters in our model: the bandwidth of the conduction band,

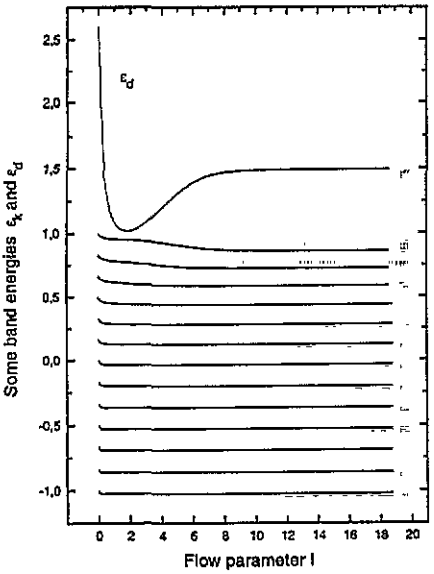

Figure 3. Free-electron fixed point. Flow of the conduction-band energies and of the impurity-site energy.

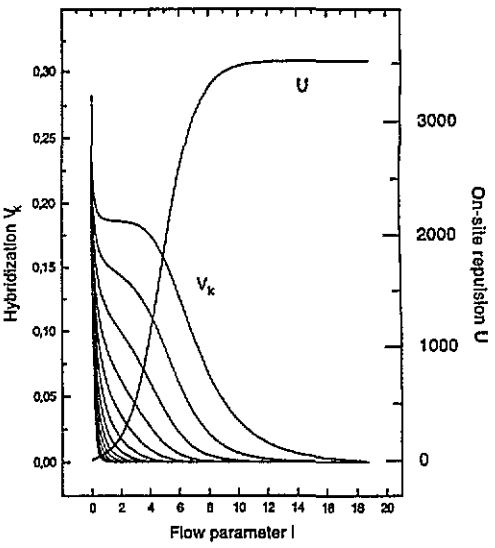

Figure 4. Free-electron fixed point. Flow of the on-site repulsion U and of the hybridization V_k.

the initial values of ϵ_d, U and of the average hybridization V. Obviously only three of these parameters can be independent since the energy scale is arbitrary. In our case the bandwidth is fixed. Of the remaining three parameters only two are really independent because the flow equations connect unitarily equivalent Hamiltonians with different values of these parameters (the bandwidth hardly changes as mentioned before for this small density of impurities). Therefore we can restrict ourselves to investigating the attraction regions for a fixed value of $V(0)$, here $V(0) = 2$.

In figure 5 the approximate boundaries of the parameter sets belonging to the local moment or the free-electron behaviour are drawn in the $(\epsilon_d(0), U(0))$-plane. In between lies the region of the strong-coupling fixed point. Since our numerical algorithm converges very slowly in this region (compare figure 4), figure 5 shall mainly give a qualitative impression of this region.

4. Relevant and irrelevant operators

In the commutator $[\eta, H]$, many terms have been neglected and it is not clear *a priori* whether or not these terms are relevant for the physical behaviour of the model. To investigate this question, we add contributions of this type to the Hamiltonian and write down the flow equations for the new Hamiltonian. A detailed derivation of the new flow equations is given in the appendix.

A simple contribution in $[\eta, H]$ that has been neglected is of the form $\sum_{k,q,\sigma} V_{k,q} : c^\dagger_{k,\sigma} c_{q,\sigma} :$. It will turn out that such a contribution is irrelevant for the model. To see this

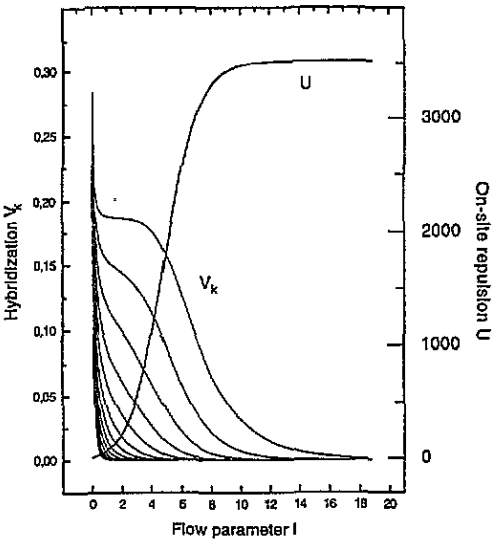

Figure 5. Approximate boundaries of the parameter sets belonging to the different fixed point.

we have to investigate the flow equations for a Hamiltonian including such a term, i.e.

$$H=\sum_{k,\sigma}\epsilon_k :c^\dagger_{k,\sigma}c_{k,\sigma}: +\sum_{\sigma}\tilde{\epsilon}_{\rm d} :d^\dagger_\sigma d_\sigma: +\sum_{k,\sigma}V_k(: c^\dagger_{k,\sigma}d_\sigma: + : d^\dagger_\sigma c_{k,\sigma}:)$$
$$+U :d^\dagger_+d^\dagger_-d_-d_+: +\sum_{k,q,\sigma}V_{k,q} :c^\dagger_{k,\sigma}c_{q,\sigma}: . \tag{4.1}$$

The flow equations are obtained from (A.8)–(A.12)

$$\frac{{\rm d}\epsilon_k}{{\rm d}\ell}=2(\epsilon_k-\tilde{\epsilon}_{\rm d})V_kV_k^{\rm r}+2\sum_q(\epsilon_k-\epsilon_q)V^2_{k,q}+2\sum_q V_{k,q}(2V_q^{\rm r}V_k-V_qV_k-V_qV_k^{\rm r}) \tag{4.2}$$

$$\frac{{\rm d}\tilde{\epsilon}_{\rm d}}{{\rm d}\ell}=2\sum_k(\tilde{\epsilon}_{\rm d}-\epsilon_k)V_kV_k^{\rm r}+2U\sum_k V_kV_k^{\rm r}(n_{\rm d}-n_k)$$
$$+\frac{1}{2}\sum_{k,q}V_{k,q}(V_q-V_q^{\rm r})(V_k-V_k^{\rm r})+U\frac{{\rm d}n_{\rm d}}{{\rm d}\ell} \tag{4.3}$$

$$\frac{{\rm d}V_k}{{\rm d}\ell}=-V_k^{\rm r}((\epsilon_k-\tilde{\epsilon}_{\rm d})^2+n_{\rm d}(1-n_{\rm d})U^2)+\sum_p(\epsilon_k-\epsilon_p)V_{k,p}V_p+\sum_p(\tilde{\epsilon}_{\rm d}-\epsilon_p)V_{k,p}V_p^{\rm r}$$
$$+\sum_p(V_kV_p^{\rm r}-V_pV_k^{\rm r})V_p+\sum_{q,p}V_{k,p}V_{p,q}(V_q-V_q^{\rm r}) \tag{4.4}$$

$$\frac{{\rm d}V_{k,q}}{{\rm d}\ell}=-(\epsilon_k-\epsilon_q)^2V_{k,q}+(\epsilon_k-\tilde{\epsilon}_{\rm d})V_k^{\rm r}V_q+(\epsilon_q-\tilde{\epsilon}_{\rm d})V_kV_q^{\rm r}+\sum_p(\epsilon_k+\epsilon_q-2\epsilon_p)V_{k,p}V_{p,q}$$
$$-\tfrac{1}{2}(V_kV_q^{\rm r}-V_qV_k^{\rm r})(\epsilon_k-\epsilon_q)+\sum_p[(V_kV_p^{\rm r}-V_pV_k^{\rm r})V_{p,q}+(V_qV_p^{\rm r}-V_pV_q^{\rm r})V_{p,k}]$$
$$+\sum_p(V_p^{\rm r}-V_p)[V_{k,p}V_q+V_{q,p}V_k] \tag{4.5}$$

$$\frac{{\rm d}U}{{\rm d}\ell}=-4\sum_k\eta_k^{(2)}V_k=4U\sum_kV_k^2. \tag{4.6}$$

First, one observes $V_{k,q}(\infty) = 0$ if $(\epsilon_k - \epsilon_q) \neq 0$. $V_{k,q}$ does not vanish for $\ell \to \infty$ if $\epsilon_k = \epsilon_q$. But this does not cause any problems, since nevertheless the second term in (4.2) tends to zero for $\ell \to \infty$. There are no diverging matrix elements in this limit. The equation for U is the same as before and $|U|$ increases. In the equation for V_k additional contributions occur, but they vanish for $\ell \to \infty$ so that V_k vanishes if $n_d = \frac{1}{2}$ or $\epsilon_k \neq \tilde{\epsilon}_d$. Finally, the additional contribution $\sum_{k,q,\sigma} V_{k,q} : c^\dagger_{k,\sigma} c_{q,\sigma} :$ to the Hamiltonian does not change the behaviour of the system. ϵ_k, $\tilde{\epsilon}_d$ and U are 'renormalized' somewhat, but the behaviour of the system remains the same. Only in the non-interacting case is $\sum_{k,q,\sigma} V_{k,q} : c^\dagger_{k,\sigma} c_{q,\sigma} :$ a relevant contribution to the Hamiltonian.

The next contribution in $[\eta, H]$ that was neglected is a term of the form

$$\sum_{k,\sigma} V_k^{(2)} (: c^\dagger_{k,\sigma} d^\dagger_{-\sigma} d_{-\sigma} d_\sigma : + : d^\dagger_\sigma d^\dagger_{-\sigma} d_{-\sigma} c_{k,\sigma} :) .$$

Such a contribution only occurs if $U \neq 0$. But if $U \neq 0$ initially U always increases. Therefore we should expect that matrix elements between states with $n_d = \frac{1}{2}$ and $n_d = 1$ are not important. This means that this contribution is likely to be irrelevant for all fixed points. To see this we add such a term to H and H^r. The flow equations are then

$$\frac{d\epsilon_k}{d\ell} = 2(\epsilon_k - \tilde{\epsilon}_d)(V_k^r V_k + n_d(1-n_d) V_k^{(2)2}) - 2n_d(1-n_d) U V_k^{(2)} (V_k + V_k^r) \tag{4.7}$$

$$\begin{aligned} \frac{d\tilde{\epsilon}_d}{d\ell} = & -2 \sum_k (\epsilon_k - \tilde{\epsilon}_d + U(n_k - n_d))(V_k^r V_k + n_d(1-n_d) V_k^{(2)2}) \\ & + 2 \sum_k ((\epsilon_k - \tilde{\epsilon}_d)(n_k - n_d) + n_d(1-n_d) U)(V_k^r + V_k) V_k^{(2)} \\ & - 2(1-2n_d) U \sum_k (n_k - n_d) V_k V_k^{(2)} + U \frac{dn_d}{d\ell} \end{aligned} \tag{4.8}$$

$$\begin{aligned} \frac{dV_k}{d\ell} = & -((\epsilon_k - \tilde{\epsilon}_d)^2 + n_d(1-n_d) U^2) V_k^r + 2n_d(1-n_d)(\epsilon_k - \tilde{\epsilon}_d) U V_k^{(2)} \\ & + \sum_p \Big((V_k V_p^r - V_p V_k^r) V_p + n_d(1-n_d) [(V_k - V_k^r) V_p^{(2)} - (V_p - V_p^r) V_k^{(2)}] V_p^{(2)} \Big) \end{aligned} \tag{4.9}$$

$$\begin{aligned} \frac{dU}{d\ell} = & 4U \sum_k V_k^r V_k - 4 \sum_k ((\epsilon_k - \tilde{\epsilon}_d) - (1-2n_d) U) V_k^{(2)} (V_k^r + V_k) \\ & + 4 \sum_k [(1 - 3n_d(1-n_d)) U - (1-2n_d)(\epsilon_k - \tilde{\epsilon}_d)] V_k^{(2)2} \end{aligned} \tag{4.10}$$

$$\begin{aligned} \frac{dV_k^{(2)}}{d\ell} = & -[n_d(1-n_d) U^2 + (\epsilon_k - \tilde{\epsilon}_d - (1-2n_d) U)^2] V_k^{(2)} + [2U(\epsilon_k - \tilde{\epsilon}_d) - (1-2n_d) U^2] V_k^r \\ & + \sum_q ((V_k - V_k^r) V_q^{(2)} - (V_q - V_q^r) V_k^{(2)}) (V_q + (1-2n_d) V_q^{(2)}) \\ & + \sum_q (V_k V_q^r - V_q V_k^r) V_q^{(2)} . \end{aligned} \tag{4.11}$$

Although these equations look complicated, they are easy to analyse. Let us first look at (4.10). U increases as long as V_k^r and $V_k^{(2)}$ do not vanish. On the other hand, the first term in (4.11) guarantees that $V_k^{(2)}$ tends to zero in the limit $\ell \to \infty$. For sufficiently

large U the dominant contribution is $\sim -U^2 V_k^{(2)}$ so that $V_k^{(2)}$ vanishes rapidly. This shows that for $n_d = \frac{1}{2}$ the behaviour of $V_k^{(2)}$ is similar to the behaviour of V_k. In (4.7), (4.8) and (4.10) the additional terms containing $V_k V_k^{(2)}$ and $V_k^{(2)2}$ are similar to the original contributions containing V_k^2. This shows that the only effect of the additional contribution $\sum_{k,\sigma} V_k^{(2)}(: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : + : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :)$ to the Hamiltonian is a renormalization of ϵ_k, $\tilde{\epsilon}_d$, and U, which also occurs if one changes, for example, the initial values of V_k. If $n_d = 0$ or $n_d = 1$ we saw that V_k does not necessarily vanish for $\ell \to \infty$. In contrast $V_k^{(2)}$ tends to zero in this case too. Furthermore, the contributions on the right-hand side of (4.7) and (4.9) containing $V_k^{(2)}$ vanish. Consequently, the behaviour of ϵ_k and V_k does not change significantly. Only $\tilde{\epsilon}_d$ and U are renormalized.

In the non-interacting case ($U = 0$) the inhomogeneity in (4.11) vanishes. Consequently, $V_k^{(2)} = 0$ if initially $V_k^{(2)}(0) = 0$. This shows that the additional contribution

$$\sum_{k,\sigma} V_k^{(2)}(: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : + : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :)$$

to the Hamiltonian is irrelevant for the fixed points described above.

Another contribution on the right-hand side of (3.12) contains

$$(: c_{k,\sigma}^\dagger c_{q,-\sigma}^\dagger d_{-\sigma} d_\sigma : + : d_\sigma^\dagger d_{-\sigma}^\dagger c_{q,-\sigma} c_{k,\sigma} :) .$$

This contribution may be analysed similarly and it turns out that it is irrelevant. This should have been expected since, as in the previous case, such a term contains matrix elements between two states with different n_d. Since U becomes large, these matrix elements tend to zero rapidly.

The last contribution in (3.12) not taken into account until now is more important. It is of the form

$$\sum_{k,q,\sigma} V_{k,q}^{(2)}(: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{q,\sigma} : - : c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_\sigma c_{q,-\sigma} :) \tag{4.12}$$

and may be written as a linear combination of a spin–spin interaction and a density–density interaction. A contribution of this form was first obtained by Schrieffer and Wolff [2]. They introduced a unitary transformation in order to eliminate the matrix elements V_k. As a result of this transformation one obtains a complicated Hamiltonian, which reduces to the original one with $V_k = 0$ and an additional contribution of the form (4.12) if $|V_k|$ is small. One should expect that these terms are important in our approach as well. To see this, we add such a term to H and H^r in (3.1) and (3.7). The flow equations are obtained as before,

$$\frac{d\epsilon_k}{d\ell} = 2(\epsilon_k - \tilde{\epsilon}_d) V_k^r V_k - \sum_q V_{k,q}^{(2)} (V_q^r - V_q) V_k (n_q - n_d) \tag{4.13}$$

$$\begin{aligned}\frac{d\tilde{\epsilon}_d}{d\ell} = &-2\sum_k (\epsilon_k - \tilde{\epsilon}_d) V_k^r V_k + 2\sum_{k,q} V_{k,q}^{(2)} (V_q^r - V_q) V_k (n_k + n_q - 2n_d) \\ &-2U \sum_k V_k V_k^r (n_k - n_d) + U \frac{dn_d}{d\ell} - \sum_{k,q} (V_k V_q^r - V_q V_k^r) V_{k,q}^{(2)} (n_k - n_q) \\ &-2(1 - 2n_d) \sum_{k,q,\sigma} (\epsilon_k - \epsilon_q)(n_k - n_q) V_{k,q}^{(2)2}\end{aligned} \tag{4.14}$$

$$\frac{dV_k}{d\ell} = -[(\epsilon_k - \tilde{\epsilon}_d)^2 + n_d(1 - n_d)U^2] V_k^r$$

$$+\sum_q(\epsilon_k-\epsilon_q)V^{(2)}_{k,q}V^{\mathrm{r}}_q(n_q-n_{\mathrm{d}})+\sum_q(\tilde{\epsilon}_{\mathrm{d}}-\epsilon_q)V^{(2)}_{k,q}V_q(n_q-n_{\mathrm{d}})$$
$$+\sum_q(V_kV^{\mathrm{r}}_q-V_qV^{\mathrm{r}}_k)V_q+Un_{\mathrm{d}}(1-n_{\mathrm{d}})\sum_q V^{(2)}_{k,q}(3V^{\mathrm{r}}_q-V_q)$$
$$+2\sum_{q,p}V^{(2)}_{k,q}V^{(2)}_{p,q}(V_p-V^{\mathrm{r}}_p)[2n_pn_q(1-n_{\mathrm{d}})+n_p+n_{\mathrm{d}}(1-2n_{\mathrm{d}})] \tag{4.15}$$

$$\frac{\mathrm{d}U}{\mathrm{d}\ell}=4U\sum_k V_kV^{\mathrm{r}}_k-\sum_{k,q}(\epsilon_k-\epsilon_q)(n_k-n_q)V^{(2)2}_{k,q}+4\sum_q V^{(2)}_{k,q}(V_q-V^{\mathrm{r}}_q)V_k \tag{4.16}$$

$$\frac{\mathrm{d}V^{(2)}_{k,q}}{\mathrm{d}\ell}=-(\epsilon_k-\epsilon_q)^2V^{(2)}_{k,q}-U(V^{\mathrm{r}}_kV_q+V^{\mathrm{r}}_qV_k)-2\sum_p V_p(V_p-V^{\mathrm{r}}_p)V^{(2)}_{k,q}$$
$$+\sum_p((2V_kV^{\mathrm{r}}_p-V_pV^{\mathrm{r}}_k-V_pV_k)V^{(2)}_{p,q}+(2V_qV^{\mathrm{r}}_p-V_pV^{\mathrm{r}}_q-V_pV_q)V^{(2)}_{p,k})$$
$$+2(1-2n_{\mathrm{d}})\sum_p(\epsilon_k+\epsilon_q-2\epsilon_p)V^{(2)}_{k,p}V^{(2)}_{p,q}. \tag{4.17}$$

To analyse these equations let us first consider the case $n_{\mathrm{d}}=\frac{1}{2}$. In this case we have $V^{\mathrm{r}}_k=V_k$ for all k and consequently only the first two terms on the right-hand side of (4.17) do not vanish. The second term is the inhomogeneity, it vanishes in the limit $\ell\to\infty$, but it yields a non-vanishing contribution to $V^{(2)}_{k,q}$ for finite ℓ. Due to the first term, this contribution will tend to zero for $\ell\to\infty$ if $\epsilon_k\neq\epsilon_q$. But if $\epsilon_k=\epsilon_q$, $V^{(2)}_{k,q}$ remains finite. It represents an antiferromagnetic interaction of the local moment in the defect state with electrons in the band. This antiferromagnetic exchange coupling is well known from the Kondo problem. In (4.16) the third term vanishes. The second term is positive and tends to zero if ℓ goes to infinity. Consequently the resulting $U(\infty)$ will be somewhat larger than before. As before, V_k vanishes rapidly due to the first term, ϵ_k and $\tilde{\epsilon}_{\mathrm{d}}$ are renormalized somewhat. This shows that in the case of the local-moment fixed point, the additional contribution (4.12) is marginal. It is important for the physical behaviour of the system, but the other parameters of the model are not changed in such a way that the system behaves completely different. We already mentioned that Schrieffer and Wolff obtained a term similar to (4.12). To be able to compare our result with the result in [2], we restrict ourselves to the symmetric case and to k-vectors near the Fermi surface. Then (4.17) yields

$$\frac{\mathrm{d}V^{(2)}_{k_{\mathrm{F}},k_{\mathrm{F}}}}{\mathrm{d}\ell}=-2UV^2_{k_{\mathrm{F}}}. \tag{4.18}$$

If V^2_k are small we can neglect contributions of higher order in V_k as in [2]. Therefore we have $U\approx U(0)$ and consequently $V_{k_{\mathrm{F}}}\approx V_{k_{\mathrm{F}}}(0)\exp(-\frac{1}{4}U^2(0)\ell)$. Inserting this in (4.18) we obtain

$$V^{(2)}_{k_{\mathrm{F}},k_{\mathrm{F}}}(\infty)=-4\frac{V^2_{k_{\mathrm{F}}}(0)}{U} \tag{4.19}$$

which is exactly the result in [2]. In the asymmetric case the analysis is more difficult but we expect that our result differs from their result in [2]. Especially if ϵ_{d} lies in the conduction band, the Schrieffer–Wolff transformation is not well defined in contrast to our transformation. We would like to mention that the Schrieffer–Wolff transformation leads to other contributions to H similar to the irrelevant trems in our case. These additional contributions were neglected in [2].

In the strong-coupling fixed point, we have $n_d = 0$ or $n_d = 1$. Furthermore, $V_k^r = 0$ for some values of k. Consequently, due to the third and fourth term on the right-hand side of (4.17), $V_{k,q}^{(2)} \to 0$ if $\ell \to \infty$ for all k and q. In this case the other parameters of the model are changed somewhat, but the contribution (4.12) vanishes. This is in contrast to the free-electron fixed point, where $n_d = 0$ or $n_d = 1$ but $V_k^r = V_k$ for all k. Here $V_{k,q}^{(2)}$ does not vanish for some values of k and q. But there is no magnetic moment in the defect state and therefore an antiferromagnetic interaction plays no role. To summarize, the contribution (4.12) is irrelevant in the strong-coupling fixed point and in the free-electron fixed point.

5. Discussion of the results

In the two preceeding sections we calculated and analysed flow equations for the Anderson model. Especially we obtained several fixed points. These fixed points and the corresponding relevant, marginal or irrelevant operators may be compared with results obtained using renormalization methods by Krishnamurty *et al* [5]. But one has to be careful since the idea of a fixed point differs in both cases. In a renormalization-group treatment a fixed point is a single point in the parameter space, whereas in our case a fixed point corresponds to a class of points in the parameter space. It will turn out that the fixed points in [5] are prototypes in the classes we obtain. Furthermore, we should mention that in our notation, n_d is a factor of 2 smaller than in [5].

The free-electron fixed point. In this case we obtain either $\epsilon_d, \epsilon_d + U > \epsilon_k$ for all k, $n_d = 0$, or $\epsilon_d, \epsilon_d + U < \epsilon_k$ for all k, $n_d = 1$. Furthermore, $V_k = 0$ for all k. This fixed point is stable, all the operators we discussed in section 4 are irrelevant. The case $n_d = 0$ corresponds to the frozen-impurity fixed point in [5], which is also stable and has only irrelevant operators. In [5] this fixed point in characterized by $\epsilon_d \to \infty$, $U = 0$ and $V_k = 0$. The physical behaviour of such a system is a prototype of the class of final parameters we called free-electron fixed point.

The strong-coupling fixed point. In this case $n_d = 0$ or $n_d = 1$, but ϵ_d or $\epsilon_d + U$ lies in the conduction band. The hybridization V_k vanishes unless $\tilde{\epsilon}_d = \epsilon_k$, for these values of k the final value of V_k is larger than its initial value. All the other operators are irrelevant in this case. It corresponds to the strong-coupling fixed point in [5] where some of the V_k tend to infinity for fixed ϵ_d and U.

The local-moment fixed point. In this case we have $n_d = \frac{1}{2}$. The defect state is occupied with a single electron, representing the local moment. $V_k = 0$ for all k in this case. The symmetric case falls into this class too. We found a marginal operator which describes an antiferromagnetic interaction of the local moment in the defect state with the electrons in the conduction band and a density–density interaction of the electron in the defect state with the electrons in the band. Due to this interaction a singlet is formed. The singlet formation takes place with electrons in the band for which $\epsilon_k = \tilde{\epsilon}_d$. The energy gain due to the singlet formation gives the Kondo temperature. If the temperature is above the Kondo temperature, triplet states are occupied. This is the usual explanation of the Kondo effect. The local-moment fixed point was found in [5] too; the antiferromagnetic interaction is marginal.

The non-interacting fixed point. It is given by $U = 0$. It is unstable with respect to the electron–electron interaction in the defect state. Other relevant operators are the additional hybridization of band electrons and the antiferromagnetic coupling between the defect state

and the band electrons. The special case where $\epsilon_d = 0$ and $V_k = 0$ is called the free-orbital fixed point in [5]. It is unstable with respect to the operators mentioned above.

In [5] another fixed point is mentioned, the so-called valence-fluctuation fixed point. It is obtained for $\epsilon_d = 0$ and $V_k = 0$, U large. This fixed point occurs in our case as well. But it is unstable with respect to the hybridization V_k, and, by definiton, unstable with respect to changes in ϵ_d. Since we introduced the flow equations to bring the Hamiltonian closer to diagonalization, the case $V_k = 0$ is trivial from our point of view.

6. Conclusions

The aim of this paper was to show that Wegner's original flow equations [1] together with a simple approximation yield approximate flow equations which are simple to analyse. The approximation consists of neglecting terms in the flow equation which do not occur in the initial Hamiltonian. From a physical point of view this may be reasonable, since all of these terms have a simple physical meaning and should occur in a more realistic model. But one does not expect significantly different behaviour of the system if one neglects these terms in the original Hamiltonian. Therefore they might be irrelevant for the flow equations too. From a mathematical point of view the approximation is not yet understood. We only showed that for irrelevant terms our results are equivalent to a second-order perturbational treatment if the off-diagonal matrix elements are small. But since $\eta \to 0$ as $\ell \to \infty$, all the matrix elements of H are functions of ℓ without any pole that tend to a certain value for $\ell \to \infty$. Also the approximate flow equations have this property. Therefore one should be able to estimate the error made by the approximation. Further investigations in this direction will be done.

On the other hand we are able to discuss the relevance of the neglected terms *a posteriori*. It is possible to introduce these terms in the flow equations and to study the effect of these terms. If a contribution is relevant, it cannot be simply included in H^r since divergencies occur. For example V_k is a relevant contribution in the strong-coupling fixed point. If a contribution does only renormalize the other matrix elements and vanishes for $\ell \to \infty$, it is irrelevant. If it does not vanish it is marginal. In our example, the Anderson model, we were able to show that the results obtained in this way agree with results from a numerical renormalization-group approach [5]. The main advantage of our approach is that flow equations are obtained without any difficulty. One simply has to calculate two commutators. Furthermore, the flow equations (3.13)–(3.16) may easily be generalized to the case of many defects or to the case of degenerate defect states. In particular, the limit where the degeneracy is infinite has been studied (see e.g. [4] and the references therein). This limit can be studied using our approach as well and it is possible to derive flow equations without any approximation. We will use this limit in a subsequent paper to test our approximation.

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Appendix A. Derivation of the flow equations in section 4

In this appendix we derive the flow equations presented in section 4. The new contribution is added to H and H^r and we calculate the new $\eta = [H, H^r]$. Then the commutator $[\eta, H]$

contains several new terms compared to (3.12). Some of these new terms are of a form different from the contributions to H. These terms are neglected. The other terms are calculated, since they contribute to the derivative of H with respect to ℓ. Then the new flow equations are given.

Appendix A.1. $\sum_{k,q,\sigma} V_{k,q} : c^\dagger_{k,\sigma} c_{q,\sigma} :$

$$H = \sum_{k,\sigma} \epsilon_k : c^\dagger_{k,\sigma} c_{k,\sigma} : + \sum_{\sigma} \tilde{\epsilon}_d : d^\dagger_\sigma d_\sigma : + \sum_{k,\sigma} V_k (: c^\dagger_{k,\sigma} d_\sigma : + : d^\dagger_\sigma c_{k,\sigma} :) + U : d^\dagger_+ d^\dagger_- d_- d_+ : + \sum_{k,q,\sigma} V_{k,q} : c^\dagger_{k,\sigma} c_{q,\sigma} : . \tag{A.1}$$

$$H^r = \sum_{k,\sigma} V^r_k (: c^\dagger_{k,\sigma} d_\sigma : + : d^\dagger_\sigma c_{k,\sigma} :) + \sum_{k,q,\sigma} V_{k,q} : c^\dagger_{k,\sigma} c_{q,\sigma} : \tag{A.2}$$

$$\eta = [H, H^r] = \sum_{k,\sigma} \eta_k (: c^\dagger_{k,\sigma} d_\sigma : - : d^\dagger_\sigma c_{k,\sigma} :) + \sum_{k,q,\sigma} \eta_{k,q} (: c^\dagger_{k,\sigma} c_{q,\sigma} : - : c^\dagger_{q,\sigma} c_{k,\sigma} :) + \sum_{k,\sigma} \eta^{(2)}_k (: c^\dagger_{k,\sigma} d^\dagger_{-\sigma} d_{-\sigma} d_\sigma : - : d^\dagger_\sigma d^\dagger_{-\sigma} d_{-\sigma} c_{k,\sigma} :) \tag{A.3}$$

$$\eta_k = (\epsilon_k - \tilde{\epsilon}_d) V^r_k + \sum_q V_{k,q} (V^r_q - V_q) \tag{A.4}$$

$$\eta_{k,q} = \tfrac{1}{2}(\epsilon_k - \epsilon_q) V^r_{k,q} + \tfrac{1}{2}(V_k V^r_q - V_q V^r_k) \tag{A.5}$$

$$\eta^{(2)}_k = -U V^r_k . \tag{A.6}$$

New contributions to $[\eta, H]$ are

$$- \sum_{k,q,\sigma} \eta_q V_{k,q} (: c^\dagger_{k,\sigma} d_\sigma : + : d^\dagger_\sigma c_{k,\sigma} :) + 2 \sum_{k,q,p,\sigma} (\eta_{k,p} V_{p,q} + \eta_{q,p} V_{p,k}) : c^\dagger_{k,\sigma} c_{q,\sigma} : - \sum_{k,q,\sigma} \eta^{(2)}_q V_{k,q} (: c^\dagger_{k,\sigma} d^\dagger_{-\sigma} d_{-\sigma} d_\sigma : + : d^\dagger_\sigma d^\dagger_{-\sigma} d_{-\sigma} c_{k,\sigma} :) . \tag{A.7}$$

The last term does not contribute to the flow equations since H does not contain a term of this form. It will be neglected. The first term contributes to the derivative of V_k, the second term to the derivative of $V_{k,q}$. Thus we obtain

$$\frac{d\epsilon_k}{d\ell} = 2\eta_k V_k + 4 \sum_q \eta_{k,q} V_{k,q} \tag{A.8}$$

$$\frac{d\tilde{\epsilon}_d}{d\ell} = -2 \sum_k \eta_k V_k + 2 \sum_k \eta^{(2)}_k V_k (n_k - n_d) + U \frac{dn_d}{d\ell} \tag{A.9}$$

$$\frac{dV_k}{d\ell} = -\eta_k (\epsilon_k - \tilde{\epsilon}_d) + 2 \sum_p \eta_{k,p} V_p + n_d (1 - n_d) \eta^{(2)}_k U - \sum_p \eta_p V_{k,p} \tag{A.10}$$

$$\frac{dV_{k,q}}{d\ell} = \eta_k V_q + \eta_q V_k - \eta_{k,q} (\epsilon_k - \epsilon_q) + 2 \sum_p (\eta_{k,p} V_{p,q} + \eta_{q,p} V_{p,k}) \tag{A.11}$$

$$\frac{dU}{d\ell} = -4 \sum_k \eta^{(2)}_k V_k . \tag{A.12}$$

Using the expression for the different matrix elements of η given above we obtain (4.2)–(4.6).

Appendix A.2. $\sum_{k,\sigma} V_k^{(2)}(:c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : + : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :)$

$$H = \sum_{k,\sigma} \epsilon_k : c_{k,\sigma}^\dagger c_{k,\sigma} : + \sum_\sigma \tilde{\epsilon}_d : d_\sigma^\dagger d_\sigma : + \sum_{k,\sigma} V_k(: c_{k,\sigma}^\dagger d_\sigma : + : d_\sigma^\dagger c_{k,\sigma} :) + U : d_+^\dagger d_-^\dagger d_- d_+ :$$
$$+ \sum_{k,\sigma} V_k^{(2)}(: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : + : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :) \tag{A.13}$$

$$H^r = \sum_{k,\sigma} V_k^r(: c_{k,\sigma}^\dagger d_\sigma : + : d_\sigma^\dagger c_{k,\sigma} :). + \sum_{k,\sigma} V_k^{(2)}(: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : + : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :) \tag{A.14}$$

$$\eta = [H, H^r] = \sum_{k,\sigma} \eta_k(: c_{k,\sigma}^\dagger d_\sigma : - : d_\sigma^\dagger c_{k,\sigma} :) + \sum_{k,q,\sigma} \eta_{k,q}(: c_{k,\sigma}^\dagger c_{q,\sigma} : - : c_{q,\sigma}^\dagger c_{k,\sigma} :)$$
$$+ \sum_{k,\sigma} \eta_k^{(2)}(: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : - : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :)$$
$$+ \sum_{k,q,\sigma} \eta_{k,q}^{(2)}(: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{q,\sigma} : - : c_{q,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :$$
$$+ : d_\sigma^\dagger c_{k,-\sigma}^\dagger d_{-\sigma} c_{q,\sigma} : - : c_{q,\sigma}^\dagger d_{-\sigma}^\dagger c_{k,-\sigma} d_\sigma :$$
$$+ : c_{q,\sigma}^\dagger c_{k,-\sigma}^\dagger d_{-\sigma} d_\sigma : - : d_\sigma^\dagger d_{-\sigma}^\dagger c_{k,-\sigma} c_{q,\sigma} :) \tag{A.15}$$

$$\eta_k = (\epsilon_k - \tilde{\epsilon}_d) V_k^r - n_d(1 - n_d) U V_k^{(2)} \tag{A.16}$$

$$\eta_{k,q} = \tfrac{1}{2}(V_k V_q^r - V_q V_k^r) \tag{A.17}$$

$$\eta_k^{(2)} = -U V_k^r + (\epsilon_k - \tilde{\epsilon}_d - (1 - 2n_d)U) V_k^{(2)} \tag{A.18}$$

$$\eta_{k,q}^{(2)} = \tfrac{1}{2}((V_k - V_k^r) V_q^{(2)} - (V_q - V_q^r) V_k^{(2)}). \tag{A.19}$$

The following new terms in $[\eta, H]$ (compared to (3.12)) contribute to the derivative of H with respect to ℓ:

$$-2\sum_{k,\sigma}(\eta_k V_k^{(2)} + (1 - 2n_d)\eta_k^{(2)} V_k^{(2)}) : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : + 2\sum_{k,\sigma} n_d(1 - n_d)\eta_k^{(2)} V_k^{(2)} : c_{k,\sigma}^\dagger c_{k,\sigma} :$$
$$+ 2\sum_{k,\sigma}((n_k - n_d)\eta_k V_k^{(2)} - n_d(1 - n_d)\eta_k^{(2)} V_k^{(2)}) : d_\sigma^\dagger d_\sigma :$$
$$+ 2\sum_{k,q,\sigma}(\eta_{k,q}^{(2)} V_q + \eta_{k,q} V_q^{(2)} + (1 - 2n_d)\eta_{k,q}^{(2)} V_q^{(2)})$$
$$\times(: c_{k,\sigma}^\dagger d_{-\sigma}^\dagger d_{-\sigma} d_\sigma : + : d_\sigma^\dagger d_{-\sigma}^\dagger d_{-\sigma} c_{k,\sigma} :)$$
$$+ 2\sum_{k,q,\sigma} \eta_{k,q}^{(2)} V_q^{(2)} n_d(1 - n_d)(: c_{k,\sigma}^\dagger d_\sigma : + : d_\sigma^\dagger c_{k,\sigma} :). \tag{A.20}$$

The flow equations are now

$$\frac{d\epsilon_k}{d\ell} = 2\eta_k V_k + 2n_d(1 - n_d)\eta_k^{(2)} V_k^{(2)} \tag{A.21}$$

$$\frac{d\tilde{\epsilon}_d}{d\ell} = -2\sum_k \eta_k V_k + 2\sum_k \left((n_k - n_d)(\eta_k^{(2)} V_k + \eta_k V_k^{(2)}) - n_d(1 - n_d)\eta_k^{(2)} V_k^{(2)}\right) + U\frac{dn_d}{d\ell} \tag{A.22}$$

$$\frac{\mathrm{d}V_k}{\mathrm{d}\ell} = -\eta_k(\epsilon_k - \tilde{\epsilon}_\mathrm{d}) + 2\sum_p(\eta_{k,p}V_p + \eta^{(2)}_{k,p}V^{(2)}_p n_\mathrm{d}(1-n_\mathrm{d})) + Un_\mathrm{d}(1-n_\mathrm{d})\eta^{(2)}_k \tag{A.23}$$

$$\frac{\mathrm{d}U}{\mathrm{d}\ell} = -4\sum_k(\eta^{(2)}_k V_k + \eta_k V^{(2)}_k + (1-2n_\mathrm{d})\eta^{(2)}_k V^{(2)}_k) \tag{A.24}$$

$$\frac{\mathrm{d}V^{(2)}_k}{\mathrm{d}\ell} = \eta_k U - \eta^{(2)}_k(\epsilon_k - \tilde{\epsilon}_\mathrm{d} - (1-2n_\mathrm{d})U) + 2\sum_q(\eta^{(2)}_{k,q}V_q + \eta_{k,q}V^{(2)}_q + (1-2n_\mathrm{d})\eta^{(2)}_{k,q}V^{(2)}_q)\,. \tag{A.25}$$

Using the matrix elements of η calculated above we obtain (4.7)–(4.11).

Appendix A.3. $\sum_{k,q,\sigma} V^{(2)}_{k,q}(:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_{-\sigma}c_{q,\sigma}: - :c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_\sigma c_{q,-\sigma}:)$

H and H^r are obtained as before, adding this term. This yields

$$\begin{aligned}
\eta = {} & \sum_{k,\sigma}\eta_k(:c^\dagger_{k,\sigma}d_\sigma: - :d^\dagger_\sigma c_{k,\sigma}:) + \sum_{k,q,\sigma}\eta_{k,q}(:c^\dagger_{k,\sigma}c_{q,\sigma}: - :c^\dagger_{q,\sigma}c_{k,\sigma}:) \\
& + \sum_{k,,\sigma}\eta^{(2)}_k(:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_{-\sigma}d_\sigma: - :d^\dagger_\sigma d^\dagger_{-\sigma}d_{-\sigma}c_{k,\sigma}:) \\
& + \sum_{k,q,\sigma}\eta^{(2)}_{k,q}(:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_{-\sigma}c_{q,\sigma}: - :c^\dagger_{q,\sigma}d^\dagger_{-\sigma}d_{-\sigma}c_{k,\sigma}: \\
& - :c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_\sigma c_{q,-\sigma}: + :c^\dagger_{q,\sigma}d^\dagger_{-\sigma}d_\sigma c_{k,-\sigma}:) \\
& + \sum_{k,q,\sigma}\eta^{(2)}_{k,q,p}(:c^\dagger_{k,\sigma}c^\dagger_{p,-\sigma}d_{-\sigma}c_{q,\sigma}: - :c^\dagger_{q,\sigma}d^\dagger_{-\sigma}c_{p,-\sigma}c_{k,\sigma}: \\
& + :c^\dagger_{k,\sigma}d^\dagger_{-\sigma}c_{p,-\sigma}c_{q,\sigma}: - :c^\dagger_{q,\sigma}c^\dagger_{p,-\sigma}d_{-\sigma}c_{k,\sigma}: \\
& - :c^\dagger_{k,\sigma}c^\dagger_{p,-\sigma}d_\sigma c_{q,-\sigma}: + :c^\dagger_{q,\sigma}d^\dagger_{-\sigma}c_{p,\sigma}c_{k,-\sigma}: \\
& - :c^\dagger_{k,\sigma}d^\dagger_{-\sigma}c_{p,\sigma}c_{q,-\sigma}: + :c^\dagger_{q,\sigma}c^\dagger_{p,-\sigma}d_\sigma c_{k,-\sigma}:)
\end{aligned} \tag{A.26}$$

$$\eta_k = (\epsilon_k - \tilde{\epsilon}_\mathrm{d})V^\mathrm{r}_k - \sum_q V^{(2)}_{k,q}(V^\mathrm{r}_q - V_q)(n_q - n_\mathrm{d}) \tag{A.27}$$

$$\eta_{k,q} = \tfrac{1}{2}(V_k V^\mathrm{r}_q - V_q V^\mathrm{r}_k) \tag{A.28}$$

$$\eta^{(2)}_k = -U\,V^\mathrm{r}_k + \sum_q V^{(2)}_{k,q}(V^\mathrm{r}_q - V_q) \tag{A.29}$$

$$\eta^{(2)}_{k,q} = \tfrac{1}{2}(\epsilon_k - \epsilon_q)V^{(2)}_{k,q} \tag{A.30}$$

$$\eta^{(2)}_{k,q,p} = \tfrac{1}{2}V^{(2)}_{k,q}(V_p - V^\mathrm{r}_p)\,. \tag{A.31}$$

The following additional terms in $[\eta, H]$ (compared to (3.12)) are of the same form as terms in H and have to be taken into account:

$$\begin{aligned}
& -\sum_{k,q,\sigma}(\eta_q V^{(2)}_{k,q} - 2\eta^{(2)}_{k,q}V_q)(n_q - n_\mathrm{d})(:c^\dagger_{k,\sigma}d_\sigma: + :d^\dagger_\sigma c_{k,\sigma}:) \\
& \qquad + 2\sum_{k,q,p,\sigma}(\eta_{k,p}V^{(2)}_{p,q} + \eta_{q,p}V^{(2)}_{p,k})(:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_{-\sigma}c_{q,\sigma}: - :c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_\sigma c_{q,-\sigma}:)
\end{aligned}$$

$$
\begin{aligned}
&-2\sum_{k,q,\sigma}\eta_{k,q}V^{(2)}_{k,q}(n_k-n_q):d^\dagger_\sigma d_\sigma:\\
&-2n_{\rm d}(1-n_{\rm d})\sum_{k,q,\sigma}\eta^{(2)}_q V^{(2)}_{k,q}(:c^\dagger_{k,\sigma}d_\sigma:+:d^\dagger_\sigma c_{k,\sigma}:)\\
&+4(1-2n_{\rm d})\sum_{k,q,p,\sigma}(\eta^{(2)}_{k,p}V^{(2)}_{p,q}+\eta^{(2)}_{q,p}V^{(2)}_{p,k})\\
&\times(:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_{-\sigma}c_{q,\sigma}:-:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_\sigma c_{q,-\sigma}:)\\
&-4(1-2n_{\rm d})\sum_{k,q,\sigma}\eta^{(2)}_{k,q}V^{(2)}_{k,q}(n_k-n_q):d^\dagger_\sigma d_\sigma:\\
&-2\sum_{k,q,\sigma}\eta^{(2)}_{k,q}V^{(2)}_{k,q}(n_k-n_q):d^\dagger_\sigma d^\dagger_{-\sigma}d_{-\sigma}d_\sigma:\\
&+4\sum_{k,q,p,\sigma}\eta^{(2)}_{p,q,k}V^{(2)}_{p,q}[n_p(1-n_q)(1-n_{\rm d})-(1-n_p)n_q n_{\rm d}]\\
&\times(:c^\dagger_{k,\sigma}d_\sigma:+:d^\dagger_\sigma c_{k,\sigma}:)\\
&-2\sum_{k,q,\sigma}\eta^{(2)}_{k,q}(\epsilon_k-\epsilon_q)(:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_{-\sigma}c_{q,\sigma}:-:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_\sigma c_{q,-\sigma}:)\\
&-4\sum_{k,q,p,\sigma}\eta^{(2)}_{k,q,p}V_p(:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_{-\sigma}c_{q,\sigma}:-:c^\dagger_{k,\sigma}d^\dagger_{-\sigma}d_\sigma c_{q,-\sigma}:). \qquad \text{(A.32)}
\end{aligned}
$$

Now the flow equations are

$$\frac{{\rm d}\epsilon_k}{{\rm d}\ell}=2\eta_k V_k \qquad \text{(A.33)}$$

$$
\begin{aligned}
\frac{{\rm d}\tilde\epsilon_{\rm d}}{{\rm d}\ell}&=-2\sum_k\eta_k V_k+2\sum_k\eta^{(2)}_k V_k(n_k-n_{\rm d})+U\frac{{\rm d}n_{\rm d}}{{\rm d}\ell}\\
&\quad-2\sum_{k,q}\eta_{k,q}V^{(2)}_{k,q}(n_k-n_q)-4(1-2n_{\rm d})\sum_{k,q,\sigma}\eta^{(2)}_{k,q}V^{(2)}_{k,q}(n_k-n_q) \qquad \text{(A.34)}
\end{aligned}
$$

$$
\begin{aligned}
\frac{{\rm d}V_k}{{\rm d}\ell}&=-\eta_k(\epsilon_k-\tilde\epsilon_{\rm d})+2\sum_q\eta_{k,q}V_q+Un_{\rm d}(1-n_{\rm d})\eta^{(2)}_k\\
&\quad-\sum_q(\eta_q V^{(2)}_{k,q}-\eta^{(2)}_{k,q}V_q)(n_q-n_{\rm d})-2n_{\rm d}(1-n_{\rm d})\sum_q\eta^{(2)}_q V^{(2)}_{k,q}\\
&\quad+4\sum_{q,p}\eta^{(2)}_{p,q,k}V^{(2)}_{p,q}[n_p(1-n_q)(1-n_{\rm d})-(1-n_p)n_q n_{\rm d}] \qquad \text{(A.35)}
\end{aligned}
$$

$$\frac{{\rm d}U}{{\rm d}\ell}=-4\sum_k\eta^{(2)}_k V_k-2\sum_{k,q}\eta^{(2)}_{k,q}V^{(2)}_{k,q}(n_k-n_q) \qquad \text{(A.36)}$$

$$
\begin{aligned}
\frac{{\rm d}V^{(2)}_{k,q}}{{\rm d}\ell}&=\eta^{(2)}_k V_q+\eta^{(2)}_q V_k-2\eta^{(2)}_{k,q}(\epsilon_k-\epsilon_q)-4\sum_p\eta^{(2)}_{k,q,p}V_p\\
&\quad+2\sum_p(\eta_{k,p}V^{(2)}_{p,q}+\eta_{q,p}V^{(2)}_{p,k})+4(1-2n_{\rm d})\sum_p(\eta^{(2)}_{k,p}V^{(2)}_{p,q}+\eta^{(2)}_{q,p}V^{(2)}_{p,k}). \qquad \text{(A.37)}
\end{aligned}
$$

As before, we obtain (4.13)–(4.17).

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