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# Flow-equations for Hamiltonians

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**Abstract.** Flow-equations are introduced in order to bring Hamiltonians closer to diagonalization. It is characteristic for these equations that matrix-elements between degenerate or almost degenerate states do not decay or decay very slowly. In order to understand different types of physical systems in this framework it is probably necessary to classify various types of these degeneracies and to investigate the corresponding physical behavior.

In general these equations generate many-particle interactions. However, for an $n$-orbital model the equations for the two-particle interaction are closed in the limit of large $n$. Solutions of these equations for a one-dimensional model are considered. There appear convergency problems, which are removed, if instead of diagonalization only a block-diagonalization into blocks with the same number of quasiparticles is performed.

**Keywords:** Many-particle problem; Flow-equations; Diagonalization.

## 1 Introduction

In order to solve a many-particle problem one would like to diagonalize the Hamiltonian and to calculate from the eigenstates and their energies the observables of interest. However, apart from a few explicitly solvable models this is not possible. Therefore one may try – and this will be done here – to transform the Hamiltonian in such a way that it becomes more and more diagonal. More precisely unitary transformations will be applied to the Hamiltonian so that the off-diagonal matrix elements become smaller and smaller.

As we will see in explicit examples there will be difficulties to reach the goal of diagonalization. The reason is that it is not easy to diagonalize between states which are almost degenerate. As is well-known perturbation theory works best, if the splitting between states is large in comparison to the interaction. Similarly here convergency will be slow for almost degenerate states. The hope is that there will develop certain asymptotic types of "almost degeneracies" which can be finally classified and investigated, and that these types of asymptotic behaviour reflect different types of physical behaviour.

This is, however, a far goal. What will be done here – always having this goal in mind – is to introduce equations which bring the Hamiltonian closer to diagonalization. In Section 2 the general flow-equation will be introduced and starting out from Jacobi's method simple – not yet many-body – examples will show how the method works.

In Section 3 the many-body problem for an $n$-orbital model will be considered as a special example, where the number $n$ of different flavors tends to infinity. In this limit

the flow-equation for the two-particle interaction becomes a closed nonlinear equation. The solution of this equation will be considered in Section 4. For reasons not yet understood there appear divergency problems.

In Section 5 a different approach will be used, where the Hamiltonian will not be required to become diagonal. Instead it will be required only, that the terms which change the number of quasiparticles, do vanish. This scheme converges better. It will be used to calculate the average occupation number in Section 6. In addition to the step function in order $n^0$ at the Fermi edge, a correction proportional to the logarithm of $k-k_F$ in order $1/n$, is obtained, which may be an indication of a power-law behaviour at the Fermi edge. In Section 7 the interaction terms which connect more than 2 quasiparticles and an aspect of their convergency behavior will be considered.

## 2 General equation and simple examples

In general the Hamiltonian is transformed by a unitary transformation. We would like to perform this transformation continuously. Thus we consider the Hamiltonian as a function of a flow parameter $l$. Its derivative with respect to $l$ is given by the generator $\eta$ of a unitary transformation, so that the basic equation reads

$$\frac{dH(l)}{dl} = [\eta(l), H(l)] \tag{2.1}$$

where $\eta$ is antihermitean since it generates a unitary transformation

$$\eta^\dagger = -\eta \ . \tag{2.2}$$

Of course, it is now crucial to choose an appropriate generator $\eta$ as function of the Hamiltonian. The numerical method by Jacobi consists of unitary transformations between two states which makes the connecting offdiagonal matrix element vanishing. If this is repeated for all offdiagonal matrix elements again and again then the offdiagonal matrix elements will become arbitrarily small. Here an infinitesimal transformation is needed. If the diagonal matrix elements are denoted by $\varepsilon$ then the choice

$$\eta_{k,k'} = (\varepsilon_k - \varepsilon_{k'}) h_{k,k'} \tag{2.3}$$

makes the off-diagonal matrix element between $k$ and $k'$ decrease (unless $\varepsilon_k = \varepsilon_{k'}$). All these unitary transformations are now performed simultaneously. This yields

$$\frac{\partial h_{k,k'}}{\partial l} = \sum_{k''} (\varepsilon_k + \varepsilon_{k'} - 2\varepsilon_{k''}) h_{k,k''} h_{k'',k'} \ . \tag{2.4}$$

The sum of the squares of the diagonal matrix elements obeys

$$\sum_k \frac{\partial \varepsilon_k^2}{\partial l} = -\sum_{k,k' \mid k \neq k'} \frac{\partial (h_{k,k'} h_{k',k})}{\partial l} = 2 \sum_{k,k'} (\varepsilon_k - \varepsilon_{k'})^2 h_{k,k'} h_{k',k} \ . \tag{2.5}$$

Thus the sum of the absolute squares of the nondiagonal elements decreases until only offdiagonal matrix elements between states with equal diagonal matrix elements are left. Note that Eq. (2.3) can be rewritten

$$\eta = [H_d, H] \tag{2.6}$$

where $H_d$ is the diagonal part of $H$.

Let us consider as an example a two-particle problem where for given total momentum the relative momenta between two particles is $k$. Suppose the diagonal matrix element increases linearly with $k$, whereas the interaction depends only on the difference $|k-k'|$. Then the sums on the right hand side of Eq. (2.4) vanish, thus $\varepsilon_k$ is independent of $l$ and the offdiagonal elements decay exponentially with $l$,

$$h_{k,k'} = h^0_{k,k'} \exp\left(-(\varepsilon_k - \varepsilon_{k'})^2 l\right) . \tag{2.7}$$

Apparently the decay is the slower the smaller the difference of the diagonal matrix-elements is. The unitary transformation itself produces wavefunctions with an energy uncertainty decreasing like $l^{-1/2}$.

Let us consider a second example which might be characteristic for a collective state. Suppose the system has a collective eigenstate of wavefunction $\phi_k$ and energy $E_0$ whereas all other states are degenerate with energy 0. Then one has

$$h_{k,k'} = E_0 \phi_k \phi^*_{k'} \tag{2.8}$$

and

$$\frac{\partial h_{k,k'}}{\partial l} = E_0^3 \phi_k \phi^*_{k'} (\phi^*_k \phi_k + \phi^*_{k'} \phi_{k'} - 2S) , \tag{2.9}$$

$$S = \sum_{k''} \phi^{*2}_{k''} \phi^2_{k''} . \tag{2.10}$$

This equation can be written as a differential equation for $\phi$,

$$\frac{\partial \phi_k}{\partial l} = E_0^2 \phi_k^2 \phi^*_k - E_0^2 S(l) \phi_k \tag{2.11}$$

or

$$\frac{\partial (\phi^*_k \phi_k)^{-1}}{\partial l} = -2E_0^2 + 2E_0^2 S(l) (\phi^*_k \phi_k)^{-1} . \tag{2.12}$$

The solution of this equation is of the form

$$(\phi^*_k \phi_k)^{-1} = (\gamma_k + C(l))/B(l) . \tag{2.13}$$

With the definition

$$I(C) = \sum_k \frac{1}{\gamma_k + C} \tag{2.14}$$

the normalization of $\phi$ yields

$$BI(C) = 1 \ . \tag{2.15}$$

From the derivative of $I$ one obtains

$$S = -B^2 I'(C) \ . \tag{2.16}$$

Insertion into the flow Eq. (2.12) yields

$$\frac{\partial C}{\partial l} = -2E_0^2/I(C) \tag{2.17}$$

with the solution

$$\sum_k \ln(\gamma_k + C) = -2E_0^2 l + \text{const.} \ , \tag{2.18}$$

which is the equation from which $C$ as a function of $l$ has to be determined. If one performs the continuum limit for $k$ then there is no real solution beyond the value of $l$ for which $C + \min(\gamma) = 0$. For discrete values of $k$ the state with minimal $\gamma_k$ will obtain increasing weight from this $l$ on whereas the other states loose their weight. This is similar to the condensation phenomenon for an ideal Bose gas at the critical point.

## 3 Flow equation for the $n$-orbital model

In this section the flow Eqs. (2.1), (2.6) will be applied to a many-body problem of electrons. If one starts out from a two-particle Hamiltonian, then apparently the generator $\eta$ contains a three-particle term and the derivative $\partial H/\partial l$ a four-particle interaction. Thus the original two-particle interaction will rapidly generate interactions between arbitrarily many particles. As a result one will in general not have any closed equations for the matrix-elements of the interaction. It will turn out useful to introduce electrons with $n$ different flavors $s$. In order to obtain closed equations the limit $n$ to infinity of this $n$-orbital model will be considered. Previously it has been observed and used, that models in the limit $n$ to infinity can be solved and that expansions around this limit are possible [1–5]. The Hamiltonian will be expressed in terms of the operators

$$N_{p,q} = \frac{1}{n} \sum_s c_{p,s}^\dagger c_{q,s} \tag{3.1}$$

with creation and annihilation operators $c^\dagger$ and $c$ and momenta $p$ and $q$. All operators will be expressed as normal-ordered polynomials of the $N_{p,q}$. Thus $N_{p,p} = n_p + :N_{p,p}:$ where $n_p$ is the occupation number for the groundstate of the free system, $n_p = \theta(k_F - |p|)$. Then one has the commutator

$$[:N_{p,q}:,:N_{r,t}:] = \frac{1}{n}\delta_{q,r}:N_{p,t}: - \frac{1}{n}\delta_{p,t}:N_{r,q}: + \frac{1}{n}\delta_{p,t}\delta_{q,r}(n_p - n_q) \tag{3.2}$$

and in leading order in $1/n$

$$[:A:,:B:] = [A,B]_1 + [A,B]_2 + O(n^{-2}) \ , \tag{3.3}$$

$$n[A,B]_1 = \sum_{p,q,r} :\frac{\partial A}{\partial N_{p,q}}\frac{\partial B}{\partial N_{q,r}} N_{p,r}: - \sum_{p,q,r} :\frac{\partial A}{\partial N_{p,q}}\frac{\partial B}{\partial N_{r,p}} N_{r,q}: \ , \tag{3.4}$$

$$n[A,B]_2 = \sum_{p,q} :\frac{\partial A}{\partial N_{p,q}}\frac{\partial B}{\partial N_{q,p}}: (n_p - n_q) \ . \tag{3.5}$$

We start out with a Hamiltonian

$$H = H_1 + H_2 + \dots \ , \tag{3.6}$$

$$H_1 = n \sum_q \varepsilon_q :N_{q,q}: \ , \tag{3.7}$$

$$H_2 = \frac{n}{2\Omega} \sum_{\delta,Q,K} v_{\delta,Q,K} :N_{Q+\delta/2,Q-\delta/2} N_{K-\delta/2,K+\delta/2}: \ , \tag{3.8}$$

where $\delta$ is the momentum transfer and $\Omega$ is the volume of the system and $H_k$ contains the $k$-particle interaction. Similarly one has

$$\eta = \eta_2 + \dots \ , \tag{3.9}$$

$$\eta_2 = \frac{n}{2\Omega} \sum_{\delta,Q,K} \eta_{\delta,Q,K} :N_{Q+\delta/2,Q-\delta/2} N_{K-\delta/2,K+\delta/2}: \ . \tag{3.10}$$

In leading order in $n$ one obtains

$$\eta_2 = [H_1, H_2 - H_{2d}]_1 + [H_{2d}, H_2]_2 \ , \tag{3.11}$$

$$\frac{\partial H_1}{\partial l} = 0 \ , \tag{3.12}$$

$$\frac{\partial H_2}{\partial l} = [\eta_2, H_1]_1 + [\eta_2, H_2]_2 \ . \tag{3.13}$$

Thus $H_1$ is constant in leading order in $n$ and the flow-equation for $H_2$ is a closed nonlinear equation. Similarly one obtains equations for $H_k$ ($k>2$), which are linear in $H_k$. The inhomogeneities of these equations depend only on the $H_m$ with $m<k$. The term $H_{2d}$ is subtracted from $H_2$ in the equation for $\eta_2$, since later nondiagonal terms in $H_d$ will be allowed.

## 4 First approach: problems

In a first step the Eqs. (2.1), (2.6) are applied literally, that is the diagonal part of the twobody-interaction is chosen

$$H_{2d} = \frac{n}{2\Omega} \sum_{Q,K} v_{0,Q,K} : N_{Q,Q} N_{K,K} : + \frac{n}{2\Omega} \sum_{\delta,Q} v_{\delta,Q,Q} : N_{Q+\delta/2,Q-\delta/2} N_{Q-\delta/2,Q+\delta/2} : \,. \tag{4.1}$$

Then one obtains for $\eta_2$

$$\eta_2 = \frac{n}{2\Omega} \sum_{\delta,Q,K} (\varepsilon_{Q+\delta/2} - \varepsilon_{Q-\delta/2} + \varepsilon_{K-\delta/2} - \varepsilon_{K+\delta/2}) v_{\delta,Q,K}$$

$$: N_{Q+\delta/2,Q-\delta/2} N_{K-\delta/2,K+\delta/2} : + \eta_{2\text{small}} \,, \tag{4.2}$$

$$\eta_{2\text{small}} = \frac{n}{2\Omega^2} \sum_{\delta,Q,K} (s_{\delta,Q} v_{\delta,Q,Q} - s_{\delta,K} v_{\delta,K,K}) v_{\delta,Q,K}$$

$$: N_{Q+\delta/2,Q-\delta/2} N_{K-\delta/2,K+\delta/2} : \,, \tag{4.3}$$

$$s_{\delta,Q} = n_{Q-\delta/2} - n_{Q+\delta/2} \,. \tag{4.4}$$

The quantity $\eta_{2\text{small}}$ has an extra factor $1/\Omega$ without a corresponding summation over a momentum. Therefore it vanishes in the thermodynamic limit and we neglect it. With the choice

$$\varepsilon_k = \frac{1}{2} k^2 \tag{4.5}$$

we have

$$\eta_{\delta,Q,K} = (Q-K) \delta v_{\delta,Q,K} \,. \tag{4.6}$$

The equation for $v$ reads

$$\frac{\partial v_{\delta,Q,K}}{\partial l} = (K-Q) \delta \eta_{\delta,Q,K} + \frac{1}{\Omega} \sum_P s_{\delta,P} (\eta_{\delta,Q,P} v_{\delta,P,K} - v_{\delta,Q,P} \eta_{\delta,P,K}) \,. \tag{4.7}$$

From the Eqs. (4.6), (4.7) it is apparent that $v$ depends only on the $v$s with the same $\delta$. We consider the behaviour for small $\delta$ and restrict the calculations to the one-dimensional case. For a linear dispersion of $\varepsilon_k$ and $2n = 2$ species of electrons one moving to the right the other to the left such a model is familiar as the Luttinger model [6–8]. It can be easily generalized to an arbitrary number $n$ of species moving in both directions. The reader will realize the coincidence of a number of results for small $\delta$ for this generalized Luttinger model with our results, which shows that in this limit of $n$ and $\delta$ only the slope of $\varepsilon_k$ at the Fermi energy that is the Fermi velocity and the interaction strengths matter. We consider only $\delta \geq 0$, since $v_{-\delta,Q,K} = v_{\delta,K,Q}$. For the region, where

$s_Q$ or $s_K$ equals $+1$ or $-1$ it is assumed that $v$ is practically constant. It is denoted by $v_{s_Q,s_K}$, similarly for $\eta$. Then one obtains

$$\eta_{+,+} = \eta_{-,-} = 0 \ , \tag{4.8}$$

$$\eta_{+,-} = 2\delta k_F v_{+,-} \ , \quad \eta_{-,+} = -2\delta k_F v_{-,+} \ , \tag{4.9}$$

$$\frac{\partial v_{+,+}}{\partial l} = \frac{\partial v_{-,-}}{\partial l} = -\frac{2\delta^2 k_F}{\pi} v_{+,-} v_{-,+} \ , \tag{4.10}$$

$$\frac{\partial v_{+,-}}{\partial l} = -\frac{2\delta^2 k_F}{\pi} A v_{+,-} \ , \tag{4.11}$$

$$\frac{\partial v_{-,+}}{\partial l} = -\frac{2\delta^2 k_F}{\pi} A v_{-,+} \ , \tag{4.12}$$

$$A = 2\pi k_F + \frac{1}{2}(v_{+,+} + v_{-,-}) \ . \tag{4.13}$$

From these equations one easily finds that $v_{+,+} - v_{-,-}$ is constant. In the following it is assumed, that it vanishes. Moreover

$$B = A^2 - v_{+,-} v_{-,+} \tag{4.14}$$

is a constant. The solution of the equations reads

$$A(l) = \frac{\sqrt{B}(A(0) + \sqrt{B} + (A(0) - \sqrt{B}) \exp(-2\gamma_1 l))}{(A(0) + \sqrt{B}) - (A(0) - \sqrt{B}) \exp(-2\gamma_1 l)} \ , \tag{4.15}$$

$$v_{+,-}(l) = \frac{2\sqrt{B} v_{+,-}(0) \exp(-\gamma_1 l)}{(A(0) + \sqrt{B}) - (A(0) - \sqrt{B}) \exp(-2\gamma_1 l)} \ , \tag{4.16}$$

$$\gamma_1 = \frac{2\delta^2 k_F \sqrt{B}}{\pi} \ . \tag{4.17}$$

For negative $B$ the solution is periodic in $l$ with vanishing denominators for special values of $l$. In this case however the system is unstable similarly as the Luttinger model. For positive $B$ one has to distinguish between positive and negative $A(0)$. For positive $A(0)$ the functions $A(l)$ and $v_{\pm,\mp}$ converge smoothly to the asymptotic values $\sqrt{B}$ and 0. For negative $A(0)$ there is however a pole for some value $l$, which makes the solution unphysical. It may be that also in this attractive case the system is unstable.

Next the components of $v_{s,K}$ are considered, where the first momentum $Q$ has $s_{\delta,Q} = \pm 1$, that is $Q$ is close to $sk_F$. Then one obtains

$$\eta_{+,K} = \delta(k_F - K) v_{+,K} \ , \tag{4.18}$$

$$\eta_{-,K} = \delta(-k_F - K) v_{-,K} \ , \tag{4.19}$$

$$\frac{\partial v_{+,K}}{\partial l} = -\delta^2(k_F-K)\left(k_F-K+\frac{1}{2\pi}v_{+,+}\right)v_{+,K}-\frac{\delta^2}{2\pi}(3k_F+K)v_{+,-}v_{-,K}\,, \quad (4.20)$$

$$\frac{\partial v_{-,K}}{\partial l} = -\delta^2(k_F+K)\left(k_F+K+\frac{1}{2\pi}v_{-,-}\right)v_{-,K}-\frac{\delta^2}{2\pi}(3k_F-K)v_{-,+}v_{+,K}\,. \quad (4.21)$$

Since for large $l$ and positive $B$ the matrix elements $v_{+,-}$ and $v_{-,+}$ tend to zero the two equations become decoupled for large $l$. Then however depending on the value of $K$ the matrix elements $v_{\pm,K}$ may increase exponentially. This is very unexpected. To the contrary one would expect that the off-diagonal matrix elements decay. The explanation of this phenomenon is an open question, which is left for further investigation. It may be connected to the neglection of terms which are smaller by a factor $1/\Omega$ or $1/n$.

## 5 Second approach: success

In the preceeding section $H_d$ has been chosen to be the diagonal part of the Hamiltonian. However a different choice is possible. We may require that $H_d$ contains those parts of the Hamiltonian which conserve the number of quasiparticles. Then $H_0$, which is a constant in addition to the Hamiltonian already written down, becomes the energy of (hopefully) the ground-state, $H_1$ contains the excitation energies of one-quasi-particles (electrons outside the Fermi-sphere or holes inside the Fermi-sea). $H_2$ contains the interaction between two quasiparticles, etc. Thus to obtain the two-quasiparticle states it would be sufficient to diagonalize a two-particle problem, which is of course much easier then to solve an $N$-particle problem. With this in mind the terms $v_{\delta,Q,K}{:}N_{Q+\delta/2,Q-\delta/2}N_{K-\delta/2,K+\delta/2}{:}$ belong to $H_{2d}$, if $s_{\delta,Q} = s_{\delta,K}$. With this definition of $H_d$ one obtains

$$\eta_{+,+} = \eta_{-,-} = 0\,, \quad (5.1)$$

$$\eta_{+,-} = \frac{\delta}{\pi}A v_{+,-}\,, \quad (5.2)$$

$$\eta_{-,+} = -\frac{\delta}{\pi}A v_{-,+}\,, \quad (5.3)$$

$$\frac{\partial v_{+,+}}{\partial l} = \frac{\partial v_{-,-}}{\partial l} = -\frac{\delta^2}{\pi^2}A v_{+,-}v_{-,+}\,, \quad (5.4)$$

$$\frac{\partial v_{+,-}}{\partial l} = -\frac{\delta^2}{\pi^2}A^2 v_{+,-}\,, \quad (5.5)$$

$$\frac{\partial v_{-,+}}{\partial l} = -\frac{\delta^2}{\pi^2}A^2 v_{-,+}\,. \quad (5.6)$$

As before $v_{+,+}-v_{-,-}$ and $B$, Eq. (4.14) are constants. The solutions read

$$A(l)^2 = \frac{BA(0)^2}{A(0)^2 - v_{+,-}(0)v_{-,+}(0)\exp(-\gamma l)}\,, \quad (5.7)$$

$$v_{+,-}(l)\,v_{-,+}(l) = \frac{B v_{+,-}(0)\,v_{-,+}(0)}{A(0)^2 \exp(\gamma l) - v_{+,-}(0)\,v_{-,+}(0)} , \tag{5.8}$$

$$\gamma = \frac{2\delta^2 B}{\pi^2} . \tag{5.9}$$

Thus for $B>0$ the matrixelement $v_{\pm,\mp}$ which stand for quasiparticle-violating processes decay for increasing $l$.

For $\eta_{\pm,K}$ and $v_{\pm,K}$ one obtains

$$\eta_{+,K} = \delta\left(k_F - K + \frac{1}{2\pi} v_{+,+}\right) v_{+,K} , \tag{5.10}$$

$$\eta_{-,K} = \delta\left(-k_F - K - \frac{1}{2\pi} v_{-,-}\right) v_{-,K} , \tag{5.11}$$

$$\frac{\partial v_{+,K}}{\partial l} = -\frac{\delta^2}{4\pi^2}(A+c_K)^2 v_{+,K} - \frac{\delta^2}{4\pi^2}(3A-c_K)\,v_{+,-}\,v_{-,K} , \tag{5.12}$$

$$\frac{\partial v_{-,K}}{\partial l} = -\frac{\delta^2}{4\pi^2}(A-c_K)^2 v_{-,K} - \frac{\delta^2}{4\pi^2}(3A+c_K)\,v_{-,+}\,v_{+,K} , \tag{5.13}$$

$$c_K = \frac{1}{2}(v_{+,+} - v_{-,-}) - 2\pi K . \tag{5.14}$$

For positive $B$ the elements $v_{\pm,\mp}$ decay exponentially and $v_{\pm,K}$ decays exponentially except at

$$K_{c,\pm} = \pm k_F \pm \frac{1}{2\pi} v_{\pm,\pm}(\infty) . \tag{5.15}$$

In the vicinity of these momenta one obtains the asymptotic behavior

$$v_{\pm,K} = v_{\pm,K_{c,\pm}}(\infty) \exp(-\delta^2 (K - K_{c,\pm})^2 l) . \tag{5.16}$$

Finally we consider $v_{Q,K}$ and obtain

$$\eta_{Q,K} = 0 , \tag{5.17}$$

$$\frac{\partial v_{Q,K}}{\partial l} = -\frac{\delta^2}{4\pi^2}[(2A + c_Q + c_K)\,v_{Q,+}\,v_{+,K} - (c_Q + c_K - 2A)\,v_{Q,-}\,v_{-,K}] . \tag{5.18}$$

Since the inhomogeneities decay exponentially, $v_{Q,K}$ approaches some finite value except at values $Q$ and $K$ at $K_{c,\pm}$. Thus one obtains asymptotically a regular part $v_{Q,K,\mathrm{reg}}$ and a diverging contribution

$$v_{Q,K}(l) = v_{Q,K,\mathrm{reg}} - \frac{(2K_{c,+} - K - Q)\, v_{K_{c,+},+}(\infty)\, v_{+,K_{c,+}}(\infty)}{2[\pi(K_{c,+} - K)^2 + (K_{c,+} - Q)^2]}$$

$$\times (1 - \exp(-\delta^2[(K_{c,+} - K)^2 + (K_{c,+} - Q)^2]\, l))$$

$$- \frac{(K + Q - 2K_{c,-})\, v_{K_{c,-},-}(\infty)\, v_{-,K_{c,-}}(\infty)}{2[\pi(K_{c,-} - K)^2 + (K_{c,-} - Q)^2]}$$

$$\times (1 - \exp(-\delta^2[(K_{c,-} - K)^2 + (K_{c,-} - Q)^2]\, l)) \ . \tag{5.19}$$

## 6 Occupation number

In this section the correction in order $1/n$ to the occupation number $\langle N_{p,p} \rangle$ will be determined. For this purpose the flow-equation

$$\frac{\partial N_{p,p}(l)}{\partial l} = [\eta(l), N_{p,p}(l)] \tag{6.1}$$

will be solved. We expand

$$N_{p,p}(l) = v_p(l) + :N_{p,p}: + \frac{1}{\Omega} \sum_{\delta > 0, Q, K} v_{\delta,Q,K}(l) :N_{Q+\delta/2, Q-\delta/2} N_{K-\delta/2, K+\delta/2}: + \ldots \ . \tag{6.2}$$

For $l = 0$ one has

$$v_p(0) = n_p \ , \quad v_{\delta,Q,K}(0) = 0 \ . \tag{6.3}$$

In order $n^0$ one obtains two contributions to the change of $v_{\delta,Q,K}$, one from the commutator of $\eta$ with $:N_{p,p}:$, the other from the commutator with the two-particle contribution,

$$\frac{\partial v_{\delta,Q,K}}{\partial l} = \eta_{\delta,Q,K}(\delta_{Q-\delta/2,p} - \delta_{Q+\delta/2,p} + \delta_{K+\delta/2,p} - \delta_{K-\delta/2,p})$$

$$+ \frac{1}{\Omega} \sum_U s_{\delta,U}(\eta_{\delta,Q,U} v_{\delta,U,K} - v_{\delta,Q,U} \eta_{\delta,U,K}) \ . \tag{6.4}$$

This contribution to $N_{p,p}(l)$ generates the only contribution of order $1/n$ to $v(l)$,

$$\frac{\partial v_p(l)}{\partial l} = \frac{1}{2n\Omega^2} \sum_{\delta,Q,K} s_{\delta,Q} s_{\delta,K} (s_{\delta,K} - s_{\delta,Q}) \eta_{\delta,K,Q} v_{\delta,Q,K} \ . \tag{6.5}$$

Therefore one has to determine $v_{\delta,Q,K}$ for $s_{\delta,Q}$ and $s_{\delta,K}$ equal $\pm 1$. With

$$v_{\delta,s,t} = \frac{1}{\Omega} \sum_{Q=sk_F-\delta/2}^{sk_F+\delta/2} \sum_{K=tk_F-\delta/2}^{tk_F+\delta/2} v_{\delta,Q,K} \tag{6.6}$$

one has

$$\frac{\partial v_{\delta,s,t}}{\partial l} = \frac{\delta}{2\pi} \eta_{\delta,s,t}(\Phi_{\delta,s,p} - \Phi_{\delta,t,d}) + \frac{\delta}{2\pi} \sum_u u(\eta_{\delta,s,u} v_{\delta,u,t} - v_{\delta,s,u} \eta_{\delta,u,t}) \tag{6.7}$$

with

$$\Phi_{\delta,s,p} = 2\Theta(sk_F - p) - \Theta(sk_F - \delta - p) - \theta(sk_F + \delta - p) \tag{6.8}$$

and

$$\frac{\partial v_p(l)}{\partial l} = -\frac{1}{n\Omega} \sum_{\delta>0} (\eta_{+,-} v_{-,+} - \eta_{-,+} v_{+,-}) \ . \tag{6.9}$$

From the Eqs. for $v_{\delta,s,t}$ it follows that

$$v_{-,-} = v_{+,+} \ , \quad v_{-,+} = v^*_{+,-} \tag{6.10}$$

$$\frac{\partial v_{+,+}}{\partial l} = -\frac{\delta}{\pi} \eta_{+,-} v_{-,+} \ , \tag{6.11}$$

$$\frac{\partial v_{+,-}}{\partial l} = -\frac{\delta}{\pi} \eta_{+,-} v_{+,+} + \frac{\delta}{2\pi} \eta_{+,-} (\Phi_{+,p} - \Phi_{-,p}) \ . \tag{6.12}$$

The solution reads

$$v_{+,+} = \frac{1}{2}(\Phi_{+,p} - \Phi_{-,p})(1 - \cosh(x)) \ , \tag{6.13}$$

$$v_{+,-} = \frac{1}{2}(\Phi_{+,p} - \Phi_{-,p}) e^{i\arg(\eta_{+,-})} \sinh(x) \ . \tag{6.14}$$

$$\frac{dx}{dl} = \frac{\delta}{\pi} |\eta_{+,-}| = \frac{\delta^2}{\pi^2} A |v_{+,-}| \ . \tag{6.15}$$

From this one obtains

$$\begin{aligned} x &= \frac{\gamma}{2} \int_0^l dl \frac{A(0) v_{+,-}(0)}{A(0)^2 \exp(\gamma l/2) - v_{+,-}(0) v_{-,+}(0) \exp(-\gamma l/2)} \\ &= \frac{1}{2} \ln \frac{(A(0)\xi - |v_{+,-}(0)|)(A(0) + |v_{+,-}(0)|)}{(A(0)\xi + |v_{+,-}(0)|)(A(0) - |v_{+,-}(0)|)} \ , \end{aligned} \tag{6.16}$$

$$\xi = \exp\left(\frac{\gamma l}{2}\right) . \tag{6.17}$$

Thus one obtains

$$\frac{\partial v_p}{\partial \xi} = -\frac{\pi}{n\Omega}\sum_{\delta>0}\frac{1}{\delta}(\Phi_{\delta,+,p}-\Phi_{\delta,-,p})\frac{A(0)^2 v_{+,-}(0)v_{-,+}(0)(\xi-1)}{\sqrt{B}(A(0)^2\xi^2 - v_{+,-}(0)v_{-,+}(0))^{3/2}} \tag{6.18}$$

and finally

$$\langle N_{p,p}\rangle = v_p(\infty) = n_p - \frac{\pi}{n\Omega}\sum_{\delta>0}\frac{1}{\delta}(\Phi_{\delta,+,p}-\Phi_{\delta,-,p})\left(\frac{A_\delta(0)}{\sqrt{B_\delta}}-1\right) . \tag{6.19}$$

From this one obtains for $p$ close to $\pm k_F$ a logarithmic correction

$$\langle N_{p,p}\rangle = n_p + \frac{1}{2n}\left(\frac{A_0(0)}{\sqrt{B_0}}-1\right)\operatorname{sign}(k_F-|p|)\ln||k_F-|p|| . \tag{6.20}$$

This can be interpreted as a power-law contribution to $\langle N_{p,p}\rangle$ of type $a\operatorname{sign}(k_F-|p|)||p|-k_F|^b$ with

$$ab = \frac{1}{2n}\left(\frac{A_0(0)}{\sqrt{B_0}}-1\right) . \tag{6.21}$$

Unfortunately only the product $ab$ can be extracted from this expression. One can however calculate the power-law behaviour for the $n$-flavor Luttinger model. If one choses the same couplings $v_{\pm,\pm}$ and the same Fermi velocity then agreement is found with Eq. (6.21) and $a = 1/2$ in leading order in $n$. Since in the limit of large $n$ it is expected that $\langle N_{p,p}\rangle$ approaches $n_p$ we conclude

$$\langle N_{p,p}\rangle = \frac{1}{2}(1+\operatorname{sign}(k_F-|p|)||p|-k_F|^b) . \tag{6.22}$$

Thus there is no discontinuity of $\langle N_{p,p}\rangle$ at the Fermi energy, which is characteristic for a Luttinger liquid.

## 7 Manybody-interactions

In this section the equations for the $m$-particle interactions with $m>2$ in leading order in $n$ are considered. They are governed by the equations

$$\eta_m = \sum_{k=1}^{m-1}[H_k, H_{m+1-k,r}]_1 + \sum_{k=2}^{m}[H_k, H_{m+2-k,r}]_2 , \tag{7.1}$$

$$H_{m,r} = H_m - H_{m,d} , \tag{7.2}$$

$$\frac{dH_m}{dl} = \sum_{k=2}^{m} [\eta_k, H_{m+1-k}]_1 + \sum_{k=2}^{m} [\eta_k, H_{m+2-k}]_2 \ . \tag{7.3}$$

We extract now out of $dH_m/dl$ and $\eta_m$ the terms which depend on $H_m$. With the parametrization

$$H_m = \frac{n}{m!\,\Omega^{m-1}} \sum_{\delta_1, Q_1, \ldots \delta_m, Q_m} v_m(\delta_1, Q_1, \ldots \delta_m, Q_m)$$

$$:N_{Q_1+\delta_1/2, Q_1-\delta_1/2} \ldots N_{Q_m+\delta_m/2, Q_m-\delta_m/2}: \ , \tag{7.4}$$

where the summation over $\delta$ runs only over those with $\sum_i \delta_i = 0$ and similarly for $\eta$ one has

$$\eta_m = (\delta k) v_{m,r} + \frac{1}{2\pi} \sum_{i,s} s\delta_i v_2(\delta_i, k_i, sk_F) v_{m,r}(sk_F \to k_i)$$

$$-\frac{1}{2\pi} \sum_{i,s} s\delta_i v_{2,r}(\delta_i, k_i, sk_F) v_m(sk_F \to k_i) + \ldots \ , \tag{7.5}$$

$$\frac{\partial v_m}{\partial l} = -(\delta k)\eta_m + \frac{1}{2\pi} \sum_{i,s} s\delta_i \eta_2(\delta_i, k_i, sk_F) v_m(sk_F \to k_i)$$

$$-\frac{1}{2\pi} \sum_{i,s} s\delta_i v_2(\delta_i, k_i, sk_F) \eta_m(sk_F \to k_i) + \ldots \ , \tag{7.6}$$

$$(\delta k) = \sum_{i=1}^{m} \delta_i k_i \ . \tag{7.7}$$

For $v_2$ and $\eta_2$ the second $\delta$ is left out. In $\eta_m$ and $v_m$ only those arguments are given which are different from those on the left hand side of the equation. In those terms containing the argument $(sk_F \to k_i)$ an average has been performed in the interval between $sk_F \to \delta_i/2$ and $sk_F + \delta_i/2$. If one restricts to those matrix elements which contain the same argument on the right hand side as on the left hand side (if $k_i$ differs less than $|\delta_i|/2$ from $sk_F$ then they are considered to be equal to $sk_F$), then one obtains

$$\frac{\partial v_m}{\partial l} = -\left((\delta k) + \sum_i \delta_i s_i v_2(\delta_i, k_i, k_i)\right)^2 v_m + \ldots \ , \tag{7.8}$$

if $v_m$ belongs to the part of $H_m$ which violates quasiparticle conservation and

$$\frac{\partial v_m}{\partial l} = -\sum_i \delta_i^2 s_i^2 v_2(\delta_i, k_F, -k_F) v_2(\delta_i, -k_F, k_F) v_m + \ldots \ , \tag{7.9}$$

if the quasiparticle number is conserved. Note that the coefficients connecting different $v_m$s contain factors which vanish for large $l$. So the equations decouple (with the ex-

ception of momenta at $K_{c,\pm}$). Since the coefficients in front of $v_m$ is the negative of a square for the case of the quasiparticle-violating contribution, it will in general decay. There are however exceptions. If all $k_i = sk_F$ with the same $s$, then due to the momentum conservation $\sum_i \delta_i = 0$ the coefficient vanishes. For $m = 3$ this corresponds to a process where two particle-hole pairs are created and one annihilated or vice versa. As long as the cost of energy is proportional to the momentum transfer this process does not cost energy and leads to degeneracies. It is this degeneracy which prevents the decay of $v_m$ in such a case. If the number of quasiparticles is conserved, then the coefficients in front of $v_m$ vanish for large $l$. Therefore they will not vanish for large $l$ as expected.

Closer inspection shows that those terms in the flow-equation for $H_m$ which do not depend on $H_m$ cannot be considered practically constant for $k_i$ in the intervals $sk_F - \delta_i/2 \ldots sk_F + \delta_i/2$. This applies for example for the contribution of $[\eta_2, H_2]_1$ in $dH_3/dl$. There are not only discontinuities at $k_3 = sk_F \pm \delta_1/2 \pm \delta_2/2 = sk_F \mp \delta_3/2$, but also at $k_3 = sk_F \pm \delta_1/2 \mp \delta_2/2$. The expressions above hold for the averages in the whole intervals. Apart from this one may consider the difference between $v_m$ for a certain value of $k_i$ in this interval and the average over this interval. This can be done independently for a set of indices $i$. Then the same equations hold, but the summation over the $i$s belonging to this set has to be omitted. Then in the case mentioned above where all $k_i = sk_F$ the coefficient in front of $v_m$ can be nonzero, so that the difference vanishes for large $l$.

## 8 Conclusion

In this paper a flow-equation for Hamiltonians has been introduced which should bring the Hamiltonian continuously closer to a diagonal form. For an $n$-orbital model it turns out that in the limit of large $n$ the equations for the two-particle interaction are closed in leading order in $n$. A first attempt (Section 4) to apply this equation to a one-dimensional $n$-orbital model turned out to be unsatisfactory since divergencies appeared, which could not be traced back to physical reasons. This has to be further investigated. In a second attempt (Sections 5 to 7) it has been required only to bring the Hamiltonian into a form which conserves the number of quasiparticles. If this is accomplished, then the problem for one, two, three quasiparticles is reduced to the diagonalization of a one-, two-, three-particle problem, instead of the original $N$-particle problem. These flow-equations worked satisfactorily. However, as already expected from a toy-example in Section 2 off-diagonal elements between degenerate states do not decay and for almost degenerate states the convergency is slow. This has to be investigated further. In order to understand different types of physical systems in this framework it is probably necessary to classify various types of these degeneracies and to investigate the corresponding physical behavior.

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Note added in proof. For the Coulomb interaction $v_\delta = ce^2 n/\delta^2$ (the constant $c$ is the full solid angle in the corresponding number of dimensions) one obtains in one dimension $v_{\delta,\pm,\pm}(l = \infty) = 2\pi\omega_{pl}/\delta$ with the plasma frequency $\omega_{pl} = (ce^2 n k_F/\pi)^{1/2} = (ce^2 n_{el})^{1/2}$. Multiplied by the prefactor $1/\Omega$ in the Hamiltonian and by the number $\delta\Omega/2\pi$ of particle-hole pairs which contribute to the plasmon it yields correctly the plasmon-frequency as collective excitation energy.