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# Flow equations and normal ordering: a survey 

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#### Abstract

First we give an introduction to the method of diagonalizing or blockdiagonalizing continuously a Hamiltonian and explain how this procedure can be used to analyse the two-dimensional Hubbard model. Then we give a short survey on applications of this flow equation on other models. Finally we outline, how symmetry breaking can be introduced by means of a symmetry breaking of the normal ordering, not of the Hamiltonian.


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## 1. Introduction

Renormalization group plays an important role both in high-energy physics and in condensed matter physics. It was invented in high-energy physics [1, 2] in order to resolve the problems with divergencies at large momenta. It was developed as a tool to define how an interaction with cut-off at some momentum $\Lambda$ has to vary as $\Lambda$ increases up to the limit infinity so that the expectation values converge to a finite limit.

For a long time, the explanation of critical behaviour was an open question in condensed matter physics. Wilson [4] showed along ideas developed by Kadanoff [3] that also this problem is solved by the renormalization group. In condensed matter, most often one does not worry about large momenta, in particular, if one considers a system on a lattice where momenta are restricted to the Brillouin zone. Then the problem of critical phenomena resides in small momenta and one has to integrate out the contributions of the interaction at momenta down to some small cut-off $\Lambda$ and finally to consider the limit where this cut-off approaches zero. This applies for bosonic degrees of freedom which have the advantage that their quantum nature is normally irrelevant so that they can be considered as classical fields.

The situation is different for fermionic degrees of freedom. They do not show a classical limit. Therefore, other methods had to be developed. The essential physics in a condensed fermionic system comes from the behaviour at the Fermi edge. Therefore, it is natural to focus on the behaviour close to the Fermi edge and to eliminate the degrees of freedom away from this Fermi edge so that the cut-off describes now the distance from the Fermi edge. This procedure was pushed forward by Shankar [5, 6]. It has been applied to fermionic systems
among others by Zanchi and Schulz [7], Salmhofer and Honerkamp [9], Halboth and Metzner [8].

There is a second approach which was started in 1993/1994. It appeared under the name of Flow equations for Hamiltonians [12] and Similarity transformation [10, 11] and is also often called Continuous unitary transformation (CUT). Głazek and Wilson and myself were at that time unaware that mathematicians in the field of control theory had developed similar ideas under the names Double Bracket Flow [14] and Isospectral Flow [13, 15]. The basic idea is to choose the Hamiltonian in a certain basis, e.g. the basis of Bloch waves and then to eliminate first the off-diagonal matrix elements between states which differ strongly in energy. This is done by a continuous unitary transformation as function of a flow-parameter $\ell$. We start from the initial Hamiltonian $H=H(0)$ and obtain a Hamiltonian $H(\ell)$ by means of a unitary transformation $U(\ell)$,

$$
\begin{equation*}
H(\ell)=U(\ell) H U^{\dagger}(\ell) \tag{1}
\end{equation*}
$$

Differentiation with respect to $\ell$ yields

$$
\begin{equation*}
\frac{\mathrm{d} H(\ell)}{\mathrm{d} \ell}=[\eta(\ell), H(\ell)] \tag{2}
\end{equation*}
$$

with the generator $\eta$ of the unitary transformation

$$
\begin{equation*}
\eta(\ell)=\frac{\mathrm{d} U(\ell)}{\mathrm{d} \ell} U^{\dagger}(\ell)=-\eta^{\dagger}(\ell) \tag{3}
\end{equation*}
$$

This is the flow equation for the Hamiltonian. The main intention of the use of these flow equations by now is not the investigation of critical phenomena, but the diagonalization or block-diagonalization of the Hamiltonians whether they describe elementary particles or strongly correlated solids. The scheme has in common with renormalization in critical phenomena that it focuses on a smaller and smaller region. It means in this case that offdiagonal matrix elements which connect two states with energy difference $\Delta \epsilon$ become small and finally negligible when the flow-parameter $\ell$ becomes large in comparison to $1 /(\Delta \epsilon)^{2}$.

Obviously $U(\ell)$ or actually $\eta(\ell)$ have to be chosen in an appropriate way. There are various ways of doing so.

## 2. Various choices for the generator

The most obvious way is to choose a generator which nearly always diagonalizes the Hamiltonian. If one chooses

$$
\begin{equation*}
\eta=\left[H^{\mathrm{d}}, H\right] \tag{4}
\end{equation*}
$$

where $H^{\mathrm{d}}$ is the diagonal part of the Hamiltonian, then we find that the sum of the squares of the off-diagonal matrix elements decays like

$$
\begin{equation*}
\sum_{k, k^{\prime} \mid k \neq k^{\prime}} \frac{\partial h_{k, k^{\prime}} h_{k^{\prime}, k}}{\partial \ell}=-2 \sum_{k, k^{\prime}}\left(\epsilon_{k}-\epsilon_{k^{\prime}}\right)^{2} h_{k, k^{\prime}} h_{k^{\prime}, k}, \tag{5}
\end{equation*}
$$

where the diagonal matrix elements are denoted by $\epsilon .{ }^{1}$ Thus the off-diagonal matrix elements decay unless (which happens only rarely) the elimination stops with a non-zero off-diagonal element between two degenerate levels ${ }^{2}$. Note, however, that in general also $\epsilon$ depends on $\ell .^{3}$

1 The flow equation now reads $\mathrm{d} H / \mathrm{d} \ell=\left[\left[H^{\mathrm{d}}, H\right], H\right]$ which explains the notion double-bracket equation.
${ }^{2}$ These argument as well as the arguments on the cost function below apply rigorously for finite matrices. For the infinite-dimensional Hilbert space they are guidelines.
${ }^{3}$ In the case of the elimination of the electron-phonon coupling these couplings decay even if the states are finally degenerate [16]. Depending on the elimination scheme such off-diagonal matrix elements can survive in the Kondo Hamiltonian below the Kondo temperature [17].

Although it seems quite desirable to diagonalize the Hamiltonian completely, there is the drawback that nearly always approximations have to be introduced. In order that they do not create too large errors, it is advisable to perform only weak unitary transformations. This can be done by bringing the Hamiltonian to a block-diagonal form. In the case of the elimination of the electron-phonon coupling, we eliminate only the matrix elements which change the number of the phonons, which is the electron-phonon coupling. In this case we are left with an effective electron-electron interaction which has the nice properties (i) that it is attractive between all pairs of electrons with total momentum zero in contrast to Fröhlich's Hamiltonian and (ii) it is instantaneous. This second property is inherent to the scheme of flow equations.

Another case where we bring the Hamiltonian in the block-diagonal form is the elimination of the contributions in an electronic system which does not conserve the number of quasiparticles (electrons above and holes below the Fermi edge). Then the eigenstates are states with fixed numbers of these quasi-particles, so that the excitation energies can be read off the one-particle contribution of the effective Hamiltonian and the two-particle excitations are now excitations determined from a two-particle problem [12].

With $H$ consisting of the diagonal and the off-diagonal part $H=H^{\mathrm{d}}+H^{\mathrm{r}}$, the generator $\eta$ may be rewritten as

$$
\begin{equation*}
\eta=\left[H, H^{\mathrm{r}}\right] . \tag{6}
\end{equation*}
$$

We are free, however, to modify $H^{\mathrm{r}}$. If we choose

$$
\begin{equation*}
H^{\mathrm{r}}=[N,[N, H]], \tag{7}
\end{equation*}
$$

where $N$ is the particle operator of the phonons or of the quasi-particles, then the particle number violating terms will be eliminated. To see this we may introduce a cost function

$$
\begin{equation*}
G(H)=\frac{1}{2} \sum g_{i j, k l} H_{j i} H_{l k}=\frac{1}{2} \operatorname{tr}\left(H H^{\mathrm{r}}\right), \quad H_{i j}^{\mathrm{r}}=\sum g_{i j, k l} H_{l k} \tag{8}
\end{equation*}
$$

where we require that $g$ is symmetric and the cost function is real,

$$
\begin{equation*}
g_{i j, k l}=g_{k l, j i}=g_{j i, l k}^{*} . \tag{9}
\end{equation*}
$$

Then one obtains

$$
\begin{equation*}
\frac{\mathrm{d} G}{\mathrm{~d} \ell}=\operatorname{tr}\left([\eta, H] H^{\mathrm{r}}\right)=\operatorname{tr}\left(\eta\left[H, H^{\mathrm{r}}\right]\right) \tag{10}
\end{equation*}
$$

If $G$ is semi-positive definite then the choice

$$
\begin{equation*}
\eta=\left[H, H^{\mathrm{r}}\right] \tag{11}
\end{equation*}
$$

yields

$$
\begin{equation*}
\frac{\mathrm{d} G}{\mathrm{~d} \ell}=\operatorname{tr}\left(\left[H, H^{\mathrm{r}}\right]\left[H, H^{\mathrm{r}}\right]\right) \leqslant 0 \tag{12}
\end{equation*}
$$

Note that $\eta$ is anti-Hermitian. The derivative $\frac{\mathrm{d} G}{\mathrm{~d} \ell}$ vanishes only, if $H^{\mathrm{r}}$ commutes with $H$. In all other cases the cost function decreases. The choice $H^{\mathrm{r}}=[N,[N, H]]$ yields the cost function

$$
\begin{equation*}
G=\frac{1}{2} \operatorname{tr}([H, N][N, H]) \tag{13}
\end{equation*}
$$

which becomes zero only if $H$ commutes with $N$.
This allows another procedure useful for systems with symmetry breaking. We may choose quite generally

$$
\begin{equation*}
H^{\mathrm{r}}=\sum_{\alpha}\left[v^{\alpha},\left[v^{\alpha}, H\right]\right] . \tag{14}
\end{equation*}
$$

If $v$ is a one-particle operator

$$
\begin{equation*}
v=\sum_{k} v_{k} c_{k}^{\dagger} c_{k}, \tag{15}
\end{equation*}
$$

then the evaluation of $[v,[v, H]]$ multiplies terms of type $c_{k_{1}}^{\dagger} c_{k_{2}}^{\dagger} \ldots c_{q_{1}} c_{q_{2}} \ldots$ in $H$ by

$$
\begin{equation*}
r_{k_{1} k_{2} \ldots q_{1} q_{2} \ldots}=\left(v_{k_{1}}+v_{k_{2}}+\cdots-v_{q_{1}}-v_{q_{2}}-\cdots\right)^{2} . \tag{16}
\end{equation*}
$$

This elimination function indicates how urgently we wish to eliminate such terms in the Hamiltonian. We have used this form of $H^{\mathrm{r}}$ in order to calculate the effective potential of the Hubbard model described by the Hamiltonian

$$
\begin{equation*}
H=-t \sum_{\text {n.n. }} c_{r^{\prime} s}^{\dagger} c_{r s}-t^{\prime} \sum_{\text {n.n.n. }} c_{r^{\prime} s}^{\dagger} c_{r s}+U \sum_{r}\left(n_{r \uparrow}-\frac{1}{2}\right)\left(n_{r \downarrow}-\frac{1}{2}\right), \tag{17}
\end{equation*}
$$

in second order in the coupling $U$ (weak coupling limit). We used the condition

$$
\begin{equation*}
-v_{-k}=v_{k}=v_{k+q_{0}} \tag{18}
\end{equation*}
$$

which transformed the Hamiltonian into a molecular-field form for the expected order parameters (superconductivity, antiferromagnetism, flux-phases, Pomeranchuk instability) that is we allowed for non-zero

$$
\begin{equation*}
\left\langle c_{k s}^{\dagger} c_{-k s^{\prime}}^{\dagger}\right\rangle, \quad\left\langle c_{k s}^{\dagger} c_{k+q_{0} s^{\prime}}\right\rangle, \quad\left\langle c_{k s}^{\dagger} c_{k s^{\prime}}\right\rangle \quad \text { and even } \quad\left\langle c_{k s}^{\dagger} c_{-k+q_{0} s^{\prime}}^{\dagger}\right\rangle . \tag{19}
\end{equation*}
$$

Depending on the couplings the above-mentioned instabilities showed up. The temperature dependence enters via normal ordering. Since the renormalization flow does not only alter twoparticle interactions but also generates higher-particle interactions, the two-particle interaction depends on the normal ordering. Moreover, the expansion of the entropy in terms of the expectation values (19) yields a temperature dependence. For more details see [18-21].

## 3. Other applications

Meanwhile the method of flow equations has been applied to many systems. Apart from those already mentioned we list the following applications: the Anderson impurity model [25, 27, 95], Fano-Anderson and Anderson lattice [83], spin-boson models and dissipation [26, $28,31,40,44,66,76-78,92$ ], qubit and the spin-boson model [97], the electron-phonon interaction and superconductivity [32, 34, 49, 52, 88, 116], superconductivity and impurities [39], the boson fermion model [50, 71, 93, 103], the Tomonaga-Luttinger model [79, 94], one-dimensional fermions [85], the Kondo model [36, 70, 84, 87, 106, 109, 113, 119, 121], Fermi and Luttinger liquid [35, 73], the sine-Gordon model [56, 69], QED [29, 30, 43], QCD and general [24, 51, 62, 68, 75, 99, 104], two-dimensional $\delta$-potential [37, 38, 55, 67, 89], limit cycles and three-body problem [82, 96], mapping of the Hubbard Model [33, 107], Heisenberg anti-ferromagnet [45, 59], spin-Peierls transition [48], spin models [58, 72, 74, 86, 90, 91, 100, 102, 105, 110, 117], RKKY interaction [54], heavy fermions [111], interacting Bosons [118, 120], the Lipkin model [44, 46, 60, 98, 101, 115], the Lipkin-Meshkov-Glick model [112, 114], Dirac particle [47], molecules [81], the Henon-Heiles Hamiltonian [53], quartic oscillator [108], complex eigenvalues [80]. It may be mentioned that the two-beam coupling in photorefractive media itself obeys the flow equation scheme [57].

The author gave short reviews on the flow equation method at several occasions [41, 42, 61, 63, 64] mainly explaining the elimination of the electron-phonon interaction and the application to an $n$-orbital model in the limit of large $n$, based mainly on [12, 16]. Stefan Kehrein prepares a book on the flow equation approach to many-body problems [122].

## 4. Symmetry breaking

In applying flow equations to a Hamiltonian one typically starts out from a Hamiltonian which does not show an explicit symmetry breaking even if the symmetry will be broken below some temperature.

The same applies for the renormalization group flows. As indicated above, in the case of flow equations one can bring the effective interaction to the molecular-field form and finally apply molecular field theory. Since we transform the interaction no divergencies appear. In the case of the fermionic renormalization group, the vertex functions will at least within weakcoupling approximations diverge at some length scale, so that the approximations become unreliable and one has to resort to other methods in this regime. Thus, it is desirable to have a way to introduce symmetry breaking from the beginning. Recently Salmhofer, Honerkamp, Metzner and Lauscher [22] have added a symmetry breaking field to the Hamiltonian and showed that this leads into the symmetry broken phase.

For the Hamiltonian flow, it is not necessary to add a symmetry breaking term to the Hamiltonian. Instead, it is sufficient to choose a normal-ordering which is symmetry broken. One can show [23] that the system will nearly always converge to the stable state, that is, in the case of symmetry breaking (that is below the critical temperature) it runs to a symmetry broken state, whereas if the symmetric state is stable (above $T_{\mathrm{c}}$ ) then it will run to the symmetric state. The basic idea is the following: normal ordering is given by the bilinear expectation values

$$
\begin{equation*}
G_{k j}=\left\langle a_{k} a_{j}\right\rangle \tag{20}
\end{equation*}
$$

where the $a_{k}$ stand for creation and annihilation operators $c_{k}^{\dagger}$ and $c_{k}$, respectively. In general, one will have normal and anomal expectation values. For given expectation values $G$ one obtains from an operator $A$ the normal-ordered one

$$
\begin{equation*}
: A_{G}:_{G}=A \tag{21}
\end{equation*}
$$

by

$$
\begin{equation*}
A_{G}=\exp \left(\sum_{k j} G_{k j} \frac{\partial^{2}}{\partial a_{j}^{\text {right }} \partial a_{k}^{\text {left }}}\right) A(a) \tag{22}
\end{equation*}
$$

In this expression the operators $a$ anticommute for fermions. Summation runs over all pairs $a$, where $a_{j}$ is to the right of $a_{k}$. An infinitesimal change in $G$ leads to a change of $A_{G}$

$$
\begin{equation*}
\delta A_{G}=A_{G+\delta G}-A_{G}=\frac{1}{2} \sum_{k j} \delta G_{k j} \frac{\partial^{2}}{\partial a_{j} \partial a_{k}} A_{G} \tag{23}
\end{equation*}
$$

Thus under the Hamiltonian flow, the Hamiltonian $H_{G}$ will change due to the unitary transformation and due to the change of normal ordering yielding

$$
\begin{equation*}
\frac{\mathrm{d} H_{G}}{\mathrm{~d} \ell}=\left[\eta, H_{G}\right]+\frac{\delta H_{G}}{\delta G} \frac{\partial G}{\partial \ell} \tag{24}
\end{equation*}
$$

As expectation values $G$ entering the normal ordering we may use the expectation values of $\exp \left(-\beta H^{0}\right)$ with the one-particle Hamiltonian

$$
\begin{equation*}
H^{0}=\sum_{k j} \frac{1}{2} \tilde{\epsilon}_{k j} a_{k}^{\dagger} a_{j} \tag{25}
\end{equation*}
$$

Besides the flow equation for the Hamiltonian, a flow equation for $H^{0}$ has to be introduced. This can be done by requiring that $\tilde{\epsilon}$ approaches the one-particle part of $H_{G}$,

$$
\begin{equation*}
H_{G}=v^{(0)}+\frac{1}{2} \sum_{k j} v_{k^{*} j}^{(1)} a_{k} a_{j}+O\left(a^{4}\right) \tag{26}
\end{equation*}
$$

where $a_{k *}=a_{k}^{\dagger}$ by means of the equation

$$
\begin{equation*}
\frac{\partial \tilde{\epsilon}_{k j}}{\partial \ell}=\gamma\left(v_{k^{*} j}^{(1)}-\tilde{\epsilon}_{k j}\right) \tag{27}
\end{equation*}
$$

with some positive constant $\gamma$.
Under the following assumptions, one can show [23] that the flow approaches a stable phase: to show this we determine the free energy with respect to the density operator $\exp \left(-\beta H^{0}\right) / Z^{0}$. If this free energy

$$
\begin{align*}
& F^{0}=\langle H\rangle_{0}-T S, \quad\langle H\rangle_{0}=v^{(0)}, \\
& S=-\frac{k_{\mathrm{B}}}{2} \operatorname{tr}(\tilde{G} \ln \tilde{G}+(1-\tilde{G}) \ln (1-\tilde{G})), \quad \quad \tilde{G}_{k j}=G_{k^{*} j} \tag{28}
\end{align*}
$$

is a local minimum against variation of $H^{0}$, then the fixed point of $H(\infty)$ is stable; if it is not a local minimum then it is unstable. Without performing the flow, that is for $\eta \equiv 0$, this procedure approaches nearly always the Hartree-Fock-Bogoliubov solution.

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