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Nuclear Physics B (Proc. Suppl.) 90 (2000) 141–146

NUCLEAR PHYSICS B
PROCEEDINGS
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# Flow equations for Hamiltonians

Franz J. Wegner* [a]

[a]Institut für Theoretische Physik der Universität Heidelberg, D-69120 Heidelberg, Germany

A method to diagonalize or block-diagonalize Hamiltonians by means of an appropriate continuous unitary transformation is reviewed.

## 1. Introduction

In the following I will describe a method for diagonalizing or block-diagonalizing Hamiltonians [1]. As an application the elimination of the electron-phonon interaction will be considered which yields the effective electronic pair interaction responsible for (low-temperature) superconductivity. Finally I will mention a number of other problems attacked by this method.

Diagonalization of a Hamiltonian is normally too difficult to be performed in one step. Instead we will consider here a procedure, which gradually decreases the off-diagonal matrix elements as a function of a parameter $l$ which I call flow-parameter. Thus we start from the initial Hamiltonian $H(0) = H$ and obtain a Hamiltonian $H(l)$ by means of a unitary transformation $U(l)$ which will become more and more (block-) diagonal as $l$ increases

$$H(l) = U(l)HU^\dagger(l). \tag{1}$$

Differentiation yields

$$\frac{dH(l)}{dl} = [\eta(l), H(l)], \tag{2}$$

with the generator

$$\eta(l) = \frac{dU(l)}{dl}U^\dagger(l) = -\eta^\dagger(l). \tag{3}$$

We call this equation the flow equation for the Hamiltonian. Obviously $U(l)$ or actually $\eta(l)$ has to be chosen in an appropriate way. In the following I will first suggest a choice for the generator $\eta$ of the unitary transformation which serves as a guideline.

The price we have to pay for the use of the flow equations is that it will generate complicated interactions in general. Starting from a problem with two-particle interactions the transformation will generate three-particle, four-particle, etc. interactions. In the original paper [1] an $n$-orbital model was considered in the limit $n \to \infty$. Although in this limit these many-particle interactions are generated, it turns out that the one-particle energies are independent of $l$ and the equations for the two-particle interaction are closed in themselves, so that an explicit calculation can be performed to a large extent. Another approach is to truncate the equations. Kehrein and Mielke observed that for systems with impurities (Anderson impurity model [2,3] and spin-boson model [4,5]) it is sufficient to keep only rather simple contributions to the Hamiltonian in order to obtain good results. Finally one can perform a perturbation expansion. This will be done in section 3 for the elimination of the electron-phonon interaction [6]. One might expect that the result agrees with Fröhlich's [7] which can be found in all textbooks of theoretical solid-state physics. His effective interaction has an energy denominator, which can vanish and gives rise to both attraction and repulsion of the electron pairs. With the present procedure we obtain in a simple way an attractive interaction between all pairs which yields very good agreement [8,9] with more sophisticated methods [10–12]. The permanent adjustment of the infinitesimal unitary transformation to the Hamiltonian yields a smoother effective interaction than conventional perturbation theory.

An interesting question is how interactions between nearly degenerate states do disappear and

*E-mail: wegner@tphys.uni-heidelberg.de


PII S0920-5632(00)00888-4

influence the final diagonal interaction. Apparently such matrix elements will decay slowly if at all. Kehrein, Mielke and Neu [4] have found for the spin-boson model that the off-diagonal matrix elements between states which are degenerate in the limit $l \to \infty$ decay (although slowly), so that the off-diagonal matrix elements are completely eliminated. The same applies for the electron-phonon interaction, if we take the change of the phonon energies with $l$ into account. This is obtained in an approximation beyond perturbation theory. Quite generally it is of interest to consider the behaviour of states with degenerate or nearly degenerate states of various interacting systems and to investigate in this way the infra-red physics of these systems. It may be, that eventually one finds different classes of systems with different characteristic infra-red behaviour.

In the following sections we consider the choice of the generator $\eta$ of the unitary transformation (section 2), the elimination of the electron-phonon interaction (section 3). In the final section 4 concluding remarks are given and a few other systems treated with this method are cited.

## 2. Generator $\eta$ of the Unitary Transformation

The generator $\eta$ of the unitary transformation should be chosen in such a way, that the off-diagonal matrix elements decay. For a finite matrix

$$\eta = [H_d, H] \tag{4}$$

is a good choice, where $H_d$ is the diagonal part of the Hamiltonian. If the diagonal matrix elements are denoted by $\epsilon$, then

$$\eta_{k,n} = (\epsilon_k - \epsilon_n) H_{k,n}. \tag{5}$$

A simple calculation yields

$$\frac{dH_{k,n}}{dl} = \sum_m (\epsilon_k + \epsilon_n - 2\epsilon_m) H_{k,m} H_{m,n}, \tag{6}$$

and

$$\frac{d}{dl} \sum_{k,n,k\neq n} H_{k,n} H_{n,k} = -\frac{d}{dl} \sum_k \epsilon_k^2$$
$$= -2 \sum_{k,n} (\epsilon_k - \epsilon_n)^2 H_{k,n} H_{n,k}. \tag{7}$$

Thus the sum of the squares of the off-diagonal matrix elements is indeed negative or zero. The procedure comes to an end, when all off-diagonal matrix elements vanish. It may be, however, that off-diagonal matrix elements survive, if the corresponding energies $\epsilon ilon$ are degenerate. Since the diagonal matrix elements themselves vary as a function of $l$, it may happen that even the off-diagonal matrix elements between asymptotically degenerate states vanish. An example will be given in section 3.3.

Although this choice of $\eta$ can serve as a guideline it is often useful or even necessary to modify $\eta$ in order to obtain reasonable results. It turns out that one should keep more than the diagonal part of two-particle interactions in electronic systems. Indeed, if one considers those contributions which conserve the number of quasi-particles (electrons above the Fermi-edge plus holes below the Fermi-edge) as diagonal, then the scheme works well, which amounts to block-diagonalization. This was found explicitly in an $n$-orbital model of interacting electrons [1]. Another example is the diagonalization of the spin-boson model [4] where a modification of the choice for $\eta$ yields equations which can be easier solved.

Independently Wilson and Głazek [13,14] introduced a scheme, where they introduce an energy parameter which decreases and they require the off-diagonal matrix elements to disappear exactly as soon as this parameter is smaller than the energy difference. The procedure I introduced yields, however, a smooth cut-off, that is a smooth disappearance of the diagonal matrix elements. They apply their scheme called similarity renormalization mainly in light-front physics [15,16].

## 3. Elimination of the electron-phonon Coupling

### 3.1. The effective electron-electron interaction

A simple example which however from the view of conventional perturbation theory yields a surprising result is the elimination of the electron-phonon coupling. This section is based on the diploma thesis of Peter Lenz and on Ref. [6]. Our

aim is to calculate the effective electron-electron interaction responsible for the superconductivity. The Hamiltonian of an electronic system coupled to phonons consists of three contributions

$$H = H_0 + H_{\mathrm{e-ph}} + H_{\mathrm{e-e}}. \tag{8}$$

Here $H_0$ is the free part

$$H_0 = \sum_q \omega_q a_q^\dagger a_q + \sum_k \epsilon_k : c_k^\dagger c_k :, \tag{9}$$

where $\omega_q$ and $\epsilon_k$ are the phonon and electron energies, resp. The electron-phonon interaction is given by

$$H_{\mathrm{e-ph}} = \sum_{k,q} M_{k,q} a_{-q}^\dagger c_{k+q}^\dagger c_k + \mathrm{h.c.}, \tag{10}$$

and the electron-electron interaction by

$$H_{\mathrm{e-e}} = \sum_{k,k',q} V_{k,k',q} : c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k : . \tag{11}$$

Here $k$ and $k'$ include the $z$-component of the spin $s$ and $s'$, resp. In all contributions of the Hamiltonian we have used normal ordering. All terms which after normal ordering are not of these types will be neglected. Here we proceed similarly as before, since we consider those terms to be diagonal which conserve the number of particles. This applies to $H_0$ and $H_{\mathrm{e-e}}$, whereas $H_{\mathrm{e-ph}}$ does not conserve the number of phonons and thus is considered to be off-diagonal. Furthermore we will assume the electron-electron interaction to be small and only the second order contribution from $H_{\mathrm{e-ph}}$ to $H_{\mathrm{e-e}}$ will be calculated. Thus we choose

$$\begin{aligned}\eta &= [H_0, H_{\mathrm{e-ph}}] \\ &= \sum_{k,q} M_{k,q}\alpha_{k,q} a_{-q}^\dagger c_{k+q}^\dagger c_k - \mathrm{h.c.},\end{aligned} \tag{12}$$

with the energy difference

$$\alpha_{k,q} = \epsilon_{k+q} - \epsilon_k + \omega_q. \tag{13}$$

This generator yields several contributions to $dH/dl = [\eta, H]$. The contribution to the change of $M$ results from $[\eta, H_0]$

$$\frac{\partial M_{k,q}(l)}{\partial l} = -\alpha_{k,q}^2 M_{k,q}(l), \tag{14}$$

with the solution

$$M_{k,q}(l) = M_q \exp(-\alpha_{k,q}^2 l), \tag{15}$$

where $M_q$ is the initial electron-phonon coupling. The contribution to the electron-phonon coupling is obtained from $[\eta, H_{\mathrm{e-ph}}]$. The terms which describe the interaction between the electron pairs (with zero momentum) obey

$$\begin{aligned}&\frac{\partial V_{k,-k,q}(l)}{\partial l} \\ &\quad = -(\alpha_{k,q} + \alpha_{-k-q,-q}) M_{k,q}(l) M_{-k-q,q}(l),\end{aligned} \tag{16}$$

with the solution

$$\begin{aligned}V_{k,-k,q}(\infty) &= V_{k,-k,q}(0) \\ &\quad - M_q^2 \frac{\omega_q}{\omega_q^2 + (\epsilon_{k+q} - \epsilon_k)^2}.\end{aligned} \tag{17}$$

Several remarks are in order, since Fröhlich's result differs from this one by a minus sign between the two squares in the denominator:

(i) The interaction from the electron-phonon coupling is attractive for all values of $k$ and $q$.

(ii) Mielke has also obtained an effective attractive interaction [8] without pole by means of Głazek and Wilson's similarity transformation [14]. The critical temperature determined from this interaction yields values very similar [8] to those determined with the method by MacMillan and Dynes [11,12] based on the Eliashberg theory [10] and close to the experimental values [9]. In contrast to the Eliashberg theory which works with a retarded effective interaction our interaction is instantaneous.

(iii) Similar sums of two squares in the denominator appear in the matrix elements $v_{K,Q}$ of the $n$-orbital model [1] and in a revised treatment of the Schrieffer-Wolf transformation [20] with the present scheme [3].

(iv) For on-shell matrix elements $V$, that is for those which obey $\epsilon_{k+q}+\epsilon_{k'-q} = \epsilon_k+\epsilon_{k'}$, Fröhlich's result and ours coincide.

(v) We observe that the permanent adjustment of $\eta(l)$ to the current $H(l)$ yields smoother interactions than conventional perturbation theory.

(vi) Perturbation theory for Hamiltonians is not uniquely defined. The reason is that within the

blocks with fixed particle numbers there can be arbitrary unitary transformations.

### 3.2. Comparison with Fröhlich's treatment

Let us now compare Fröhlich's and our treatment. Fröhlich introduces a transformation

$$H^{\rm Fr} = e^{-S} H e^{S} = H + [H,S] + \frac{1}{2}[[H,S],S] + \dots$$
$$= H_0 + H_{\rm e-ph} + [H_0,S] + [H_{\rm e-ph},S]$$
$$+ \frac{1}{2}[[H_0,S],S] + \dots \qquad (18)$$

He assumes $S$ to be of the order of the electron-phonon coupling and requires the contribution in first order, that is $H_{\rm e-ph}+[H_0,S]$, to vanish. This yields

$$S^{\rm Fr} = -\sum_{k,q} M_q \left( \frac{a^\dagger_{-q}}{\alpha_{k,q}} - \frac{a_q}{\alpha_{k+q,q}} \right) c^\dagger_{k+q} c_k. \qquad (19)$$

Our treatment yields

$$\exp(-S^{\rm LW}) = T_l \exp\left[ \int dl\, \eta(l) \right], \qquad (20)$$

where $T_l$ is an ordering of $l$, since $\eta$'s with different argument do not commute. An expansion in powers of $\eta$ yields

$$S^{\rm LW} = -\int_0^\infty dl\, \eta(l) - \frac{1}{2}\int_0^\infty dl \int_0^l dl' [\eta(l),\eta(l')]$$
$$+ \dots \qquad (21)$$

The first term agrees with Fröhlich's $S^{\rm Fr}$. The second term yields the difference due to the permanent adjustment of $\eta$ to $H$.

### 3.3. Asymptotics of $\omega_q(l)$

By now we have not considered a variation of the one-particle energies with $l$. For the phonon-energies $\omega_q(l)$ one has the flow equation

$$\frac{\partial \omega_q(l)}{\partial l} = 2\sum_k M^2_{k,q}(l)\alpha_{k,q}(l)(n_{k+q} - n_k), \qquad (22)$$

$$M_{k,q}(l) = M_q \exp\left[ -\int_0^l dl' \alpha^2_{k,q}(l') \right]. \qquad (23)$$

This yields a nonlinear integro-differential equation for $\omega_q(l)$. Comparable equations were obtained before by Kehrein, Mielke and Neu [4] for the tunneling frequency. They obtained the asymptotic behaviour $\partial lta(l) = \partial lta(\infty) + 1/(2\sqrt{l})$. Lenz found that the general asymptotic behaviour obeys $\omega(l) = \omega(\infty) + c(l)/\sqrt{l}$ for the electron-phonon system [6], where $c(l)$ is a periodic function in $\ln(l)$ and the average of $c^2$ equals $1/4$. This decay to the asymptotic value is sufficiently slow, so that even the off-diagonal matrix elements $M$, for which $\alpha(\infty) = 0$, vanish.

## 4. Concluding remarks and other applications

For the electron-phonon coupling in superconductivity, it has been shown, how the idea of flow equations for Hamiltonians can be applied in order to obtain an effective block-diagonal interaction between the electrons. A different model of super conductivity investigated by means of flow equations is the (localized) boson- (itinerant) Fermi-system ([17]).

The first not trivial system to which this scheme was applied is the $n$-orbital model [1]. In this model the flow equations for the two-particle interaction close, although three-, four- and higher particle-interactions are generated. Using the unitary transformation one can determine the average occupation number in the $n$-orbital model, which yields a correction in order $1/n$. The result is compatible with that for the Luttinger model [18], which can easily be generalized to $n$ orbitals. In the Luttinger model one finds a power law behavior of the occupation number both above and below the Fermi edge. The occupation number itself is a continuous function of the energy at the Fermi energy. Similar calculations in dimensions $d > 1$ [19] indicate, that there is a jump of the occupation number at least for small interactions in agreement with the idea of a Landau liquid.

As already mentioned, this scheme has also been applied to two impurity models, the Anderson impurity model and the spin-boson model. An interesting subject only briefly mentioned for the operator of occupancy in the $n$-orbital model is the question, what happens to operators under the flow equations. It has been investigated for the spin-boson model [4,5]. The interesting

observation is that the spin operator completely transforms into a linear combination of boson creation and annihilation operators. From this one sees explicitly that quasi-particles may be quite different from bare particles. This transformation allows the calculation of the time-dependent spin-correlation function. The results for intermediate time scales is in good agreement with NIBA, whereas for longer time scales (where NIBA fails to predict the correct asymptotic behaviour) they are in good agreement with the Shiba-relation. Thus this procedure covers ranges otherwise only covered by different approaches. In the case of the electron-phonon coupling [21] the phonon-creation operator transforms into an electron-hole pair which allows the determination of the phonon damping. Kehrein and Mielke have investigated the question of dissipation in the framework of the flow equations [22,23].

Some other applications are: the elimination of the coupling between states with different double-occupancy in the Hubbard model [24] and the diagonalization of the Hamiltonian of the Heisenberg antiferromagnet near the classical limit [25] by Stein. Here a different generator of the unitary transformation is used, which orders the states according to their eigenvalues, a method also used by Mielke for band matrices [26], which he applied to the Lipkin model and the spin-boson model. Other applications to the Lipkin model are by Pirner and Friman [27] and by Stein [28]. Some further applications are to a Dirac particle in an external magnetic field [29], to the Henon-Heiles Hamiltonian [30], to the spin-Peierls transition [31], to dimerized and frustrated $S = 1/2$ chains [32], and to the derivation of the Ruderman-Kittel-Yosida interaction [33].

Another choice of $\eta$ is presently used to investigate the Hubbard model [34]. One may rewrite (4)

$$\eta = [H, H_r], \tag{24}$$

with $H_r = H - H_d$. Instead of using this expression one may introduce an elimination factor $r$, by which the terms of $H$ are multiplied in order to obtain $H_r$. This factor indicates how urgently the corresponding terms should be eliminated. Then in first order such terms vanish like $\exp(-r\alpha^2 l)$, where $\alpha$ is the energy difference, which in the case of the electron-phonon coupling was given in (13). This allows to reduce the Hamiltonian of the Hubbard model in the limit $l \to \infty$ to that, which makes the Hartree-Fock-Bogoliubov-approximation exact. Application in second order perturbation theory yields terms in the BCS-channel which for $d_{x^2-y^2}$-pairing is attractive and strongest, for $d_{xy}$-, $p$- and $s_{xy(x^2-y^2)}$-pairing is less attractive. Second-order perturbation yields hardly an attractive contribution to the repulsive first order term for $s_1$-pairing.

Recently the crossover from weak to strong coupling in the sine-Gordon model has been determined by flow equations [35,36]. A new and interesting ingredient of this calculation is the introduction of vertex-operators which enriches the possibilities of the method and which has also been applied to the anisotropic Kondo-model [37]. With a similar method the spin-boson model can be treated ([38]). Both in the sine-Gordon model and in the spin-boson model a special coupling allows the reduction to an interaction-free model.

An instructive example of renormalization is a two-dimensional particle in a contact potential [39].

The observation, that the flow equations converge or yield only mild divergences in the interaction, when we restrict ourselves to block-diagonalization is important. In particular if the eigenstates are far from being reminiscent to extended states as in the case of the bound states of positronium it is hardly possible to perform the diagonalization completely. The elimination of the off-diagonal interaction works well down to an energy uncertainty of the order of Rydberg [40]. Below this uncertainty one has to use other approaches or one restricts oneself (from the beginning) to the elimination of the coupling to the photon field, that is to the terms which do not conserve the number of photons. In this case one can carry through the scheme to arbitrary small energy differences (at least in second order in the coupling) [41,42]. I will not list all the contributions to light-front physics, but I refer the reader to the review by Perry [43], which summarizes some of the results.

**Acknowledgment**

This work was supported in part by the German Science Foundation DFG.

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