

# Flow equations for band–matrices<sup>\*</sup>

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**Abstract.** Continuous unitary transformations can be used to diagonalize or approximately diagonalize a given Hamiltonian. In the last four years, this method has been applied to a variety of models of condensed matter physics and field theory. With a new generator for the continuous unitary transformation proposed in this paper one can avoid some of the problems of former applications. General properties of the new generator are derived. It turns out that the new generator is especially useful for Hamiltonians with a banded structure. Two examples, the Lipkin model, and the spin–boson model are discussed in detail.

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## 1 Introduction

The diagonalization of a given Hamiltonian is one of the important goals in any quantum mechanical problem. Apart from few explicitly solved models it is only possible approximatively or numerically. Four years ago, Wegner [1] proposed flow equations for Hamiltonians to bring a given Hamiltonian closer to diagonalization. Technically, the approach is based on a continuous sequence of infinitesimal unitary transformations applied to the Hamiltonian. The infinitesimal unitary transformations are chosen so that the off-diagonal matrix elements become smaller. In principle the flow equations proposed by Wegner finally yield a diagonal matrix, except for the situation close to resonances, where few off-diagonal matrix elements may still be large. This will be made more precise later. Unfortunately it turned out that for a realistic Hamiltonian in an infinite-dimensional Hilbert space, the situation may be more difficult. Wegner discussed as an example interacting electrons in one dimension. The first problem in such a system is, that during the flow higher interactions are generated. Wegner solved this problem by passing to an  $n$ -orbital model, where, in the large  $n$ -limit, the flow equations can be closed. The second problem is, that even then it is not possible to diagonalize the Hamiltonian completely. Instead he used a block–diagonalization. With this modified approach he was able to solve the flow equations.

Later Wegner's flow equations have been applied to various models of condensed matter physics. A class of

models where the flow equations yield very accurate results are dissipative quantum systems [2,3]. It was also possible to treat the electron–phonon problem with this method [4,5], for which one can obtain accurate values for the transition temperature [6]. The reason why the approach is so successful is that it provides a consistent renormalization scheme for Hamiltonians. This has first been pointed out by Glazek and Wilson [7], who developed an essentially equivalent method a few months later. Their method has been used to treat problems from quantum chromo dynamics [8,9].

Flow equations are a useful tool to treat systems with various energy scales and to renormalize a given Hamiltonian, but it is difficult to apply them to a finite matrix or to a Hamiltonian with a simple structure. Although it may be possible to choose the transformation in such a way that some of the higher interactions are not generated (this has been done in the treatment of dissipative quantum systems in [2]), one cannot avoid in general that the Hamiltonian loses its initially simple structure. This point has been discussed in detail by Richter [10]. He applied the flow equations to a simple model, the spin–boson model, and used it to test various truncation schemes. The aim of the present work is to propose a different set of flow equations that has the property that a band diagonal matrix or Hamiltonian keeps its band diagonal structure during the flow.

In the following section, I introduce the new generator for the continuous unitary transformation and I show that it can be used to diagonalize a given Hamiltonian. The main property of the new generator is that band diagonal Hamiltonians remain band diagonal. I derive some properties of the new flow equations.

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<sup>\*</sup> Dedicated to J. Zittartz on the occasion of his 60th birthday

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In Sections 3 and 4 I apply the flow equations to two simple models: the Lipkin model and the spin–boson model. The Lipkin model has a finite Hilbert space, the Hamiltonian can be written in the form of two tridiagonal matrices. The spin–boson model can as well be written as two tridiagonal matrices, but the Hilbert space is infinite. The aim of this paper is to show that the new set of flow equations is useful if one wants to deal with simple finite or infinite matrices. Therefore I only derive some results for the spectra of these models, but I do not discuss the physics of these models in detail. In both cases the reader may consult the references for the physical background of the models. For the Lipkin model, all results presented here are well known and have been obtained by various other methods. For the spin–boson model I derive a formula for higher eigenvalues that has been derived so far only within a first order perturbational treatment. The new result is that this formula has a much wider range of validity.

Section 5 contains the conclusions together with a critical discussion of the possible range of applicability of the new flow equations.

## 2 Generalities

In this section I deal with a Hamiltonian that is given by a finite or infinite, real, symmetric matrix

$$H = (h_{nm}), \quad h_{nm} = h_{mn}. \quad (2.1)$$

An extension to complex, hermitian or normal matrices is easily done. In general, flow equations for a Hamiltonian are constructed by a continuous unitary transformation written in a differential form,

$$\frac{dH}{d\ell} = [\eta, H]. \quad (2.2)$$

$\eta$  is the generator of the infinitesimal unitary transformation, it is an anti-hermitian operator that depends on  $H$  and therefore implicitly on the flow parameter  $\ell$ . Wegner [1] proposed to choose  $\eta = [H_d, H]$ , where  $H_d$  is the diagonal part of the Hamiltonian. With this choice of  $\eta$  one can show that  $\eta \rightarrow 0$  for  $\ell \rightarrow \infty$ . The flow equations yield a final matrix with the property that  $h_{nm}(h_{nn} - h_{mm}) = 0$ . This means that either the off-diagonal matrix elements  $h_{nm}$  vanish or that for a finite  $h_{nm}$  the difference of the corresponding diagonal matrix elements  $h_{nn} - h_{mm}$  must vanish. Thus the Hamiltonian is diagonalized except for some possible resonances. As already mentioned in the introduction this choice of  $\eta$  has one disadvantage: if the initial matrix has a simple structure, it loses this structure for finite  $\ell$ . This becomes clear if one takes a band diagonal Hamiltonian, *i.e.*

$$h_{nm}(\ell = 0) = 0 \quad \text{if } |n - m| > M. \quad (2.3)$$

Taking

$$\eta = (\eta_{nm}), \quad (2.4)$$

one obtains flow equations for the matrix elements

$$\frac{dh_{nm}}{d\ell} = \sum_k (\eta_{nk} h_{km} - h_{nk} \eta_{km}) \quad (2.5)$$

which in general do not conserve (2.3). Therefore I propose the new generator

$$\eta_{nm} = -\eta_{mn} = \text{sign}(n - m) h_{nm}, \quad \eta_{nn} = 0. \quad (2.6)$$

With this choice the flow equations for the off-diagonal matrix elements are

$$\begin{aligned} \frac{dh_{nm}}{d\ell} = & -\text{sign}(n - m)(h_{nn} - h_{mm})h_{nm} \\ & + \sum_{k \neq n, m} (\text{sign}(n - k) + \text{sign}(m - k)) h_{nk} h_{km}. \end{aligned} \quad (2.7)$$

Due to the sum of the two sign–functions the second term vanishes if  $|n - m| > M$ . This shows that the new generator preserves the band diagonal structure. For the diagonal matrix elements one obtains

$$\frac{dh_{nn}}{d\ell} = 2 \sum_{k \neq n} \text{sign}(n - k) h_{nk} h_{kn}. \quad (2.8)$$

The main question is now whether the new choice of  $\eta$  can be used to diagonalize the Hamiltonian. This is indeed the case for finite matrices ( $1 \leq n \leq N$ ) or semi–infinite matrices ( $1 \leq n$ ). For the sum of the first  $r$  diagonal matrix elements one obtains the differential equation

$$\frac{d}{d\ell} \sum_{n=1}^r h_{nn} = -2 \sum_{n=1}^r \sum_{k>r} h_{nk} h_{kn} < 0. \quad (2.9)$$

This quantity decays as a function of  $\ell$ . I assume that  $H$  is bounded from below. Then  $\sum_{n=1}^r h_{nn}$  is bounded from below by the sum of lowest  $r$  eigenvalues of  $H$ . Therefore its derivative must vanish in the limit  $\ell \rightarrow \infty$ , *i.e.*

$$\lim_{\ell \rightarrow \infty} h_{nk} h_{kn} = 0. \quad (2.10)$$

Furthermore, if  $h_{nm}$  tends to zero, one must have  $\text{sign}(n - m)(h_{nn} - h_{mm}) < 0$  for sufficiently large values of  $\ell$ . Thus the diagonal matrix elements are ordered for large  $\ell$ .

Some properties of the flow equations with the new choice (2.6) of the generator are:

- The final matrix is diagonal, even if it contains degeneracies.
- The matrix remains banded,  $h_{nm} = 0$  if  $|n - m| > M$ .
- $h_{nn}(\infty) \geq h_{mm}(\infty)$  for  $n > m$  and for irreducible matrices. If the matrix is reducible, each of the irreducible blocks can be treated separately.
- The asymptotic behaviour of  $h_{nm}$  for large  $\ell$  is known:  $h_{nm} \propto \exp(-|h_{nn}(\infty) - h_{mm}(\infty)| \ell)$ .

The last property follows directly from the flow equations. For large values of  $\ell$ , the diagonal matrix elements are in the correct order and no level crossings occur for

larger values of  $\ell$ . The second term in (2.7) falls off faster than  $\propto \exp(-|h_{nn}(\infty) - h_{mm}(\infty)|\ell)$  so that the asymptotic behaviour is determined by the first term. For Wegner's choice of  $\eta$ , one cannot exclude non-vanishing off-diagonal matrix elements due to degeneracies of diagonal matrix elements, and the asymptotic behaviour of the matrix elements for large  $\ell$  is less clear.

Let me now discuss the application of the new flow equations to two examples.

### 3 Example 1: Lipkin model

The Lipkin model [11] is a toy model of nuclear physics that describes in its simplest version two shells for the nucleons and an interaction between nucleons in different shells. It serves as a standard example for testing of various approximations. Recently Pirner and Friman [12] applied flow equations to this model. As usual new interactions are generated and they used a suitable truncation to close the flow equations. They showed that for a large number of particles  $N$  the truncated flow equations yield the exact result whereas for small  $N$  deviations occur. Furthermore the flow equations are only applicable for small couplings. For larger couplings the model shows a transition from a state with the same symmetry properties as the Hartree–Fock state to a state with different properties [13]. I will come back to this point later.

A suitable representation for the Lipkin model is in terms of pseudo-spin operators [12].

$$H(\ell = 0) = \xi_0 J_z + V_0(J_+^2 + J_-^2). \quad (3.1)$$

$H$  commutes with  $\hat{J}^2 = J_z^2 + \frac{1}{2}(J_+J_- + J_-J_+)$  and  $\hat{J}^2$  has the eigenvalues  $J(J+1)$  as usual. The pseudo-spin operators form the usual angular momentum algebra

$$[J_z, J_\pm] = \pm J_\pm, \quad [J_+, J_-] = 2J_z. \quad (3.2)$$

It can easily be shown that in the basis where  $\hat{J}^2$  and  $J_z$  are diagonal the Hamiltonian decays into two tridiagonal matrices.

$$H = (h_{nm})_{n,m=0\dots J \text{ or } J-1 \text{ or } J-1/2}. \quad (3.3)$$

The dimension of the matrices depends on  $J$ . If  $2J$  is even, one of the two matrices has dimension  $J$ , the other  $J+1$ , if  $2J$  is odd, both matrices have the dimension  $J+1/2$ . The matrix elements are

$$h_{nn} = \epsilon_n, \quad h_{nn+1} = \delta_n, \quad h_{nm} = 0 \text{ if } |n-m| > 1 \quad (3.4)$$

with

$$\epsilon_n(0) = \xi_0(-J+2n) \quad (3.5)$$

$$\delta_n(0) = V_0 \sqrt{J(J+1) - (J-2n)(J-2n-1)} \\ \times \sqrt{J(J+1) - (J-2n-1)(J-2n-2)} \quad (3.6)$$

or

$$\epsilon_n(0) = \xi_0(-J+2n+1) \quad (3.7)$$

$$\delta_n(0) = V_0 \sqrt{J(J+1) - (J-2n-1)(J-2n-2)} \\ \times \sqrt{J(J+1) - (J-2n-2)(J-2n-3)}. \quad (3.8)$$

The flow equations are in both cases

$$\frac{d\epsilon_n}{d\ell} = -2\delta_n^2 + 2\delta_{n-1}^2 \quad (3.9)$$

$$\frac{d\delta_n}{d\ell} = -\delta_n(\epsilon_{n+1} - \epsilon_n). \quad (3.10)$$

A first possibility is to solve these equations iteratively. One can start with the *ansatz*  $\epsilon_n^{(0)}(\ell) = \epsilon_n(0)$  and  $\delta_n^{(0)}(\ell) = \delta_n(0) \exp(-2\xi_0\ell)$ . Inserting these expressions on the right hand side of the flow equations yields a first iterative solution, which can again be used to obtain the next iterative solution and so on. When one uses this procedure it may be useful to write the flow equation for  $\delta_n$  in the form  $\frac{d \ln \delta_n}{d\ell} = -\epsilon_{n+1} + \epsilon_n$ . This procedure reproduces simply perturbation theory, which works well for small  $V_0$  and not too large  $J$  (*i.e.* not too large particle numbers).

A simple non-perturbative solution can be obtained in the limit of large  $J$ ; this corresponds to the limit of a large particle number. The two different cases for the initial conditions above yield

$$\delta_n(0)^2 - \delta_{n-1}(0)^2 = 32V_0^2 J^2 \left(n + \frac{1}{4}\right) \left(1 + O(1/J)\right), \quad (3.11)$$

or

$$\delta_n(0)^2 - \delta_{n-1}(0)^2 = 32V_0^2 J^2 \left(n + \frac{3}{4}\right) \left(1 + O(1/J)\right). \quad (3.12)$$

With the *ansatz*

$$\epsilon_n(\ell) = a(\ell)n + b(\ell) \quad (3.13)$$

the flow equations can be written as

$$\delta_n(\ell) = f(\ell)\delta_n(0) \quad (3.14)$$

where

$$\frac{df}{d\ell} = -af, \quad (3.15)$$

and

$$\frac{da}{d\ell} = -64V_0^2 J^2 f^2. \quad (3.16)$$

For the last two equations the quantity

$$a^2 - 64V_0^2 J^2 f^2 \quad (3.17)$$

is conserved. Since  $f \rightarrow 0$  for  $\ell \rightarrow \infty$ , this yields directly

$$a(\infty) = \sqrt{4\xi_0^2 - 64V_0^2 J^2} \quad (3.18)$$

This solution exists for  $4JV_0 < \xi_0$ . Taking the first case from above one has

$$\frac{db_1}{d\ell} = \frac{1}{4} \frac{da}{d\ell} \quad (3.19)$$

with the solution

$$b_1(\infty) = -\left(J + \frac{1}{2}\right)\xi_0 + \frac{1}{4}\sqrt{4\xi_0^2 - 64V_0^2 J^2}. \quad (3.20)$$

For the second case one obtains

$$\frac{db_2}{d\ell} = \frac{3}{4} \frac{da}{d\ell} \quad (3.21)$$

and

$$b_2(\infty) = -\left(J + \frac{1}{2}\right)\xi_0 + \frac{3}{4}\sqrt{4\xi_0^2 - 64V_0^2 J^2}. \quad (3.22)$$

This yields directly the approximate spectrum

$$\epsilon_{n1,2} = \sqrt{4\xi_0^2 - 64V_0^2 J^2} \left(n + \frac{1}{2} \pm \frac{1}{4}\right) - \left(J + \frac{1}{2}\right)\xi_0 \quad (3.23)$$

and the gap between the ground state and the first excited state

$$\epsilon_{02} - \epsilon_{01} = \sqrt{\xi_0^2 - 16V_0^2 J^2}. \quad (3.24)$$

This result has been obtained by Pirner and Friman [12] as well. It is also well-known from RPA. Nevertheless the above formulation of the flow equations has certain advantages.

1. It is quite easy to obtain perturbation theory using the flow equations. With the conventional formulation of the flow equations this in principle possible, but one has to introduce many higher interactions if one wants to obtain higher orders in perturbation theory. In the present formulation the flow equations (3.9, 3.10) are closed and the iterative solution is easily constructed.
2. The formulation of the flow equations is not restricted to  $4JV_0 < \xi_0$ . Although the perturbative solution and the approximate solution for large  $J$  shown here are limited to this regime, the flow equations (3.9, 3.10) can be solved (at least numerically) for  $4JV_0 > \xi_0$  as well.
3. The flow equations in the present form may be used to derive a systematic  $1/J$ -expansion. To do this one has to use a polynomial *ansatz* for  $\epsilon_n$  as a function of  $n$  instead of the linear *ansatz* above, and one has to take higher orders in  $\delta_n^2 - \delta_{n-1}^2$  into account.

Since the aim of the present paper is only to show that the new proposal for the continuous unitary transformation is useful if one wants to treat band-diagonal Hamiltonians, I do not follow the lines suggested in these points.

## 4 Example 2: spin-boson model

As a second example I discuss the spin-boson model described by the Hamiltonian

$$H(\ell = 0) = -\frac{\Delta}{2}\sigma_x + \frac{\lambda}{2}\sigma_z(b + b^\dagger) + \omega b^\dagger b. \quad (4.1)$$

It has a wide range of possible applications, especially in atomic physics where the spin describes a two level atom that is coupled to a *e.g.* laser field. Due to its long history there exists an enormous amount of work that has already been published on this model, so that it is impossible to review or cite all these papers. A good overview may be found in the paper by Graham *et al.* [14]. More recently this model has been discussed in connection with quantum chaos [15, 16]. Together with the usual flow equations the model has been used to test several approximation schemes [10]. It turned out that the ground state and the low lying excited states as well as dynamical properties can be calculated very accurately using traditional flow equations. If one is interested in quantum chaos, an accurate knowledge of high eigenvalues is necessary.

The Hamiltonian (4.1) can be written as two tridiagonal infinite matrices. The flow equations are therefore the same as for the Lipkin model,

$$\frac{d\epsilon_n}{d\ell} = -2\delta_n^2 + 2\delta_{n-1}^2, \quad (4.2)$$

and

$$\frac{d\delta_n}{d\ell} = -\delta_n(\epsilon_{n+1} - \epsilon_n), \quad (4.3)$$

but with different initial conditions:

$$\delta_n(0) = \frac{\lambda}{2}\sqrt{n+1}, \quad (4.4)$$

$$\epsilon_n(0) = n\omega \pm (-1)^n \frac{\Delta}{2}. \quad (4.5)$$

It is very easy to solve these equations for  $\Delta = 0$ . One obtains

$$\begin{aligned} \epsilon_n &= n\omega + \epsilon_0, & \epsilon_0 &= -\frac{\lambda^2}{4\omega} \left(1 - \exp(-2\omega\ell)\right), \\ \delta_n &= \frac{\lambda}{2}\sqrt{n+1} \exp(-\omega\ell). \end{aligned} \quad (4.6)$$

In principle it is possible to use this solution to obtain an expansion for small  $\Delta$ . A perturbative treatment for small  $\Delta$  has been given to first order by Graham *et al.* [14], and the flow equations yield the same result. Therefore I will not reproduce this solution here. A second possibility is an iterative solution for small  $\lambda$ . It yields a perturbative solution valid for small  $n$ . Similarly ordinary perturbation theory is valid only if  $n$  is small ( $n \ll (\omega \pm \Delta)^2 / \lambda^2$ ). Instead I try to obtain an asymptotic expression for  $\epsilon_n$  that is valid for large  $n$ . To do this, I make the following *ansatz*

$$\epsilon_n = n\omega - \frac{\lambda^2}{4\omega} (1 - \exp(-2\omega\ell)) \pm (-1)^n \frac{\Delta}{2} f_n(\ell), \quad (4.7)$$

and

$$\delta_n^2 = \frac{\lambda^2}{4}(n+1)\exp(-2\omega\ell) \pm (-1)^n \frac{\Delta}{2} g_n(\ell). \quad (4.8)$$

This *ansatz* yields flow equations for  $f_n$  and  $g_n$

$$\frac{df_n}{d\ell} = -2(g_n + g_{n-1}) \quad (4.9)$$

$$\begin{aligned} \frac{dg_n}{d\ell} &= \frac{\lambda^2}{2}(n+1)\exp(-2\omega\ell)(f_{n+1} + f_n) \\ &\quad - 2\omega g_n \mp \Delta(-1)^n g_n(f_{n+1} + f_n). \end{aligned} \quad (4.10)$$

It is now useful to introduce the new variable

$$x = 1 - \exp(-2\omega\ell) \quad (4.11)$$

instead of the flow parameter  $\ell$ . In the following I take  $f_n$  and  $g_n$  as functions of  $x$ . The flow equations are rewritten as

$$\omega(1-x)\frac{df_n}{dx} = -g_n - g_{n-1}, \quad (4.12)$$

$$\begin{aligned} 2\omega(1-x)\frac{dg_n}{dx} &= \frac{\lambda^2}{2}(n+1)(1-x)(f_{n+1} + f_n) \\ &\quad - 2\omega g_n \mp \Delta(-1)^n g_n(f_{n+1} + f_n), \end{aligned} \quad (4.13)$$

with the initial conditions

$$f_n(0) = 1, \quad g_n(0) = 0. \quad (4.14)$$

These equations are still exact. For large  $n$  one has  $g_{2n+2} \approx g_{2n}$  and  $g_{2n+1} \approx g_{2n-1}$ . As a consequence one obtains  $f_{2n+1} \approx f_{2n}$ . This yields

$$\omega(1-x)\frac{df_{2n}}{dx} \approx \omega(1-x)\frac{df_{2n+1}}{dx} = -g_{2n} - g_{2n+1}, \quad (4.15)$$

$$\begin{aligned} 2\omega(1-x)\frac{dg_{2n}}{dx} &\approx 2\lambda^2 n(1-x)f_{2n} \\ &\quad - 2\omega g_{2n} \mp 2\Delta g_{2n} f_{2n}, \end{aligned} \quad (4.16)$$

$$\begin{aligned} 2\omega(1-x)\frac{dg_{2n+1}}{dx} &\approx 2\lambda^2 n(1-x)f_{2n} \\ &\quad - 2\omega g_{2n+1} \pm 2\Delta g_{2n+1} f_{2n}. \end{aligned} \quad (4.17)$$

Taking the derivative of the first equation, and using the sum of the second and the third to express the derivative of  $g_{2n} + g_{2n+1}$  by  $f_{2n}$  I obtain for large  $n$  (*i.e.*  $2n+1 \approx 2n$ )

$$(1-x)\frac{d^2 f_n}{dx^2} = -2\frac{\lambda^2}{\omega^2} n f_n. \quad (4.18)$$

The general solution of this differential equation can be expressed using Bessel functions

$$\begin{aligned} f_n(x) &= \sqrt{1-x} \left[ a J_1 \left( \frac{2\lambda}{\omega} \sqrt{n(1-x)} \right) \right. \\ &\quad \left. + b Y_1 \left( \frac{2\lambda}{\omega} \sqrt{n(1-x)} \right) \right]. \end{aligned} \quad (4.19)$$

Using the initial conditions  $f_n(0) = 1$  and  $f'_n(0) = 0$ , one obtains

$$\begin{aligned} a &= \pi \frac{\lambda}{\omega} \sqrt{n} Y_0 \left( \frac{2\lambda}{\omega} \sqrt{n} \right), \\ b &= -\pi \frac{\lambda}{\omega} \sqrt{n} J_0 \left( \frac{2\lambda}{\omega} \sqrt{n} \right). \end{aligned} \quad (4.20)$$

This yields the complete solution for  $\epsilon_n(\ell)$ . I am interested in the limit  $\ell \rightarrow \infty$ , which corresponds to  $x = 1$ . Using the behaviour of the Bessel function for small arguments one obtains

$$f_n(1) = -J_0 \left( \frac{2\lambda}{\omega} \sqrt{n} \right). \quad (4.21)$$

This yields the final expression for the eigenvalues for large  $n$

$$\epsilon_n(\ell = \infty) = n\omega - \frac{\lambda^2}{4\omega} \mp (-1)^n \frac{\Delta}{2} J_0 \left( \frac{2\lambda}{\omega} \sqrt{n} \right). \quad (4.22)$$

Using the asymptotic behaviour of the Bessel function, one obtains

$$\begin{aligned} \epsilon_n(\ell = \infty) &= n\omega - \frac{\lambda^2}{4\omega} \\ &\quad \mp (-1)^n \frac{\Delta}{2n^{1/4}} \sqrt{\frac{\omega}{\pi\lambda}} \cos \left( \frac{2\lambda}{\omega} \sqrt{n} - \frac{1}{4}\pi \right). \end{aligned} \quad (4.23)$$

Except for a misprint (the factor  $n^{-1/4}$  is missing in the last term) this expression coincides with the result in [14]. Graham *et al.* performed a first order perturbational treatment in  $\Delta$  and expanded the result to obtain (4.23) for large  $n$ . Thus, in their approach, the validity of (4.23) is unclear.

How accurate are (4.22, 4.23)? A first condition is obtained from a consistency check of the above assumption  $f_{n+1}(x) \approx f_n(x)$ . This assumption must be true for all  $x$  and all  $\lambda/\omega$ . Due to  $2\sqrt{n+1}\lambda/\omega \approx 2\sqrt{n}\lambda/\omega + \lambda/(\omega\sqrt{n})$  one must have

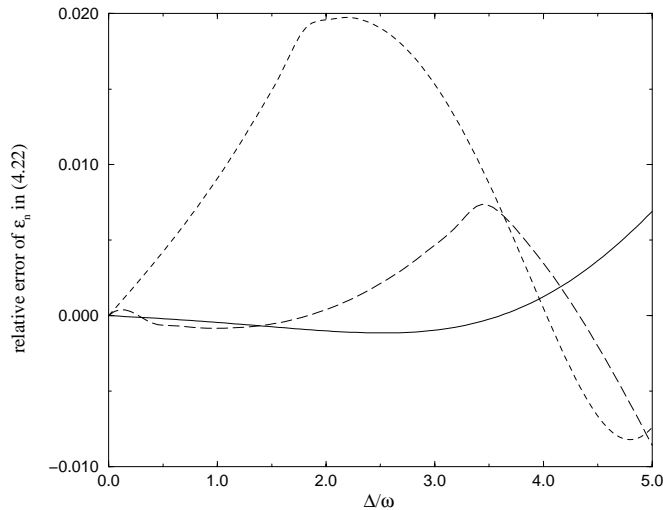
$$\frac{\lambda}{\omega\sqrt{n}} \ll 1. \quad (4.24)$$

But this is not the only condition one needs. A similar consistency check has to be done for  $g_n$ . It is more complicated since it depends on  $\Delta$ . Fortunately there is a more simple possibility to determine the range of applicability for (4.22, 4.23), which is equivalent to the consistency check proposed above. From the general considerations in Section 2 one knows that the flow equations yield  $\epsilon_n(\ell = \infty) \leq \epsilon_{n+1}(\ell = \infty)$ . This means that one must have

$$\omega > \frac{\Delta}{2} \left| J_0 \left( \frac{2\lambda}{\omega} \sqrt{n} \right) - J_0 \left( \frac{2\lambda}{\omega} \sqrt{n+1} \right) \right|. \quad (4.25)$$

For large  $\frac{\lambda}{\omega}\sqrt{n}$  this yields the condition

$$\frac{\Delta}{2\omega} \sqrt{\frac{\lambda}{\pi\omega}} \frac{1}{n^{3/4}} < 1. \quad (4.26)$$



**Fig. 1.** The relative error of the asymptotic expression for the eigenvalue compared to the exact result as a function of  $\Delta/\omega$  for  $\lambda/\omega = 4.0$ . The short dashed line is  $n = 10$ , the long dashed line  $n = 15$  and the solid line  $n = 20$ .

Equations (4.24, 4.26) show that within a wide range of parameters (4.22, 4.23) are applicable. But one should be careful using (4.23) for small  $\lambda$ . Equation (4.23) has a relative error  $O(\frac{\omega}{2\lambda\sqrt{n}})$  compared to (4.22) so that for small  $\lambda$  (4.22) yields better results. For  $\lambda = 0$ , (4.22) yields the exact solution (which is of course trivial), whereas (4.23) is not defined. Only in the limit  $\lambda \rightarrow 0$  and  $\Delta\lambda/\omega^2 = \text{const.}$  it is not possible to apply (4.22). But this regime can be treated with perturbation theory for small  $\lambda$ .

The accuracy of (4.22) is very high, even for small  $n$  and large  $\Delta$ . It can be tested numerically if one compares (4.22) with the exact numerical solution of the flow equations. This is done in Figure 1. We show the relative error of the asymptotic formula (4.22) plotted as a function of  $\Delta/\omega$ . The coupling is  $\lambda/\omega = 4.0$ . For small  $n$  the error is relatively large (up to 2% for  $n = 10$ ), whereas it is smaller for larger  $n$ . The parameters are chosen so that for  $n = 10$  the left hand side of (4.24) equals 1.3 and is therefore too large. The left hand side of (4.26) equals 0.5 for the worst case shown, *i.e.*  $n = 10$  and  $\Delta = 5\omega$ . A relative error less than 0.1% is obtained if the left hand side of (4.26) is less than 0.1 and for  $n \gtrsim \lambda^2/\omega^2$ .

The main result of this section is clearly the expression for  $\epsilon_n(\ell = \infty)$  given above. But one does not only know the eigenvalues of the Hamiltonian, the complete flow (4.19) is known as well. This allows to reconstruct the continuous unitary transformation that diagonalizes the Hamiltonian. Therefore it is even possible to calculate other observables in the transformed basis. In principle it is possible to combine this result with the results of Richter [10], which are very accurate for small  $n$ . Then one should be able to obtain accurate values for dynamical correlation functions of the model. But the goal of the present calculations was to show that the new flow equations proposed in this paper

are indeed useful if one wants to deal with band-diagonal matrices or Hamiltonians. Therefore I do not follow this line.

## 5 Conclusions

The flow equations proposed in this paper seem to be useful if one wants to solve a given model. The two examples showed that solutions can be obtained at least approximately or in some limits. Some of the advantages of the new flow equations have already been pointed out. 1) The matrix is finally in a diagonal form, even if degeneracies occur. 2) If the Hamiltonian has initially a banded structure, this form is preserved. 3) The asymptotic behaviour of the equations is known. Another advantage is that with the new flow equations one can obtain accurate results for higher eigenvalues as well. But there are also some disadvantages, which may be important in other systems

1. Although asymptotically off-diagonal matrix elements decay faster if the difference of the corresponding diagonal matrix elements is larger, the new generator does not separate different energy scales automatically. For small  $\ell$  it is not guaranteed that off-diagonal matrix elements corresponding to large energy differences decay fast. Therefore the new flow equations do not provide a renormalization scheme.
2. An important property of a Hamiltonian one wants to solve using the new flow equations is that it must have a pure point spectrum. Hamiltonians with continuous spectra cannot be treated that way. It is for instance not possible to apply the new generator to a dissipative quantum system.
3. If the diagonal matrix elements of the initial Hamiltonian are not in the correct order (*i.e.*  $h_{nn} \leq h_{mm}$  if  $n < m$ ) the flow equations will reorder the diagonal matrix elements. This may cause a problem, because in such a case the analytical treatment of the flow equations becomes more difficult.

The first two points mentioned above show that the new generator cannot be applied successfully to the kind of problems that have been treated so far using flow equations. In all these problems one has several different energy scales and continuous spectra, and one needs a renormalization scheme to obtain useful results. In this sense the new generator provides a complementary set of flow equations. It can be applied to problems that cannot be treated with the original flow equations, but problems that can be treated with the original flow equations are not within the range of possible applications of the new scheme.

What kind of problems can be treated with the new flow equations? It became already clear that Hamiltonians with a banded structure are good candidates. But even for Hamiltonians without such a structure the present approach may be useful. If one has for instance a problem for which all diagonal matrix elements are of the same order of magnitude, the usual flow equations are difficult to apply.

The reason is that differences of diagonal matrix elements are small and that therefore the flow is very slow. This does not happen with the new flow equations, since the flow of the diagonal matrix elements is only determined by the magnitude of the off-diagonal matrix elements. A class of possible candidates are therefore disordered systems.

In general one can say that the new flow equations can be applied to single or few particle systems. It may therefore be useful in nuclear or atomic physics.

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