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Moyal implementation of flow equations—a non-perturbative approach to quantum many-body systems

J N Kriel, F G Scholtz and J D Thom

Institute of Theoretical Physics, University of Stellenbosch, South Africa

E-mail: hkriel@sun.ac.za, fgs@sun.ac.za and nthom@sun.ac.za

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Abstract

We show how Wegner's flow equations can be reformulated as ordinary differential equations through the use of the Moyal bracket. In finite-dimensional Hilbert spaces the introduction of the Moyal bracket leads naturally to the identification of a small expansion parameter, namely the inverse of the dimensionality of the space. This expansion corresponds to a non-perturbative treatment of the coupling constant. In the case of infinite-dimensional spaces \hbar plays the role of the small parameter and the Moyal formulation then allows for a semi-classical treatment of the flow equation. We demonstrate these statements for the Lipkin and Dicke models as well as for the symmetric x^4 and double-well potentials.

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1. Introduction

Wegner's flow equations [1] present an interesting alternative approach to the analysis of quantum many-body systems and has indeed found a considerable range of applications. These include the treatment of the electron–phonon coupling [2], the spin-boson Hamiltonian [3], the Hubbard model [4] and several spin models [5–9]. A comprehensive overview of these and other applications can be found in [10, 11].

In [12, 13] it was suggested that these flow equations may present a viable non-perturbative approach to quantum many-body systems. This suggestion was based on the analysis of the Lipkin model, where it was observed that the flow equations admit a systematic expansion in the inverse number of particles. This expansion treated the coupling constant in a non-perturbative fashion, which allowed for an accurate description even at the quantum phase transition. The way in which the small expansion parameter was identified in these two references was, however, not very systematic. Here we attempt to give a general procedure,

based on the Moyal bracket, for implementing the flow equation in a way in which this small parameter appears quite naturally. Exploiting the presence of this parameter enables us to recast the flow equation, which is an operator equation, into the form of an ordinary partial differential equation, which is more tractable both analytically and numerically. In contrast, an operator treatment of the flow equation generally leads to an infinite set of coupled differential equations in order to reflect the new operators which are generated during the flow. There is no systematic way to truncate this set, apart from an expansion in the coupling constant, which we know will invariably fail at large coupling or in the presence of a quantum phase transition. In the formulation presented here, however, the natural appearance of a small parameter immediately suggests a systematic truncation, which is non-perturbative in the coupling constant.

We organize the paper as follows. In section 2 we briefly review the philosophy behind the flow equation. This section also serves to set our notation and conventions. In section 3 we introduce the Moyal bracket, indicate the emergence of the small expansion parameter and finally show how the flow equation can be reformulated in this framework as a differential equation. In section 4 we present two examples of many-body systems, the Lipkin and Dicke models, for which the small expansion parameter is the inverse particle number. In section 5 we consider the quartic and double-well potentials as examples of infinite-dimensional quantum systems. In these cases \hbar plays the role of the small parameter, and this approach is therefore tantamount to a semi-classical expansion. We end with conclusions in section 6.

2. The flow equation

The central notion in Wegner's flow equations [1] is the transformation of a Hamiltonian H into a simplified form through a sequence of consecutive infinitesimal unitary transformations. It is the continuous evolution of H under these transformations that we refer to as the flow of the operator. The transformations are constructed to bring about decoupling in H , which results in a final Hamiltonian exhibiting a diagonal, or block diagonal, form. We are led to consider a family of unitary transformations $U(\ell)$ which is continuously parametrized by the flow parameter $\ell \in [0, \infty)$. $U(\ell)$ constitutes the net effect of all the infinitesimal transformations applied up to the point in the flow labeled by ℓ . At the beginning of the flow $U(0)$ is just the identity operator. The evolution of $U(\ell)$ is governed by

$$\frac{dU(\ell)}{d\ell} = -U(\ell)\eta(\ell), \quad (1)$$

where $\eta(\ell)$ is the anti-Hermitian generator of the transformation. Applying $U(\ell)$ to H produces the transformed Hamiltonian $H(\ell) = U^\dagger(\ell)HU(\ell)$ for which the flow equation is

$$\frac{dH(\ell)}{d\ell} = [\eta(\ell), H(\ell)]. \quad (2)$$

Similarly, an observable O flows according to

$$\frac{dO(\ell)}{d\ell} = [\eta(\ell), O(\ell)]. \quad (3)$$

The choice of $\eta(\ell)$ plays a central role in this formalism, since it determines the form of $H(\ell)$ at finite ℓ as well as the nature of the fixed point in the $\ell \rightarrow \infty$ limit.

One popular choice of the generator is $\eta(\ell) = [G, H(\ell)]$, where G is a fixed ℓ -independent, Hermitian operator of which the eigenstates are known. It is straightforward to show that $H(\ell)$ converges to a form which commutes with G . The proof rests on the observation that

$$\frac{d}{d\ell} \text{tr}(H(\ell) - G)^2 = -2 \text{tr}([G, H(\ell)]^\dagger [G, H(\ell)]) < 0, \quad (4)$$

where the positivity of the trace norm has been used. It follows that $\text{tr}(H(\ell) - G)^2$ is a monotonically decreasing function of ℓ that is bounded from below by 0, and so its derivative must vanish in the $\ell \rightarrow \infty$ limit. Since the right-hand side of (4) is just the trace norm of $\eta(\ell) = [G, H(\ell)]$, we conclude that $\eta(\infty) = 0$. In the case of infinite-dimensional spaces the traces in (4) may diverge and some form of regularization may be required. Any proper regularization that preserves the positivity of the trace norm will, however, not alter the above argument, making it also valid if the operators are not necessarily of the trace class. Choosing G to be diagonal leads to a block-diagonal structure for $H(\infty)$, where only states corresponding to equal diagonal matrix elements of G can be connected. In particular, a non-degenerate choice of G yields a complete diagonalization of H . Furthermore, it can be shown [14] that the eigenvalues of H , as they appear on the diagonal of $H(\infty)$, will have the same ordering as the eigenvalues (diagonal matrix elements) of G . We summarize this by saying that the flow equation generates a transformation that maps the eigenstates of H onto the eigenstates of G in an order preserving fashion. It is worth noting that this ordering can only take place within subspaces that are irreducible under G and H , since the flow equation clearly cannot mix states that are not connected by either H or G .

The second class of generators we consider are the so-called form preserving (or particle conserving) generators [5, 6, 15]. If H possesses a band block diagonal structure (see below) these generators will ensure that this structure is preserved during the flow. Not only this is computationally favorable (since fewer nonzero matrix elements are generated), but it also allows for a clear physical interpretation of the resulting Hamiltonian $H(\infty)$. These generators have been applied to a wide range of models [5–8, 15–18].

To construct such a generator, we first introduce an operator Q with integer eigenvalues q_i which will serve as a labeling device for different subspaces in the Hilbert space. Each eigenvalue is associated with a subspace of corresponding eigenvectors, which we call a Q -sector. The Hamiltonian H is said to have a band block diagonal structure with respect to Q if there exists an integer N such that $\langle i | H | j \rangle$ is zero for all $|i\rangle$ and $|j\rangle$ from the q_i and q_j sectors whenever $|q_i - q_j| > N$. In other words, H does not connect Q -sectors differing by more than N . It is possible to split the Hamiltonian into three parts: one leaves Q unchanged while two others either increase or decrease Q :

$$H = T_0 + \underbrace{\sum_{n=1}^N T_n}_{T_+} + \underbrace{\sum_{n=1}^N T_{-n}}_{T_-}, \tag{5}$$

where T_n is such that it changes Q by n . This is formally expressed as $[Q, T_n] = nT_n$. We would like the flow equations to bring H into a form that commutes with Q while preserving the structure of (5) during the flow as

$$H(\ell) = T_0(\ell) + \sum_{n=1}^N T_n(\ell) + \sum_{n=1}^N T_{-n}(\ell), \tag{6}$$

where $T_+(\ell) = \sum_{n=1}^N T_n(\ell)$ and $T_-(\ell) = \sum_{n=1}^N T_{-n}(\ell)$. The generator that achieves this is

$$\eta(\ell) = T_+(\ell) - T_-(\ell). \tag{7}$$

It can be shown [15] that the flow generated by $\eta(\ell)$ converges to a final Hamiltonian that conserves Q .

3. Moyal formulation of the flow equation

The practical implementation of the flow equation method is hampered by the difficulty of solving the operator differential equation. This is due to the generation of additional operators during the flow that were not present in the original Hamiltonian and this results in an extremely large set of coupled differential equations for the coupling constants of these new terms. Generally, some kind of approximation is required in order to continue. The usual approach consists of replacing $H(\ell)$ by a simpler parametrized form for which the flow equation closes on a set of coupled equations of a tractable size. A particular parametrization is usually selected on the basis of a perturbative approximation, or by using some knowledge of the relevant degrees of freedom in the problem. This approach is generally only valid for a limited range of the coupling constant and tends to break down when the system exhibits non-perturbative features, i.e. non-analytic behavior in the coupling constant.

We will introduce a new approach to this problem which allows the flow equation to be treated non-perturbatively. Central to this method is the use of non-commutative variables together with the Moyal bracket to recast the flow equation as a regular partial differential equation. Two variations of this approach arise naturally, and both are based on an expansion in an appropriate small parameter. In the first case this parameter is the inverse of the system size, or more generally the dimensionality of the Hilbert space, which is a natural parameter to use when studying the thermodynamic limit. Such expansions have been used in the context of flow equations in [13, 19–24]. In the second instance the expansion is made in orders of \hbar , and is therefore semi-classical in nature.

Although similar in spirit to the method described in [13], the Moyal bracket-based approach greatly clarifies the conceptual framework and simplifies the calculations. Furthermore, this approach can be extended to other models in a straightforward and natural manner.

3.1. $1/D$ -expansion

Let \mathcal{H} denote the D -dimensional Hilbert space of the Hamiltonian under consideration. First we construct a basis for the space of linear operators acting on \mathcal{H} . This is done in terms of a pair of specially chosen operators which lead to the representation of operators as scalar functions. The operator product is then realized in terms of differential operators acting on these functions.

Let h and g be two unitary operators that act irreducibly on \mathcal{H} and satisfy the exchange relation

$$hg = e^{-i\theta} gh. \quad (8)$$

Since g is unitary, its eigenvalues are pure phases. Let $e^{i\sigma}$ be one such eigenvalue, and consider the action of gh on the corresponding eigenstate $|\sigma\rangle$:

$$gh|\sigma\rangle = e^{i\theta} hg|\sigma\rangle = e^{i(\theta+\sigma)} h|\sigma\rangle. \quad (9)$$

We see that $h|\sigma\rangle$ is again an eigenstate of g with the eigenvalue $e^{i(\theta+\sigma)}$. Since g and h act irreducibly on \mathcal{H} , all the eigenstates of g can be obtained by the repeated application of h to $|\sigma\rangle$. Furthermore, we may scale g so that it possesses an eigenvalue equal to 1.

It follows that the eigenvalues and eigenstates of g take the form

$$g|n\rangle = e^{i\theta n} |n\rangle \quad \text{where } n = 0, 1, 2, \dots, D-1, \quad (10)$$

while h acts as a ladder operator between these states:

$$gh|n\rangle = e^{i\theta} hg|n\rangle = e^{i\theta(n+1)} h|n\rangle \implies h|n\rangle \propto |n+1\rangle. \quad (11)$$

The allowed values of θ are found by taking the trace on both sides of $h^{-1}gh = e^{i\theta}g$, which leads to the requirement

$$\text{tr}(g) = \sum_{n=0}^{D-1} e^{in\theta} = 0. \tag{12}$$

This fixes θ at an integer multiple of $2\pi/D$. We choose $\theta = 2\pi/D$ since this ensures that g is non-degenerate, which is crucial for the construction that follows.

Our aim is to represent flowing operators in terms of g and h . The main result in this regard is that the set

$$\mathcal{P} = \{D^{-\frac{1}{2}}g^n h^m : n, m = 0, 1, 2, \dots, D - 1\} \tag{13}$$

constitutes an orthonormal basis for the space of linear operators acting on \mathcal{H} . The orthogonality of \mathcal{P} follows from applying the trace inner product in the g -basis to two members of \mathcal{P} :

$$\text{tr}[(g^n h^m)^\dagger g^{n'} h^{m'}] = \delta_{m,m'} \text{tr}[g^{(n'-n)}] = \delta_{m,m'} \sum_{q=0}^{D-1} e^{iq(n'-n)\theta} = \delta_{m,m'} \delta_{n,n'} D. \tag{14}$$

This, together with the observation that the dimension of the complex linear operator space equals $|\mathcal{P}| = D^2$, proves the claim.

Consider two arbitrary operators U and V expressed in the \mathcal{P} -basis as

$$U = \sum_{n,m} C_{n,m} g^n h^m \quad \text{and} \quad V = \sum_{n',m'} C'_{n',m'} g^{n'} h^{m'}, \tag{15}$$

where $C_{n,m}$ and $C'_{n',m'}$ are complex scalar coefficients. We use the convention of always writing the h 's to the right of the g 's. The product of U and V then gives

$$UV = \sum_{n,m,n',m'} C_{n,m} C'_{n',m'} g^{m+m'} h^{n+n'} e^{-inm'\theta}. \tag{16}$$

Note the similarity in form between this product and the product of functions of regular commuting variables. Only the phase factor, the result of imposing our ordering convention on the product, distinguishes the two. In fact, we may treat g and h as regular commuting variables provided that we modify the product rule to incorporate this phase. Convenient variables for this procedure are α and β , which are related to g and h (now treated as scalars) through $g = e^{i\alpha}$ and $h = e^{i\beta}$. Having replaced operators by functions of α and β the modified product rule is given by

$$U(\alpha, \beta) * V(\alpha, \beta) \equiv U(\alpha, \beta) e^{i\theta \overleftarrow{\partial}_\beta \overrightarrow{\partial}_\alpha} V(\alpha, \beta), \tag{17}$$

where the α and β derivatives act to the right and left respectively. This is seen to be of the correct form by using the fact that both g and h are eigenfunctions of ∂_α and ∂_β :

$$U(\alpha, \beta) e^{i\theta \overleftarrow{\partial}_\beta \overrightarrow{\partial}_\alpha} V(\alpha, \beta) = \sum_{n,m,n',m'} C_{n,m} C'_{n',m'} e^{im\alpha} e^{in'\beta} \underbrace{e^{i\theta \overleftarrow{\partial}_\beta \overrightarrow{\partial}_\alpha}}_{e^{-i\theta m'n}} e^{im'\alpha} e^{in'\beta} \tag{18}$$

which agrees with (16).

The $*$ -operation is known as the Moyal product [25], while the corresponding commutator $[U, V]_* = U * V - V * U$ is the Moyal bracket. When $H(\ell)$ and $\eta(\ell)$ are represented in this manner the flow equation becomes a partial differential equation in α, β and ℓ :

$$\frac{dH(\alpha, \beta, \ell)}{d\ell} = [\eta(\alpha, \beta, \ell), H(\alpha, \beta, \ell)]_*. \tag{19}$$

The same procedure may be applied, completely unchanged, to an arbitrary observable O . The flow equation for O is simply (3) rewritten in terms of the Moyal bracket. In its exact form this formulation is not of much practical value, since the operator exponent involved in the Moyal product is very difficult to treat either analytically or numerically. A significant simplification can be achieved by expanding the operator exponent to first order in θ , which is known to scale like the inverse of the dimension of the Hilbert space. We expect this to be a very good approximation provided that the derivatives do not bring about factors of the order of D . This translates into a smoothness condition: we require that the derivatives of the relevant functions remain bounded in the thermodynamic limit as D goes to infinity.

Using this approximation the Moyal product becomes, to leading order,

$$U * V = UV + i\theta U_{\beta} V_{\alpha}, \quad (20)$$

while the Moyal bracket reads

$$[U, V]_* = i\theta(U_{\beta} V_{\alpha} - V_{\beta} U_{\alpha}). \quad (21)$$

Partial derivatives are indicated by the subscript shorthand. The form of the flow equation is now largely fixed, up to the specific choice of the generator.

The remaining problem is that of constructing the initial condition $H(0)$ in terms of g and h (or equivalently α and β) in such a way that the smoothness requirements are met. The reader may have noticed that we have not specified how the realization of g and h should be constructed on \mathcal{H} . Put differently, there is no obvious rule which associates a specific basis of \mathcal{H} with the eigenstates of g . It seems reasonable that this freedom may allow us to construct smooth initial conditions through an appropriate choice of basis, whereas a different choice could produce very poorly behaved functions. We know of no way to proceed on such general terms, and instead tackle this problem on a case-by-case basis.

An useful generalization of this formalism involves introducing multiple $\{g, h\}$ pairs. This would be a natural choice when \mathcal{H} is a tensor product of Hilbert spaces $\mathcal{H}_i (i = 1, \dots, m)$, each of which is of a high dimension. We can introduce m pairs of operators $\{g_i, h_i\}$ which satisfy $h_i g_i = e^{-i\theta_i} g_i h_i$ and $h_i g_j = g_j h_i$ for all $i \neq j$. In the same way as before this leads to m pairs of scalar variables $\{\alpha_i, \beta_i\}$ for which the product rule, to first order in the θ_i 's, is

$$U(\alpha, \beta) * V(\alpha, \beta) = UV + i \sum_{j=1}^m \theta_j U_{\beta_j} V_{\alpha_j}, \quad (22)$$

while the Moyal bracket becomes

$$[U(\alpha, \beta), V(\alpha, \beta)]_* = i \sum_{j=1}^m \theta_j (U_{\beta_j} V_{\alpha_j} - V_{\beta_j} U_{\alpha_j}). \quad (23)$$

3.2. Semi-classical approximation

The formulation we present next is based on a semi-classical approximation with the relevant small parameter being \hbar . This approach to the flow equation is very closely related to the Wigner–Weyl–Moyal [25, 26] formalism, which is based on the construction of a mapping between quantum operators and functions of classical phase space coordinates.

Let us formalize some of these notions in the context of a single particle in three dimensions. The relevant Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^3)$, and the position and momentum operators satisfy the standard commutation relations

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij} \quad i, j = 1, 2, 3. \quad (24)$$

We first introduce the characteristic operator [27]

$$U(\mathbf{t}, \mathbf{s}) = e^{i\mathbf{t}\cdot\hat{\mathbf{p}}} e^{i\mathbf{s}\cdot\hat{\mathbf{x}}}, \tag{25}$$

where $\mathbf{t} = (t_1, t_2, t_3) \in \mathbb{R}^3$, $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$ and similar for $\mathbf{s} \in \mathbb{R}^3$ and $\hat{\mathbf{p}}$. Varying the arguments of $U(\mathbf{t}, \mathbf{s})$ over their domains produces a set of operators analogous to \mathcal{P} in (13), where the discrete powers n and m have been replaced by the continuous labels \mathbf{t} and \mathbf{s} . We again find both completeness and orthogonality with respect to the trace norm:

$$\begin{aligned} \text{tr}[U(\mathbf{t}', \mathbf{s}')^\dagger U(\mathbf{t}, \mathbf{s})] &= \int d\mathbf{x} \langle \mathbf{x} | e^{-i\mathbf{s}'\cdot\hat{\mathbf{x}}} e^{-i\mathbf{t}'\cdot\hat{\mathbf{p}}} e^{i\mathbf{t}\cdot\hat{\mathbf{p}}} e^{i\mathbf{s}\cdot\hat{\mathbf{x}}} | \mathbf{x} \rangle \\ &= \frac{1}{(2\pi\hbar)^3} \int d\mathbf{x} d\mathbf{p} e^{i\mathbf{p}\cdot(\mathbf{t}-\mathbf{t}')} e^{i\mathbf{x}\cdot(\mathbf{s}-\mathbf{s}')} \\ &= \frac{1}{\hbar^3} \delta(\mathbf{t}-\mathbf{t}') \delta(\mathbf{s}-\mathbf{s}'). \end{aligned} \tag{26}$$

Using this result we can represent an operator $A(\hat{\mathbf{x}}, \hat{\mathbf{p}})$ as

$$A(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = \int d\mathbf{t} d\mathbf{s} \tilde{A}(\mathbf{t}, \mathbf{s}) U(\mathbf{t}, \mathbf{s}) \tag{27}$$

where

$$\tilde{A}(\mathbf{t}, \mathbf{s}) = \hbar^3 \text{tr}[U(\mathbf{t}, \mathbf{s})^\dagger A(\hat{\mathbf{x}}, \hat{\mathbf{p}})] \tag{28}$$

is a scalar function. Now consider the product of two operators written in this manner:

$$A(\hat{\mathbf{x}}, \hat{\mathbf{p}}) B(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = \int d\mathbf{t} d\mathbf{s} d\mathbf{t}' d\mathbf{s}' \tilde{A}(\mathbf{t}, \mathbf{s}) \tilde{B}(\mathbf{t}', \mathbf{s}') U(\mathbf{t} + \mathbf{t}', \mathbf{s} + \mathbf{s}') e^{-i\mathbf{t}'\cdot\mathbf{s}} \tag{29}$$

The non-commutativity of $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$ gives rise to the scalar factor $e^{-i\mathbf{t}'\cdot\mathbf{s}}$, which is the only element distinguishing this product from one of the regular scalar functions. We conclude, as before, that the position and momentum operators may be treated as scalar variables provided that we modify the product rule to incorporate this phase. This leads to the Moyal product

$$A(\mathbf{x}, \mathbf{p}) * B(\mathbf{x}, \mathbf{p}) = A(\mathbf{x}, \mathbf{p}) e^{i\hbar \overleftarrow{\partial}_x \cdot \overrightarrow{\partial}_p} B(\mathbf{x}, \mathbf{p}), \tag{30}$$

where $\mathbf{x}, \mathbf{p} \in \mathbb{R}^3$ and $\overleftarrow{\partial}_x \cdot \overrightarrow{\partial}_p = \sum_i \overleftarrow{\partial}_{x_i} \overrightarrow{\partial}_{p_i}$. Note that an expansion of the exponential is controlled by \hbar . To leading order the Moyal bracket is given by

$$[A(\mathbf{x}, \mathbf{p}), B(\mathbf{x}, \mathbf{p})]_* = i\hbar \sum_{i=1}^3 (A_{x_i} B_{p_i} - A_{p_i} B_{x_i}), \tag{31}$$

where the subscripts denote partial derivatives. In the Moyal formulation the Hamiltonian and generator can therefore be replaced by scalar functions $H(\mathbf{x}, \mathbf{p}, \ell)$ and $\eta(\mathbf{x}, \mathbf{p}, \ell)$, while the flow equation is given in terms of the Moyal bracket by

$$\frac{dH(\mathbf{x}, \mathbf{p}, \ell)}{d\ell} = [\eta(\mathbf{x}, \mathbf{p}, \ell), H(\mathbf{x}, \mathbf{p}, \ell)]_* \tag{32}$$

When solved to leading order in \hbar this equation describes the renormalization of the Hamiltonian within a semi-classical approximation.

4. Examples in finite dimensions

In the following two sections we show how the leading-order approximation of the flow equation can be applied to two simple, but non-trivial, many-body systems.

4.1. Example 1: the Lipkin model

The Lipkin–Meshov–Glick [28] model describes N fermions distributed over two degenerate energy levels. Interactions bring about scattering of fermion pairs between the levels. The Hamiltonian may be written in terms of pseudo-spin operators as

$$H = J_z + \frac{\lambda}{2N}(J_+^2 + J_-^2), \quad (33)$$

where λ is the coupling constant and J_z , J_+ and J_- are the $su(2)$ generators. The factor of $1/N$ ensures that the Hamiltonian is extensive, i.e. scales like N . Together with the second-order Casimir operator $J^2 = J_z^2 + J_z + J_- J_+$, these satisfy the regular $su(2)$ commutation relations

$$[J_z, J_\pm] = \pm J_\pm, \quad [J_+, J_-] = 2J_z \quad \text{and} \quad [J^2, J_\pm] = [J^2, J_z] = 0. \quad (34)$$

Since $[H, J^2] = 0$, the Hamiltonian acts within irreducible representations of $su(2)$ where states are labeled by the eigenvalues of J^2 and J_z , i.e., $J^2|j, m\rangle = j(j+1)|j, m\rangle$ and $J_z|j, m\rangle = m|j, m\rangle$ for $m = -j, \dots, j$. The Hamiltonian therefore assumes a block diagonal structure of sizes $2j+1$. The low-lying states occur in the multiplet $j = N/2$. We fix j at this value throughout, and use the shorthand $|m\rangle \equiv |j, m\rangle$ for the basis states. The eigenstate of H with energy E_n is denoted by $|E_n\rangle$, where $E_n \leq E_{n+1}$. Interactions cause particle–hole excitations across the gap, and at $\lambda = \pm 1$ the model exhibits a phase transition from an undeformed first phase to a deformed second phase. The two phases are distinguished by the order parameter $\Omega \equiv 1 + \langle E_0 | J_z | E_0 \rangle / j$ which is nonzero only within the second phase. Further discussion of this model and its features can be found in [28]. Other applications of the flow equations to the Lipkin model appear in [4, 12, 13, 29–31]. A $1/N$ expansion of the flow equation was also used in [19, 23] to study aspects of finite-size scaling.

We follow [29] and choose the generator as

$$\eta(\ell) = [J_z, H(\ell)]. \quad (35)$$

Let us examine the consequences of this choice. Firstly, since J_z is non-degenerate, we expect the final Hamiltonian $H(\infty)$ to be diagonal in the spin basis. Furthermore, the eigenvalues of H will appear on the diagonal of $H(\infty)$ in the same order as in J_z , i.e. increasing from top to bottom. Secondly, note that H possesses a band diagonal structure in the J_z basis. This choice of $\eta(\ell)$ ensures that the band diagonality is preserved during flow, and so $H(\ell)$ will only connect states of which the spin projection differ by 0 or 2.

The Moyal formulation allows the flow equation to be rewritten as the differential equation

$$\frac{\partial H}{\partial \ell} = \theta(H_{\beta\beta}H_\alpha - H_\beta H_{\beta\alpha}), \quad (36)$$

where subscripts denote partial derivatives. We still need to construct the initial condition for this equation. To do so we note that the Hamiltonian is a function solely of the $su(2)$ generators. Since the commutator of operators and Moyal bracket of functions are isomorphic, it follows that we can construct the initial Hamiltonian in the Moyal formulation by finding three functions $J_z(\alpha, \beta)$, $J_+(\alpha, \beta)$ and $J_-(\alpha, \beta)$ which satisfy the $su(2)$ commutation relations with respect to the Moyal bracket $[\cdot, \cdot]_*$, i.e. by constructing a representation of the $su(2)$ algebra in the Moyal formulation.

The Moyal formalism allows this essentially algebraic problem to be reduced to one of solving a set of differential equations. We begin by making the following ansatz for the forms of these functions:

$$J_+ = e^{i\beta} f(\alpha), \quad J_- = e^{-i\beta} f(\alpha) \quad \text{and} \quad J_z = p(\alpha). \quad (37)$$

This ansatz implies an unitary representation and is based on the interpretation of $h = e^{i\beta}$ as a ladder operator which connects states labeled by the eigenvalues of $g = e^{i\alpha}$. Substituting these forms into the commutation relations $[J_z, J_{\pm}]_* = \pm J_{\pm}$ and $[J_+, J_-]_* = 2J_z$ produces

$$\theta \frac{d}{d\alpha} p(\alpha) = 1 \quad \text{and} \quad -\theta \frac{d}{d\alpha} f^2(\alpha) = 2p(\alpha), \tag{38}$$

where $\theta = 2\pi/D$ and $D = 2j + 1$. These equations are easily solved to obtain

$$p(\alpha) = \frac{\alpha}{\theta} + a_1 \quad \text{and} \quad f^2(\alpha) = -\frac{\alpha^2}{\theta^2} - 2a_1 \frac{\alpha}{\theta} + a_2. \tag{39}$$

Here a_1 and a_2 are integration constants that we fix by requiring that the second-order Casimir operator assumes a constant value corresponding to the $j = N/2$ -irrep:

$$J^2 = j(j + 1) = \frac{1}{2}(J_+ * J_- + J_- * J_+) + J_z * J_z = a_2 + a_1^2. \tag{40}$$

This constraint can be satisfied to leading order in j by setting $a_2 = 0$ and $a_1 = -j$. Finally, we arrive at

$$J_+ = e^{i\beta} \sqrt{\frac{2j\alpha}{\theta} - \frac{\alpha^2}{\theta^2}}, \quad J_- = e^{-i\beta} \sqrt{\frac{2j\alpha}{\theta} - \frac{\alpha^2}{\theta^2}} \quad \text{and} \quad J_z = \frac{\alpha}{\theta} - j. \tag{41}$$

It follows from (10) and $g = e^{i\alpha}$ that $\alpha \in [0, 2j\theta] \subset [0, 2\pi)$ since $\theta = 2\pi/(2j + 1)$, and the natural domain of α/θ is therefore $[0, 2j]$. We will use the scaleless variable $x = \alpha/(j\theta) - 1 \in [-1, 1]$ in what follows. The $su(2)$ representation now becomes

$$J_+ = j e^{i\beta} \sqrt{1 - x^2}, \quad J_- = j e^{-i\beta} \sqrt{1 - x^2} \quad \text{and} \quad J_z = jx. \tag{42}$$

By substituting the representation (42) into the Lipkin Hamiltonian (33) we obtain the initial condition, to leading order in j , as

$$H(x, \beta, 0) = jx + \frac{j\lambda}{2}(1 - x^2) \cos(2\beta). \tag{43}$$

The band diagonality of $H(\ell)$ should be reflected in the form of the solution of the flow equation. We note that scattering between states with different spin projections is associated with the $\cos(2\beta)$ term. This suggests that $H(\ell)$ has the form

$$H(x, \beta, \ell) = j[n_0(x, \ell) + n_1(x, \ell) \cos(2\beta)], \tag{44}$$

where n_0 and n_1 are scalar functions. Note that a factor of j , responsible for the extensivity of the Hamiltonian, has been factored out. Upon substituting this form into the flow equation we obtain

$$\frac{\partial n_0}{\partial \ell} = -4n_1 \frac{\partial n_1}{\partial x} \quad \text{and} \quad \frac{\partial n_1}{\partial \ell} = -4n_1 \frac{\partial n_0}{\partial x}, \tag{45}$$

while the flow of an observable O is given by

$$\frac{\partial O}{\partial \ell} = 2 \sin(2\beta) \frac{\partial n_1}{\partial x} \frac{\partial O}{\partial \beta} - 4 \cos(2\beta) n_1 \frac{\partial O}{\partial x}. \tag{46}$$

These equations agree with those derived in [13], although the interpretation of the constituents differs. Next we turn to the matter of extracting the spectrum and expectation values from the solutions of these equations. Since the eigenvalues of H appear on the diagonal of $H(\infty)$ in increasing order, we conclude that $U^\dagger(\infty)|E_n\rangle = |-j + n\rangle$, i.e. the n 'th excited state is mapped to the eigenstate of J_z with spin projection $m = -j + n$. The eigenvalues are given by

$$E_n = \langle E_n | H | E_n \rangle = \langle -j + n | H(\infty) | -j + n \rangle. \tag{47}$$

To calculate this expectation value we note that representation (42) allows $n_0(x, \infty)$, and therefore $H(\infty)$ itself, to be viewed as functions of J_z only. The second matrix element of (47) amounts to simply replacing each occurrence of J_z in $H(\infty)$ by $-j + n$, or equivalently, replacing x by $-1 + n/j$ in $n_0(x, \infty)$. To summarize

$$E_n = j n_0(x = -1 + n/j) \quad \text{for} \quad n = 0, 1, \dots, 2j. \quad (48)$$

The expectation values of a Hermitian observable O may be found using a similar procedure. Since $\langle E_n | O | E_n \rangle = \langle -j + n | O(x, \beta, \infty) | -j + n \rangle$, the quantities of interest are the diagonal elements of the transformed observable $O(x, \beta, \infty)$. The form of $J_{\pm}(\alpha, \beta)$ suggests that $O(\ell)$ may be written as

$$O(x, \beta, \ell) = \sum_{n=0}^{\infty} f_n(x, \ell) \cos(n\beta), \quad (49)$$

where $\cos(n\beta)$ corresponds to an off-diagonal term proportional to $J_+^n + J_-^n$. In particular, the $f_0(x, \infty)$ term contains the desired information about the diagonal entries. Since each f_n may be considered as a function of J_z , we conclude that

$$\langle E_n | O | E_n \rangle = f_0(x = -1 + n/j, \ell = \infty). \quad (50)$$

4.1.1. Numeric results. Solving the flow equations (45) and (46) numerically produces very accurate results for both the spectrum and order parameter. These equations have already been studied in detail in [13], and we only state two results here. Figure 1(a) shows $n_0(x, \ell)$ at large ℓ for three values of the coupling constant λ . At this point in the flow the off-diagonal part of $H(\ell)$ represented by n_1 is already of the order of 10^{-20} , and may be dropped. In order to compare the prediction of (47) with exact results, we calculate the spectrum for $j = 1000$ using direct diagonalization and plot the pairs $(x = -1 + n/j, E_n^{\text{exact}}/j)$ for $n = 0, \dots, j$ as dots. We observe an excellent correspondence for all states and in both phases, with an average error of about 0.05%. Choosing $O(x, \beta, 0) = jx$ equation (46) allows us to calculate the groundstate expectation value of J_z , and therefore also the order parameter $\Omega \equiv 1 + \langle E_0 | J_z | E_0 \rangle / j$. Figure 1(b) shows the result of this calculation together with the exact values for $j = 1000$.

4.2. Example 2: the Dicke model

As a second example we treat the Dicke model [32] using a two-step approach. The flow equation will be applied twice, first to derive an effective Hamiltonian H_{eff} which conserves the number of elementary excitations in the system (see below) and then a second time to diagonalize H_{eff} for a fixed number of these excitations. For this purpose we use the form preserving generator [5, 6, 15]. Previous applications of the flow equations to the Dicke model appeared in [24], and also made use of a $1/N$ expansion.

The Dicke model describes the interaction of N two-state atoms with a single bosonic mode. In terms of collective spin operators the Hamiltonian [33, 34] reads

$$H = J_z + b^\dagger b + \frac{\lambda}{\sqrt{N}} (J_+ + J_-)(b^\dagger + b). \quad (51)$$

Here J_z and J_{\pm} are the $su(2)$ generators in the $j = N/2$ representation, while b^\dagger and b are the creation and annihilation operators of the bosonic mode. The coupling constant λ controls the dipole interaction strength. When $\lambda < 0.5$ the model is in the normal phase [33] and we will restrict ourselves to this case. The $1/\sqrt{N}$ factor ensures that the Hamiltonian remains extensive when the bosonic mode is macroscopically occupied, i.e. when $\langle b^\dagger b \rangle \sim N$.

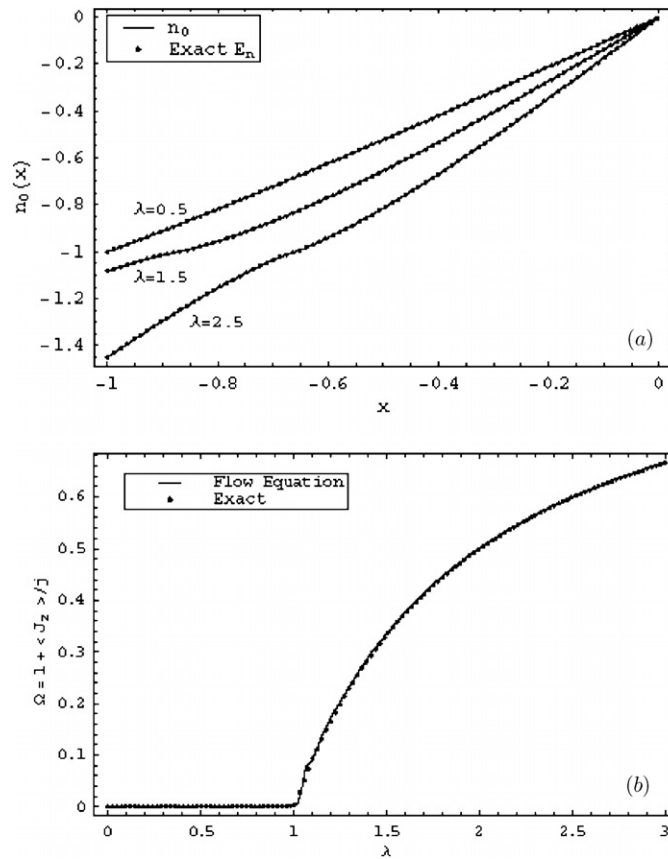


Figure 1. (a) The solution $n_0(x, \ell)$ of equation (45) at large ℓ . The dots represent the exact spectrum for $j = 1000$. For clarity only every twelfth eigenvalue is shown. (b) The order parameter Ω as a function of λ .

Central to our treatment is the operator $Q \equiv J_z + \hat{n} + j$, which acts as a counting operator for the number of elementary excitations or energy quanta in the system. We see that the Hamiltonian (51) contains terms which either increase or decrease the number of excitations by two, or leave it unchanged.

4.2.1. Variables and representations. To account for the model’s two independent degrees of freedom we introduce two pairs of operators $\{g, h\}$ and $\{g', h'\}$ as described in section 3.1. These satisfy the exchange relations

$$hg = e^{-i\theta} gh \quad \text{and} \quad h'g' = e^{-i\theta'} g'h', \tag{52}$$

while operators coming from different pairs commute. As before we proceed to treat these operators as scalar variables and replace the operator product by the Moyal product

$$U * V = UV + i(\theta U_\beta V_\alpha + \theta' U_{\beta'} V_{\alpha'}), \tag{53}$$

where $g = e^{i\alpha}$, $h = e^{i\beta}$, $g' = e^{i\alpha'}$ and $h' = e^{i\beta'}$. The pair g, h is used to represent the spin degree of freedom through the $su(2)$ representation constructed in equation (42) in terms of $x_s = \alpha/(j\theta) - 1 \in [-1, 1]$ and β :

$$J_+ = j e^{i\beta} \sqrt{1 - x_s^2}, \quad J_- = j e^{-i\beta} \sqrt{1 - x_s^2} \quad \text{and} \quad J_z = j x_s. \tag{54}$$

We use the second pair $\{g', h'\}$ to construct an approximate representation of the boson algebra. Since only infinite-dimensional representations of the boson algebra exist, a construction in terms of the finite-dimensional operators g' and h' must constitute an approximation to the exact case. One such construction is

$$b = h'^{\dagger} \sqrt{\bar{g}'}, \quad b^{\dagger} = \sqrt{\bar{g}'} h' \quad \text{and} \quad b^{\dagger} b = \hat{n} = \bar{g}', \tag{55}$$

where $\bar{g}' = -i \log(g')/\theta' = \alpha'/\theta' = \text{diag}(0, 1, 2, \dots, D - 1)$ and $\theta' = 2\pi/D$ with D being the dimension of the truncated boson Fock-space. See the discussion after (41) for details. Denoting the eigenstates of $\bar{g}' = \hat{n}$ by $|n\rangle$, $n = 0, 1, \dots, D - 1$ we see that $b|n\rangle = \sqrt{n}|n - 1\rangle$ and $b^{\dagger}|n\rangle = \sqrt{n + 1}|n + 1\rangle$ for $0 \leq n < D - 1$. (See equations (10) and (11).) The creation operator b^{\dagger} maps the highest state $|D - 1\rangle$ to zero, since $h'|D - 1\rangle = |0\rangle$ and $\bar{g}'|0\rangle = 0$. This amounts to a truncation of the boson Fock-space, and the operators in (55) agree with the truncated forms of the exact infinite-dimensional operators. Proceeding as before, we treat g' and h' as scalars and define α' and β' through $g' = e^{i\alpha'}$ and $h' = e^{i\beta'}$. The representation now becomes

$$b = e^{-i\beta'} \sqrt{\alpha'/\theta' + 1}, \quad b^{\dagger} = e^{i\beta'} \sqrt{\alpha'/\theta'} \quad \text{and} \quad b^{\dagger} b = \alpha'/\theta' \tag{56}$$

which satisfies, to leading order in θ' , the desired commutation relation with respect to the Moyal bracket: $[b, b^{\dagger}]_* = 1$. It is clear that D controls the Fock-space cutoff, and therefore the domain of $b^{\dagger} b = \alpha'/\theta'$. We introduce the variable $x_b = \alpha'/(j\theta') \in [0, C]$, where $C = D/j$ may be chosen arbitrarily large and plays a spectator role in what follows. The representation can now be rewritten as

$$b = \sqrt{j} e^{-i\beta'} \sqrt{x_b + 1/j}, \quad b^{\dagger} = \sqrt{j} e^{i\beta'} \sqrt{x_b} \quad \text{and} \quad b^{\dagger} b = j x_b. \tag{57}$$

It is also useful to define

$$T_q \equiv J_+ b + J_- b^{\dagger} \quad \text{and} \quad x_q \equiv T_q / j^{3/2}. \tag{58}$$

Note that T_q conserves Q and that x_q is scaleless with respect to j . In terms of these variables the Hamiltonian, to leading order in j , is

$$H(x_s, \beta, x_b, \beta') = j [x_s + x_b + \lambda \sqrt{2x_b(1 - x_s^2)} (\cos(\beta - \beta') + \cos(\beta + \beta'))], \tag{59}$$

while the Moyal bracket in (23) becomes

$$[U, V]_* = i(U_{\beta} V_{x_s} - V_{\beta} U_{x_s} + U_{\beta'} V_{x_b} - V_{\beta'} U_{x_b}) / j. \tag{60}$$

4.2.2. Step one. Using the flow equation we wish to transform H into an effective Hamiltonian $H_{\text{eff}} \equiv H(\ell = \infty)$ which commutes with Q and therefore conserves the number of elementary excitations [5, 15]. We choose the generator as $\eta(\ell) = [Q, H(\ell)]$ since this ensures that Q and H_{eff} commute while also restricting the operators appearing in $H(\ell)$ to those which change Q maximally by 2. Unfortunately, the complexity of the resulting non-perturbative flow equation does not permit a direct numerical solution. Instead, we proceed by solving the equation to finite order in the coupling λ . This step is most easily performed using a symbolic processor

such as *Mathematica*. We only state the result up to fourth order here. The details of this calculation can be found in [35]. For $H_{\text{eff}} = \sum_{n=0}^{\infty} \lambda^n H_{\text{eff}}^{(n)}$, we find that

$$\begin{aligned} H_{\text{eff}}^{(0)} / j &= \hat{n} + J_z \\ H_{\text{eff}}^{(1)} / j &= T_q / \sqrt{2} \\ H_{\text{eff}}^{(2)} / j &= (J_z^2 + 2\hat{n}J_z - 1) / 4 \\ H_{\text{eff}}^{(3)} / j &= -T_q(\hat{n} + 4J_z) / (8\sqrt{2}) \\ H_{\text{eff}}^{(4)} / j &= (7T_q^2 + 20J_z - 2\hat{n} + 38\hat{n}J_z^2 + 20J_z^3) / 64, \end{aligned} \tag{61}$$

where, to aid interpretation, we temporarily abuse notation by writing J_z, \hat{n}, T_q for the scaleless variables x_s, x_b, x_q . Note that during the flow new off-diagonal terms involving T_q were generated. We also point out that to first order the effective Hamiltonian is

$$H_{\text{eff}} = J_z + \hat{n} + \frac{\lambda}{\sqrt{2}j} (J_+ b + J_- b^\dagger), \tag{62}$$

which is precisely the RWA approximation in which the model was originally studied; see [33] and references therein.

In order to verify these results we explicitly construct the submatrices corresponding to individual Q -sectors for finite j and to high orders in coupling λ . The resulting matrices are maximally of size $(2j + 1) \times (2j + 1)$. Figure 2 shows the results obtained for the excitation energies $\Delta E_1 = E_1 - E_0$ and $\Delta E_3 = E_3 - E_0$ by applying direct diagonalization to these submatrices. For comparison the first-order (RWA) results and those obtained by diagonalizing H directly are also shown. We observe very good agreement between the exact values and those obtained using H_{eff} .

4.2.3. Step two. Since sectors with different numbers of elementary excitations (i.e. Q eigenvalues) have been decoupled in H_{eff} we may treat each sector individually. When restricted to a single sector the operator J_z is non-degenerate, and the flow generated by $\eta(\ell) = [J_z, H_{\text{eff}}(\ell)]$ will result in a complete diagonalization of H_{eff} . We illustrate this procedure for the first-order case in (62). The initial condition is given by

$$H_{\text{eff}}(x_s, \beta, x_b, \beta', \ell = 0) = j[x_s + x_b + \lambda\sqrt{2x_b(1 - x_s^2)} \cos(\beta - \beta')]. \tag{63}$$

Since we consider Q to be fixed we may set $x_s + x_b + 1 = Q/j \equiv q$. In fact, x_b may be eliminated from the initial condition, leaving

$$H_{\text{eff}}(x_s, \beta, \ell = 0) = j[q - 1 + \lambda\sqrt{2(q - 1 - x_s)(1 - x_s^2)} \cos(\beta)], \tag{64}$$

where β' has been set to zero. Here $q = Q/j$ acts as a parameter labeling the relevant Q -sector. The form of both the initial condition and the flow equation is completely analogous to that of the Lipkin model, and the methods of section 4.1 may be applied here virtually unchanged. The final result is a set of functions $n^{(q)}(x_s)$ corresponding to the diagonal part of $H_{\text{eff}}(\infty)$ for different values of $q = Q/j$. Identifying x_s with J_z/j the eigenvalues for the $Q = qj$ sector are given by $E_n = n_0(x = -1 + n/j, \ell = \infty)$ for $n = 0, 1, \dots, \min(2j, Q)$. Figures 2(c) and (d) show the results of carrying out this procedure numerically. We again find very good agreement with the exact results of the RWA Hamiltonian.

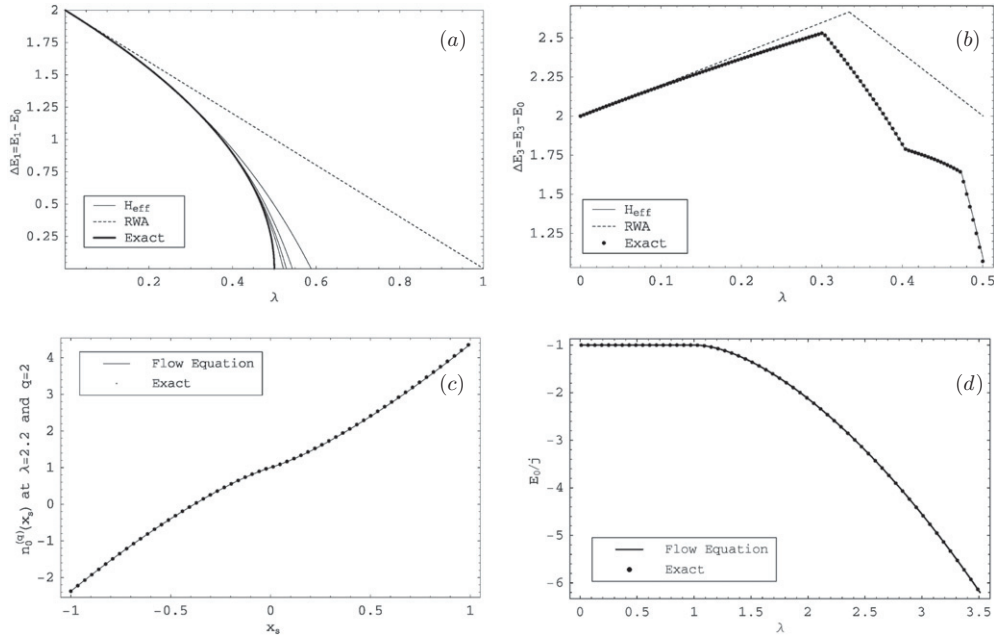


Figure 2. (a) The gap ΔE_1 versus λ . The four solid lines correspond to the results obtained using H_{eff} up to orders of 5, 10, 15, 20 in λ as they appear from right to left. The bold line corresponds to the exact result that $\Delta E_1 = \sqrt{1 - 2\lambda}$ for $j = \infty$ [33]. (b) The gap ΔE_3 versus λ . H_{eff} was constructed for $j = 100$ up to order 15 in λ . The kinks are due to level crossings. (c) The function $n_0^{(q)}(x)$ for $q = Q/j = 2$ and $\lambda = 2.2$ in the $\ell \rightarrow \infty$ limit. (d) The ground state energy together with the exact result for $j = 200$. The exact results shown in figures (c) and (d) are for the first-order effective Hamiltonian in (62).

5. Examples in infinite dimensions: the semi-classical approximation

5.1. Example 1: the quadratic potential

It is well known that in the WKB and path integral formalisms the quadratic potential can be solved exactly. This is due to the absence of higher order corrections in \hbar . It is straightforward to show that the semi-classical flow equations share this property. Let $H = \hat{p}^2 + \epsilon \hat{x}^2$ be a quadratic Hamiltonian and consider the flow generated by $H_0 = \hat{p}^2 + \hat{x}^2$. It is clear that at $\ell = 0$ the Moyal bracket truncates at linear order in \hbar . Indeed, this also holds at $\ell > 0$ since the flowing Hamiltonian retains its quadratic form with only the scalar coefficients flowing toward renormalized values. It follows that the leading-order approximation of the Moyal bracket is exact and that the fixed point $H(\infty) = \sqrt{\epsilon}(\hat{p}^2 + \hat{x}^2)$ is an exact diagonalization of the quadratic Hamiltonian. Further details on the flow equation treatment of this model appear in [36].

5.2. Example 2: the quartic oscillator potential

Next we consider a quadratic potential with an additional quartic term. Flow equations have also been applied to this potential in [36] using both Wegner's and the form preserving generator together with variational techniques. The full Hamiltonian is given by

$$H = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 + \frac{\lambda}{2}\hat{x}^4. \quad (65)$$

Two length scales appear naturally, one associated with the harmonic oscillator terms and the second with the quartic interaction. The former is $L = \sqrt{\hbar/(m\omega)}$, while we define the latter as $L_0 = \sqrt{\hbar_0/(m\omega)}$, where $\hbar_0 = m^2\omega^3/\lambda$. Note that L_0 is independent of \hbar but does depend on the strength of the quartic interaction. We introduce dimensionless position and momentum operators through a rescaling by this second length scale:

$$\hat{x} \rightarrow L_0\hat{x} \quad \text{and} \quad \hat{p} \rightarrow \frac{\hbar_0}{L_0}\hat{p}. \tag{66}$$

The rescaled operators then commute as

$$[\hat{x}, \hat{p}] = i\frac{\hbar}{\hbar_0} = i\alpha. \tag{67}$$

The ratio of length scales squared, α , assumes the role of the parameter in which we expand the Moyal product. The Hamiltonian in the Moyal form now reads

$$H = p^2 + x^2 + x^4, \tag{68}$$

where the energy is expressed in units of $\hbar_0\omega/2$. Note that λ has been absorbed into the length and energy scales, and no longer appears as an explicit parameter in H .

We choose the generator as $\eta(\ell) = [H_0, H(\ell)]_*$ with $H_0 = p^2 + x^2$. H_0 is a regular harmonic oscillator with a non-degenerate spectrum: $H_0|n\rangle = \alpha(2n + 1)|n\rangle$. This is not the optimal choice of generator, since the flowing Hamiltonian will not retain its band diagonal form in the harmonic oscillator basis. Despite this complication the resulting functions are sufficiently well behaved to allow the flow equations to be solved successfully. We contrast this situation with that of the following section on the double-well potential where significantly more sophisticated choices of the generator and basis are necessary, despite Hamiltonian's similar form to the present case. This emphasizes that the construction of the flow equations are not determined solely by the form of the Hamiltonian, but also by the physical consequences of different parameter choices.

The flow equation and the initial conditions can be simplified significantly by transforming to new variables q and θ according to $x = \sqrt{q} \cos(\theta)$ and $p = \sqrt{q} \sin(\theta)$. After a trivial rescaling of ℓ the flow equations read

$$\frac{dH(q, \theta, \ell)}{d\ell} = H_q H_{\theta\theta} - H_\theta H_{q\theta} \tag{69}$$

along with the initial condition

$$H(q, \theta, 0) = q + q^2 \cos^4(\theta). \tag{70}$$

Since H_0 is non-degenerate we expect $H(\infty)$ to be diagonal in the harmonic oscillator basis with eigenvalues appearing in increasing order. As before we conclude that for an eigenvalue E_n and eigenstate $|E_n\rangle$ it holds that

$$E_n = \langle E_n | H | E_n \rangle = \langle n | H(\infty) | n \rangle. \tag{71}$$

Since $H(\infty)$ is diagonal it will be a function of $q = H_0$ only, and the θ dependence should vanish. We can then find E_n by replacing each instance of H_0 by its eigenvalue

$$E_n = \langle n | H(H_0, \infty) | n \rangle = H(q = \alpha(2n + 1), \infty) \quad n = 0, 1, 2, \dots \tag{72}$$

We emphasize that equations (69) and (68) treat the coupling constant λ non-perturbatively, even though λ appears in the expansion parameter α . This apparent contradiction is resolved by keeping in mind that the flow equation in (69) was derived in a semi-classical approximation and that at no stage do we neglect terms based solely on the powers of λ they contain. This point becomes clear by noting that due to the scale transformation, both the dimensionless

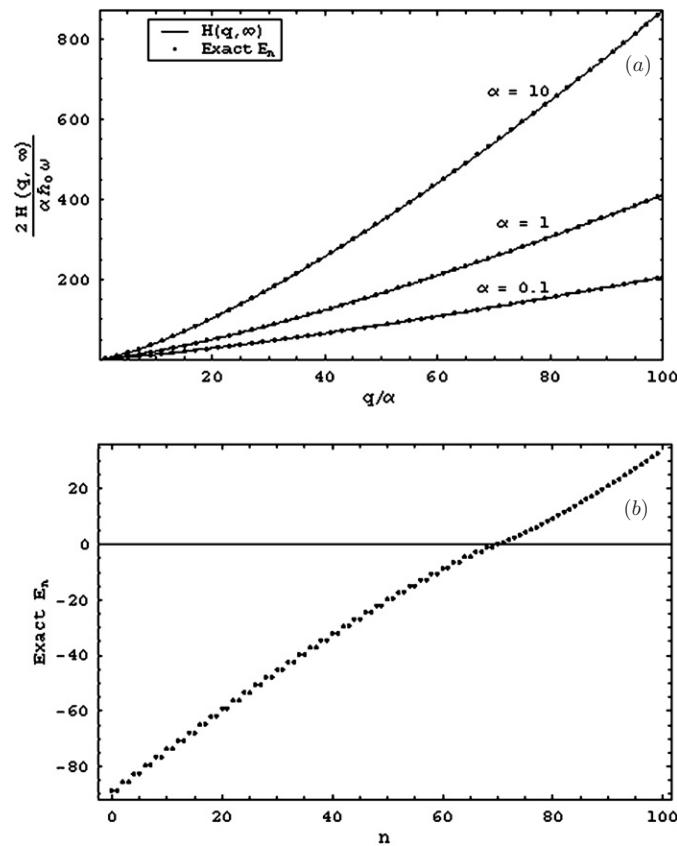


Figure 3. (a) The first fifty exact eigenvalues for the quartic potential for $\alpha = 0.1, 1, 10$ as obtained using the flow equations. (b) The first hundred exact eigenvalues for the SDW potential with $\epsilon \ll -1$. Note that the degenerate pairs lead to step-like behavior in the spectrum.

Moyal variables x and p are in fact proportional to $\sqrt{\lambda}$. In contrast to a regular perturbative expansion we do not limit the powers of λ (and therefore x and p) appearing in $H(x, p, \ell)$, but rather treat it as a completely general function. Were we to transform the resulting function $H(x, p, \infty)$ back to non-dimensional variables the λ dependency would become explicit, and non-perturbative nature of the result would be clear.

5.2.1. Numerical results. Equation (69) is a $(2 + 1)$ -dimensional PDE which we solve numerically. It was found that transforming to $r = \sqrt{q}$ aided in the stability of the numerical methods. The flow equation was integrated until the θ dependence was sufficiently small, at which point the Hamiltonian is almost completely diagonal. Figure 3(a) shows the flow equation results for the spectrum together with exact values for a number of α values. For $\alpha = 0.1$, the relative error was about 2.83% for the ground state and dropped to 0.000481% for the last (50th) eigenvalue appearing in the figure. On average the relative error was less than 0.1%. We note that even at seemingly large values of α the agreement with exact results is very good. This suggests that in the power series of $H(q, \infty)$ around $\alpha = 0$ the coefficients of higher order terms are very small, and dominate even high powers of α .

Table 1. A comparison of the energy eigenvalues obtained via the WKB and flow equation methods. All energies are given in units of $\alpha\hbar_0\omega/2$.

		Method			Relative error (%)	
		Exact	WKB	Flow equations	WKB	Flow equations
$\alpha = 0.1$	E_0	1.065 285 510	1.035 155 662	1.035 098 939	2.83	2.83
	E_1	3.306 872 013	3.285 483 080	3.285 517 078	0.647	0.644
	E_2	5.747 959 269	5.730 954 235	5.731 013 951	0.296	0.295
	E_{48}	198.284 6571	198.281 9353	198.283 7052	0.001 37	0.000 0178
	E_{49}	203.498 0353	203.495 3503	203.497 0574	0.001 32	0.000 0356
$\alpha = 1$	E_0	1.392 351 642	1.250 768 760	1.250 057 196	10.2	10.2
	E_1	4.648 812 704	4.592 560 473	4.592 609 691	1.21	1.21
	E_2	8.655 049 958	8.613 057 729	8.613 165 445	0.485	0.484
	E_{48}	395.416 9465	395.411 1175	395.437 8920	0.001 47	0.005 30
	E_{49}	406.200 9974	406.195 2475	406.222 2788	0.001 42	0.005 24
$\alpha = 10$	E_0	2.449 174 072	2.061 139 563	2.063 524 463	15.8	15.7
	E_1	8.599 003 455	8.489 468 733	8.492 548 519	1.27	1.23
	E_2	16.635 921 49	16.545 823 60	16.540 478 11	0.542	0.574
	E_{48}	836.811 5578	836.799 0299	836.090 9037	0.001 50	0.0861
	E_{49}	859.837 0953	859.824 7368	858.949 8280	0.001 44	0.103

Since both the semi-classical flow equation and the WKB method [37] are based on expansions in \hbar , it would be interesting to compare their results for the quartic potential. This is the content of table 1, which shows that the flow equation results are very close to those of the WKB for both the low-lying and excited states. The weaker performance of the flow equations at high energies is believed to be mainly due to discretization and edge effects which plague the numerical solutions of the PDEs.

5.3. Example 3: the 1D symmetric double-well potential

As a final example we consider the quartic oscillator with a negative x^2 term

$$H(\hat{p}, \hat{x}) = \hat{p}^2 + (1 + \epsilon)\hat{x}^2 + \hat{x}^4, \tag{73}$$

where $\epsilon < -1$. The dimensionless operators \hat{x} and \hat{p} were introduced in the previous section and satisfy $[\hat{x}, \hat{p}] = i\alpha$, with α being an expansion parameter. All energies are expressed in units of $\hbar_0\omega/2$. This Hamiltonian is the well-known symmetric double-well potential consisting of two energy minima with depth $-(1 + \epsilon)^2/4$. Classically, one would expect the low-lying eigenstates to occur in degenerate pairs localized in each of the two wells. This picture is perturbed by quantum tunneling effects which lift the degeneracies slightly at low energies. As one moves up the spectrum, the splitting grows until the two sets merge as the central hump at $E = 0$ is crossed. The greater the well depth the closer the low-lying eigenvalues are to being completely degenerate. These almost-degenerate states occur in pairs which are respectively even and odd under parity transformations. Ideally we would like to obtain the energy splitting of these pairs, since this is a truly non-perturbative phenomenon.

The similar form of this Hamiltonian and the quartic oscillator may suggest that the flow equation of the previous section is also applicable here. However, this approach will eventually fail due to the lack of smoothness of the relevant functions. This can be understood by considering figure 3(b), which shows the exact eigenvalues obtained through numerical diagonalization. The almost degenerate pairs lead to step-like behavior in the spectrum as a function of the state label $n = 0, 1, 2, \dots$. If $E_n = H(q = \alpha(2n + 1), \infty)$, this implies

that $H(q, \infty)$ is not slowly varying on a length scale of α , which violates the smoothness condition and renders our truncation of the Moyal bracket invalid. The origin of this behavior is the fact that H and H_0 are not irreducible on the entire Hilbert space and this allows different subspaces to flow independently. In this case it is not possible to describe the flow of independent subspaces with the same smooth function of Moyal variables. To overcome this problem we first identify the two subspaces concerned by writing H in terms of boson creation and annihilation operators as

$$H(a^\dagger, a) = \alpha(2n + 1) + \epsilon \frac{\alpha}{2}(2n + 1) + \frac{\alpha^2}{4}(3 + 6n + 6n^2) + a^\dagger a^\dagger \left[\epsilon \frac{\alpha}{2} + \frac{\alpha^2}{2}(3 + 2n) \right] + \text{h.c.} \\ + a^\dagger a^\dagger a^\dagger a^\dagger \frac{\alpha^2}{4} + \text{h.c.} \tag{74}$$

Here we have made the substitutions

$$x = \sqrt{\frac{\alpha}{2}}(a^\dagger + a), \quad p = i\sqrt{\frac{\alpha}{2}}(a^\dagger - a) \quad \text{and} \quad n = a^\dagger a. \tag{75}$$

This form makes it clear that H only changes the number of boson by 0, 2 or 4 and that there is no mixing of subspaces with an even or odd number of bosons. It follows that the even and odd sectors flow independently, and should be described by separate functions of Moyal variables. We can identify these functions by introducing an appropriate basis for each sector. To be exact, we perform the following mapping:

$$\text{old basis} \quad \begin{cases} \text{even:} & |2n\rangle \\ \text{odd:} & |2n + 1\rangle \end{cases} \rightarrow |n\rangle \text{ new basis}, \quad n = 0, 1, 2, 3, \dots \tag{76}$$

The $|n\rangle$ states are themselves harmonic oscillator states with creation and annihilation operators B^\dagger and B ladder between them

$$B^\dagger |n\rangle = \sqrt{n + 1} |n + 1\rangle \quad \text{and} \quad B |n\rangle = \sqrt{n} |n - 1\rangle. \tag{77}$$

In terms of the original bosonic operators these are given by

$$B^\dagger = \frac{1}{\sqrt{2\hat{n} - 2}} a^\dagger a^\dagger, \quad B = aa \frac{1}{\sqrt{2\hat{n} - 2}} \quad \text{and} \quad \hat{N} = B^\dagger B = \frac{\hat{n}}{2} \tag{78}$$

in the even sector, and

$$B^\dagger = \frac{1}{\sqrt{2\hat{n}}} a^\dagger a^\dagger, \quad B = aa \frac{1}{\sqrt{2\hat{n}}} \quad \text{and} \quad \hat{N} = B^\dagger B = \frac{\hat{n} - 1}{2} \tag{79}$$

in the odd sector. It is straightforward to show that B and B^\dagger obey $[B, B^\dagger] = 1$. Having found separate descriptions for each sector, we return to the position-momentum picture by introducing \hat{X} and \hat{P} as

$$B^\dagger = \frac{1}{\sqrt{2\alpha}}(\hat{X} - i\hat{P}) \quad \text{and} \quad B = \frac{1}{\sqrt{2\alpha}}(\hat{X} + i\hat{P}), \tag{80}$$

where $\hat{N} = B^\dagger B = (2\alpha)^{-1}(\hat{P}^2 + \hat{X}^2 - \alpha)$. To find the Moyal representation of H in terms of X and P for a particular sector we need to write $H(a^\dagger, a)$ of (74) in terms of B and B^\dagger and then transform to \hat{X} and \hat{P} . In the resulting expression we order the \hat{X} 's to the right of the \hat{P} 's and then replace them by the Moyal variables X and P . The final ordering procedure can be carried out using the following two identities which are valid up to linear order in α .

- (1) Let $m_i = m_i(X, P)$ $i = 1, \dots, k$ be a set of functions of Moyal variables. The Moyal product $m_1 * m_2 * \dots * m_k$ is given by

$$m_1 * m_2 * \dots * m_k = \left(\prod_{j=1}^k m_j \right) \left[1 + i\alpha \sum_{j<l} \frac{1}{m_j m_l} \frac{\partial m_j}{\partial X} \frac{\partial m_l}{\partial P} \right] + O(\alpha^2). \tag{81}$$

(2) Let $m = m(X, P)$ be another such function representing the (properly ordered) operator $\hat{m} = m(\hat{X}, \hat{P})$. Applying the result above to the Taylor series of a function f gives the Moyal representation of $f(\hat{m})$ as

$$f(m) + \frac{1}{2}[m * m - m^2]f^{(2)}(m) + O(\alpha^2). \tag{82}$$

Using these results the initial conditions follow from a straightforward but tedious calculation. We find that

$$H_E(q, \theta, 0) = H^{(0)} - \frac{\alpha}{2}H^{(1)} \quad \text{and} \quad H_O(q, \theta, 0) = H^{(0)} + \frac{\alpha}{2}H^{(1)}, \tag{83}$$

where

$$H^{(0)} = \frac{q}{2}(4 + 2\epsilon + 3q) + q(\epsilon + 2q)\cos(\theta) + \frac{q^2}{2}\cos(2\theta) \tag{84}$$

$$H^{(1)} = (2 + \epsilon + 3q) + (\epsilon + 4q)\cos(\theta) + q\cos(2\theta) \tag{85}$$

and $X = \sqrt{q}\cos(\theta)$ and $P = \sqrt{q}\sin(\theta)$ as before. The initial condition also contains terms proportional to $i\alpha$ which have been dropped in the expression above. We argue that this is permitted, based on the following two observations. First, note that these terms cannot affect the real part of $H(\ell)$ to lower than second order in α since their product, although real, always contains α^2 . Secondly, it is known that $H(\infty)$ is diagonal and a function of \hat{N} only. It follows that the Moyal representation of $H(\infty)$ has the form of (82) where the imaginary part is the result of our ordering convention for \hat{X} and \hat{P} . For the purposes of evaluating $H(\hat{N}, \infty)$ at $\hat{N} = 0, 1, 2, \dots$ it is clear that only the real part of $H(q, \infty)$ is needed and we may therefore neglect the imaginary terms from the outset. We also note that in both sectors $H(0)$ is of the form

$$H(q, \theta, 0) = n_0(q, 0) + n_1(q, 0)\cos(\theta) + n_2(q, 0)\cos(2\theta). \tag{86}$$

This concludes the calculation of the initial conditions. We now turn to the construction of an appropriate generator. The two main considerations here are the form of $H(\ell)$ during the flow and the nature of the fixed point $H(\infty)$. In particular, we want $H(\infty)$ to be diagonal in the \hat{N} basis and $H(\ell)$ to have the form of (86). The form preserving generator of section 2 with $Q = \hat{N}$ meets these requirements, and is represented in terms of Moyal variables as

$$\eta(\ell) = T_+(\ell) - T_-(\ell) = -i[n_1(q, \ell)\sin(\theta) + n_2(q, \ell)\sin(2\theta)]. \tag{87}$$

This is seen to be the correct form by noting that $\cos(\theta)$ and $\cos(2\theta)$ are proportional, up to factors involving q , to $a + a^\dagger$ and $aa + a^\dagger a^\dagger$ respectively. Substituting these expressions into the flow equation

$$\frac{dH}{d\ell} = i\alpha(H_\theta\eta_q - \eta_\theta H_q) \tag{88}$$

gives

$$\begin{aligned} \frac{dn_0}{d\ell} &= -\frac{1}{2}\frac{\partial n_1^2}{\partial q} - \frac{\partial n_2^2}{\partial q} \\ \frac{dn_1}{d\ell} &= -n_1\frac{\partial n_0}{\partial q} - 2n_2\frac{\partial n_1}{\partial q} - n_1\frac{\partial n_2}{\partial q} \\ \frac{dn_2}{d\ell} &= -2n_2\frac{\partial n_0}{\partial q}. \end{aligned} \tag{89}$$

Note that we only consider the flow equation to lowest order, whereas the initial conditions include higher order corrections. Our treatment of these corrections is therefore not entirely consistent, but despite this the results exhibit the correct qualitative behavior.

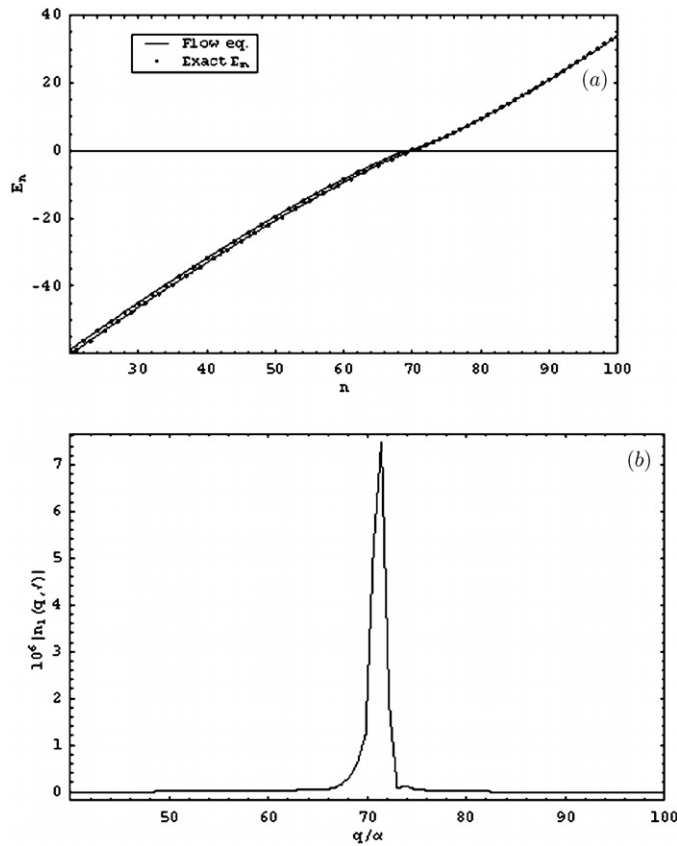


Figure 4. (a) First hundred eigenvalues of the SDW potential with $\epsilon = -20$ and $\alpha = 1/4$. Both the exact and flow equation values are shown. The two solid lines correspond to the solutions of the odd and even sectors. (b) The off-diagonal function $n_1(q, \ell)$ at $\ell \gg 0$ for the odd sector.

Since $[\hat{N}, H(\infty)] = 0$, we expect that $n_1(q, \infty) = n_2(q, \infty) = 0$. Following the same argument as in the previous example we conclude that within a specific sector

$$E_N^{\text{even/odd}} = n_0(\alpha(2N + 1), \infty) \quad \text{where } N = 0, 1, 2, \dots \quad (90)$$

By combining the results of the two sectors we find that $E_n = E_{n/2}^{\text{even}}$ and $E_n = E_{(n-1)/2}^{\text{odd}}$ when n is even and odd respectively.

5.3.1. Numerical results. Figure 4(a) illustrates how the solutions of the flow equation in the two sectors are combined to obtain the first 100 eigenvalues of H . It is clear that the near degeneracy of odd–even pairs at negative energies is easily dealt with by treating each sector individually. Also note that, to lowest order, the initial conditions of the two sectors in (83) are the same, and the absence of degeneracy at positive energies must therefore be due to the higher order corrections we included in the initial conditions. The accuracy of the flow equation results is very good away from $E = 0$, with typical relative errors of a fraction of a per cent. The loss of accuracy at $E = 0$ coincides with the very slow convergence of the flow equation at this point. Figure 4(b) shows the off-diagonal function $n_1(q, \ell)$ at large ℓ exhibiting a sharp spike at the point where the eigenvalues change the sign. The reason for

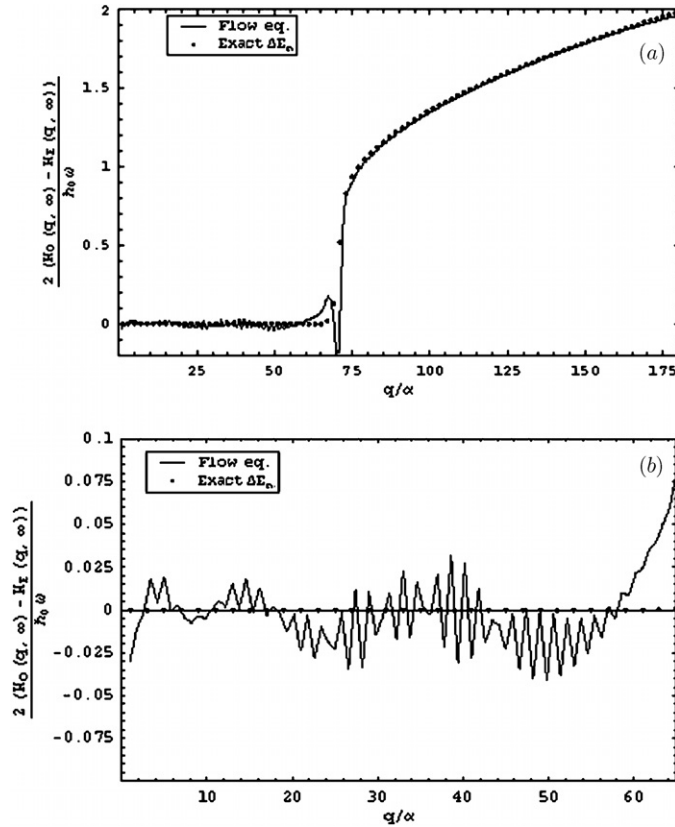


Figure 5. (a) The splitting of odd–even pairs found using the flow equations, together with the exact results. Here $\epsilon = -20$ and $\alpha = 1/4$. (b) Close up of the region $q/\alpha \in [0, 64]$

this slow convergence is that this is a point of inflection of $n_0(q, \infty)$ where the derivative, and therefore the gap between successive eigenvalues, tends to zero. It is well known [1] that the off-diagonal matrix element m_{ij} of $H(\ell)$ decays like $\exp(-(E_{i-1} - E_{j-1})\ell^2)$ at large ℓ , which implies very slow convergence in the presence of degeneracies. The WKB method also suffers a marked decrease in accuracy at this transition point.

From figures 4(a) and 5(a) it is clear that the flow equations correctly predict the presence of near degenerate pairs at negative energy. However, it is not presently known if the very small splitting of these pairs can be calculated using this method. As we see in figures 5(a) and 5(b) numerical errors dominate the gap calculation at $E < 0$ and make any prediction of the splitting impossible. Furthermore, since this is such a small effect, one may be forced to also include higher order corrections in the flow equation itself.

6. Conclusions

We have presented several examples that show quite convincingly that the Moyal implementation of flow equations presents a viable non-perturbative approach to quantum many-body systems. The main advantage of this approach is the natural appearance of a small parameter, either the inverse of the dimensionality of the Hilbert space or \hbar , and a

systematic method of expansion in this parameter. This expansion treats the coupling constant non-perturbatively, i.e., it amounts to summing, at a given order in this expansion, certain classes of diagrams in perturbation theory to all orders.

There are, however, a number of practical difficulties facing this approach. These are (1) the construction of the initial conditions (2) large derivatives that prevent the truncation of the flow equation to lowest order and (3) numerical accuracy in solving for small non-perturbative quantities, such as the ground state splitting in the symmetric double-well potential. Possible resolutions of, at least, the first two problems have been suggested. For the first problem, the algebraic approach presented in section 4, which constructs Moyal based representations of the algebra of operators in terms of which the Hamiltonian is written, offers a very viable possibility. The reason for this is that, generically, any one- plus two-body Hamiltonian is linear and quadratic in the generators of some (possibly infinite-dimensional) algebra. The second problem can, in many instances, be avoided by finding the invariant subspaces of the Hamiltonian. Generically, the function appearing in the flow equation behaves smoothly on these subspaces, but any attempt to describe these subspaces simultaneously is doomed to failure as the flow in the decoupled subspaces is, in principle, completely uncorrelated. The numerical implementation of the flow equations remains, in general, problematic. However, it was also clearly demonstrated that a judicious choice of generator may considerably simplify the flow equation, thereby rendering it amenable to accurate numerical analysis. Unfortunately, no generic algorithm to identify this generator exists, and it must be done on a case by case basis.

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