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The quartic oscillator: a non-perturbative study by continuous unitary transformations

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Abstract
The quantum quartic oscillator is investigated in order to test the many-body technique of the continuous unitary transformations. The quartic oscillator is sufficiently simple to allow a detailed study and comparison of various approximation schemes. Due to its simplicity, it can be used as a pedagogical introduction to the unitary transformations. Both the spectrum and the spectral weights are discussed.

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1. Introduction

Quantum many-body systems often can be simplified considerably by choosing an appropriate basis. This is the first step where the qualitative understanding of the system enters. If the problem is first formulated in a basis which is not optimum for the subsequent treatment it is reasonable to change the basis. This is a unitary transformation. Famous examples of such changes of basis are the fermionic one that leads to the wavefunction of the superconducting BCS phase or the bosonic Bogoliubov transformation which leads to the spin waves in a Heisenberg quantum antiferromagnet. These examples refer to mean-field treatments. The complete solution of a many-body problem by a simple analytical transformation is rarely possible.

Ten years ago, the proposal was made to use unitary transformations beyond the single particle level [1–3]. The unitary transformation is performed in a continuous fashion whence the name continuous unitary transformation (CUT). This means that it is parametrized by a continuous parameter l running from 0 to ∞. At $l = 0$ the Hamiltonian is unchanged and at $l = \infty$ it is in its final form. The fundamental idea is that the transformation at a later stage, i.e., at larger values of l, can take into account the changes introduced already at an earlier stage. The transformation can be set up such that processes at larger energy are treated

before those at lower energies. Then the transformation has properties similar to Wilson's renormalization group approach [4]. The objective is of course to simplify the model by the transformation. At best, the final Hamiltonian has become diagonal.

The aim of the present paper is to illustrate the CUT approach, and to study it for a simple model where exact (numerical) data are also easily accessible. The simplicity of the model permits us to present the equations on the basic level and also to go to higher orders. Our presentation is intended to serve as an introduction to the CUT method. This will enable the interested reader to generalize the approach to more elaborate models.

The model of our choice is the quantum anharmonic oscillator which is defined by the usual quadratic kinetic energy and a potential with quadratic and quartic parts. We will abbreviate the oscillator comprising both a quadratic and a quartic part in the potential by QO; the one which has only a quartic one is called the pure quartic oscillator (PQO). This model has often been investigated as a testbed for more complicated situations, e.g., it was used to test other renormalization treatments [5, 6].

The bottom line of our investigation is that the CUT method works extremely well providing very good quantitative results. The starting point of the CUTs can easily be optimized by incorporating prior understanding of the physics of the underlying model. Then only very moderate effort suffices to obtain satisfactory results.

Following this introduction, we present basic facts and insights about the CUTs. In section 3 results for the energetically lowest states of the QO and the PQO will be shown for various ways to conduct the transformation. Spectral weights will also be computed in this section. In section 4 we discuss in which way the CUT approach can be systematically improved. Section 5 concludes the article.

2. Basics about the CUTs

Before addressing the anharmonic oscillator, it is worthwhile to study the harmonic oscillator in order to become familiar with the CUTs.

2.1. Method

A given Hamiltonian H can be diagonalized by a suitable unitary transform U ($UU^\dagger = \mathbb{I}$). But it is usually a very hard task to find this transform U. The idea of Wegner [1] (and independently of Głazek and Wilson [2, 3]) was to diagonalize the Hamiltonian in a continuous way starting from the original Hamiltonian $H = H(0)$. A flowing Hamiltonian is defined by $H(l) = U^\dagger(l)HU(l)$ depending on the parameter l such that H ($l = \infty$) is decisively simpler.

The continuous transform is equivalent to performing infinitely many infinitesimal unitary transforms $\mathrm{e}^{-\eta(l)\,\mathrm{d}l}$ with the generator $\eta(l) = -U^\dagger(l)\partial_l U(l)$. The flow equation

$$\partial_l H(l) = [\eta(l), H(l)] \tag{1}$$

defines the change of the Hamiltonian. Of course, the whole transformation $U(\infty) = \mathcal{L}\exp\left(-\int_0^\infty \eta(l)\,\mathrm{d}l\right)$ can also be given in one formal expression. Note, however, that this requires the use of the l-ordering operator $\mathcal{L}$ which sorts from left to right according to ascending values of l. This means that the whole transformation operator can be extremely complicated. For simple models, however, the explicit transformation can also be written down.

The crucial point is to choose the generator η which leads to a simplification of the Hamiltonian. Wegner proposed to take the commutator between the diagonal part H_d and the non-diagonal part H_nd in a given basis. This means that the generator reads

$\eta_{\mathrm{W}}(l) = [H_{\mathrm{d}}(l), H_{\mathrm{nd}}(l)] = [H_{\mathrm{d}}(l), H(l)]$. In the basis of the eigenstates of H_{d} the generator thus reads

$$\eta_{i,j}(l) = (\varepsilon_i(l) - \varepsilon_j(l))H_{i,j}(l). \tag{2}$$

For finite matrices, this choice was proven [1] to achieve

$$[H_{\mathrm{d}}(\infty), H(\infty)] = 0. \tag{3}$$

If $H_{\mathrm{d}}(\infty)$ is non-degenerate this equation implies that $H(\infty)$ is diagonal. Otherwise it implies block-diagonality with respect to the degenerate subspaces of $H_{\mathrm{d}}(\infty)$. An extension of this proof to infinite matrices is given in appendix A. Note that there is an enormous freedom in what one considers to be diagonal and non-diagonal. For practical calculations the only restriction on H_{d} should be that it can easily be diagonalized.

For Hamiltonians of the form of band matrices, Mielke proposed another generator involving the sign of the difference of the vector indices (see below). This generator preserves the band structure during the flow [7] which is not the case for Wegner's generator. Independently, Knetter and Uhrig observed that a generator based on the sign of the difference of the particle number allows the construction of particle-number conserving effective Hamiltonians [8, 9]. If Q is the operator counting the number of elementary excitations and the matrix elements of η in the eigen basis of Q are chosen to be

$$\eta_{i,j}(l) = \mathrm{sgn}(q_i(l) - q_j(l))H_{i,j}(l) \tag{4}$$

then the final Hamiltonian satisfies $[Q, H(\infty)] = 0$. Furthermore, one can show that this type of generator sorts the eigen values in ascending order of the particle number of the corresponding eigen vectors [7, 9]. Analogous generators were also used by Stein [10, 11] for models where the sign-function is not required since only one finite absolute value of $\Delta q := q_i - q_j$ occurs. For instance, if $\Delta q = 0, \pm 2$ the sign-function only changes the scale of l. But for $\Delta q = 0, \pm 2, \pm 4$ the sign is essential.

In the following, the generators of Wegner's type will be denoted by the subscript W; the generators characterized by the sign as introduced by Mielke, Knetter and Uhrig will be denoted by the subscript MKU. Any coefficient g without argument appearing in the Hamiltonian or in the generator stands for the running coefficient $g(l)$. Their initial values are denoted by $g^{(\mathrm{B})}$ (bare) and their final values by $g^{(\mathrm{R})}$ (renormalized).

2.2. Two solvable models

We illustrate the above for easily solvable models, namely a two-level system and a harmonic oscillator. The Hamiltonians read

$$H_2 = E\mathbb{I} - \frac{\omega}{2}\sigma^z + \frac{e}{2}\sigma^x, \tag{5a}$$

$$H_{\mathrm{HO}} = E\mathbb{I} + \omega a^\dagger a + \frac{d}{2}(a^{\dagger 2} + a^2), \tag{5b}$$

where σ^i are Pauli matrices, and a and $a^\dagger$ are bosonic annihilation and creation operators satisfying the commutation relation $[a, a^\dagger] = 1$.

Let us first consider the two-level system. The counting operator is $Q = (\mathbb{I} - \sigma^z)/2$. Hence, the MKU generator is given by $\eta_{\mathrm{MKU}} = -(e/2)\,\mathrm{i}\sigma^y$. The flow equations read

$$\partial_l E = 0 \tag{6a}$$

$$\partial_l \omega = e^2 \tag{6b}$$

$$\partial_l e = -\omega\, e. \tag{6c}$$

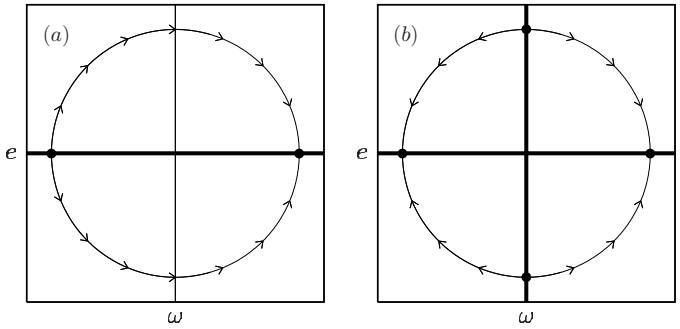

Figure 1. Flows for the two-level system. (*a*) Depicts the flow from the MKU generator; (*b*) the one from Wegner's generator. Thick lines represent lines of fixed points; the dots represent the fixed points of the particular circular trajectory shown. The arrows indicate the direction of the flows for increasing l.

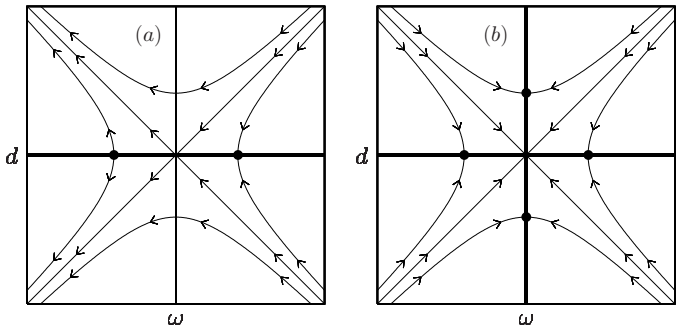

Figure 2. Flows for the bosonic oscillator. (*a*) MKU generator and (*b*) Wegner's generator. Thick lines represent lines of fixed points, and the dots represent the fixed points reached for the particular hyperbolic trajectories shown. The arrows indicate the direction of the flows for growing l.

The diagonal part of the Hamiltonian is the one proportional to ω. Thus Wegner's generator is found to be equal to $\eta_{\mathrm{W}} = [H_{\mathrm{d}}, H_{\mathrm{nd}}] = [-(\omega/2)\sigma^z, (e/2)\sigma^x] = \omega\eta_{\mathrm{MKU}}$. So the flow equations are the same as above if we rescale the continuous parameter $l \to l'$ with $\mathrm{d}l' = \omega(l)\,\mathrm{d}l$ and $l'(l=0) = 0$. The flow trajectories in (ω, e) space are circles since $\omega^2 + e^2 = R^2$ is a constant of the flow, see figure 1. Thus the diagonalized Hamiltonian has the coefficients $\omega^{(\mathrm{R})} = \sqrt{R} = \sqrt{\omega^{(\mathrm{B})2} + e^{(\mathrm{B})2}}$ and $E^{(\mathrm{R})} = E^{(\mathrm{B})}$.

Second, we consider the bosonic oscillator for which the counting operator is $Q = a^\dagger a$. So the MKU generator is $\eta_{\mathrm{MKU}} = d/2(a^{\dagger 2} - a^2)$ and the flow equations read

$$\partial_l E = -d^2 \tag{7a}$$

$$\partial_l \omega = -2d^2 \tag{7b}$$

$$\partial_l d = -2\omega d. \tag{7c}$$

The canonical choice of the diagonal part is $H_{\mathrm{d}} = \omega a^\dagger a$. Thus we have again $\eta_{\mathrm{W}} = \left[\omega a^\dagger a, d/2\left(a^{\dagger 2} + a^2\right)\right] = \omega\eta_{\mathrm{MKU}}$ so that the flow trajectories of both generators are the same. The expression $\omega^2 - d^2$ is a constant of the flow so that the trajectories are hyperbolae as shown in figure 2. For a Hermitian Hamiltonian bounded below, i.e., $\omega > |d|$ (see

below), the final coefficients of the diagonalized Hamiltonian read $\omega^{(\mathrm{R})} = \sqrt{{\omega^{(\mathrm{B})}}^2 - {d^{(\mathrm{B})}}^2}$ and $E^{(\mathrm{R})} = E^{(\mathrm{B})} + (\omega^{(\mathrm{B})} - \omega^{(\mathrm{R})})/2$. The energy is found by integration of $\partial_l E = \partial_l \omega/2$.

As expected from the rescaling $\mathrm{d}l \to \mathrm{d}l' = \omega\,\mathrm{d}l$ the topologies of both flows are the same. The directions are the same for positive values of ω. Only for negative values of ω do the directions differ. The coincidence of the topologies of the flows for both choices of the generator is special to the simple systems under study here. It is not a general feature for more complicated, generic Hamiltonians.

2.3. Remarks

First, we want to stress that the CUTs exactly diagonalize these simple Hamiltonians. Note that for the harmonic oscillator, the CUTs are infinitesimal Bogoliubov transformations whose total effect corresponds to the single-step Bogoliubov transformation diagonalizing the Hamiltonian [12]. This was to be expected since there is only one unique way, except for phases, to diagonalize non-degenerate problems.

Second, we see that Wegner's generator always leads to a fixed point. This does not need to correspond to a final diagonal Hamiltonian when there are degeneracies as is the case for $\omega = 0$. In contrast, the MKU generator is not sensitive to degeneracies, but it does not always lead to a fixed point. A fixed direction may occur as seen in figure 2(a)[4]. The flow in figure 2(a) is similar to the Kosterlitz–Thouless flow. The fixed directions are reached when the Hamiltonian is unbounded below, i.e. $\omega < |d|$. In this case the proof of convergence indeed fails[5]. A possible cure for this problem is to diagonalize $-H$, or what amounts to the same, to revert the flows [12]. Physically, Hamiltonians unbounded below occur only for open physical systems whose treatment requires special care. This is beyond the scope of the present investigation. It is a general feature that Wegner's generator always leads to a fixed point and that it is stopped by degeneracies. In contrast the MKU generator is insensitive to degeneracies, but it may fail to converge to a fixed point.

3. The quartic oscillator

3.1. Model and notation

The Hamiltonian of the anharmonic oscillator under study is in first quantization

$$H = \tfrac{1}{2}(P^2 + \omega^2 X^2) + \lambda X^4, \tag{8}$$

where λ is a positive constant. We will consider two cases. For $\omega = 0$, we consider the pure quartic oscillator (PQO) for which a rescaling $X \to X/\alpha$, $P \to \alpha P$ and $H \to H/\alpha^2$ leads to a unique Hamiltonian. Choosing $\alpha^6 = 6\lambda$ it reads

$$H = \tfrac{1}{2}P^2 + \tfrac{1}{6}X^4. \tag{9}$$

For $\omega \neq 0$, we use another rescaling to bring the Hamiltonian in the form

$$H = \tfrac{1}{2}(P^2 + X^2) + \lambda X^4. \tag{10}$$

The Hamiltonian (10) will be called QO in the following.

Both Hamiltonians have been studied numerically, see for instance [13]. Nowadays, they can be diagonalized numerically on a workstation in seconds, so that we can easily check the quality of our approximations.

[4] See [17] for a detailed discussion of fixed directions.

[5] The proofs of convergence that can be found for the MKU generator [7, 9] and for Wegner's generator [1] are valid for finite matrices. In appendix A, the proof of convergence for Wegner's generator is extended to infinite matrices.

For both Hamiltonians, we introduce annihilation and creation operators

$$a(\sigma) = \frac{1}{\sqrt{2}}\left(\frac{X}{\sigma} + \mathrm{i}\sigma P\right) \tag{11a}$$

$$a^\dagger(\sigma) = \frac{1}{\sqrt{2}}\left(\frac{X}{\sigma} - \mathrm{i}\sigma P\right), \tag{11b}$$

where σ is a free parameter which will be determined later. Recall that the QO reduces to the conventional harmonic oscillator for $\lambda = 0$. It is diagonalized by using $\sigma = 1$ in equation (11). The Hamiltonians will be used in their normal-ordered form. Normal ordering is done with respect to the bosonic vacuum which depends on the value of σ. The $a^\dagger$ operators are put to the left of the a operators. Thus the general form of the Hamiltonians reads

$$H = g_{0,0} + g_{0,1}a^\dagger a + g_{0,2}a^{\dagger 2}a^2 + a^{\dagger 2}(g_{2,0} + g_{2,1}a^\dagger a) + (g_{2,0} + g_{2,1}a^\dagger a)a^2 + a^{\dagger 4}g_{4,0} + g_{4,0}a^4. \tag{12}$$

For brevity of the notation, we do not denote the explicit dependence of the couplings and operators on σ in the above equation. The coupling constants $g_{i,j}$ have two indices which indicate the powers of $a^\dagger$ and a in the corresponding operator. For instance, $g_{i,j}$ is associated with the operator $a^{\dagger i} \cdot a^{\dagger j}a^j$ and with its Hermitian conjugate.

For illustration we consider the harmonic oscillator (5). The ground state energy is given by $E = g_{0,0}$, the single-particle energy by $\omega = g_{0,1}$ and the Bogoliubov term by $d/2 = g_{2,0}$. For the PQO, the bare values of the coupling constants are

$$g^{(\mathrm{B})}_{0,0}(\sigma) = \frac{1}{4}\left(\frac{1}{\sigma^2} + \frac{1}{2}\sigma^4\right) \tag{13a}$$

$$g^{(\mathrm{B})}_{0,1}(\sigma) = \frac{1}{2}\left(\frac{1}{\sigma^2} + \sigma^4\right) \tag{13b}$$

$$g^{(\mathrm{B})}_{0,2}(\sigma) = \frac{1}{4}\sigma^4 \tag{13c}$$

$$g^{(\mathrm{B})}_{2,0}(\sigma) = \frac{1}{4}\left(-\frac{1}{\sigma^2} + \sigma^4\right) \tag{13d}$$

$$g^{(\mathrm{B})}_{2,1}(\sigma) = \frac{1}{6}\sigma^4 \tag{13e}$$

$$g^{(\mathrm{B})}_{4,0}(\sigma) = \frac{1}{24}\sigma^4. \tag{13f}$$

For the QO, they are found to be

$$g^{(\mathrm{B})}_{0,0}(\sigma) = \frac{1}{4}\left(\frac{1}{\sigma^2} + \sigma^2 + 3\lambda\sigma^4\right) \tag{14a}$$

$$g^{(\mathrm{B})}_{0,1}(\sigma) = \frac{1}{2}\left(\frac{1}{\sigma^2} + \sigma^2 + 6\lambda\sigma^4\right) \tag{14b}$$

$$g^{(\mathrm{B})}_{0,2}(\sigma) = \frac{3}{2}\lambda\sigma^4 \tag{14c}$$

$$g^{(\mathrm{B})}_{2,0}(\sigma) = \frac{1}{4}\left(-\frac{1}{\sigma^2} + \sigma^2 + 6\lambda\sigma^4\right) \tag{14d}$$

$$g^{(\mathrm{B})}_{2,1}(\sigma) = \lambda\sigma^4 \tag{14e}$$

$$g^{(\mathrm{B})}_{4,0}(\sigma) = \tfrac{1}{4}\lambda\sigma^4. \tag{14f}$$

3.2. Perturbative results

We start by analysing the QO by perturbative schemes. The results shall serve as reference for the following more sophisticated approaches.

The first approach is to expand perturbatively in λ around the diagonal Hamiltonian for $\sigma = 1$. It is known that the resulting series is not convergent but asymptotic [13]. Yet the results may approximate the exact ones if they are restricted to low orders in λ. In this sense, we computed the first three renormalized eigen energies $E^{(\mathrm{R})}_0$, $E^{(\mathrm{R})}_1$ and $E^{(\mathrm{R})}_2$ to second order in λ. Their bare values are $E^{(\mathrm{B})}_0 = g^{(\mathrm{B})}_{0,0}$, $E^{(\mathrm{B})}_1 = g^{(\mathrm{B})}_{0,0} + g^{(\mathrm{B})}_{0,1}$ and $E^{(\mathrm{B})}_2 = g^{(\mathrm{B})}_{0,0} + 2g^{(\mathrm{B})}_{0,1} + 2g^{(\mathrm{B})}_{0,2}$. From the approximate first three eigen energies we deduce the renormalized diagonal coefficients of the Hamiltonian $g^{(\mathrm{R})}_{0,0}$, $g^{(\mathrm{R})}_{0,1}$, $g^{(\mathrm{R})}_{0,2}$. Figure 3 displays the relative errors of these coefficients compared to the exact values, i.e., $r_i = \left[g^{(\mathrm{R})}_{0,i} - g^{(\mathrm{ex})}_{0,i}\right] \big/ g^{(\mathrm{ex})}_{0,i}$. The curves are labelled 2O-PT for second order perturbation theory. As expected, the errors grow very quickly on increasing λ.

Instead of passing tediously to higher orders of λ we choose another route. We consider all terms which preserve the number of quanta as diagonal. This means all terms with equal numbers of creation and annihilation operators are kept in the diagonal Hamiltonian. Then we perform second order perturbation theory around this diagonal part in all the off-diagonal contributions, i.e., the terms which change the number of bosonic quanta. For concreteness, we give the resulting expression for the ground-state energy

$$g^{(\mathrm{R})}_{0,0}(\sigma) = g^{(\mathrm{B})}_{0,0}(\sigma) - \frac{{g^{(\mathrm{B})}_{2,0}}^2(\sigma)}{2\left(g^{(\mathrm{B})}_{0,1}(\sigma) + g^{(\mathrm{B})}_{0,2}(\sigma)\right)} - \frac{{g^{(\mathrm{B})}_{4,0}}^2(\sigma)}{4\left(g^{(\mathrm{B})}_{0,1}(\sigma) + 3g^{(\mathrm{B})}_{0,2}(\sigma)\right)}. \tag{15}$$

Now, we exploit the freedom to choose σ. Five choices are studied:

- $\sigma_{\mathrm{HF}} = 1$. This choice diagonalizes the harmonic part of the Hamiltonian (10). Hence we denote this scheme 2O-HF since it represents second order perturbation around the Hartree–Fock Hamiltonian.
- σ is chosen to fulfil $\partial_\sigma g^{(\mathrm{B})}_{0,0}(\sigma) = 0$, i.e., a stationary point of the bare approximate ground state energy is chosen. It can be checked that this is the same as having $g_{2,0}(\sigma) = 0$ vanish. So the bilinear part of the whole bare Hamiltonian is diagonal. This scheme is denoted by 2O-VAR-$g^{(\mathrm{B})}_{0,0}$ since it represents second order perturbation around the stationary point of $g^{(\mathrm{B})}_{0,0}$. Conventionally, this choice is called second order perturbation around the self-consistent Hartree–Fock Hamiltonian.
- In analogy to the previous choice we require that the bare *single-particle energy* is stationary, $\partial_l g^{(\mathrm{B})}_{0,1} = 0$. This choice is called 2O-VAR-$g^{(\mathrm{B})}_{0,1}$.
- Instead of looking for stationary points of the bare parameters, we can look for the stationary points of renormalized parameters. We denote by 2O-VAR-$g^{(\mathrm{R})}_{0,0}$ the second order perturbation around the stationary point of the renormalized ground state energy $\partial_\sigma g^{(\mathrm{R})}_{0,0}(\sigma) = 0$.
- We call 2O-VAR-$g^{(\mathrm{R})}_{0,1}$ the analogous variation of the renormalized single-particle energy.

On the mean-field level it is well established to look for stationarity in order to define the optimum choice of parameters. To do the same for higher order results, here second order, is justified by the argument that in an exact calculation the result does *not* depend on σ. The value of σ only defines a starting point of the calculation. If the calculation is exact it does

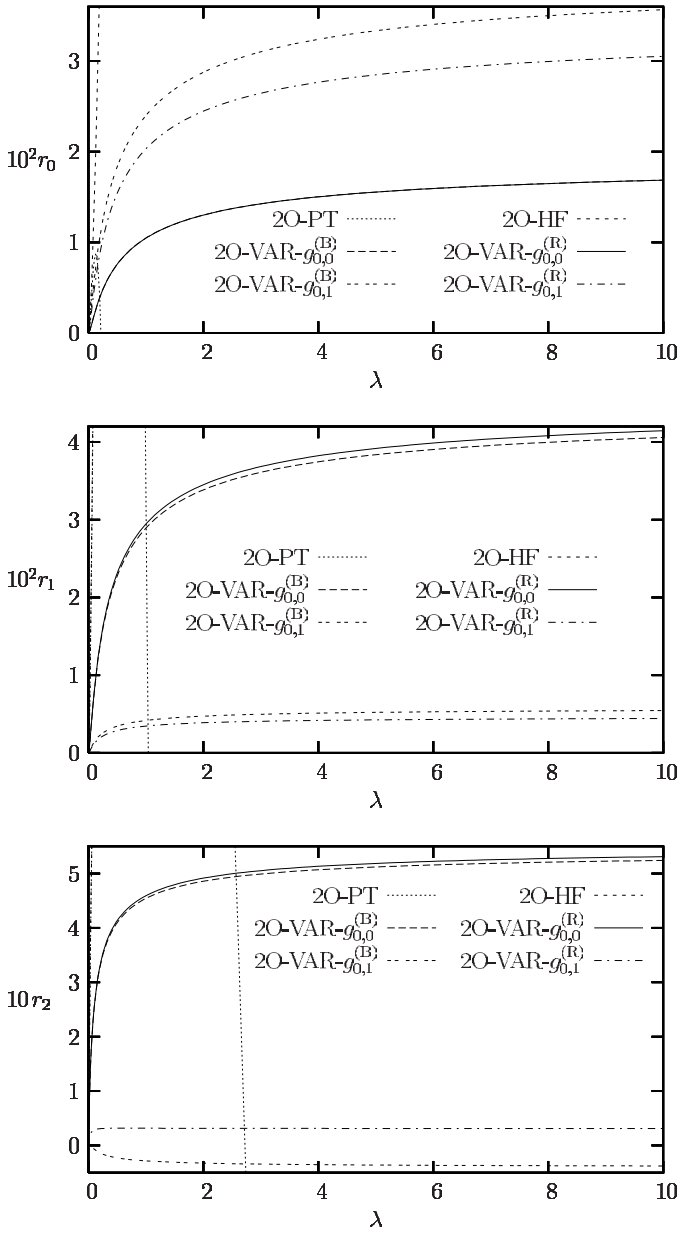

Figure 3. Relative errors r_0, r_1 and r_2 of the first three diagonal coefficients $g^{(R)}_{0,0}$, $g^{(R)}_{0,1}$, $g^{(R)}_{0,2}$ (see text) for five different computation schemes. For the second order perturbation theory (2O-PT) r_1 reaches a maximum value $\simeq$23% for $\lambda \sim 0.5$ (outside the graph) and then decreases again; r_2 reaches a maximum value $\simeq$300% for $\lambda \sim 1.1$. For the second order calculation around the Hartree–Fock Hamiltonian (2O-HF), all r_i grow very fast. The results of the second order calculation around the optimum bare value of the ground state energy (2O-VAR-$g^{(B)}_{0,0}$) and the one around the optimum value of the renormalized $g^{(R)}_{0,0}$ (2O-VAR-$g^{(R)}_{0,0}$) are always very close to each other. For r_0 they cannot be distinguished.

not depend on the starting point. Hence it is stationary with respect to the variation of the parameters defining the starting point. An approximate treatment, however, will not show this

Table 1. Comparison of the four variational second order calculations for the purely quartic oscillator.

	$10^2 r_0$	$10^2 r_1$	$10^2 r_2$
2O-VAR-$g^{(\mathrm{B})}_{0,0}$	1.94	4.47	54.5
2O-VAR-$g^{(\mathrm{R})}_{0,0}$	1.94	4.57	55.3
2O-VAR-$g^{(\mathrm{B})}_{0,1}$	4.01	0.59	−4.07
2O-VAR-$g^{(\mathrm{R})}_{0,1}$	3.45	0.47	3.08

independence of the starting point. The best that can be achieved is stationarity [14] which therefore defines the optimum starting point.

The results obtained for these five choices are represented in figure 3. Clearly, the 2O-HF result leads to no improvement compared to the 2O-PT result. The four other choices using a variational criterion lead to much better results. Apart from the ground state energy where the 2O-VAR-$g^{(\mathrm{R})}_{0,0}$ scheme is the best, the overall best choice is the 2O-VAR-$g^{(\mathrm{R})}_{0,1}$ scheme, especially for r_2. Note that there is no big difference between 2O-VAR-$g^{(\mathrm{R})}_{0,0}$ and 2O-VAR-$g^{(\mathrm{B})}_{0,0}$. On average, the 2O-VAR-$g^{(\mathrm{R})}_{0,0}$ scheme computes the $g^{(\mathrm{R})}_{0,i}$ coefficients with an accuracy ranging from half a per cent to a few per cent. Thus we conclude from these calculations that the use of a variational criterion is always very rewarding. We will also use such a criterion to choose the starting point of the CUT approaches.

Finally, we address the PQO without any harmonic part. It represents the $\lambda \to \infty$ limit of the QO considered before. Of course, neither a direct perturbative approach nor a Hartree–Fock approach is defined. But all the other approaches can be used for the PQO without conceptual difficulty. The results are given in table 1. Again, it turns out that the stationary point of the single-particle energy leads to the best results. The error in the interaction value analysed by r_2 is reduced by a factor of 10 compared to the stationary point of the ground state energy. The deviation in the ground state energy is smallest at its stationary points, but only doubled when the single-particle energy is made stationary.

3.3. Non-perturbative results

3.3.1. Spectrum. Let us consider the Hamiltonian given in equation (12). Performing an infinitesimal unitary transformation generates some new terms in the Hamiltonian which were not present before. Focusing, however, on the states at low energies the new terms with at least six bosonic operators will be of minor importance. They represent processes which involve at least three particles. Hence we discard the new terms for the moment once they have been brought into normal-ordered form. Recall that on normal-ordering higher order terms, terms of lower order occur. These are kept since they matter for the low-lying states.

If the flowing Hamiltonian is truncated in this way it stays in the form of equation (12). It is natural to view all terms conserving the number of bosons, namely $g_{0,0} + g_{0,1}a^\dagger a + g_{0,2}a^{\dagger 2}a^2$, as the diagonal part H_d. The non-conserving term makes up the non-diagonal part of the Hamiltonian. With this choice, Wegner's generator $\eta_\mathrm{W} = [H_\mathrm{d}, H_\mathrm{nd}]$ is computed. It is found to comprise terms of the form $a^{\dagger 4}a^2 - a^{\dagger 2}a^4$ and $a^{\dagger 5}a - a^\dagger a$ [5] which are not present in the initial Hamiltonian. Hence we omit them also in the generator[6] which reads

$$\eta = \eta_{2,0}(a^{\dagger 2} - a^2) + \eta_{2,1}(a^{\dagger 3}a - a^\dagger a^3) + \eta_{4,0}(a^{\dagger 4} - a^4), \tag{16}$$

[6] We also performed computations where these terms are kept in the generator. The ensuing results are worse than those obtained without these terms.

Table 2. Comparison of the four variational CUT calculations for the PQO with Wegner's or MKU generator.

	$10^2 r_0$	$10^2 r_1$	$10^2 r_2$
W-VAR-$g^{(\mathrm{B})}_{0,0}$	0.127	0.000 876	−15.8
W-VAR-$g^{(\mathrm{R})}_{0,0}$	−0.0815	−0.195	−1.86
W-VAR-$g^{(\mathrm{B})}_{0,1}$	−0.0612	−0.279	−4.83
W-VAR-$g^{(\mathrm{R})}_{0,1}$	−0.0426	−0.287	−6.22
MKU-VAR-$g^{(\mathrm{B})}_{0,0}$	0.0492	−0.136	−16.5
MKU-VAR-$g^{(\mathrm{R})}_{0,0}$	−0.0608	−0.232	−0.951
MKU-VAR-$g^{(\mathrm{B})}_{0,1}$	−0.0555	−0.289	−3.51
MKU-VAR-$g^{(\mathrm{R})}_{0,1}$	−0.0352	−0.315	−6.97

where for Wegner's generator

$$\eta_{2,0} = 2(g_{0,1} + g_{0,2})g_{2,0} \tag{17a}$$

$$\eta_{2,1} = 2(g_{0,1} + 3g_{0,2})g_{2,1} + 4g_{0,2}g_{2,0} \tag{17b}$$

$$\eta_{4,0} = 4(g_{0,1} + 3g_{0,2})g_{4,0}. \tag{17c}$$

For the MKU generator the coefficients can be read off from the Hamiltonian

$$\eta_{2,0} = g_{2,0} \tag{18a}$$

$$\eta_{2,1} = g_{2,1} \tag{18b}$$

$$\eta_{4,0} = g_{4,0}. \tag{18c}$$

It is one of the advantages of the MKU generator that it always has a simpler form than Wegner's generator, as exemplified here for the quartic oscillator. This was not obvious for the quadratic oscillator or the two-level system which are too simple to exhibit this general feature. The flow equations read

$$\partial_l g_{0,0} = -4\eta_{2,0}g_{2,0} - 48\eta_{4,0}g_{4,0} \tag{19a}$$

$$\partial_l g_{0,1} = -4\eta_{2,0}(2g_{2,0} + 3g_{2,1}) - 12\eta_{2,1}(g_{2,0} + g_{2,1}) - 192\eta_{4,0}g_{4,0} \tag{19b}$$

$$\partial_l g_{0,2} = -12\eta_{2,0}g_{2,1} - 12\eta_{2,1}(g_{2,0} + 3g_{2,1}) - 144\eta_{4,0}g_{4,0} \tag{19c}$$

$$\partial_l g_{2,0} = -2\eta_{2,0}(g_{0,1} + g_{0,2} + 6g_{4,0}) - 24\eta_{2,1}g_{4,0} - 12\eta_{4,0}(g_{2,0} + 2g_{2,1}) \tag{19d}$$

$$\partial_l g_{2,1} = -4\eta_{2,0}(g_{0,2} + 2g_{4,0}) - 4\eta_{4,0}(2g_{2,0} + 9g_{2,1}) - 2\eta_{2,1}(g_{0,1} + 3g_{0,2} + 18g_{4,0}) \tag{19e}$$

$$\partial_l g_{4,0} = -2\eta_{2,0}g_{2,1} + 2\eta_{2,1}g_{2,0} - 4\eta_{4,0}(g_{0,1} + 3g_{0,2}). \tag{19f}$$

The derivation of these expressions is presented in appendix B.

We start with the results for the PQO. All the results for the eight possible computational schemes are presented in table 2. The eight schemes are made up from two possible generators (W or MKU) and from the four choices of which quantity is made stationary, see previous section. We have to mention that $g^{(\mathrm{R})}_{0,0}$ and $g^{(\mathrm{R})}_{0,1}$ display both a local minimum and a local maximum, i.e., there are two choices for the stationary point. Here only the local minima are considered.

The comparison of tables 1 and 2 reveals that the CUT results are always much more accurate than the second order calculations performed in section 3.2. This is of course expected and does not depend on the chosen variational scheme. For instance, the ground state energy is mostly given to an accuracy of less than 0.1%, to be compared to the 2% of the second order calculations. Yet the calculation is straightforward. Only six differential equations need to be solved which can be done by any computer algrebra program. This proves that the CUTs lead to a significant improvement.

To vary the renormalized quantities instead of the bare ones modifies the CUT results more than it modified the second order results in table 1. In the CUT calculations, the stationary points of the ground state energy provide the best results. This is in contrast to the finding in the perturbative results where the stationary points of the single-particle energy were optimum. We stress that the variation of the renormalized quantities is superior to the variation of the bare ones if the focus is set not only on the ground state energy but in particular on the single-particle and two-particle energies.

In comparison, the results for the two choices of the generator are very similar. The MKU generator works a little better, for instance for the variation of the renormalized ground state energy. We attribute this to the fact that it avoids the appearance of terms which create or annihilate more than four bosons. Hence there are some terms which are not created so that they do not need to be neglected in the truncation scheme. But this effect is obviously fairly small for the system under study.

From these observations we will restrict our computations for the QO to the schemes which are based on stationarity, i.e., we do not show the direct Hartree–Fock calculation. We performed such calculations and the results were unsatisfactory. The flow equations did not even converge to a diagonal Hamiltonian fixed point for $\lambda \gtrsim 4$. This illustrates again that the starting point should not be too far away from the exact result[7].

Furthermore, we show results only for the MKU generator. Its results are representative for similar calculations based on Wegner's generator. They are shown in figure 4. Moreover, the MKU generator is easier to implement (compare equations (17) and (18)). This fact will be of importance for calculations comprising more terms (see below).

The accuracy of the results is very impressive in view of the simplicity of the numerical effort. As for the PQO the variation of the renormalized, i.e., final ground state energy yields the best results if the focus includes the two-particle energies whose accuracy is given by r_2.

Finally, a remark about another possible choice of the generator is in order since its generalizations have been used in more complex physical situations, e.g. in [15, 16]. Using the W-VAR-$g^{(\mathrm{B})}_{0,0}$ scheme, the quadratic off-diagonal coefficient $g_{2,0}$ vanishes at $l = 0$. But it will become finite in the course of the flow. It is possible to modify Wegner's generator to keep this coefficient zero during the flow. To this end, the $\eta_{2,0}$ coefficient of the generator is changed. It is chosen to be $\eta_{2,0} = -72 g_{2,1} g_{4,0}(g_{0,1} + 3g_{0,2})/(g_{0,1} + g_{0,2} + 6g_{4,0})$ instead of $2(g_{0,1} + g_{0,2})g_{2,0}$. This choice has two major advantages. First, the coefficient $g_{2,0}$ does not need to be traced. Second, we find that it converges faster to its diagonal Hamiltonian. For the PQO, the accuracies are found to be $10^2 r_0 = 0.005\,69$, $10^2 r_1 = 1.53$ and $10^2 r_2 = -13.6$. Thus we obtain the best value of the ground state energy with this scheme but also the worst value of the single-particle energy. The value of the interaction is as inaccurate as it is for the

[7] A particularly drastic illustration of this statement is the attempt to derive the spectrum of the harmonic oscillator starting from free particles, even though no truncations are necessary. Consider $H = (P^2 + \delta\omega^2 X^2)/2$ with $\delta\omega^2$ being small. One may try to choose the P^2 term as the diagonal part of the Hamiltonian and the X^2 term as the non-diagonal part. Writing $H(l) = [\alpha(l)P^2 + \beta(l)X^2]/2$, it is found that $\eta_{\mathrm{W}} = -2\mathrm{i}\alpha\beta(XP + PX)$ so that the flow equations $\partial_l \alpha = 2\alpha^2\beta$ and $\partial_l \alpha = -2\alpha^2\beta$ result. Thus $\alpha\beta$ is a constant, and as $\beta \to 0, \alpha \to \infty$. Of course, this was to be expected since the spectrum of a harmonic oscillator is discrete so that it cannot be mapped one-to-one to the continuous spectrum of P^2.

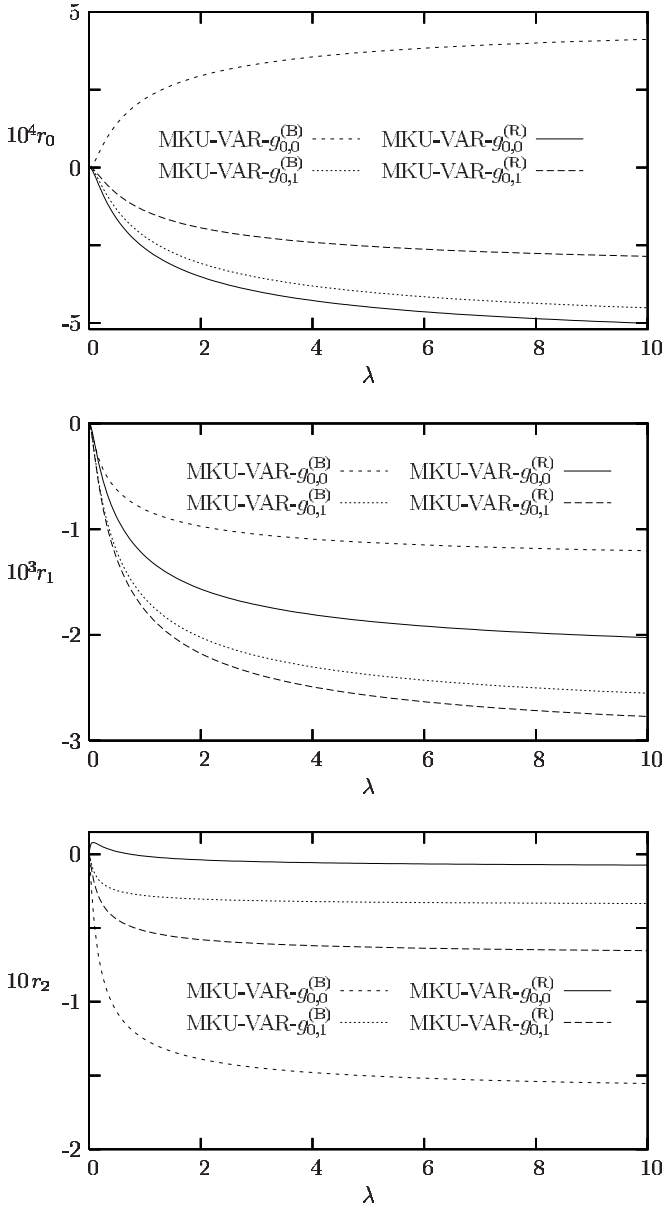

Figure 4. Relative errors r_0, r_1 and r_2 of the first three diagonal coefficients $g^{(R)}_{0,0}$, $g^{(R)}_{0,1}$, $g^{(R)}_{0,2}$ (see text) for four variation schemes based on the MKU generator.

W-VAR-$g^{(B)}_{0,0}$ scheme. Furthermore, we have lost the possibility of varying the initial value of the parameter σ since it is fixed to unity by the condition $g_{2,0} = 0$. An adapted choice of σ will be important in dealing with more terms so that we consider it a caveat that σ is already fixed. In summary, this variant yields very reasonable results, but it is not the optimum choice.

3.3.2. Spectral weights. Apart from the spectrum of the oscillator, one is also interested in the computation of the Green function and of the spectral weights. The retarded Green

function is defined as

$$G(t) = -\mathrm{i}\langle 0|[X(t), X(0)]|0\rangle\Theta(t), \tag{20}$$

where $X(t) = \exp(\mathrm{i}Ht)X\exp(-\mathrm{i}Ht)$, $|0\rangle$ is the ground state. The Fourier transform of the Green function reads

$$G(\omega) = \int_{-\infty}^{+\infty} \mathrm{d}t\, G(t)\exp(\mathrm{i}\omega t) \tag{21}$$

$$= \sum_n |\langle n|X|0\rangle|^2 \left(\frac{1}{\omega - (E_n - E_0) + \mathrm{i}0+} - \frac{1}{\omega + (E_n - E_0) + \mathrm{i}0+}\right). \tag{22}$$

We have denoted the eigenstates of the Hamiltonian by $|n\rangle$ with eigen energies E_n, i.e. $H|n\rangle = E_n|n\rangle$. We will focus on the computation of the spectral weights $J_n := |\langle n|X|0\rangle|^2$. They can be found trivially after the transformation since then the eigenstates are the states with a given number of bosons

$$|0\rangle = U(\infty)|0\rangle_0 \tag{23a}$$

$$|n\rangle = U(\infty)|n\rangle_0 \tag{23b}$$

$$= U(\infty)\frac{1}{n!}a^{\dagger n}|0\rangle_0. \tag{23c}$$

So we need the transformed observable $X(l) = U^\dagger(l)XU(l)$ which satisfies the same flow equation as the Hamiltonian

$$\partial_l X(l) = [\eta(l), X(l)] \tag{24}$$

with initial condition $X(0) = (\sigma/\sqrt{2})(a^\dagger + a)$. Here again, an infinite hierarchy of terms appears when $X(l)$ is commuted with $\eta(l)$. We will restrict the calculation to the lowest non-trivial truncation scheme

$$X(l) = \alpha_{1,0}(l)(a^\dagger + a) + \alpha_{1,1}(l)(a^{\dagger 2}a + a^\dagger a^2) + \alpha_{3,0}(l)(a^{\dagger 3} + a^3). \tag{25}$$

The flow equations of the α coefficients are found to be

$$\partial_l\alpha_{1,0} = -2[\eta_{2,0}(\alpha_{1,0} + \alpha_{1,1} + 3\alpha_{3,0}) + 3\eta_{2,1}\alpha_{3,0} + 12\eta_{4,0}\alpha_{3,0}] \tag{26a}$$

$$\partial_l\alpha_{1,1} = -2[\eta_{2,0}(2\alpha_{1,1} + 3\alpha_{3,0})] - 3[\eta_{2,1}(\alpha_{1,0} + 2\alpha_{1,1} + 6\alpha_{3,0}) + 12\eta_{4,0}\alpha_{3,0}] \tag{26b}$$

$$\partial_l\alpha_{3,0} = -2\eta_{2,0}\alpha_{1,1} + \eta_{2,1}\alpha_{1,0} - 4\eta_{4,0}(\alpha_{1,0} + 3\alpha_{1,1}). \tag{26c}$$

Note that this set of equations is linear in the α coefficients since the coefficients in the generator are determined from the flow of the Hamiltonian. So for the computation of the observables the g coefficients are given and only a linear set of differential equations, though with non-constant coefficients, has to be solved.

The first three J coefficients can be obtained from (26); they read $J_1 = \alpha_{1,0}^2(\infty)$, $J_2 = 0$ due to the identical parity of the $|0\rangle$ and $|2\rangle$ states and $J_3 = 6\alpha_{3,0}^2(\infty)$. The parity of the states in real-space representation is expressed in second quantization by the fact that the boson number is changed only by multiples of two. In figure 5, the results obtained in this way, for the MKU generator, are compared to the numerically exact ones. The relative errors $s_{1/3} = \left[J_{1/3} - J_{1/3}^{(\mathrm{ex})}\right]/J_{1/3}^{(\mathrm{ex})}$ are plotted. For $\lambda = 10$, the error in J_1 is of the order of a few tenth of a per cent. The error in J_3 is about 10%. Note that the weight J_1 $\left(J_1^{(\mathrm{ex})}(\lambda = 10) = 1.297 \times 10^{-1}\right)$ dominates and that the weight of J_3 $\left(J_3^{(\mathrm{ex})}(\lambda = 10) = 3.469 \times 10^{-4}\right)$ is smaller by more than two orders of magnitude so that the errors in the

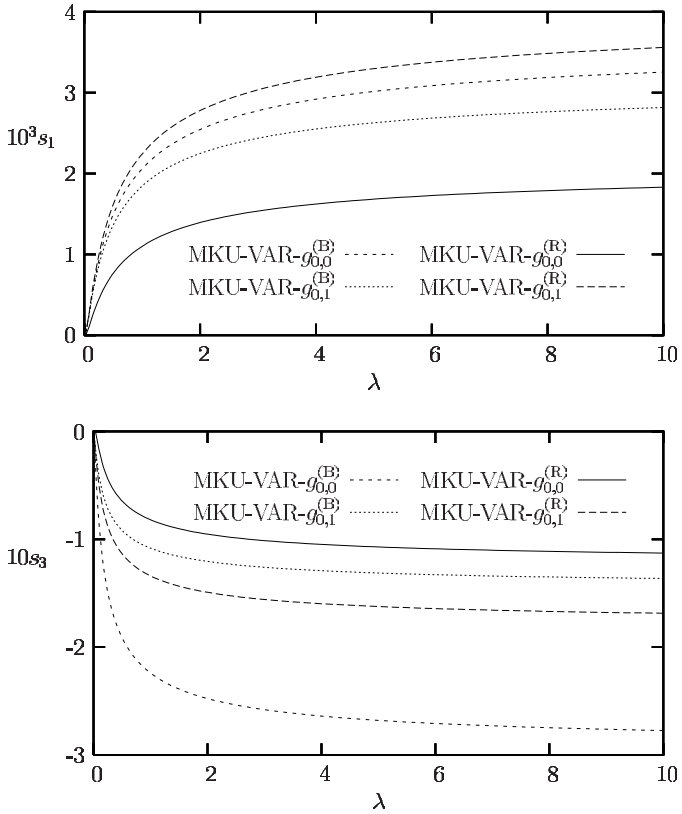

Figure 5. Relative errors s_1 and s_3 of the CUT calculation for the spectral weights J_1 and J_3 (see text) for four variation schemes based on the MKU generator.

Table 3. Relative errors s_1 and s_3 of the CUT calculation for the spectral weights J_1 and J_3 of the PQO for four variation schemes based on the W and MKU generators.

	$10^3 s_1$	$10 s_3$
W-VAR-$g^{(B)}_{0,0}$	2.77	−1.99
W-VAR-$g^{(R)}_{0,0}$	2.02	−1.00
W-VAR-$g^{(B)}_{0,1}$	3.58	−1.15
W-VAR-$g^{(R)}_{0,1}$	3.96	−1.24
MKU-VAR-$g^{(B)}_{0,0}$	3.71	−2.94
MKU-VAR-$g^{(R)}_{0,0}$	2.12	−1.23
MKU-VAR-$g^{(B)}_{0,1}$	3.17	−1.46
MKU-VAR-$g^{(R)}_{0,1}$	4.06	−1.80

absolute scale are equally small. We attribute the relatively large deviations in J_3 to the low order of the truncation scheme used for the observables and for the Hamiltonian where no three-particle energy was included.

For the PQO, the relative errors of the computation of the spectral weights are given in table 3 for MKU and W generators. The exact values for the spectral weights are $J_1^{(\mathrm{ex})} = 0.521$

and $J_3^{(\mathrm{ex})} = 0.00\,152$, showing that even for the PQO the lowest excited state has most of the spectral weight.

It is very interesting to compare the various variational schemes. The result from the energies is confirmed. The by far best result is obtained from the variation of the renormalized ground state energy. This fact strongly suggests adopting this scheme also in more complex situations. The variation of the bare ground state energy, equivalent to the CUT treatment around the self-consistent mean-field calculation, also yields satisfactory results. It is easier to realize, which may become essential for extended systems. Finally, let us note that both generators give results which are similar, as was already the case for the spectrum. Wegner's generator works a little better for the spectral weights than the MKU generator, whereas it was the inverse for the spectrum.

4. Extended truncation schemes

In this section, we only consider the PQO of equation (9) to keep the presentation concise. The question investigated is how the truncation scheme used so far can be extended to improve the results for the spectrum in a systematically controlled fashion. For simplicity, we stick to the MKU generator.

4.1. Structure of the flow equations

Using the MKU generator, the Hamiltonian retains its band structure during the flow so that no terms changing the boson number by more than four arise. Hence the generalization of equation (12) reads

$$H = g_{0,i} M_i + g_{2,i} a^{\dagger 2} M_i + g_{2,i} M_i a^2 + g_{4,i} a^{\dagger 4} M_i + g_{4,i} M_i a^4, \tag{27}$$

where summation over the repeated index i from 0 to ∞ is understood. The same convention is used in the following unless upper bounds for the indices are explicitly discussed. The operator $M_i = a^{\dagger i} a^i$ appearing in equation (27) is the normal-ordered form of the ith power of the number operator $Q = a^\dagger a$. In Wegner's scheme the flowing Hamiltonian would contain terms creating or destroying *any* even number of the excitations. The MKU generator is given by

$$\eta_{\mathrm{MKU}} = g_{2,i} a^{\dagger 2} M_i - g_{2,i} M_i a^2 + g_{4,i} a^{\dagger 4} M_i - g_{4,i} M_i a^4. \tag{28}$$

The flow equations are found by commuting η_{MKU} with H. The derivation of these equations is included in appendix B where the relations needed for Wegner's scheme are also given. The flow equations have the general form

$$\partial_l g_{0,k} = -\left[\beta^{0,2,2}_{k,i,j} g_{2,i} g_{2,j} + \beta^{0,4,4}_{k,i,j} g_{4,i} g_{4,j}\right] \tag{29a}$$

$$\partial_l g_{2,k} = -\left[\beta^{2,0,2}_{k,i,j} g_{0,i} g_{2,j} + \beta^{2,2,4}_{k,i,j} g_{2,i} g_{4,j}\right]. \tag{29b}$$

$$\partial_l g_{4,k} = -\left[\beta^{4,0,4}_{k,i,j} g_{0,i} g_{4,j}\right] \tag{29c}$$

Let us for example consider the g_0 which appear in the part of the Hamiltonian conserving the number of excitations. They are renormalized only by the commutation of one operator creating $n = 2\,(4,$ resp.$)$ excitations and of one operator destroying $n = 2\,(4,$ resp.$)$ excitations.

4.2. Truncation schemes

In the numerical integration of the differential equations, we can keep only a finite number of couplings. We denote by m_0, m_2 and m_4 the number of g_0, g_2 and g_4 couplings kept. For

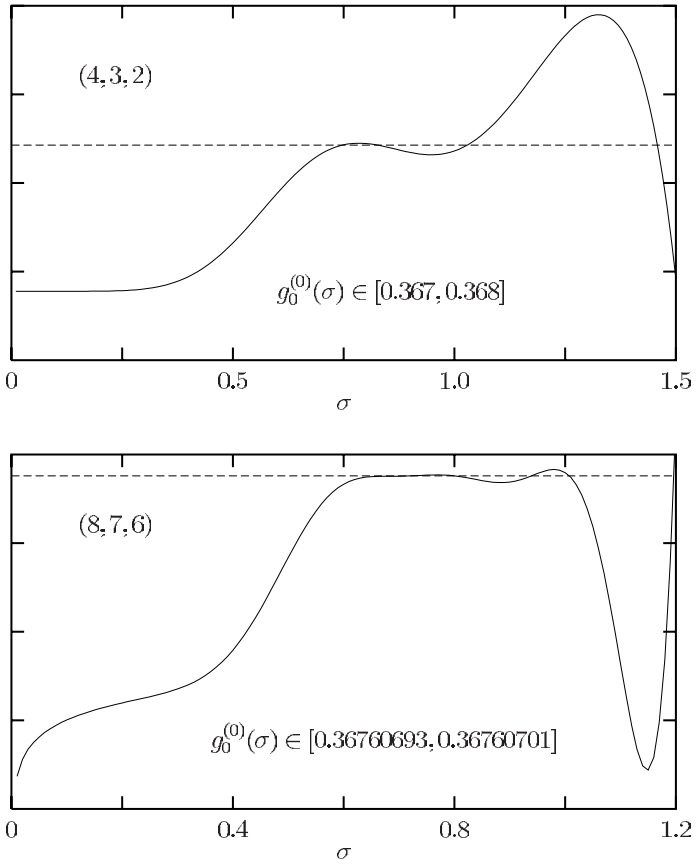

Figure 6. Ground state energy of the PQO as a function of σ for the two schemes (4, 3, 2) and (8, 7, 6). The dashed line represents the exact ground state energy.

the g_0 couplings, this means that we keep the couplings $g_{0,0}, \ldots, g_{0,m_0-1}$. We will call the truncation scheme defined by the three numbers m_0, m_2 and m_4 the '(m_0, m_2, m_4) scheme'. For example, the truncation scheme used in section 3.3.1 is the (3, 2, 1) scheme.

One question arising is how to choose the truncation scheme. This is a very difficult question which to our knowledge has no general answer. Starting from a Hamiltonian of the form (m_0, m_2, m_4) and commuting it once with the corresponding MKU generator, new terms are generated which belong to the $(\max[2m_2, 2(m_4 + 1)], \max[m_0 + m_2 - 2, m_2 + m_4], m_0 + m_4 - 2)$ scheme. Starting from the initial (3, 2, 1) scheme, for instance, the following schemes are generated

$$\begin{aligned}(3, 2, 1) &\to (4, 3, 2) \to (6, 5, 4) \\ &\to (10, 9, 8) \to (18, 17, 16) \to \cdots. \end{aligned} \tag{30}$$

These schemes are all of the type $(N, N-1, N-2)$. So we decide to consider the schemes of this family. Additionally, the terms of this family have the nice property that in each class changing the number of excitations Q by 0, 2 or 4 the maximum number of creation and annihilation operators is equal to $2(N-1) = 2(m_0 - 1) = 2 + 2(m_2 - 1) = 4 + 2(m_4 - 1)$.

4.3. Results

We have checked that including more terms in the Hamiltonian, i.e., increasing N in the $(N, N-1, N-2)$ scheme, results in a continuously improved accuracy for the low-lying energy levels. In figure 6 we illustrate results for the ground-state energy on passing from the scheme $(4, 3, 2)$ to the scheme $(8, 7, 6)$. For both truncation schemes, the ground-state energy is plotted as a function of the parameter σ (see section 3). Clearly, a plateau behaviour develops around a value of σ smaller than 1. Note in particular that the magnitude of the scale on which the ground state energy changes is shrinking strikingly from the $(4, 3, 2)$ to the $(8, 7, 6)$ scheme. This finding agrees perfectly with our previous argument on the independence of an exact calculation of the starting point, see section 3.2. Hence an improved calculation should approach this independence gradually. This means that the dependence of the quantities computed decreases as the accuracy of the calculational scheme is enhanced. This is exactly what we can observe. The fact that values of σ below 1 are preferred is plausible. The X^4 part of the potential squeezes the eigenstates more than does the harmonic potential.

Figure 6 also shows another feature. The results deteriorate if σ becomes too big. In fact, the flows even diverge above some critical value of σ. For the $(4, 3, 2)$ scheme this value is $\sigma_c \simeq 1.52$ and for the $(8, 7, 6)$ scheme it is $\sigma_c \simeq 1.21$. These divergences originate in the error induced by the truncation of the flow equations. The values of σ_c decrease on increasing N. For the values we investigated (up to 25) the values of σ_c remained finite.

These results suggest that there is no uniform convergence as the limit $N \to \infty$ is taken. For any practical calculation, however, this is no serious limitation since the values of N cannot be chosen very large. In particular, in spatially extended systems, $N = 3$ or 4 will be the maximum which can be treated.

5. Summary and conclusion

In this paper, we presented a detailed investigation of the quantum quartic oscillator by perturbative and non-perturbative, renormalizing treatments. We applied continuous unitary transformations to determine the spectrum as well as the spectral weights of the quartic oscillator. This model served as the simplest interacting quantum model. So the method could be illustrated in a simple and transparent setting. The calculations presented may guide future investigations of spatially extended systems such as, for instance, interacting spin waves in quantum antiferromagnets.

We demonstrated that it is rewarding to ally the CUTs with a variational principle. Thereby, an optimum reference state can be chosen with respect to which the necessary truncations introduce only very small errors. It is to be expected that this is also true for other renormalizing schemes.

In the CUT treatment presented tracing only six couplings achieved a remarkable accuracy. Without a reasonably chosen reference state, however, the CUT procedure does not succeed. Information on the spectral weights complements the information needed for the Green functions. Only a little additional effort is needed to obtain the required coefficients.

We compared two generator schemes (Wegner (W), equation (2) and Mielke–Knetter–Uhrig (MKU), equation (4)). The W generators always lead to a fixed point while the MKU generators may fail to converge. But the W generators are stopped by degeneracies so that no significant simplification is reached. The MKU generators are easier to write down and to implement than the W generators. In their performance they are similar for the quartic oscillator. For the energies the MKU is slightly better than the W generator. For the spectral

weights it is the inverse. The experience with more complex, extended systems [18, 19] indicates that the MKU generator is very powerful if the energy eigenvalues are sorted in ascending order of the particle number Q.

Finally, we discussed how the truncation scheme for the continuous unitary transformation can be extended to improve the accuracy of the approach in a systematically controlled way. Our results show that this is indeed possible. Although no uniform convergence can be expected, the description of the low-lying states can be gradually improved by keeping more terms in the flow.

Ideally, our presentation will serve as seed for future investigations of more complex systems by the approach discussed here.

Acknowledgments

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Appendix A. Proof of convergence of Wegner's flow for infinite matrices

The proof of convergence given in [1] is only valid for finite matrices since it makes use of the invariance of the trace of $H^2(l)$ in the flow. But the trace is not generally defined for infinite systems. So the proof as given in [1] works for the two-level system (5*a*), but it does not work for the bosonic oscillator (5*b*) whose eigenvalues grow like n.

But the proof can be slightly modified so that it works for infinite matrices as well. The idea is inspired from statistical mechanics. A regularization is needed which makes the higher lying eigenvalues contribute less. To this end, one can study $\exp(-\beta H(l))$ instead of H for an arbitrary but fixed $\beta > 0$. Since $\exp(-\beta H)$ and H commute there is a certain basis in which both are diagonal. So the aim is to diagonalize $\exp(-\beta H(l))$ which guarantees the diagonality of H up to possible degeneracies.

The generator is modified

$$\eta_\beta(l) = \frac{1}{\beta^2}[\exp(-\beta H(l))|_{\mathrm{d}}, \exp(-\beta H(l))|_{\mathrm{nd}}]. \tag{A1}$$

Then Wegner's proof can be used with H replaced by $\exp(-\beta H)$. The division by β^2 in η only changes the scale of l. But it is useful since it ensures $\lim_{\beta\to 0}\eta_\beta = \eta_{\mathrm{W}}$. Thus one recovers in this 'high-temperature' limit the generator proposed by Wegner. Hence the flow equation $\partial_l \exp(-\beta H(l)) = [\eta_\beta(l), \exp(-\beta H(l))]$ can be reduced to the usual one $\partial_l H(l) = [\eta_{\mathrm{W}}(l), H(l)]$ because it does not matter whether the unitary transformation is applied to the whole function or to its argument.

So the use of $\beta > 0$ serves only to induce convergence. For $\beta \to 0$ all states of the Hilbert space matter as before.

Appendix B. Flow equations

B.1. Basic relation for commutators of bosonic operators

The computation of the commutator of the generator with the Hamiltonian or the observables basically involves commutators $[a^n, a^{\dagger p}]$. It suffices to consider $n \leqslant p$ since, if $n \geqslant p$,

one can use the relation $[a^n, a^{\dagger p}] = [a^p, a^{\dagger n}]^\dagger$. Such a commutator is computed using basic counting arguments, and one finds ($M_i = a^{\dagger i} a^i$)

$$[a^n, a^{\dagger p}] = a^{\dagger p-n} \sum_{c \geqslant 1} \left(c! C_n^c C_p^c\right) M_{n-c}, \tag{B1}$$

$C_n^p = n!/[p!(n-p)!]$ being the usual binomial coefficient for $p \leqslant n$, and being 0 otherwise. The sum in (B1) is performed over the number c of contracted a and $a^\dagger$ operators.

B.2. Derivation of the flow equations

Here the evaluation of the commutator of the generator with the Hamiltonian is addressed. Note that for Wegner's generator the first task is to compute the generator, given by the commutator of two parts of the Hamiltonian. As the computation of η_W is qualitatively not different from the computation of $[\eta, H]$ we will not discuss it here but focus on the MKU generator. We will however use notation which is more general than that used in the main text, and that is easily transferable to Wegner's generator.

The flowing Hamiltonian has the form

$$H = H_0 + \sum_{k=2,4} \left(H_k^+ + H_k^-\right), \tag{B2}$$

with $H_k^- = \left(H_k^+\right)^\dagger$ and

$$H_0 = \sum_{i \in \mathbb{N}} g_{0,i} M_i \text{ and } H_k^+ = \sum_{i \in \mathbb{N}} g_{k,i} a^{\dagger k} M_i. \tag{B3}$$

For Wegner's generator, the sum over k in (B3) would extend over all non-negative even integers. The MKU generator simply reads

$$\eta_{\text{MKU}} = \sum_{k=2,4} \left(\eta_k^+ - \eta_k^-\right) = \sum_{k=2,4} \left(H_k^+ - H_k^-\right), \tag{B4}$$

from which one deduces the flow equations

$$\partial_l H_0 = 2\left(\left[H_2^+, H_2^-\right] + \left[H_4^+, H_4^-\right]\right) \tag{B5a}$$

$$\partial_l H_2^+ = \left[H_2^+, H_0\right] + 2\left[H_4^+, H_2^-\right] \tag{B5b}$$

$$\partial_l H_4^+ = \left[H_4^+, H_0\right]. \tag{B5c}$$

As an example, let us now outline the computation of the commutator $\left[H_p^+, H_n^-\right]$ for $n \leqslant p$. It is equal to

$$\sum_{i',i''} g_{p,i'} g_{n,i''} [a^{\dagger p} M_{i'}, M_{i''} a^n] \tag{B6a}$$

$$= a^{\dagger p-n} \sum_{i',i''} g_{p,i'} g_{n,i''} \sum_c \mathcal{A}^{p,n}_{i',i'',c} M_{i'+i''+n-c} \tag{B6b}$$

$$= a^{\dagger p-n} \sum_i M_i \left(\sum_{i',c} \mathcal{A}^{p,n}_{i',i-i'-n+c,c} g_{p,i'} g_{n,i-i'-n+c} \right), \tag{B6c}$$

where we defined

$$\mathcal{A}^{p,n}_{i',i'',c} = c! \left[C_{i'}^c C_{i''}^c - C_{i'+p}^c C_{i''+n}^c\right]. \tag{B7}$$

In (B6*c*), the i runs over $\mathbb{N}$, but the sums over i' and c are performed on a finite set of positive numbers, because $C_n^p = 0$ if $p > n$. Note that by setting $n = 0$ in (B6*c*), one obtains $\left[H_p^+, H_0\right]$

Collecting everything gives

$$\partial_l g_{0,i} = 2 \sum_{i',c} \left[\mathcal{A}^{2,2}_{i',i-i'-2+c,c} g_{2,i'} g_{2,i-i'-2+c} + \mathcal{A}^{4,4}_{i',i-i'-4+c,c} g_{4,i'} g_{4,i-i'-4+c}\right] \tag{B8a}$$

$$\partial_l g_{2,i} = \sum_{i',c} \left[\mathcal{A}^{2,0}_{i',i-i'+c,c} g_{2,i'} g_{0,i-i'+c} + 2\mathcal{A}^{4,2}_{i',i-i'-2+c,c} g_{4,i'} g_{2,i-i'-2+c}\right] \tag{B8b}$$

$$\partial_l g_{4,i} = \sum_{i',c} \left[\mathcal{A}^{4,0}_{i',i-i'+c,c} g_{4,i'} g_{0,i-i'+c}\right]. \tag{B8c}$$

The flow of the observable $X(l)$ can be computed in the same way. One has

$$X = \sum_{k \in 2\mathbb{N}+1} \left(X_k^+ + X_k^-\right), \tag{B9}$$

with $X_k^- = \left(X_k^+\right)^\dagger$ and

$$X_k^+ = \sum_{i \in \mathbb{N}} \alpha_{k,i} a^{\dagger k} M_i. \tag{B10}$$

The flow equations are found to be

$$\partial_l X_1^+ = \left[H_2^+, X_1^-\right] - \left[H_2^-, X_3^+\right] + \left[H_4^+, X_3^-\right] - \left[H_4^-, X_5^+\right] \tag{B11a}$$

$$\partial_l X_3^+ = \left[H_2^+, X_1^+\right] - \left[H_2^-, X_5^+\right] + \left[H_4^+, X_1^-\right] - \left[H_4^-, X_7^+\right] \tag{B11b}$$

$$\partial_l X_{k\geqslant 5}^+ = \left[H_2^+, X_{k-2}^+\right] - \left[H_2^-, X_{k+2}^+\right] + \left[H_4^+, X_{k-4}^+\right] - \left[H_4^-, X_{k+4}^+\right]. \tag{B11c}$$

These equations can be written in an explicit form, as we did in transforming (B5) into (B8). But we refrain from doing so, since they would be more complicated than (B8). All relations needed to derive them are contained in this appendix.

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