APPLICATION OF A NUMERICAL RENORMALIZATION GROUP PROCEDURE TO AN ELEMENTARY ANHARMONIC OSCILLATOR*

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The canonical quantum Hamiltonian eigenvalue problem for an anharmonic oscillator with a Lagrangian $L = \dot{\phi}^2/2 - m^2\phi^2/2 - gm^3\phi^4$ is numerically solved in two ways. One of the ways uses a plain cutoff on the number of basis states and the other employs a renormalization group procedure. The latter yields superior results to the former because it allows one to calculate the effective Hamiltonians. Matrices of effective Hamiltonians are quite small in comparison to the initial cutoff but nevertheless yield accurate eigenvalues thanks to the fact that just eight of their highest-energy matrix elements are proper functions of the small effective cutoff. We explain how these cutoff-dependent matrix elements emerge from the structure of the Hamiltonian and the renormalization group recursion, and we show that such small number of cutoff-dependent terms is sufficient to renormalize any band-diagonal Hamiltonian.

1. Introduction

The purpose of this article is to show that a renormalization group procedure (RGP) of Hamiltonians, based on Gaussian elimination of basis states [1], provides a convenient approach to the Hamiltonian matrix diagonalization problem for an elementary oscillator with quartic anharmonicity

$$ H \;=\; \frac{\dot{\phi}^2}{2} + \frac{m^2\phi^2}{2} + gm^3\phi^4 \,, \tag{1} $$

where $g > 0$ is a dimensionless coupling constant and the units are chosen such that $\hbar = 1$ and $c = 1$. By "elementary" we mean that we consider ϕ

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* Based on the author's bachelor thesis, University of Warsaw, July 2010.

a single variable, describing only one mode of a scalar field. Thus, instead of a quantum field theory problem, we have a simple quantum mechanics problem. The utility of RGP results from the band-diagonal structure of the oscillator's Hamiltonian. Having written the initial Hamiltonian in the second-quantized form

$$H = m \left[a^\dagger a + g \left(a^\dagger + a \right)^4 \right] \tag{2}$$

(the irrelevant constant $+m/2$ was suppressed), the Hamiltonian matrix is obtained by evaluating matrix elements in the basis of normalized eigenstates of $H_0 = ma^\dagger a$.

In general, band-diagonal structure of a Hamiltonian corresponds to the situation, when an interaction cannot mix the states belonging to distinct energy scales. Such an interaction is much easier to understand then the one which does not possess this property. For this reason, building a unitary transformation which decouples states distinct in energy from each other may be the main part of solving a Hamiltonian eigenvalue problem involving interactions of the latter kind. The examples of methods dealing with such unitary decoupling are the similarity renormalization group (SRG) scheme [2, 3] and (closely related) Wegner's flow equation [4–6]. Both methods bring (arbitrarily chosen) initial Hamiltonian to a band-diagonal form. The oscillator Hamiltonian possesses a band diagonal structure from the beginning, *i.e.*, without any need for using SRG to make it so. Thus, this paper can be considered as dealing with the second stage of solving the eigenvalue problem after the band diagonal structure is already achieved.

Namely, in this paper we address the problem of precise and systematic numerical calculation of small eigenvalues of the band-diagonal Hamiltonian, using the one in Eq. (2) as an example. We show that the Wilsonian RGP in the case of any band-diagonal Hamiltonian is reduced to a recursive relation for only a few (six in the considered example) independent Hamiltonian matrix elements. Thus, what we do here may be considered a convenient tool for analysing band-diagonal Hamiltonians emerging from aforementioned methods. Further discussion of this possibility in the case of realistic field-theoretic Hamiltonians can be found in [3], see Appendix A there.

In zero-dimensional oscillator there are no ultraviolet divergences, so the renormalization issues in this model are limited to finite cutoff dependence. Such finite cutoff dependence strictly disappears from the smallest eigenvalues when the cutoff is sent to infinity. Thus, there is no need to introduce diverging counterterms. Nevertheless, RGP is still of great value, because it *gets rid of the spurious finite cutoff dependence of small Hamiltonian eigenvalues*, even for very small cutoffs. The numerical recipe is very fast, precise

and nonperturbative. So, it is valid for all values of g. The low-energy spectra of the Hamiltonian (2) obtained with RGP method will be compared with the corresponding spectra obtained by simply cutting off the initial Hamiltonian at the same small cutoff, for different values of g.

RGPs are extensively used as numerical tools since Wilson has delivered the algorithm [7] for treating the systems in which Kondo effect [8] appears. The algorithm considered in this paper resembles the one considered in [7], but does not include a logarithmic discretization of any conduction band. It does, however, deal with a discrete set of states that is similar to an infinite set of intervals of pion momentum in [9] and a discrete set in [1]. Ref. [10] provides an overview of applications of numerical RGPs to the quantum impurity systems. Here, we show that an appropriate numerical RGP can be always applied to any quantum Hamiltonian that is band-diagonal. In particular, we have in mind systems of particles for which SRG renders a Hamiltonian of the band-diagonal form [3].

Our approach is not the only one possible in the case of a quartic oscillator. Another approach, based directly on SRG, was presented in [11]. In the case of oscillator, the procedure of Ref. [11] is simple and an effective generator of SRG transformation is found using specific simplifications. Most of the work is done analytically. However, for an arbitrary band-diagonal Hamiltonian such simple generator does not exist and numerical calculations based on SRG are complex. In fact, in such circumstances they are less effective then these based on Wilsonian RGP that are presented in this article using the example of quartic oscillator.

The paper is organized as follows. The RGP carried out in this article is described in Section 2. The resulting evolution of Hamiltonian matrix elements is described in Section 3. Section 4 compares results obtained using RGP with results obtained using a plain cutoff (PC) of the Hamiltonian matrix, without inclusion of any corresponding changes in its matrix elements. The PC procedure has no *a priori* justification for general Hamiltonians but works for large enough cutoffs for band-diagonal Hamiltonians, see Section 4 for details. The effective Hamiltonians we obtain are described in Section 5. Section 6 concludes the article with a summary of accuracy achieved using the RGP.

2. Description of RGP carried out in this article

We set $m = 1$ and denote $H_{\mathrm{I}} = (H - H_0)/g$. In the basis of normalized eigenstates of H_0, $|k\rangle = (k!)^{-1/2}(a^\dagger)^k|0\rangle$, H has matrix elements

$$
\begin{aligned}
H_{kl} \equiv \langle k|H|l\rangle \;=\; & \left[k + 3g\left(2k^2 + 2k + 1\right)\right]\delta_{kl} \\
& + g(4l + 6)\sqrt{(l+1)(l+2)}\,\delta_{k(l+2)} \\
& + g(4k + 6)\sqrt{(k+1)(k+2)}\,\delta_{l(k+2)} \\
& + g\sqrt{(l+1)(l+2)(l+3)(l+4)}\,\delta_{k(l+4)} \\
& + g\sqrt{(k+1)(k+2)(k+3)(k+4)}\,\delta_{l(k+4)} \,.
\end{aligned}
\tag{3}
$$

Due to the Kronecker delta functions most of the matrix elements are zero and the Hamiltonian matrix is band-diagonal with only five near-diagonals different from zero.

As the first step of RGP, we define the Hamiltonian with a big cut-off N, *i.e.*, we reduce the space of states to the one spanned by the set $\{|0\rangle, |1\rangle, \ldots, |N\rangle\}$ and write the Hamiltonian as $(N+1) \times (N+1)$ matrix with elements given by Eq. (3).

Then, we denote $\langle k|\psi\rangle = \psi_k$ and write the resulting Hamiltonian matrix eigenvalue equation in the form

$$
\sum_{l=0}^{N} H_{kl}\psi_l \;=\; E\psi_k \,.
\tag{4}
$$

We extract ψ_N from the highest energy equation, $k = N$, in the set (4) of $N+1$ equations, and use it in the remaining N equations in the set (4) with $k < N$. This is essentially Gaussian elimination. The resulting set of only N equations is

$$
\sum_{l=0}^{N-1} \left(H_{kl} + \frac{H_{kN}H_{Nl}}{E - H_{NN}}\right)\psi_l \;=\; E\psi_k \,.
\tag{5}
$$

Taking into account that $H = H_0 + gH_\mathrm{I}$, we arrive at the equation

$$
\sum_{l=0}^{N-1} \Big(H_{0\,kl} + gH_{\mathrm{I}\,kl} + \underbrace{g^2 \frac{H_{\mathrm{I}\,kN}H_{\mathrm{I}\,Nl}}{E - (H_{0\,NN} + gH_{\mathrm{I}\,NN})}}_{gH_{\mathrm{I}\,kl}^{(1)}(E)}\Big)\psi_l \;=\; E\psi_k \,,
\tag{6}
$$

which is an eigenvalue problem for a new matrix with elements $H_{0\,kl} + gH_{\mathrm{I}\,kl}^{(1)}(E)$. We call it the matrix of effective Hamiltonian. It can be used as a starting point for the next Gaussian elimination step, but we notice that there appears a difficulty: $H_\mathrm{I}^{(1)}$ depends on an unknown eigenvalue E.

However, we are interested only in small eigenvalues of H, so small that they are negligible when compared with $H_{0\,NN} + gH_{I\,NN}$. The latter is the highest-index diagonal matrix element of H that appears in the denominator on the left-hand side in Eq. (6). Thus, we bypass the difficulty by introducing the approximation

$$E - (H_{0\,NN} + gH_{I\,NN}) \approx -(H_{0\,NN} + gH_{I\,NN}). \tag{7}$$

This approximation limits our ability to precisely calculate eigenvalues E using our RGP to lowest eigenvalues. For this price we can do as many Gaussian steps as we like, using the relation

$$H_{I\,kl}^{(j+1)} = H_{I\,kl}^{(j)} - g\frac{H_{I\,kn}^{(j)}H_{I\,nl}^{(j)}}{H_{0\,nn} + gH_{I\,nn}^{(j)}}, \tag{8}$$

with $n = N - j$, provided that we keep satisfying condition (7) for every step number j. We may suppose that for some $M = N - j$, $H_{0\,MM} + gH_{I\,MM}^{(N-M)} \approx E$ and the condition (7) may be eventually violated. On the other hand, we can continue a calculation assuming the simplification and using the approximate Gaussian steps to eliminate states $|N\rangle, |N-1\rangle, \ldots, |n+1\rangle$ down to a small n. We analyse results of such steps for a set of smallest eigenvalues for which the violation of our approximation appears quite small.

From now on, the interaction Hamiltonian reduced in size by performing $N - n$ approximate Gaussian steps (in other words the renormalized interaction Hamiltonian) is denoted by $H_I^{RG}(n)$. On the other hand, a Hamiltonian matrix reduced to the same size with a PC is denoted by $H_I^{PC}(n)$. This means that both $H_I^{RG}(n)$ and $H_I^{PC}(n)$ are $(n+1) \times (n+1)$ matrices but their matrix elements are different. The matrix elements of $H_I^{RG}(n)$ are to be calculated and the matrix elements of $H_I^{PC}(n)$ are directly given by the right-hand side of Eq. (3) as the terms proportional to g.

Note that some matrix elements of the renormalized matrix depend on N and n. If the dependence on N were divergent or otherwise significant, it would have to be removed by counterterms in $H^{(0)}$. Since in our model there are no divergences, and the limit of $N \to \infty$ is easily achieved for small eigenvalues, one can simply use some big N and calculate the corresponding matrices of operators $H^{RG}(n)$. N sufficiently large for working without counterterms to be valid, is determined in Sec. 4. $H^{RG}(n)$ will have some matrix elements that vary with n. The only variation we study here is the one obtained assuming condition (7). A more precise study than the one described here would be required to identify consequences of a finite ratio E/H_{nn}.

3. RGP evolution of Hamiltonian matrix elements

3.1. General band-diagonal Hamiltonian

Matrix elements of interaction part of any band-diagonal Hamiltonian can be written in the form

$$H_{I\,kl} = \sum_{i=-m}^{m} h_i(k)\delta_{k-l,i}, \qquad (9)$$

for some integer m. From Eq. (8) follows that $H_{I\,kl}^{\mathrm{RG}}(N-1) \neq H_{I\,kl}^{\mathrm{RG}}(N) \equiv H_{I\,kl}^{\mathrm{PC}}(N)$ only for such k that $H_{I\,kN}^{\mathrm{RG}}(N) \neq 0$ and $H_{I\,Nl}^{\mathrm{RG}}(N) \neq 0$. This implies both $k,l \geq N-m$. Thus, after first Gaussian step, done in approximation (7) or exactly, H_I^{RG} is still band-diagonal. Moreover, only matrix elements situated in $m \times m$ submatrix in highest-energy corner of $H_I^{\mathrm{RG}}(N-1)$ can be different then corresponding matrix elements of $H_I^{\mathrm{PC}}(N-1)$. We see, that we can repeat this reasoning recursively, with N changed into n (the highest index after some number of Gaussian steps).

Thus, we can conclude that $H^{\mathrm{RG}}(n)$ is band-diagonal for any n, and that not more then m^2 its matrix elements, located in the high-energy corner, does really depend on n. Eq. (8) allows to write down the set of (conjugated) recursions for these matrix elements. Numerical iteration of such a set can be easily done using computer.

3.2. Oscillator example

First, we see that in the case of oscillator's Hamiltonian (3), $m = 4$. Further, from Eqs. (3) and (8) we see, that no new nonzero matrix elements appear in the 4×4 submatrix in the high-energy corner during the Gaussian step. Thus, only eight matrix elements depend on n. Finally, the symmetry of Hamiltonian matrix is preserved by RGP transformation, so there are only six independent functions of n in $H_I^{\mathrm{RG}}(n)$. To number them, we introduce a function

$$i(k,l) = \begin{cases} j & \text{for} \quad k=l=n-(j-1) & \text{and} \quad j \in \{1,2,3,4\}, \\ 5 & \text{for} \quad (k,l)=(n,n-2) & \text{or} \quad (k,l)=(n-2,n), \\ 6 & \text{for} \quad (k,l)=(n-1,n-3) & \text{or} \quad (k,l)=(n-3,n-1), \end{cases} \qquad (10)$$

and denote

$$\xi_{i(k,l)}(n) = \frac{H_{I\,kl}^{\mathrm{RG}}(n)}{H_{I\,kl}^{\mathrm{PC}}}. \qquad (11)$$

This means that $\xi_i(n=N) = 1$ and the deviation of $\xi_{i(k,l)}(n)$ from unity is the relative correction to $H_{I\,kl}^{\mathrm{PC}}$ resulting from RGP. Values of $g\xi_i$ are effective coupling constants in the highest-energy 4×4 submatrix of $H_I^{\mathrm{RG}}(n)$.

From Eq. (8), we obtain a set of recursions for coefficients $\xi_i(n)$. In the case of oscillator, six conjugated first order recursive equations can be simply split into two sets of three equations of the second order. One such set is

$$\xi_1(n-2) \;=\; \xi_3(n) - g\frac{f_{02}^2}{f_{22}}\frac{\xi_5(n)^2}{n + gf_{00}\xi_1(n) - E}\,, \tag{12}$$

$$\xi_3(n-2) \;=\; 1 - g\frac{f_{04}^2}{f_{44}}\frac{1}{n + gf_{00}\xi_1(n) - E}\,, \tag{13}$$

$$\xi_5(n-2) \;=\; 1 - g\frac{f_{02}f_{04}}{f_{24}}\frac{\xi_5(n)}{n + gf_{00}\xi_1(n) - E}\,, \tag{14}$$

where $f_{kl} = H_{I\,(n-k)(n-l)}$ are functions of n, explicitly known from Eq. (3). The second set is almost identical. The only differences are that all down indices are increased by one and $(n-1)$ appears instead of n in the denumerator on the right-hand side. For large n the two sets evolve nearly identically. It is evident that the coefficients $\xi_i(n)$ are easy to calculate numerically.

4. Comparison of RGP and PC

In Eq. (6), we can see that $H_{\mathrm{I}}^{\mathrm{PC}}(n)$ can be interpreted as $H_{\mathrm{I}}^{\mathrm{PC}}(N)$ after $N - n$ Gaussian steps performed in the approximation

$$H_{\mathrm{I}\,kl} + g\frac{H_{\mathrm{I}\,kN}H_{\mathrm{I}\,Nl}}{E - H_{NN}} \;\approx\; H_{\mathrm{I}\,kl}\,. \tag{15}$$

This approximation neglects terms obtained in the approximation (7). Therefore, we can predict, that the results obtained using the RGP will be more accurate then the ones obtained using the PC.

It is not clear how to compare the accuracies of the two procedures, since we do not know the exact eigenvalues of the infinite Hamiltonian. However, in our simple model, we can very precisely calculate small eigenvalues of the Hamiltonian numerically diagonalizing $H^{\mathrm{PC}}(M)$ for some big cutoff M.

In all computations, the numbers were handled with precision of 53 binary places (almost 16 decimal places). The numerical calculations show that for $M \in [200, 1000]$ and $g \in \{0.01, 0.1, 1, 10\}$ the three smallest eigenvalues, denoted E_0, E_1, E_2, do not depend on M with a relative precision 10^{-10}. For this reason, we can consider them to be accurate results and define the (relative) accuracy of RGP and PC as $|E_i^{\mathrm{RG}}(n) - E_i|/E_i$ and $|E_i^{\mathrm{PC}}(n) - E_i|/E_i$, respectively. Also for this reason $N = 200$ will be considered sufficiently large initial cutoff and it will be used as a starting point for RGP described in previous sections.

We shall illustrate our results on examples with three different values of the initial coupling constant: $g = 0.01$, $g = 1$ and $g = 10$. These values are chosen because each one illustrates a different regime of RGP results. $g = 0.01$ illustrates how RGP works in the case of interactions which only slightly change eigenvalues of H_0. $g = 10$ illustrates how RGP works in the case of interactions dominating the system (which manifest itself in eigenvalues much different then those of H_0). $g = 1$ illustrates the intermediate situation. The results are discussed separately for different values of g.

4.1. Results for $g = 0.01$

For $g = 0.01$, the accurate eigenvalues are $E_0 = 0.1687726041$, $E_1 = 1.716925770$ and $E_2 = 3.602838696$. Both procedures, RGP and PC, give precise results. Even for n as small as $n = 10$, E_0 is recovered with accuracy 4×10^{-10} and E_1 and E_2 are recovered with accuracy 2×10^{-8} in the case of RGP. In the case of PC, the accuracy of these three eigenvalues is about 10^{-7}. We see that RGP increases accuracy of predicting E_0 about 500 times. Also E_1^{RG} and E_2^{RG} are calculated about 5 times more precisely then E_1^{PC} and E_2^{PC}. Nevertheless, accuracy obtained with PC is also brilliant.

4.2. Results for $g = 1$

For $g = 1$ and $n = 10$, eigenvalues E_1^{PC} and E_2^{PC} differ from eigenvalues E_1^{RG} and E_2^{RG} much more then for $g = 0.01$. We can say that the difference is qualitative. The correct eigenvalues are $E_1 = 3.521565666$ and $E_2 = 7.263980184$. E_2^{RG} has accuracy 3%, while E_2^{PC} only 21%. For E_1, the difference is 0.25% to 6% in favor of RGP.

The correct ground state energy is $E_0 = 0.6487889141$. The errors are 2×10^{-4} in RGP and 6×10^{-3} in PC. Both values can be considered satisfactory if the required accuracy is of the order of 1%.

4.3. Results for $g = 10$

Utility of RGP is most clearly visible in the case of $g = 10$. This is giant, but still realistic coupling. For example the pion–nucleon coupling constant is about 13 [12]. Moreover, there is no *a priori* reason for values of couplings emerging from SRG procedure to be small.

The accurate eigenvalues in this case are $E_0 = 1.826275924$, $E_1 = 7.790412053$ and $E_3 = 15.70695963$. The results for eigenvalue E_0, obtained with RGP and with PC, as a function of cutoff n are plotted in Fig. 1. One sees that PC with highest index smaller than ~ 15 produces a huge error in the eigenvalue. In the same cutoff region, RGP still gives a reasonable value of E_0.

For $n = 10$, E_0^{RG} has accuracy 0.35%, which is about 100 times better than 33% obtained with PC. These results prove that as long as $E \ll H_{nn} \sim n^2$, RGP gives a reasonable estimation of an eigenvalue. Even for $n = 4$, RGP reproduces E_0 with 5.5% accuracy while PC introduces about 230% of error.

For $n = 4$, the eigenvalues E_1 and E_2 are obtained with poor accuracy. In RGP, E_1^{RG} and E_2^{RG} have errors 11% and 43%, respectively. Obtaining E_1^{PC} and E_2^{PC} does not make any sense.
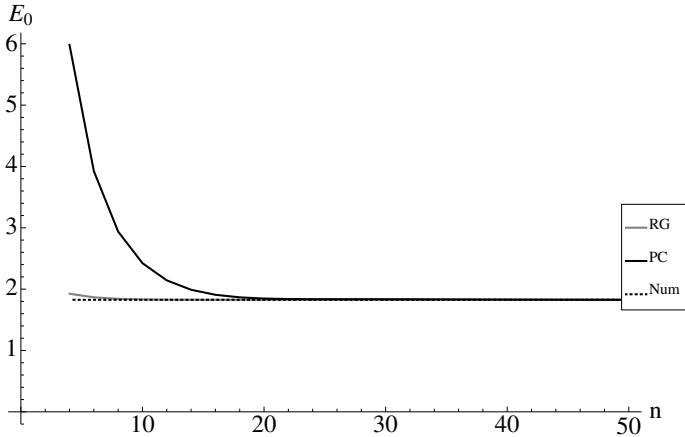

Fig. 1. The ground state energy of H for $g = 10$ determined with RGP and PC, compared with the value achieved in the accurate numerical calculation (Num).

5. Effective Hamiltonians

The important question is how it happens that the RGP produces a better result then PC. In PC, there appears a non-physical parameter n. If n is not large enough, even small eigenvalues depend on n. The key idea behind the RGP is to base physical predictions (in this case the small eigenvalues of H) on the effective theory whose Hamiltonian $H_{\mathrm{I}}^{\mathrm{RG}}(n)$ is calculated from the initial one, instead of plainly cutting off the initial theory to the arbitrary number of states.

As it was explained in Sec. 3, in the case of band-diagonal Hamiltonian most of the matrix elements of the effective Hamiltonian stay invariant under the RGP transformation given by Eq. (8).

The ratios of the changed terms in $H_{\mathrm{I}}^{\mathrm{RG}}(n)$ to the corresponding terms in $H_{\mathrm{I}}^{\mathrm{PC}}$ for $g = 10$ are presented in Fig. 2. One can see that for $n < N$

$$0 < \xi_1 \approx \xi_2 < \xi_5 \approx \xi_6 < \xi_3 \approx \xi_4 < 1 \,. \tag{16}$$

This means that these renormalized matrix elements are smaller then the original ones, but the sign remains unchanged. The approximate equalities correspond to the observation made in Sec. 3 that the six evolving matrix elements form two similar independent subsets.

Within the 4×4 highest-energy corner of the Hamiltonian matrix, the closer is the matrix element to the cutoff corner, the bigger is the necessary correction. It is worth noticing that although ξ_i considerably depart from unity, they still very weakly depend on n. Calculations for various g show that they also weakly depend on g.
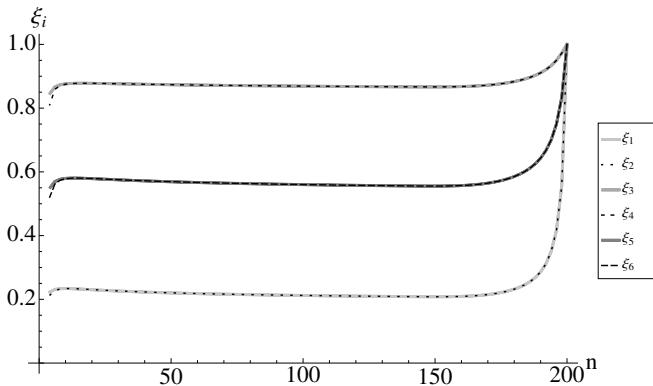

Fig. 2. The ratios of renormalized matrix elements to the original ones, ξ_i, as functions of n, obtained for the initial cutoff $N = 200$ and $g = 10$, see Eq. (11).

6. Conclusion

We have considered a simple version of RGP in application to an elementary Hamiltonian of a single-mode scalar field with an anharmonic interaction term proportional to φ^4. We have calculated the ground state and two least excited states energies and compared results obtained using RGP to the results obtained using PC.

Our results show that when the coupling constant g is large, the RGP is much more accurate than the PC procedure. For $g = 10$, RGP reproduces E_0 with 5.5% accuracy in a 5×5 matrix, which can be considered a reasonable estimate. Such small matrices provide a model of small spaces of states that one can handle nonperturbatively using computers in realistic theories. In the matrix of the same size, PC gives the result with an enormous error (about 230%). RGP is significantly more accurate also for small values of g.

In the presented oscillator model, the improvement due to RGP is achieved through a calculation of eight cutoff-dependent terms (only six of them being different) in the effective Hamiltonians with small cutoffs. A small number of terms is an unavoidable consequence of the band-diagonal structure of the initial Hamiltonian. This feature make RGP a potentially convenient tool for analysing band-diagonal Hamiltonians, in particular these emerging form applying SRG to some realistic field-theoretic Hamiltonians.

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