Operator method for solution of the Schrödinger equation with the rational potential

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The eigenvalue problem for one-dimensional Schrödinger equation with the rational potential is numerically solved by the operator method. We show that the operator method, applied for solving the Schrödinger equation with the nonpolynomial structure of the Hamiltonian, becomes more efficient if a nonunitary transformation of the Hamiltonian is used. We demonstrate on numerous examples that this method can handle both perturbative and nonperturbative regimes with very high accuracy and moderate computational cost.

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I. INTRODUCTION

In this paper we generalize the operator method for solving the Schrödinger equation (SE) with a nonpolynomial structure of the Hamiltonian. As an example of such a problem we consider one-dimensional Hamiltonian with the rational potential

\[ V_L(x) = \frac{x^2}{2} + \frac{\lambda x^{2L}}{1+gx^2}. \]  

(1)

The problem chosen is of interest in different areas of physics, i.e. laser physics\cite{1} and non-linear quantum field theory\cite{2}. It can be also exploited for verifying new nonperturbative methods, which allow us to find approximate solution of the Schrödinger equation in the whole range of Hamiltonian parameters. Such methods can be used for treating many physical problems of current interest. The test problem chosen is very suitable for these purposes because the SE

\[ \left[ \frac{p^2}{2} + V_L(x) - E \right] |\psi\rangle = 0, \]  

(2)

can be solved exactly if some algebraic relations between parameters \( g \) and \( \lambda \) are assumed\cite{3,4,5}. The exact solutions allow to find out the accuracy of approximate methods.

The Schrödinger equation with the potentials \( V_1(x) \) and \( V_2(x) \) has been treated by different approaches based on finite-difference schemes, variational and asymptotic methods\cite{6,7,8,9,10,11,12,13}. To the best of our knowledge there is only one work\cite{13}, where the case \( L > 2 \) was studied in the wide range of the parameter \( \alpha = g/\lambda \) by very efficient method of finite-differences. The case \( L = +3 \) has been studied for \( g \ll 1, \lambda \ll 1 \) by using the Padé-approximant and hypervirial methods\cite{14}. Three-dimensional generalization of Eq.(2) can be found in Ref.\cite{15}.

In the present paper the SE Eq.(2) is solved by the operator method (OM), developed by Komarov and Feranchuk\cite{16}. The OM has been successfully applied to different problems\cite{17,18,19,20}, but the most problems considered had a polynomial structure of the Hamiltonian. The polynomial structure allows one to calculate matrix elements of the SE equation analytically in the Fock basis\cite{16}. But this simple analytical scheme can not be directly applied to the nonpolynomial equation Eq.(2). We can still perform the OM calculations\cite{17}, but some extra numerical scheme must be exploited to calculate matrix elements. This problem can be resolved by the use of the nonunitary transformation \( C \)

\[ |\psi\rangle = C |\varphi\rangle, \quad C = (1 + gx^2), \]  

(3)

which leads to the following expression for Eq.(2)

\[ \left[ \frac{p^2}{2} + \frac{x^2}{2} + g \left( \frac{p^2 x^2}{2} + \frac{x^4}{2} \right) + \lambda x^{2L} - (1 + gx^2)E \right] |\varphi\rangle = 0. \]  

(4)

So we transformed the nonpolynomial operator equation Eq.(2) to the polynomial one Eq.(4), where the operator at the left side is nonhermitian with respect to the scalar product

\[ \langle \phi | \psi \rangle = \int dx \, \phi^* (x) \psi (x). \]  

(5)
The idea of using nonunitary transformations was recently suggested in Ref. [21]. It was also developed in Ref. [22] as nonhermitian technique of canonical transformations. The basic idea is that the commutation relation \( [x, p] = i \) can be preserved by any unitary transformation, but the same is also true if we make use of the similarity transformation \( X = C x C^{-1}, P = C p C^{-1} \). Below we show that the polynomial operator equation Eq. (1) is very easy to handle within the framework of the operator method in order to find both the exact numerical and approximate analytical solutions. The OM allows us to treat the problem in the wide range of Hamiltonian parameters \( g \) and \( \lambda \), where the SE Eq. (2) has a discrete energy spectrum, i.e. when \( -\infty < L \leq +1, |\lambda| < +\infty, g \geq 0; L > +2, \lambda \geq 0, g \geq 0; L = +2, \lambda > -g/2, g \geq 0 \). Below we present results of our nonperturbative calculations for four cases \( 1 \leq L \leq 4 \).

II. ITERATIVE SCHEME OF THE OPERATOR METHOD

In this section we apply the operator method for solving the equation Eq. (1) using the scheme developed in Ref. [16]. If we introduce the annihilation operator \( a(\omega) \), the creation operator \( a^+ (\omega) \) and the excitation number operator \( n(\omega) = a^+ (\omega) a(\omega) \)

\[
a^+ (\omega) = \frac{1}{\sqrt{2}\omega} (\omega x - ip), \quad a(\omega) = \frac{1}{\sqrt{2}\omega} (\omega x + ip),
\]

which satisfy the commutation relations

\[
[a(\omega), a^+(\omega)] = 1, \quad [a(\omega), n(\omega)] = a(\omega), \quad [a^+(\omega), n(\omega)] = -a^+(\omega),
\]

one have for Eq. (1)

\[
(L' - E L'')(\varphi) = 0, \quad (L' = \left( \frac{1}{4\omega} + \frac{\omega}{4} \right) (2n + 1) + \frac{3g}{8\omega^2} (2n^2 + 2n + 1) + \frac{g}{8} (2n^2 + 2n - 1) + \frac{g}{8} (\frac{1}{\omega^2} - 1),
\]

\[
\times \left( a^+ a^2 + 2a^4 + a^2 + \frac{3g}{4\omega^2} + \frac{g}{2\omega^2} n \right) (a^2 + a^4) - \frac{g}{\omega^2} a^2
\]

\[
+ \frac{g}{2} (a^2 - a^4) + \lambda x^{2L},
\]

\[
L'' = 1 + \frac{g}{2\omega} (a^2 + a^4 + 2n + 1),
\]

where \( x^{2L} \) is written below for the four particular cases \( 1 \leq L \leq 4 \)

\[
x^2 = \frac{1}{2\omega} (2n + 1) + \frac{1}{2\omega} (a^2 + a^2),
\]

\[
x^4 = \frac{3}{4\omega^2} (1 + 2n + 2n^2) + \frac{1}{4\omega^2} (a^4 + a^4 + (4n - 2) a^2 + (4n + 6) a^2),
\]

\[
x^6 = \frac{5}{8\omega^3} (3 + 8n + 6n^2 + 4n^3) + \frac{1}{8\omega^3} (a^6 + a^6 + (6n - 9) a^4 + (6n + 15) a^4 + 15 (1 - n + n^2) a^2 + 15 (3 + 3n + n^2) a^2),
\]

\[
x^8 = \frac{1}{16\omega^4} (105 + 280n + 350n^2 + 140n^3 + 70n^4)
\]

\[
+ \frac{1}{16\omega^4} (a^8 + a^8 + (8n - 20) a^6 + (8n + 28) a^6 + (98 - 84n + 28n^2) a^4 + (210 + 140n + 28n^2) a^4
\]

\[
+ (-28 - 196n - 84n^2 + 56n^3) a^2 + (420 + 532n + 252n^2 + 56n^3) a^2).
\]

Any degree of \( x^2 \) can be derived by the use of a recursive relation between \( x^{2L} \) and \( x^{2L-2} \). The normalized eigenvectors \( |n, \omega \rangle \) of the excitation number operator \( n \) are

\[
|n, \omega \rangle = \frac{(a^+ (\omega))^n}{\sqrt{n!}} |0, \omega \rangle, \quad a(\omega) |0, \omega \rangle = 0.
\]
In contrast to the equation Eq. (2) we can calculate the matrix elements of the equation Eq. (8) exactly in the Fock basis Eq. (15). The eigenvector \( |\varphi\rangle \) can be represented in the Fock basis Eq. (16) as

\[
|\varphi\rangle = \sum_{p=0}^{\infty} C_p |p,\omega\rangle,
\]

with the coefficient \( C_p \) to be defined by the equation Eq. (8). The arguments of \( a^\dagger(\omega) \), \( a(\omega) \), \( n(\omega) \) and \( |n,\omega\rangle \) will be omitted in order to simplify all expressions. Substitute Eq. (16) in Eq. (8) and find its projection on bra-vector \( \langle k,\omega | \)

\[
C_k \langle k|L'|k\rangle - C_k \langle k|L''|k\rangle E + \sum_{p\neq k} C_p \langle k|L'|p\rangle - E \sum_{p\neq k} C_p \langle k|L''|p\rangle = 0.
\]

The system of the linear equations Eq. (17) can be solved by the iterative method of the form 20

\[
C_{k,k\neq n}^{(s)} = -\sum_{p=k-m, p\neq k}^{k+m} C_{p}^{(s-1)} \langle k|L'|p\rangle - E_{n}^{(s-1)} \sum_{p=k-m, p\neq k}^{k+m} C_{p}^{(s-1)} \langle k|L''|p\rangle,
\]

\[
E_{n}^{(s)} = \frac{\langle n|L'|n\rangle + \sum_{p=n-m, p\neq n}^{n+m} C_{p}^{(s-1)} \langle n|L'|p\rangle}{\langle n|L''|n\rangle + \sum_{p=n-m, p\neq n}^{n+m} C_{p}^{(s-1)} \langle n|L''|p\rangle},
\]

\[
C_k^{(0)} = \delta_{n,k}
\]

where \( C_k^{(s)} \) is the coefficient of the eigenvector expansion and \( E_n^{(s)} \) is the energy of \( n \)-level calculated in \( s \)-th iteration; \( m = 2L; s = 0, 1, \ldots, s_{\text{max}} \). The results of numerical calculations of the energy eigenvalues for the ground \( (n = 0) \) and first excited \( (n = 1) \) states in the wide range of values of \( g, \lambda \) are summarized in Tables 1-4. For convenience of the comparison with the results in Refs. 12,14 we present our results in the form 20 \( \lambda \), 20 \( E \). As is clear from Table 1 and Table 2, where some exact eigenvalues are given, the accuracy of the operator method is very high \( |E_n^{(s_{\text{max}})} - E_n|/E_n < 10^{-15} \). But the case \( g \gg 1, \lambda \gg 1 \) needs the increase of the iteration number \( s_{\text{max}} \). So it is important to make use of the parameter \( \omega \), which allows us to speed up the convergence of the iterative scheme. Since the exact eigenvalues of the Hamiltonian do not depend on the choice of \( \omega \), the following condition has to be satisfied for exact energy eigenvalues20:

\[
\frac{\partial E_n}{\partial \omega} = 0.
\]

Because \( E_n \) is equal to \( E_n^{(\infty)}(\omega) \), a good accuracy can be achieved at the extremum point \( \omega_{\text{extr}} \) of the function \( E_n^{(s_{\text{max}})}(\omega) \) (see Fig. 1). Notice that this statement is only valid in the case of large iteration number. As soon as the iteration number is relatively small \( E_n^{(s_{\text{max}})}(\omega) \) is described by an oscillating function crossing \( E = E_n \) (exact) for some values of \( \omega \) (see Fig. 1 and Ref. 19). In the case of large iteration number the magnitude of oscillations is very small and goes to zero quickly (see Fig. 1).

We emphasize that even for small number of iterations the points of extremum are near the exact energy eigenvalue and belong to the range of stable convergence of the iterative scheme. They can be chosen as starting values for \( \omega \). As is clear from Table 2 the values of \( s_{\text{max}} \) and \( \omega \) must be increased for excited states. Large values of \( g \) and \( \lambda \) require the increase of \( \omega \) as well. Such behavior is typical for all potentials \( V_L(x) \). Different criteria for choosing \( \omega \) can be also found in Refs. 16,17,19.

We’d like to notice that the normalized eigenfunctions \( \Psi_n(x) \) of the original SE Eq. (2) can be easily calculated

\[
\Psi_n(x) = \frac{\psi_n(x)}{\sqrt{\langle \psi_n|\psi_n \rangle}} \approx \frac{1}{N} (1 + gx^2) \sum_{k=0}^{s_{\text{max}}} C_k^{(s_{\text{max}})} \langle x|k,\omega \rangle
\]

\[
N^2 = \langle \psi_n|\psi_n \rangle \approx \int_{-\infty}^{\infty} dx (1 + gx^2)^2 \left[ \sum_{k=0}^{s_{\text{max}}} C_k^{(s_{\text{max}})} \langle x|k,\omega \rangle \right]^2.
\]

The polynomial structure of the operator equation Eq. (4) also allows us to obtain some analytical expressions for the energy eigenvalues with the explicit dependence on all parameters. Such expressions can be found by making a limited number of iterations with any system of computer algebra like Maple or Mathematica.
III. CONCLUSION

The Schrödinger equation with the rational potential was solved by the operator method. The energy of the ground state and the first excited state were calculated with very high accuracy without any limitations on the parameters of the Hamiltonian. The numerical solutions are in excellent agreement with the exact solutions known for some values of $g$ and $\lambda$. The criteria for choosing the convergence parameter $\omega$ was analyzed. So we have shown that the spectrum of the original nonpolynomial Schrödinger equation Eq.(2) is identical to the one of the polynomial operator equation Eq.(4). The results obtained demonstrate that the operator method is very efficiently for solving the problems with the nonpolynomial structure of the Hamiltonian if the nonunitary transformation is used. The application of the operator method to the three-dimensional nonpolynomial Hamiltonian is straightforward.

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### TABLE I: Energy eigenvalues for $V_1(x)$.

| $2\lambda/g$ | 100/10 | 10/10 | 10/100 |
|--------------|--------|-------|--------|
| $2E_0(OM)$   | 5.79394230019270 | 1.5800223729150 | 1.08406335494411 |
| $2E_1(OM)$   | 11.5721967757092 | 3.87903683088257 | 3.09831695088943 |
| $2\lambda/g$ | -2.494002/0.499 | -1.585842/0.339 | -0.0402/0.01 |
| $2E_0(OM)$   | 0.0020000000000000 | 0.322000000000000 | 0.980000000000000 |
| $2E_0(\text{exact})$ | 0.0020000000000000 | 0.322000000000000 | 0.980000000000000 |

### TABLE II: Energy eigenvalues for $V_2(x)$.

| $2\lambda/g$ | 0.1/1 | 0.1/0.1 | 1/0.1 |
|--------------|-------|---------|-------|
| $2E_0(OM)$   | 1.02514716380525 | 1.0552977725788 | 1.3605917324177 |
| $\omega/s_{\text{max}}$ | 3.0/69 | 1.74/20 | 2.90/22 |
| $2E_1(OM)$   | 3.09577659167734 | 3.24865072344241 | 4.49215757165382 |
| $\omega/s_{\text{max}}$ | 2.9/70 | 1.56/20 | 2.82/22 |
| $2\lambda/g$ | 100/10 | 10/10 | 10/100 |
| $2E_0(OM)$   | 2.90257776978742 | 1.35977466215783 | 1.04797115328336 |
| $\omega/s_{\text{max}}$ | 16.6/115 | 11.0/200 | 27.3/1400 |
| $2E_1(OM)$   | 9.21596081849447 | 4.15798607191020 | 3.1454441596743 |
| $\omega/s_{\text{max}}$ | 16.3/125 | 10.4/210 | 25.7/1700 |
| $\alpha/g$  | 0.001/0.02 | 0.005/0.1 | 0.01/0.1 |
| $E_0(OM)$    | 0.50712699243485 | 0.503010339434091 | 0.507093239851 |
| $E_0(\text{14})$ | 0.50712699243485 | 0.503010339434091 | 0.507093239851 |
| $E_1(OM)$    | 1.503492319497928 | 1.5139227239619 | 1.53457040870676 |
| $E_1(\text{14})$ | 1.503492319497928 | 1.5139227239619 | 1.53457040870676 |

### TABLE III: Energy eigenvalues for $V_3(x)$.

| $2\lambda/g$ | 100/10 | 10/10 | 10/100 |
|--------------|--------|-------|--------|
| $2E_0(OM)$   | 2.32812938769652 | 1.36685074612832 | 1.06484795071250 |
| $2E_1(OM)$   | 8.25858912303721 | 4.57644754780293 | 3.3056177307224 |
| $\lambda/g$ | $10^{-4}/10^{-3}$ | $10^{-4}/0.01$ | $5 \times 10^{-4}/2.5 \times 10^{-3}$ |
| $E_0(OM)$    | 0.500186311611817 | 0.500180733817835 | 0.500186311611817 |
| $E_0(\text{14})$ | 0.500186311611817 | 0.500180733817835 | 0.500186311611817 |
| $E_1(OM)$    | 1.503492319497928 | 1.5139227239619 | 1.53457040870676 |
| $E_1(\text{14})$ | 1.503492319497928 | 1.5139227239619 | 1.53457040870676 |
| $\alpha/g$  | 0.5215/0.2607543752089 | 0.5215/0.2607543752089 | 0.5215/0.2607543752089 |
| $2E_0(OM)$   | 1.8657366612601 | 1.8657366612601 | 1.8657366612601 |
| $2E_0(\text{exact})$ | 1.8657366612601 | 1.8657366612601 | 1.8657366612601 |
TABLE IV: Energy eigenvalues for $V_4(x)$.

| $2\lambda/g$ | 100/10 | 10/10 | 10/100 |
|-------------|--------|-------|--------|
| $2E_0$ (OM) | 2.14407957597610 | 1.41752810562730 | 1.10864569823789 |
| $2E_1$ (OM) | 3.59432196739250 | 4.9694962368201 | 3.59432196739250 |
| $2\lambda/g$ | 10/0 | 1000/0 | 10000/0 |
| $2E_0$(OM) | 2.1145462194213 | 4.94948744003274 | 7.77827221431110 |
| $2E_0$(13) | 2.11454621942129 | 4.949487440032743 | 7.778272214311099 |

FIG. 1: The ground state energy $2E_0^{(s)}$ as a function of $\omega$ for $L = +2$, $2E_0$(exact) = 1.1865736661201, $2\lambda = 0.500008389662453$, $g = 0.26075437208969$. 