Optimal choice of a parameter for the operator method of the solution of the Schrodinger equation

Optimal choice of a parameter for the operator method of the solution of the Schrödinger equation

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Abstract. The rate of convergence of the operator method iterative series as a function of the variational parameter is investigated numerically. The optimal method of calculation of this parameter is proposed.

The operator method (OM) of the approximate solution of the Schrödinter equation was introduced by Feranchuk and Komarov (1982, 1984). This method gives a uniformly convergent series for eigenvalues and eigenstates of the Hamiltonian for arbitrary values of its parameters. Casewell (1979) used a similar approach but his method of calculation of the perturbation series was essentially based on the characteristic features of the anharmonic oscillator.

We recall that, according to the OM, the Hamiltonian $\hat{\mathcal{H}}(\hat{x}, \hat{p}, \lambda)$ of the arbitrary system must be put in the second quantised form through the canonical transformation

$$\hat{x} = [1/(2\omega)^{1/2}](a^+ + a) \qquad \hat{p} = \mathrm{i}(\omega/2)^{1/2}(a^+ - a) \tag{1}$$

with arbitrary parameter ω. Here $\hat{x}$ and $\hat{p}$ are the coordinate and momentum operators, a and a^+ are the annihilation and creation operators respectively and λ is the Hamiltonian parameter.

Then $\hat{\mathcal{H}}(a, a^+, \lambda)$ is divided into two parts

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0(\omega, \hat{n}, \lambda) + \hat{V}(\omega, a, a^+, \lambda) \tag{2}$$

where $\hat{\mathcal{H}}_0(\omega, \hat{n}, \lambda)$ contains all the terms which commute with the particle number operator $\hat{n} = a^+ a$ and its eigenvalues and eigenstates are easily calculated. The perturbation theory (PT) with respect to the operator $\hat{V}(\omega)$ leads to rapidly convergent series for all eigenvalues E_n and any coupling constant λ, if the parameter ω is chosen in an optimal way.

Originally, we found $\omega = \omega_{n0}$ from the condition

$$\partial E_n^{(0)} / \partial \omega = 0 \tag{3}$$

where $E_n^{(0)}(\omega, \lambda)$ is the eigenvalue of the Hamiltonian $\hat{\mathcal{H}}_0$. This condition follows from the obvious demand that the accurate eigenvalue E_n of the Hamiltonian (2) could not depend on the artificial parameter ω, that is

$$\partial E_n / \partial \omega \equiv 0. \tag{4}$$

Equation (4) becomes equation (3) in the zeroth-order approximation with respect to the operator $\hat{V}$.

Fernandez *et al* (1984) have recently found one of the most accurate results for eigenvalues of the quantum anharmonic oscillator (QAO) by means of the OM. Their numerical calculations have shown that equation (3) leads to a good approximation for E_n only in the lowest orders of PT, but calculation of E_n with high accuracy demands that we choose the optimal value $\omega = \omega_{nb} \neq \omega_{n0}$. These authors found ω_{nb} by means of a numerical examination of various values of ω from some interval. It is clear that this method is not sufficiently effective.

In the present paper we shall investigate numerically the convergence of the PT series for different ω and shall introduce the regular method of calculation of ω_{nb} for any order of PT. We shall carry our specific calculations for the QAO problem which is described by the following Hamiltonian

$$\hat{\mathscr{H}} = \hat{\mathscr{H}}_0 + \hat{V}$$

$$\hat{\mathscr{H}}_0 = \frac{1}{4}\left(\omega + \frac{1}{\omega}\right)(2\hat{n}+1) + \frac{3\lambda}{4\omega^2}(1+2\hat{n}+2\hat{n}^2)$$

$$\hat{V} = \frac{1}{4}\left(\frac{1}{\omega}-\omega\right)(a^{+2}+a^2) + \frac{\lambda}{4\omega^2}[6(a^{+2}+a^2)+a^{+4}+a^4+4(a^+a^3+a^{+3}a)].$$

In the representation of the eigenfunctions of the operator $\hat{n}$

$$\hat{n}|n\rangle = n|n\rangle, \qquad n = 0, 1, 2, \ldots$$

the non-zeroth matrix elements of the operators $\hat{\mathscr{H}}_0$ and $\hat{V}$ are

$$\langle n|\hat{\mathscr{H}}_0|m\rangle = \mathscr{H}_{0n}\delta_{mn} \qquad \mathscr{H}_{0n} = \frac{1}{4}\left(\omega+\frac{1}{\omega}\right)(2n+1) + \frac{3\lambda}{4\omega^2}(1+2n+2n^2)$$

$$\langle n+2|\hat{V}|n\rangle = \langle n|\hat{V}|n+2\rangle = [(n+1)(n+2)]^{1/2}\frac{\omega(\omega^2-1)-\lambda(4n+6)}{4\omega^2}$$

$$\langle n+4|\hat{V}|n\rangle = \langle n|\hat{V}|n+4\rangle = \frac{\lambda}{4\omega^2}\left(\frac{(n+4)!}{n!}\right)^{1/2}.$$

Let us find the accuracy eigenvector $|\psi_n\rangle$ and eigenvalue E_n of the Hamiltonian (2)

$$\hat{\mathscr{H}}|\psi_n\rangle = E_n|\psi_n\rangle$$

in the following form

$$|\psi_n\rangle = \sum_{j=0}^{\infty} C_{nj}|j\rangle \tag{5}$$

with the normalisation condition

$$\langle n|\psi_n\rangle = 1 \qquad C_{nn} = 1.$$

Then the OM gives in the zeroth approximation

$$C_{nj}^{(0)} = \delta_{nj} \qquad E_n^{(0)} = \mathscr{H}_{0n} \tag{6}$$

and the perturbation series with respect to the operator $\hat{V}(\omega)$ leads to the following recursive equations (Fernandez *et al* 1984)

$$E_n^{(s)} = \sum_{j\neq n} C_{nj}^{(s-1)}\langle n|\hat{V}|j\rangle \qquad s \geq 2 \tag{7}$$

$$C_{nj}^{(s)} = -(\mathscr{H}_{0j}-\mathscr{H}_{0n})^{-1}\left(\sum_{k\neq j} C_{nk}^{(s-1)}\langle j|\hat{V}|k\rangle - \sum_{p=1}^{s-1} C_{nj}^{(p)}\sum_{k\neq n} C_{nk}^{(s-p-1)}\langle n|\hat{V}|k\rangle\right) \qquad n\neq j$$

$$\tag{8}$$

where

$$C_{nj} = \sum_{s=1}^{\infty} C_{nj}^{(s)}(\omega) \qquad E_n = \sum_{s=0}^{\infty} E_n^{(s)}(\omega) \qquad E_n^{(1)} = 0. \qquad (9)$$

The parameter ω is still arbitrary, but in accordance with Feranchuk and Komarov (1984) its optimal value ω_{nb} corresponds to a partial summation of PT series and essentially affects the rate of convergence of the series (9). In order to introduce the regular method of the calculation of ω_{nb} let us consider the following partial sums

$$S_n^{(m)}(\omega) = \sum_{s=0}^{m} E_n^{(s)}(\omega) \qquad m = 0, 1, 2 \dots \qquad (10)$$

as functions of ω. This proves (see figure 1) that $S_n^{(m)}(\omega)$ for the QAO problem becomes a constant E_n, when $m \to \infty$. This limit transition is very peculiar because the value $S_n^{(m)} - E_n$ is an oscillating function of ω but an amplitude of the oscillation vanishes. The positions of extrema of the function $S_n^{(m)}(\omega)$ essentially change for different m and condition (4) becomes ambiguous. At the same time there are values of the parameter ω such that $S_n^{(m)}(\omega)$ coincides with its limit value E_n. This affirmation is correct for $m \geq 2$, if $n = 0, 1$, and for $m \geq 0$, if $n \geq 2$. This permits us to propose the following numerical method of the regular calculation of the optimal value ω_{nb}: let us
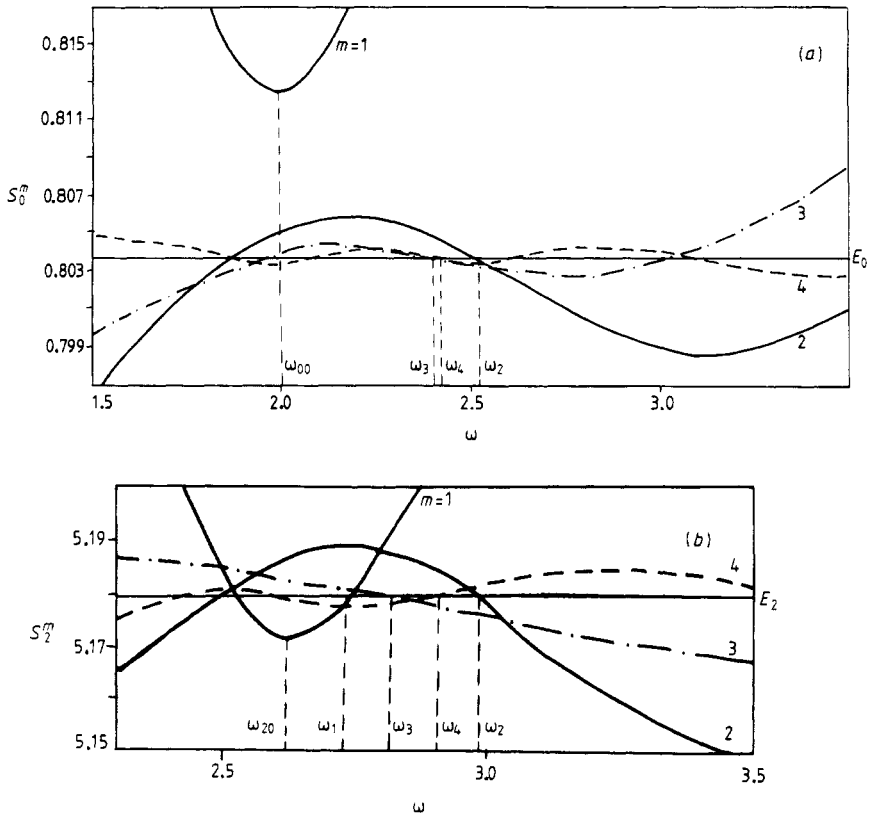

Figure 1. Dependence of the partial sums of OM perturbation series for the QAO problem on the parameter ω: (a) the ground state ($n = 0$); (b) the second excited state ($n = 2$).

determine it as a root of the equation

$$E_n^{(0)}(\omega_{nb}) + E_n^{(2)}(\omega_{nb}) = E_n \qquad \text{if } n = 0, 1$$
$$E_n^{(0)}(\omega_{nb}) = E_n \qquad\qquad \text{if } n \geq 2. \tag{11}$$

It is obvious that the accurate value E_n is unknown beforehand and in reality ω_{nb} is calculated as the following limit value

$$\omega_{nb} = \lim_{m \to \infty} \omega_{nb}^{(m)} \qquad \omega_{nb} > \omega_{n0} \tag{12}$$

where for every eigenvalue its own parameter $\omega_{nb}^{(m)}$ is that root of the equation

$$\sum_{s=3}^{m} E_n^{(s)}(\omega_{nb}^{(m)}) = 0 \qquad \text{if } n = 0, 1$$
$$\sum_{s=2}^{m} E_n^{(s)}(\omega_{nb}^{(m)}) = 0 \qquad \text{if } n \geq 2 \tag{13}$$

which is nearest to the value ω_{n0}. Here ω_{n0} is defined by equation (3).

Equation (13) gives an unambiguous numerical method for the calculation of ω_{nb} and the sequence $\omega_{nb}^{(m)}$ converges to ω_{nb} sufficiently rapidly (see figure 2). This procedure
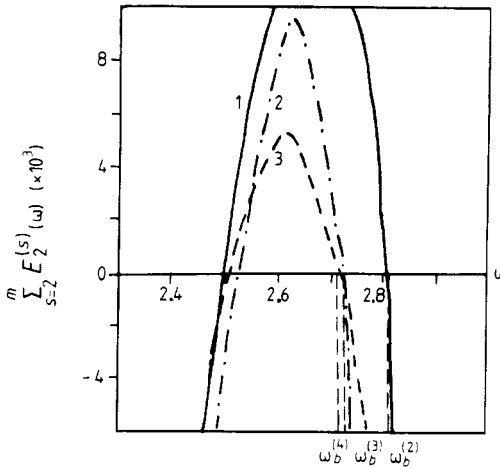

Figure 2. Successive values of the optimal parameter $\omega_{0b}^{(m)}$.

acquires a clear meaning if you consider the graphical presentation of the perturbation series introduced by Feranchuk and Komarov (1984) for the QAO problem. Indeed, if condition (11) is fulfilled for every iteration then the recursive equations (7) are essentially simplified:

$$C_{nj}^{(s)} = -(\mathcal{H}_{0j} - \mathcal{H}_{0n})^{-1} \sum_{k \neq j} C_{nk}^{(s-1)} \langle j | \hat{V} | k \rangle \qquad n \geq 2. \tag{14}$$

It is easy to make sure that this series corresponds to bound diagrams only, i.e. the choice $\omega = \omega_{nb}$ leads to the disappearance of the unbound diagrams.

Figure 3 shows the successive terms of the iterative series defined by equations (9), (13) and (14) for the eigenvalues of the QAO problem. Their decrease as a function of s signifies that this series rapidly converges as the geometric progression with
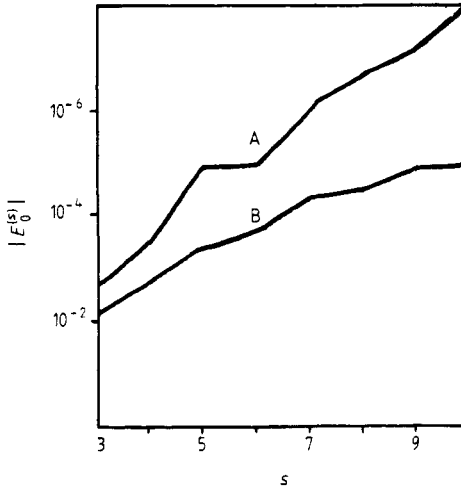
Figure 3. Successive terms of OM perturbation series with A optimal, ω_{0b} and B, fixed ω. $\lambda = 1$.

denominator $q \sim \frac{1}{8}$. At the same time the rate of convergence of the OM series with any fixed ω, which was considered by Fernandez *et al* (1984), is essentially smaller $(q \sim \frac{1}{3})$. Several eigenvalues of the QAO problem are compared with their accurate values in table 1.

Table 1. Comparison of the eigenvalues for the QAO problem, calculated by means of the operator method, with its accurate values E_n.

λ	E_0	$E_0^{(0)} + E_0^{(2)}(\omega_{0b}^{(8)})$	$E_0^{(0)} + E_0^{(2)}(\omega_{0b}^{(9)})$	$\omega_{0b}^{(9)}$
1	0.803 770 65	0.803 770 79	0.803 770 71	2.517 0107
50	2.499 708 77	2.499 710 45	2.499 709 57	8.770 4769

	E_2	$E_2^{(0)}(\omega_{2b}^{(8)})$	$E_2^{(0)}(\omega_{2b}^{(9)})$	$\omega_{2b}^{(9)}$
1	5.179 291 69	5.179 293 28	5.179 292 02	3.011 8979
50	17.436 992 1	17.437 008 2	17.436 995 8	10.712 937

We realise that the modification of the OM, described in this paper, is required for rigorous mathematical reasons, and it can still be considered as a practical calculation algorithm. However, we have tried it for several examples, besides the QAO problem, and it proves very efficient for calculation of the high-order corrections for eigenvalues by means of the operator method.

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