An analytical description of some quantum systems in periodic external fields and

quasistationary systems

An analytical description of some quantum systems in periodic external fields and quasistationary systems

I D Feranchuk, L I Komarov and I V Nechipor

Department of Physics, Byelorussian State University, Minsk-80, USSR

Abstract. The peculiarities of the operator method in solving the Schrödinger equation with periodic potentials are discussed. Approximate analytical solutions of the Mathieu equation and Schrödinger equations for a two-level system are found on the basis of the operator method. An analogous method is used for the analytical estimation of the quasistationary state energy and width.

1. Introduction

The operator method (OM) for the approximate solution of the Schrödinger equation in the whole range of Hamiltonian parameters was developed by Feranchuk and Komarov (1982, 1984). In the present paper we shall use the main ideas of the OM in order to solve the Schrödinger equation for specific Hamiltonians which have space or time periodicity.

According to Feranchuk and Komarov (1984), the essential characteristics of the OM which define its efficiency in different problems are the following: (i) a special choice of the basis set $\psi_n^{(0)}(\omega_n)$ of the eigenfunctions, which are non-orthogonal in general and contain the set of the variational parameters ω_n, different for various n; (ii) a definite method of separating the zeroth-order Hamiltonian $\hat{H}_0$ out of the exact operator $\hat{H}$; (iii) calculation of the series for eigenfunctions and eigenvalues of $\hat{H}$ which are uniformly convergent in the whole range of the Hamiltonian parameters.

In the majority of examples discussed by Feranchuk and Komarov (1982, 1984), the transition from coordinate representation to the second quantised form was used. In this case the particle-number operator eigenfunctions $|n, \omega_n\rangle$ were chosen as the functions $|\psi_n^{(0)}(\omega_n)\rangle$. In particular, the Mathieu equation eigenvalue problem was considered with the help of such an approach. However, the results contained infinite sums and did not have a simple analytical form.

Undoubtedly, the choice of the functions $|n, \omega_n\rangle$ as a full set is not the only possible one. In general, this choice is conditioned by the algebraic character of the calculations of the OM high-order corrections. Sometimes, however, it is expedient to complicate such calculations if the choice of a more adequate basis permits us to improve radically the accuracy of the zeroth-order approximation. Such a situation arises in describing quantum systems in periodic fields, which we examine in the present paper. In § 2 we shall consider specific features of the OM in solving the Mathieu equation, for which detailed quantitative calculations exist (see, for example, Abramowitz and Stegun 1979). This fact permits us to estimate the accuracy of the approach.

The quasi-energy method is a very handy way of describing quantum systems which are in an external periodic field (see, for example, the review by Zeldovitch (1973) and references therein). The problem of the evolution of a two-level system in a monochromatic linearly polarised field is a good model for many physical problems. The numerical solutions of these problems and approximate analytical formulae for quasi-energies in the different limits defined by the large or small values of non-dimensional parameters of the system are well known (see, for example, Fainstein *et al* (1978) and Finkelstein (1985) and references therein). However, analytical expressions for eigenfunctions and quasi-energies of two-level systems which are correct with sufficient accuracy in the whole range of the parameters are of great interest because these functions and the quasi-energy spectrum are often used as a basis for investigating real atomic systems (see, for example, Liaptsev and Zuev 1985). Therefore, § 3 is devoted to deducing the zeroth-order approximation formulae for quasi-energies and eigenfunctions of two-level systems on the basis of the OM. It is shown that these formulae give a sufficiently accurate solution of the problem.

In § 4 we shall show that an analogous method leads to sufficiently simple formulae for real, E', and imaginary, E'', parts of the quasistationary state energies. We prove that these formulae give a uniformly fitted approximation for eigenvalues, both in the case of exponentially small E'' and in the case where $E'' \sim E'$.

We shall also discuss the regular procedure which permits us to improve the zeroth-order approximation for the problem considered in this paper.

2. Approximate solution of the Mathieu equation

Let us consider the canonical form of the Mathieu equation, corresponding to the Schrödinger equation for a particle with mass $m = \frac{1}{2}$ in a one-dimensional periodic potential field:

$$(\hat{H} - E)\psi \equiv (\hat{p}^2 + h \cos 2x - E)\psi(x) = (-d^2/dx^2 + h \cos 2x - E)\psi(x) = 0. \tag{1}$$

We shall consider the eigenvalues E corresponding to the periodic solutions

$$\psi(x + 2\pi) = \psi(x) \qquad \psi(x + \pi) = \pm\psi(x). \tag{2}$$

Without any additional suppositions about the potential amplitude h we put the operator $\hat{H}$ into a form similar to the harmonic oscillator Hamiltonian:

$$\hat{H} = \hat{p}^2 + 2h \cos^2 x - h \tag{3}$$

and introduce two canonical conjugate operators

$$a = \hat{p} - i\sqrt{2h} \cos x \qquad a^+ = \hat{p} + i\sqrt{2h} \cos x. \tag{4}$$

These operators define two basic functions

$$|\psi^{(\pm)}\rangle = \exp(\pm\sqrt{2h} \sin x) \qquad a|\psi^{(-)}\rangle = 0 \qquad a^+|\psi^{(+)}\rangle = 0. \tag{5}$$

The commutator of the operators a and a^+ is more complicated than the analogous one for the harmonic oscillator considered by Feranchuk and Komarov (1982). This is why they do not factorise the Hamiltonian $\hat{H}$ and the functions (5) are not accurate solutions of equation (1). Nevertheless, it is possible to build some set of the basic functions ψ_n with their help, which will serve as a foundation for the OM construction. Feranchuk and Komarov (1982, 1984) used a one-parametric unitary transformation of the initial creation and annihilation operators in order to consider quantum systems more complicated than the harmonic oscillator. This transformation allowed them to

introduce the arbitrary parameter ω into the basic function set. We shall perform an analogous transformation on the operators (4) which corresponds to the following substitution of functions:

$$\psi^{(\pm)} \to \psi_\nu^{(\pm)} = \exp(\pm \tfrac{1}{2}\nu \sin x) \tag{6}$$

where ν is a parameter which will be defined later. To construct the whole spectrum of periodic solutions of equation (1), one has to take into account the wavefunction symmetry (2) and consider the algorithm for calculating the excited states. To provide the conditions (2) it is necessary to use odd and even linear combinations of (6). As a result, the approximate normalised periodic solutions of equation (1), corresponding to the smallest eigenvalues E_0, E_1, have the following form:

$$|\psi_{0\nu}\rangle = \frac{1}{(I_0 + 1)^{1/2}} \cosh(\tfrac{1}{2}\nu \sin x)$$

$$\tag{7}$$

$$|\psi_{1\nu}\rangle = \frac{1}{(I_0 - 1)^{1/2}} \sinh(\tfrac{1}{2}\nu \sin x).$$

Here $I_0(\nu)$ is the zeroth-order Bessel function with imaginary argument and the normalising and orthogonalisation conditions are defined by the scalar product (Abramowitz and Stegun 1979)

$$\langle \psi_{\alpha,\nu} | \psi_{\beta,\nu} \rangle = \int_0^{2\pi} dx\, \psi_{\alpha,\nu}^*(x) \psi_{\beta,\nu}(x) = \pi \delta_{\alpha\beta}.$$

As will be shown later, the simple analytical functions $|\psi_{0\nu}\rangle$ and $|\psi_{1\nu}\rangle$ are approximate representations of the Mathieu functions Ce_0 and Se_1 (Abramowitz and Stegun 1979) if the parameter ν is chosen in an optimal way.

The complicated form for the commutators of the operators a and a^+ in the present case does not permit us to find the excited system states and perturbation operator matrix elements purely algebraically, as is done in using the oscillator wavefunctions. Nevertheless, one can find without difficulty the necessary quantity of the functions $|\psi_{n,\nu}\rangle$ of the full set using linear combinations of (7) multiplied by polynomials over powers of $\cos x$ using well known orthogonalisations (Tikhonov and Samarsky 1972).

We emphasise that, in accordance with the OM scheme, the parameter ν_n will take different values for different n. This being so, different functions of the full set $|\psi_{n,\nu_n}\rangle$ will not in general be orthogonal. The above-mentioned orthogonalisation of the wavefunctions with fixed parameter ν is necessary to provide a correct symmetry and a number of zero points of wavefunctions for excited states.

We remark that the solution of the Mathieu equation corresponding to non-zero quasimomentum k does not have definite parity. Therefore one has to use linear combinations of basic functions (6) with variational coefficients for the approximation of such a solution.

We adduce also the normalised functions $|\psi_{2\nu}\rangle$ and $|\psi_{3\nu}\rangle$ of two excited states which give an analytical approximation for the Mathieu functions Ce_1 and Se_2:

$$|\psi_{2,\nu}\rangle = \frac{1}{[(1/\nu)I_1 + \tfrac{1}{2}]^{1/2}} \cos x \cosh(\tfrac{1}{2}\nu \sin x)$$

$$I_1 = \frac{\partial I_0}{\partial \nu}. \tag{8}$$

$$|\psi_{3,\nu}\rangle = \frac{1}{[(1/\nu)I_1 - \tfrac{1}{2}]^{1/2}} \cos x \sinh(\tfrac{1}{2}\nu \sin x)$$

These functions correspond to the eigenvalues $E_{2,3}$.

Now let us pass to the choice of the parameter ν_n. According to Feranchuk and Komarov (1984) and Fernandez *et al* (1985), one can represent the result of an operation of the Hamiltonian $\hat{H}$ on the definite wavefunction in the following form:

$$\hat{H}|\psi_{n,\nu}\rangle \equiv (\hat{H}_{0n} + \hat{V}_n)|\psi_{n,\nu}\rangle = E_n(\nu)|\psi_{n\nu}\rangle + \sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \beta^m V_{nm}|\psi_{n+m,\nu}\rangle \tag{9}$$

where $\hat{H}_{0n}$ is the $\hat{H}$ operator diagonal part with function $|\psi_{n\nu}\rangle$ being the eigenfunction for this part with eigenvalue $E_n(\nu)$. The operator $\hat{V}_n$ transforms the function $|\psi_{n,\nu}\rangle$ into wavefunctions of different states with numbers $n' \neq n$. According to the OM, the value $E_n(\nu_{n0})$ determines the zeroth-order approximation $E_n^{(0)}$ of the precise eigenvalue E_n for a definite choice of the parameter $\nu = \nu_{n0}$. To calculate the high-order approximation corrections it is necessary to use perturbation theory with respect to the operator $\hat{V}_n$. For example, in order to calculate the pth-order correction to $E_n^{(0)}$ one should take into account the matrix elements of transitions V_{nm} to the states with n' differing from n for $|m| \leq p$ in the perturbation theory formulae. To account for this circumstance we have introduced the arbitrary parameter β into the matrix elements of the operator $\hat{V}_n$ (one has to put β equal to unity at the end of the calculation).

In this case the coefficients C_{nk} of the expansion of the exact state vector $|\psi_n\rangle$ in the basic functions $|\psi_{k,\nu}\rangle$

$$|\psi_n\rangle = \sum_k C_{nk}|\psi_{k,\nu}\rangle$$

are defined by the following recurrence system:

$$C_{nk}^{(i)} = [E_n^{(i-1)} - E_k(\nu)]^{-1}\left(\nu_{nm}(\delta_{m,1} + \delta_{m,-1})\delta_{m,k-n} + \sum_{\substack{|m| \leq i-1 \\ m \neq 0}} \sum_j C_{nj}^{(i-|m|)} V_{jm}\delta_{k,j+m} \right) \tag{10}$$

where $C_{nk} = \sum_{i=0}^{\infty} C_{nk}^{(i)}$. The exact eigenvalue is obtained using the expression

$$E_n^{(i)} = E_n(\nu)\delta_{i,0} + \sum_{\substack{|m| \leq i-1 \\ m \neq 0}} C_{nm+n}^{(i-|m|)} V_{nm}$$

$$E_n = \sum_{i=0}^{\infty} E_n^{(i)}. \tag{11}$$

Calculating the OM high-order corrections for the Mathieu equation with the help of basis $|\psi_{n,\nu}\rangle$ has no principal difficulties.

A good zeroth-order approximation for Mathieu equation solutions is not a coincidence. Let us find the first non-zero correction to the energy $E_0^{(0)}$. According to formulae (10) and (11) this correction is defined by the transition from the ground state to the state $|\psi_{4\nu_0}\rangle$. The normalised wavefunction $|\psi_{4\nu_0}^{(0)}\rangle$ has the following form:

$$|\psi_{4\nu_0}^{(0)}\rangle = \frac{(2/\nu)I_1 + 1 - 2(1+I_0)\cos^2 x}{(1+I_0)[\frac{3}{2} + (12/\nu^2)I_2 - (2I_1/\nu+1)^2/(I_0+1)]^{1/2}}\cosh(\tfrac{1}{2}\nu\sin x)$$

$$I_2 = I_0 - (2/\nu)I_1$$

where

$$\langle \psi_{4\nu_0}^{(0)}|\psi_{k\nu_0}^{(0)}\rangle = 0 \qquad k \leq 3.$$

Then the corrections $E_0^{(2)}$ and $|\psi_{0\nu_0}^{(1)}\rangle$ are defined by the formulae

$$E_0^{(2)} = -\frac{|\langle \psi_{4\nu_0}^{(0)}|\hat{H}|\psi_{0\nu_0}^{(0)}\rangle|^2}{\langle \psi_{4\nu_0}^{(0)}|\hat{H}|\psi_{4\nu_0}^{(0)}\rangle - E_0^{(0)}} \qquad |\psi_{0\nu_0}^{(1)}\rangle = -\frac{\langle \psi_{4\nu_0}^{(0)}|\hat{H}|\psi_{0\nu_0}^{(0)}\rangle}{\langle \psi_{4\nu_0}^{(0)}|\hat{H}|\psi_{4\nu_0}^{(0)}\rangle - E_0^{(0)}}|\psi_{4\nu_0}^{(0)}\rangle.$$

For example, we obtain $E_0^{(2)} = -5.78 \times 10^{-5}$ for $h = 10$ which accounts for $\sim 0.001\%$ of $E_0^{(0)}$ and $|\psi_{0\nu_0}^{(1)}(\pi/2, 5)\rangle = 2.05 \times 10^{-3}$.

We shall not consider the detailed calculations of the high-order corrections because the OM zeroth-order approximation provides very high accuracy both for eigenvalues and for eigenfunctions of the Mathieu equation and two-level systems.

To choose the parameter ν_n in the OM zeroth-order approximation we use the fact that exact eigenvalues of equation (1) do not depend on the parameter ν introduced artificially, i.e. the following condition must be satisfied:

$$\partial E / \partial \nu = 0. \tag{12}$$

This condition in the zeroth-order approximation gives an equation for calculation of the parameter ν_n:

$$\frac{\partial E_n(\nu_n)}{\partial \nu_n} = \frac{\partial}{\partial \nu_n} \int_0^{2\pi} \psi_{n,\nu_n}^* \hat{H} \psi_{n,\nu_n} \, dx = 0. \tag{13}$$

For the ground state ($n = 0$) equation (13) leads to the same result as the variational principle on the class of functions $|\psi_{0\nu}\rangle$ gives. However, it is impossible to consider it as a consequence of the variational principle for excited states, because in differentiating over the single parameter ν_n for every n we do not take into account the orthogonality conditions of the function $|\psi_{n,\nu_n}\rangle$ with all functions corresponding to the index $n' < n$. In the ordinary variational solution these conditions demand the introduction of n parameters in the trial function for the nth excited state.

Thus, (9) and (13) lead to two equations for computing the parameter ν_n and the zeroth-order approximation $E_n^{(0)} = E_n(\nu_n)$ of the eigenvalue E_n for every n. The approximate wavefunction is determined by the simple formulae (7) and (8) after substitution of the solution ν_n of equation (13). Let us give as an example the corresponding equations for the states with $n = 0, 1, 2, 3$:

$$E_{0,1} = \frac{1}{I_0 \pm 1} \left[\mp \tfrac{1}{8} \nu^2 + \tfrac{1}{4} \nu I_1 + h_{0,1} \left(\frac{2}{\nu} I_1 - I_0 \right) \right] \tag{14}$$

$$h_{0,1} = \frac{\nu}{4} \frac{I_0^2 - 1 \pm I_1(\tfrac{1}{2}\nu \mp I_1)}{I_1(2I/\nu - I_0) + (I_0 \pm 1)[I_1(1 + 4/\nu^2) - 2I_0/\nu]} \tag{15}$$

$$E_{2,3} = \frac{1}{2I_1/\nu \pm 1} \{ \pm 1 \mp \tfrac{3}{16} \nu^2 + \tfrac{3}{2} I_0 - I_1/\nu$$
$$- h_{2,3}[\mp \tfrac{1}{2} - 12 I_0/\nu^2 + (2/\nu)(1 + 12/\nu^2) I_1] \} \tag{16}$$

$$h_{2,3} = \frac{I_1^2 - I_0^2 + (2/\nu) I_0 I_1 - \tfrac{1}{8} \nu^2 \pm (2/\nu) I_1 \pm I_0(\tfrac{1}{8}\nu^2 - 1)}{(8/\nu^2) I_0^2 \pm I_0(1 + 16/\nu^2) - (8/\nu^2) I_1^2(1 + 4/\nu^2) \mp (2/\nu) I_1(3 + 16/\nu^2)}. \tag{17}$$

The transcendental equations (14)–(17) can be solved in obvious form and the dependence $E_n^{(0)}(h)$ can be found in the limits $h \gg 1$ and $h \ll 1$. For example, one can find for the case of $n = 0$

$$h \simeq \tfrac{1}{4} \nu^2 \qquad E_0^{(0)} \simeq \tfrac{1}{16}(\tfrac{1}{8}\nu^4 - h\nu^2) \approx -\tfrac{1}{8} h^2 \qquad h \ll 1$$

$$h \simeq \tfrac{1}{8} \nu^2 \qquad E_0^{(0)} \simeq \tfrac{1}{4}\nu(I_1/I_0) + h[(2/\nu)(I_1/I_0) - 1] \simeq -h + \sqrt{2h} \qquad h \gg 1. \tag{18}$$

These results coincide with corresponding asymptotic expansions of the accurate eigenvalue $E_0(h)$.

It is not difficult to verify that the main terms of the asymptotic expansions are reproduced exactly for other states as well. The characteristic feature of the solutions

Table 1. Comparison of the exact periodic solution and eigenvalues of the Mathieu equation (Abramowitz and Stegun 1979) with the OM zeroth approximation.

	h_0	E_0	$Ce_0(0, \tfrac{1}{2}h_0)$	$Ce_0(\tfrac{1}{2}\pi, \tfrac{1}{2}h_0)$
Exact	10	-5.800	4.48×10^{-2}	1.335
Solution	30	-22.513	1.93×10^{-3}	1.550
$\nu_0 = 8.331$	10	-5.800	4.14×10^{-2}	1.333
$\nu_0 = 14.944$	30	-22.513	1.76×10^{-3}	1.550
	h_1	E_1	$Se_1'(0, \tfrac{1}{2}h_1)$	$Se_1(\tfrac{1}{2}\pi, \tfrac{1}{2}h_1)$
Exact	10	-5.790	1.75×10^{-1}	1.337
Solution	30	-22.513	1.39×10^{-2}	1.550
$\nu_1 = 8.370\,64$	10	-5.790	1.70×10^{-1}	1.337
$\nu_1 = 14.944\,164$	30	-22.513	1.32×10^{-2}	1.550
	h_2	E_2	$Ce_1(0, \tfrac{1}{2}h_2)$	$Ce_1'(\tfrac{1}{2}\pi, \tfrac{1}{2}h_2)$
Exact	10	1.858	2.57×10^{-1}	-3.469
Solution	30	-8.101	1.50×10^{-2}	-5.764
$\nu_2 = 6.783\,55$	10	1.867	2.28×10^{-1}	-3.388
$\nu_2 = 13.772\,105$	30	-8.100	1.17×10^{-2}	-5.740
	h_3	E_3	$Se_2'(0, \tfrac{1}{2}h_3)$	$Se_2'(\tfrac{1}{2}\pi, \tfrac{1}{2}h_3)$
Exact	10	2.099	7.33×10^{-1}	-3.641
Solution	30	-8.099	9.18×10^{-2}	-5.766
$\nu_3 = 7.212$	10	2.100	7.09×10^{-1}	-3.615
$\nu_3 = 13.7793$	30	-8.099	8.06×10^{-2}	-5.742

obtained by the OM is their ability to approximate the exact solution in the whole range of the coupling constant. That is why the powers of h appearing in the next terms of the series (18) are the same as in the accurate asymptotic series but with negligible differing coefficients. Table 1 shows the accuracy provided by the functions $|\psi_{n, \nu_n}\rangle$ and $E_n^{(0)}(h)$ for intermediate values of h.

It should be remarked that during concrete calculations it is convenient to consider ν as an independent quantity defining the function $E_n^{(0)}(h)$ in parametric form. It permits one to avoid solving equation (15) or (17) for every fixed h but use it to calculate $h(\nu)$. The results listed in table 1 show that rather simple formulae such as (14)–(17) determine eigenvalues of the Mathieu equation with an accuracy $\sim 10^{-4}$. Correct asymptotic behaviour and symmetry properties of simple functions such as (7) and (8) can also provide enough accuracy for many practical calculations with Mathieu functions (see table 1).

3. Quasi-energies and wavefunctions of the two-level system

Let us consider the Schrödinger equation for a two-level atom in a periodic linearly polarised field. For this we shall use the notation of the paper of Fainstein *et al* (1978):

$$\hat{H}|\psi(\tau)\rangle \equiv \left[-i\omega \frac{\partial}{\partial \tau} + \tfrac{1}{2}E\sigma_3 - F\sigma_1 \cos \tau \right] |\psi(\tau)\rangle = \mathscr{E}|\psi(\tau)\rangle. \tag{19}$$

Here σ_i are the Pauli matrices, $\mathscr{E}$ is the quasi-energy, the value E determines the distance between unexcited atom levels, the parameter F proportional to the transition dipole matrix elements determines the amplitude of the atom interaction with external field and ω is the frequency of this field. The method, used previously to find the approximate solution for the Mathieu equation can be used in the case defined by equation (19).

However, it is necessary to use functions different from (6) to construct the state vector basic set containing the arbitrary parameter λ. In the case considered one can choose the basic functions in the following spinor form:

$$|\psi^{\pm}\rangle = \exp(\pm i\lambda \sin \tau)\chi_{\pm} \qquad \chi_{+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \chi_{-} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{20}$$

Let us build a linear combination of the spinors (20) for lower quasi-energetic zones $\mathscr{E}_{n0}(n = 1, 2)$ in such a way that it could reproduce the precise solution of equation (19) in the quasiclassical limit ($F \gg 1$) and in the limit of weak coupling ($F \ll 1$). Wavefunctions of the form $|\psi_{n,\lambda}(\tau)\rangle = C_1\chi_1 + C_2\chi_2\, e^{i\tau}$ satisfy the conditions

$$\chi_1 = \begin{pmatrix} \cos \varphi \\ -i \sin \varphi \end{pmatrix} \qquad \chi_2 = \begin{pmatrix} \sin \varphi \\ i \cos \varphi \end{pmatrix} \qquad \varphi = \lambda \sin \tau \tag{21}$$

where $C_{1,2}$ are arbitrary coefficients. The other branches of the quasi-energy spectrum can be obtained by the functions containing polynomials over the powers of the function $\exp(i\tau)$ as factors before the spinors in (21). The orthogonalisation of these functions must be fulfilled, taking into account the scalar production definition (Zeldovich 1973)

$$\langle\!\langle \psi_\alpha(\tau)|\psi_\beta(\tau)\rangle\!\rangle = \int_0^{2\pi} \mathrm{d}\tau\langle\psi_\alpha(\tau)|\psi_\beta(\tau)\rangle.$$

Later we shall only discuss the states corresponding to the quasi-energies $\mathscr{E}_{n0}$. Let us now separate from $\hat{H}$ the part which is diagonal relative to the function (21). As a result we obtain the following system for determining the coefficients $C_{1,2}$:

$$\begin{aligned}
\mathscr{E}C_1 &= \tfrac{1}{2}E(\mathscr{J}_0(2\lambda)C_1 + i\mathscr{J}_1(2\lambda)C_2) + \tfrac{1}{2}i(F - \omega\lambda)C_2 \\
\mathscr{E}C_2 &= \omega C_2 - \tfrac{1}{2}E(\mathscr{J}_0(2\lambda)C_2 + i\mathscr{J}_1(2\lambda)C_1) - \tfrac{1}{2}i(F - \omega\lambda)C_1
\end{aligned} \tag{22}$$

where $\mathscr{J}_0$ and $\mathscr{J}_1$ are Bessel functions with real argument.

The condition of existence of the non-trivial solution of the system (22) defines the zeroth-order approximation for the quasi-energy:

$$A_{1,2} \equiv \mathscr{E}_{1,2}^{(0)}/E = \tfrac{1}{2}(\omega/E \pm \{[\omega/E - \mathscr{J}_0(2\lambda)]^2 + [\omega\lambda/E - F/E - \mathscr{J}_1(2\lambda)]^2\}^{1/2}) \tag{23}$$

if the parameter λ is calculated by means of the equation arising from the condition $\partial\mathscr{E}_{n0}(\lambda)/\partial\lambda = 0$, or

$$2\mathscr{J}_1(2\lambda)(\omega/E - \mathscr{J}_0(2\lambda)) + \left[\frac{\omega}{E} + 2\left(\frac{\mathscr{J}_1(2\lambda)}{2\lambda} - \mathscr{J}_0(2\lambda)\right)\right]\left(\frac{\omega}{E}\lambda - \frac{F}{E} - \mathscr{J}_1(2\lambda)\right) = 0. \tag{24}$$

Here we have taken into account the recursive formulae

$$\mathscr{J}_0'(2\lambda) = -\mathscr{J}_1(2\lambda) \qquad \mathscr{J}_0''(2\lambda) = \mathscr{J}_1(2\lambda)/2\lambda - \mathscr{J}_0(2\lambda).$$

The normalised wavefunctions of the system are defined by the simple analytical formulae

$$|\psi_{1,2}^{(0)}(\tau)\rangle = C_1\chi_1(\tau) + C_2\chi_2(\tau)\,e^{i\tau}$$

$$C_1 = i\,\frac{F/E + \mathcal{J}_1(2\lambda) - \omega\lambda/E}{\Delta} \qquad C_2 = \frac{2A - \mathcal{J}_0(2\lambda)}{\Delta} \tag{25}$$

$$\Delta = (2A - \mathcal{J}_0(2\lambda))^2 + (\mathcal{J}_1(2\lambda) + F/E - \omega\lambda/E)^2.$$

Equations (23)–(25) reproduce correctly the main terms of the well known asymptotic expansions for quasi-energies in the corresponding limits. For example, we can find from equation (24) in the limit $F \gg \omega$

$$\lambda \simeq \frac{F}{\omega} + \frac{E}{\omega}\,\mathcal{J}_1\!\left(\frac{2F}{\omega}\right) + \mathrm{O}\!\left[\left(\frac{\omega}{F}\right)^{1/2}\right] \tag{26}$$

so that

$$\mathcal{E}_{1,0} = \frac{E}{2}\left(\frac{2}{\pi x_0}\right)^{1/2}\cos(x_0 - \tfrac{1}{4}\pi)$$

$$\mathcal{E}_{2,0} = \omega - \frac{E}{2}\left(\frac{2}{\pi x_0}\right)^{1/2}\cos(x_0 - \tfrac{1}{4}\pi) \qquad x_0 = 2F/\omega.$$

In the resonance limit $F \ll E$, $\omega \simeq E$ we find

$$\lambda \simeq F/(\omega + E) \qquad \mathcal{E}_{1,2;0} = \tfrac{1}{2}\{\omega \pm [(\omega - E)^2 + \tfrac{1}{4}F^2]^{1/2}\}$$

that also coincides with the known result (Zeldovich 1973). In addition, the formulae obtained give sufficient accuracy in the intermediate range of the Hamiltonian parameter. This is demonstrated by figure 1, where the curves obtained by means of the analytical formulae (23) and (24) are compared with the results of numerical calculations carried out by Fainstein *et al* (1978).
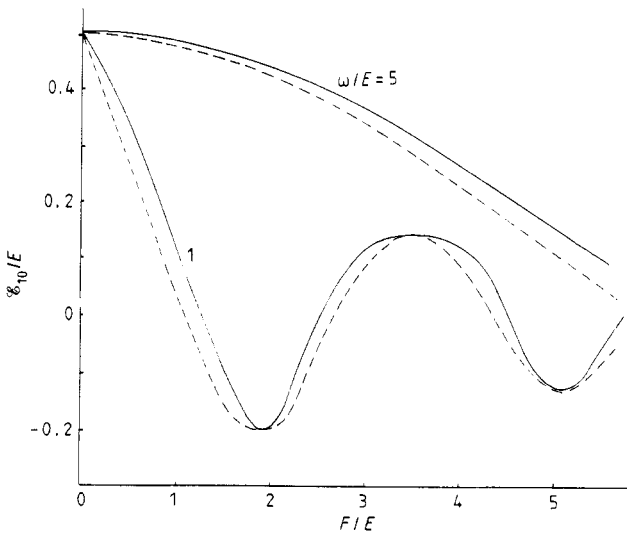

Figure 1. Comparison of the numerical calculation of quasi-energies $\mathcal{E}_{10}$ of Fainstein *et al* (1978) (broken curve) and OM zeroth approximation $\mathcal{E}_{10}^{(0)}$ for the same values (full curve) as a function of the external field magnitude. The quasi-energies are measured in units of *E*.

4. The estimation of the quasistationary state energy

Let us consider another group of problems connected with calculating the real, E'_n, and imaginary, E''_n, parts of the Hamiltonian eigenvalues E_n for quasistationary states (QS). The most widespread method of analytical estimation for these quantities, based on the quasiclassical approximation (see, for example, Sanchez and Bejarano 1986), is suitable only in the range of exponentially small values of E''_n. On the other hand, the precise numerical computations of E'_n and E''_n based on the complex coordinate rotation method (Farrelly and Reinhardt 1983) demand a great deal of calculation, especially in the range $E'_n \gg E''_n$. This is why the method which allows us to obtain sufficiently accurate estimations for E_n for any correlation between E'_n and E''_n and a comparatively small volume of calculations is of great interest for different applications.

Let us take a simple example of the system with Hamiltonian

$$\hat{H} = \tfrac{1}{2}(\hat{p}^2 + x^2) - \lambda x^4 \qquad \lambda > 0. \tag{27}$$

Its spectrum consists of QS. As is generally known, in this case the quantity E''_n corresponds to an essential singularity for $\lambda \to 0$, concerned with the exponentially small potential barrier penetration. Firstly, let us find eigenfunctions of the operator (1) with the help of OM in the simple form discussed by Feranchuk and Komarov (1982). For this purpose one has to pass to the second quantised representation

$$\hat{x} = (1/\sqrt{2\omega})(a^+ + a) \qquad \hat{p} = \mathrm{i}(\tfrac{1}{2}\omega)^{1/2}(a^+ - a) \qquad [aa^+] = 1 \tag{28}$$

supposing that the parameter ω may be complex valued, which is equivalent to a complex-valued coordinate rotation. As has been shown by Feranchuk and Komarov (1984), the analytical continuation of the state vector and creation and annihilation operators on complex-valued ω is carried out by the following operator:

$$\hat{R}(\omega, 1) = \exp[\tfrac{1}{4}(a_1^{+2} - a_1^2) \ln \omega] \tag{29}$$

where a_1 and a_1^+ are the operators corresponding to the parameter $\omega = 1$

$$a = \hat{R}^{-1} a_1 \hat{R} \qquad |0, \omega\rangle = \hat{R}(\omega, 1)|0, 1\rangle \qquad a_1|0, 1\rangle = 0. \tag{30}$$

It should be remarked that both the operators a_ω and a_ω^+ and the vectors $\langle \omega, 0|$ and $|0, \omega\rangle$ are not Hermitian conjugate with each other for an arbitrary complex-valued ω. In particular, the expression

$$\{|0, \omega\rangle\}^+ = \{\langle \omega, 0|\}^* \tag{31}$$

is satisfied. In the OM zeroth-order approximation we find the following equation for the eigenvalues of the operator (1) (Feranchuk and Komarov 1982):

$$E_n^{(0)} = \langle \omega, n|\hat{H}|n, \omega\rangle = \tfrac{1}{4}(\omega + 1/\omega)(2n + 1) - (3\lambda/4\omega^2)(1 + 2n + 2n^2) \tag{32}$$

the parameter ω being defined for every n by the equation $\partial E_n^{(0)}/\partial \omega = 0$, i.e.

$$(\omega^3 - \omega)(2n + 1) + 6\lambda(1 + 2n + 2n^2) = 0. \tag{33}$$

As has been shown by different examples by Feranchuk and Komarov (1982), the OM zeroth-order approximation allows one to find eigenvalues with an accuracy $\sim 1\%$. That is why it is possible to expect that equations (32) and (33) give a sufficiently good evaluation of energy for $\lambda > \lambda_b$ when $E''_n \gtrsim 0.01 E'_n$. In fact, the complex-valued solutions of equation (33) satisfying the condition $\omega' > 0$ appear for values of λ satisfying

the inequality

$$\lambda > \frac{2n+1}{9\sqrt{3}(2n^2+2n+1)} = \lambda_b. \tag{34}$$

Table 2(a) compares the results of calculations on the basis of equations (32) and (33) for $\lambda = 0.1$, satisfying condition (34), with the exact values of E_n obtained numerically (Farrelly and Reinhardt 1983). The results show that in the range $\lambda > \lambda_b$ the OM zeroth-order approximation provides the same accuracy of the QS energy calculation as for the stationary states ($\lambda < 0$) discussed by Feranchuk and Komarov (1982). In order to define more exactly the real and imaginary parts of $E_n^{(0)}$ we should take into account the second-order correction calculated for $\omega = \omega_0' + i\omega_0''$ by the formulae obtained by Feranchuk and Komarov (1982). For example, we find for the ground state $E_0^{(0)} + E_0^{(2)} = 0.397 + i0.046$, where $\lambda = 0.1$. This result can be compared with the exact value of E_0 given in table 2(a). Calculation of the OM high-order corrections demands numerical computation and it is not the purpose of this paper to perform it.

The aim of the paper is to obtain simple analytical formulae permitting us to estimate eigenvalues in the zeroth-order approximation. Due to this fact we use the method developed in the previous sections in the range $\lambda < \lambda_b$. For that we introduce, as in solving the Mathieu equation, two operators

$$\hat{A}_{\pm} = \frac{1}{\sqrt{2}} \hat{p} \pm i(\tfrac{1}{2}x^2 - \lambda x^4)^{1/2} \tag{35}$$

and use solutions of the equation $\hat{A}_{\pm}\psi_0^{(\mp)} = 0$, in which an arbitrary parameter ν will be introduced for creation of the zeroth-order approximation basic functions. To estimate the ground-state eigenvalue of the operator $\hat{H}$ we choose the eigenfunction zeroth approximation in the form of a linear combination of the functions $\psi_{0\nu}^{(\pm)}$:

$$|\psi_{0\nu}\rangle = \begin{cases} \frac{1}{\sqrt{2}} \exp\left(i\frac{\pi}{4} + \frac{\nu}{\lambda}(1 - 2\lambda x^2)^{3/2} \right) + \frac{1}{\sqrt{2}} \exp\left(-i\frac{\pi}{4} - \frac{\nu}{\lambda}(1 - 2\lambda x^2)^{3/2} \right) & |x| \leq 1/\sqrt{2\lambda} \\ \exp[i(\nu/\lambda)(2\lambda x^2 - 1)^{3/2}] & |x| > 1/\sqrt{2\lambda}. \end{cases} \tag{36}$$

The coefficients of $|\psi_{0\nu}\rangle$ are chosen in such a way that they contain only the diverging wave for $x \to \infty$ and are continuous with the first and the second derivatives at the

Table 2. (a) Comparison of the results of calculations of the eigenvalues of the Hamiltonian $H = (p^2 + x^2)/2 - \lambda x^4$ on the basis of formulae (31) and (32) with the exact values of E_n obtained by Farrelly and Reinhardt (1983). (b) Comparison of the outcome of the calculations of $E_0^{(0)}$ using formula (38) with the exact values of $E_0(\lambda)$.

(a)	$\lambda = 0.1$	E_n'	E_n''	Re $E_n^{(0)}$	Im $E_n^{(0)}$
	$n = 0$	0.397	0.045	0.384	0.042
	$n = 1$	1.096	0.340	1.074	0.353
	$n = 2$	1.753	0.969	1.769	0.971
(b)	λ	E_0'	Re $E_0^{(0)}(\lambda)$	E_0''	Im $E_0^{(0)}(\lambda)$
	0.025	0.479	0.480	7.8×10^{-6}	8.2×10^{-6}
	0.03	0.474	0.475	6.2×10^{-5}	6.8×10^{-5}
	0.05	0.450	0.456	3.3×10^{-3}	4.2×10^{-3}
	0.1	0.397	0.402	4.5×10^{-2}	7.4×10^{-2}

point $x = (1/2\lambda)^{1/2}$. The vectors $|\psi_{n\nu}\rangle$ for the excited states can be represented as a product of the Hermite polynomial $H[(\nu/3)^{1/2}x]$ and the vector $|\psi_{0\nu}\rangle$. $E_0^{(0)}(\nu)$ in the zeroth approximation is defined from the equation

$$\langle \psi_{0\nu} | (\hat{H} - E_0^{(0)}(\nu)) | \psi_{0\nu} \rangle = 0. \tag{37}$$

By analogy with (31) the vector $\langle \psi_{0\nu} |$ for complex-valued ν is defined by the following expression:

$$\langle \psi_{0\nu} | = \{ | \psi_{0\nu} \rangle^+ \}^*.$$

As a result, equation (37) assumes the following form:

$$
\begin{aligned}
\phi(\nu) \equiv \frac{1}{\sqrt{2\lambda}} \int_0^1 \frac{t \, dt}{\sqrt{1-t^2}} \Bigg\{ & \frac{i}{2} \Bigg[\exp\left(\frac{2\nu}{\lambda} t^3\right) \left(\frac{1-36\nu^2}{4\lambda} t^2(1-t^2) + \frac{3\nu}{t}(2t^2-1) - E_0 \right) \\
& - \exp\left(-\frac{2\nu}{\lambda} t^3\right) \left(\frac{1-36\nu^2}{4\lambda} t^2(1-t^2) - \frac{3\nu}{t}(2t^2-1) - E_0 \right) \Bigg] \\
& + \frac{1-36\nu^2}{4\lambda} t^2(1-t^2) - E_0 \Bigg\} + \frac{1}{\sqrt{2\lambda}} \int_0^\infty \frac{z \, dz}{\sqrt{1+z^2}} \exp\left(i \frac{2\nu}{\lambda} z^3\right) \\
& \times \left(\frac{1-36\nu^2}{4\lambda} z^2(1+z^2) + \frac{3i\nu}{z}(2z^2+1) - E_0 \right) = 0
\end{aligned}
\tag{38}
$$

with the parameter ν defined by the condition $\partial E / \partial \nu = 0$.

Since equations (32) and (33) provide a sufficiently good approximation for E_n for $\lambda \geqslant 0.1$, we consider (38) for the case of $\lambda \leqslant 0.1$ only (i.e. $\lambda \ll 1$), when it is essentially simplified and permits us to find $E_0^{(0)}(\nu)$ in the obvious form

$$
\begin{aligned}
E_0^{(0)}(\nu) \simeq & F(\nu) - 4i \left(\frac{6\nu}{\pi}\right)^{1/2} \frac{\exp(-2\nu/\lambda)}{\sqrt{2\lambda}} \left(\frac{1-36\nu^2}{30\lambda} - F(\nu) \right) \\
& - 4 \left(\frac{6\nu}{\pi}\right)^{1/2} \exp(-2\nu/\lambda) \Gamma(\tfrac{1}{3}) \frac{\nu^{2/3}}{2^{5/6}\lambda^{1/6}} \exp(i\tfrac{1}{6}\pi) + O(\lambda^{1/6}) \exp(-2\nu/\lambda)
\end{aligned}
$$

$$
F(\nu) = \frac{1}{24\nu} + \frac{3}{2}\nu - \frac{\lambda}{48\nu^2}. \tag{39}
$$

The solution of the equation $\partial E_0^{(0)} / \partial \nu = 0$ gives

$$\nu_0 \equiv \nu_0(\lambda) = \tfrac{1}{6}(1 - \tfrac{3}{2}\lambda) + \dots$$

and as a result we obtain the following formula for the ground-state energy:

$$E_0^{(0)} \simeq \tfrac{1}{2} - \tfrac{3}{4}\lambda - \tfrac{9}{4}\lambda^2 + O(\lambda^3) + i \exp(-1/3\lambda) \left(\frac{e}{2\pi}\right)^{1/2} \left(\frac{8}{5\sqrt{\lambda}} - \frac{\Gamma(\tfrac{1}{3})}{3^{2/3}\lambda^{1/6}} + O(\lambda^{1/6}) \right). \tag{40}$$

We note that the parameter ν_0 contains the correction $\Delta\nu \sim \exp(-1/3\lambda)$. However, if we put ν_0 into equation (39), the change of energy $E_0^{(0)}$ conditioned by this correction is proportional to $(\Delta\nu)^2$ because $F'(\nu_0) = 0$ by definition. The outcome of the calculation by formula (39) is compared with the exact values of $E_0(\lambda)$ in table 2(b), which shows that the asymptotic formula (40) gives a sufficiently good approximation for $E_0(\lambda)$ in the range of $\lambda < \lambda_b$, which can be improved upon taking into account subsequent terms in the expansion of formula (37) over powers of $\lambda^{1/3}$.

5. Conclusion

The results obtained in the present paper indicate the wide possibilities appearing in the use of the operator method for solving the Schrödinger equation with a periodic potential in space or time. We believe that the method described here can be used for investigation of physical systems with Hamiltonians outside the limits of the particular examples discussed here. At the same time, we realise that the empirical computational procedures considered here demand serious mathematical substantiation of convergence and research into the limits of their applicability.

References

Abramowitz M and Stegun I A 1979 *Handbook of Mathematical Functions* (New York: Dover)
Fainstein A G, Manakov N L and Rapoport L P 1978 *J. Phys. B: At. Mol. Phys.* **11** 2561–78
Farrelly D and Reinhardt W P 1983 *J. Phys. B: At. Mol. Phys.* **16** 2103–17
Feranchuk I D and Komarov L I 1982 *Phys. Lett.* **88A** 211–5
—— 1984 *J. Phys. A: Math. Gen.* **17** 3111–33
Fernandez F M, Meson A M and Castro E A 1985 *Phys. Lett.* **111A** 104–7
Finkelstein V Yu 1985 *Zh. Exp. Teor. Fiz.* **88** 1527–47
Liaptsev A V and Zuev A N 1985 *Opt. Spectrosc.* **58** 970–8
Sanchez A M and Bejarano J D 1986 *J. Phys. A: Math. Gen.* **19** 887–901
Tikhonov A N and Samarsky A A 1972 *Mathematical Physics Equations* (Moscow: Nauka)
Zeldovich Ya B 1973 *Usp. Fis. Nauk* **110** 139–51