IOP PUBLISHING PHYSICA SCRIPTA

Phys. Scr. **77** (2008) 045004 (7pp) doi:10.1088/0031-8949/77/4/045004

Quasilinearization approach to the resonance calculations: the quartic oscillator

E Z Liverts[1], R Krivec[2] and V B Mandelzweig[1]

[1] Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel
[2] Theoretical Physics Department, J Stefan Institute, 1001 Ljubljana, Slovenia

E-mail: liverts@phys.huji.ac.il

Received 16 January 2008
Accepted for publication 15 February 2008
Published 14 March 2008
Online at stacks.iop.org/PhysScr/77/045004

Abstract

We pioneered the application of the quasilinearization method (QLM) to resonance calculations. The quartic anharmonic oscillator $(kx^2/2) + \lambda x^4$ with a negative coupling constant λ was chosen as the simplest example of the resonant potential. The QLM has been suggested recently for solving the bound state Schrödinger equation after conversion into Riccati form. In the quasilinearization approach the nonlinear differential equation is treated by approximating the nonlinear terms by a sequence of linear expressions. The QLM is iterative but not perturbative and gives stable solutions to nonlinear problems without depending on the existence of a smallness parameter. The choice of zero iteration is based on general features of solutions near the boundaries. Comparison of our approximate analytic expressions for the resonance energies and wavefunctions obtained in the first QLM iteration with the exact numerical solutions demonstrate their high accuracy in the wide range of the negative coupling constant. The results enable accurate analytic estimates of the effects of the coupling constant variation on the positions and widths of the resonances.

PACS numbers: 03.65.Ca, 03.65.Ge, 03.65.Sq, 03.65.Db

1. Introduction

The concept of quasi-stationary (metastable) states and resonances plays a fundamental role in quantum mechanics. Metastable states arise as resonances in scattering reactions when the particle enters the classically forbidden region by tunneling effect. Such a quasi-bound state, observed in atomic and molecular collisions, can be described with a complex energy eigenvalue

$$E = E_r - i\Gamma/2. \quad (1)$$

The resonance width Γ for the resonance energy E_r was found long ago by Gamow [1]. It was shown that a purely outgoing wave, known as the Gamow–Siegert [2] boundary condition, determines the resonance spectrum. This is a computationally difficult boundary condition and therefore resonance states have been studied by complex scaling or complex coordinate rotation methods [3–11]. However, these successful techniques are not without disadvantages. They involve the necessity of choosing the basis set (which should be sufficiently large), or the rotation angle.

A novel two-potential approach to tunneling problems was recently proposed by Gurvitz and Kalbermann [12]. In their approach the 'unperturbed' bound states are required as input. However, such states do not exist in some cases. For instance, they are not available in the case of large coupling constant λ of the quartic anharmonic oscillator (QAO) considered below.

One should also mention a very powerful method of summation of divergent series [13] which is based on generating the perturbation series used in the construction of the so-called 'intelligent approximants'. This approach was successfully applied to resonance calculations in both quartic and cubic anharmonic oscillators with negative coupling constants.

Quantum anharmonic oscillator has been, and continues to be, the subject of intensive theoretical study, due to the variety of its applications in different fields of physics. The most used example is the QAO. The Schrödinger equation for it has

the form

$$-\tfrac{1}{2}\psi''(x)+V(x)\psi(x)=E\psi(x), \tag{2}$$

where

$$V(x)=\frac{k}{2}x^2+\lambda x^4. \tag{3}$$

For $\lambda>0$, the QAO exhibits bound states, whereas for $\lambda<0$ it forms resonance states.

In what follows we use the atomic unit system ($m=e=\hbar=1$).

Complex eigenvalues E of the QAO resonances were first calculated by Bender and Wu [14]. Their approach was further developed in the papers [15] using the Rayleigh–Schrödinger perturbation theory and Wentzel–Kramers–Brillouin (WKB) methods.

In this paper, we pioneer the application of the quasilinearization method (QLM) to the resonance calculations. QLM has been suggested recently for solving the Schrödinger equation for bound states after conversion into the Riccati form [16–20]. In the QLM the nonlinear differential equation is treated by approximating the nonlinear terms by a sequence of linear expressions. The QLM is iterative but not perturbative and gives stable solutions to nonlinear problems without depending on the existence of a smallness parameter. The choice of the zeroth iteration is based on general features of solutions near the boundaries. The precise form of the zeroth iteration is not important in view of the very fast quadratic convergence of the quasilinear iterations.

Recently, we used the QLM for analytic calculations of the bound-state energies and wavefunctions of the quartic and pure quartic oscillators [17] that correspond to the positive coupling constant λ in the potential (3). The goal of the present paper is to employ the QLM for computation of the resonant states, which appear in the QAO at negative values of λ. One should emphasize, that also here, in analogy with the bound state case, the first QLM iteration provides an approximate but very accurate analytic presentation of both resonance energies and resonance wavefunctions. The next iterations could serve for precise numerical computation of these quantities.

2. Quasiclassical solution and the asymptotic behavior

First of all, we resort to the basic quasiclassical (WKB) wavefunction:

$$\psi_{\mathrm{WKB}}(x)\simeq\frac{\mathrm{const}}{\sqrt{p(x)}}\exp\left(-\mathrm{i}\int p(x)\mathrm{d}x\right) \tag{4}$$

with

$$p(x)=\sqrt{2\left[E-U(x)\right]}. \tag{5}$$

It is very important to stress that one should take the minus sign in the exponent, if we consider, for example, a particle which tends to escape by tunneling to the region of negative potential energy to reach $x=-\infty$ ('outgoing' condition).

For the logarithmic derivative of the quasiclassical wavefunction (4), we have

$$y_{\mathrm{WKB}}(x)\equiv\frac{\psi'_{\mathrm{WKB}}(x)}{\psi_{\mathrm{WKB}}(x)}=-\mathrm{i}p(x)-\frac{p'(x)}{2p(x)}, \tag{6}$$

where prime denotes the first derivative in variable x.

The necessary condition for validity of the quasiclassical approximation has the form (see, e.g. [21]):

$$\left|\frac{U'(x)}{p^3(x)}\right|\ll 1. \tag{7}$$

It is easy to verify that for the QAO potential (3) one has:

$$\lim_{x\to\pm\infty}\frac{V'(x)}{[E-V(x)]^{3/2}}=0. \tag{8}$$

This limit relation confirms the validity of condition (7) at sufficiently large x for QAO.

Substituting the potential (3) into the rhs of equation (6) one obtains:

$$y_{\mathrm{WKB}}(x,E)=\frac{x\left(k+4\lambda x^2\right)}{2\left(2E-kx^2-2\lambda x^4\right)}-\mathrm{i}\sqrt{2E-x^2\left(k+2\lambda x^2\right)},\quad(x\leqslant 0). \tag{9}$$

The latter expression enables us to find the behavior of the logarithmic derivative $y(x)$ at infinity which is antisymmetric for both symmetric and antisymmetric solutions:

$$\mathrm{Re}\left\{y(x)\right\}\simeq-\frac{1}{x},\quad(x\to\pm\infty), \tag{10}$$

$$\mathrm{Im}\left\{y(x)\right\}\simeq\pm\sqrt{-2\lambda}x^2,\quad(x\to\pm\infty). \tag{11}$$

3. QLM iteration scheme for resonances

It is well known that the one-dimensional Schrödinger equation for the wavefunction $\psi(x)$ can be easily transformed into the Riccati equation

$$y'(x)+y^2(x)=2\left[U(x)-E\right], \tag{12}$$

for the logarithmic derivative $y(x)=\psi'(x)/\psi(x)$ and arbitrary potential $U(x)$.

For the complex energy E defined by equation (1) in the tunneling/resonance problems, $y(x)$ in general is a complex function:

$$y(x)=\alpha(x)+\mathrm{i}\beta(x). \tag{13}$$

The QLM enables one to solve the exact Riccati equation (12) by the iteration procedure using the approximate equation [18–20]:

$$y'_{n+1}(x)+2y_{n+1}(x)y_n(x)=y_n^2(x)+2\left[U(x)-E_n\right]. \tag{14}$$

where E_n is the energy of the nth iteration. Let us consider a solution of this equation at the first iteration ($n=0$). The general solution can be written in the form:

$$y_1(x)=C\mathrm{e}^{-2\int_{x_0}^{x}y_0(t)\mathrm{d}t}+\int_{x_0}^{x}\mathrm{e}^{-2\int_{s}^{x}y_0(t)\mathrm{d}t}\left[y_0^2(s)+2U(s)-2E_0\right]\mathrm{d}s, \tag{15}$$

where x_0 and C are arbitrary constants and E_0 is the zero iteration energy. Only one of the constants x_0, C is independent, of course. Setting $x=x_0$ in equation (15), one obtains:

$$C=y_1(x_0). \tag{16}$$

Using equation (16), it is easy to rewrite the solution (15) in the form:

$$y_1(x) = \mathrm{e}^{-2\int_{x_0}^{x} y_0(t)\mathrm{d}t} \times \left\{ y_1(x_0) + \int_{x_0}^{x} \mathrm{e}^{2\int_{x_0}^{s} y_0(t)\mathrm{d}t} \left[y_0^2(s) + 2U(s) - 2E_0 \right] \mathrm{d}s \right\}. \tag{17}$$

Both even and odd solutions to the Riccati equation (12) with the symmetric potential (3), in view of the antisymmetry of the logarithmic derivative, satisfy the following Dirichlet boundary condition at the origin:

$$y(0) = 0. \tag{18}$$

Putting $x_0 = 0$ in the rhs of equation (17) and using the condition (18) one obtains the QLM logarithmic derivative of the first order in the form:

$$y_1(x) = \int_0^x \mathrm{e}^{2\int_x^s y_0(t)\mathrm{d}t} \left[y_0^2(s) + 2V(s) - 2E_0 \right] \mathrm{d}s. \tag{19}$$

Note that according to equation (10) the QAO exhibits very slow convergence of the corresponding wavefunction $|\psi(x)| \sim \exp[\int \mathrm{Re}\{y(x)\}\,\mathrm{d}x] \simeq x^{-1}$ at infinity. This circumstance does not enable one to use equation (19) directly for the calculation of the complex zero iteration resonance energy E_0, as it was done previously for bound states by setting y_1 at infinity equal to zero [19].

Therefore, we propose instead to match the QLM approximation (19) with the quasiclassical expression (9), which is valid at large $|x|$. Note that expression (9) is valid only for nonpositive x. Hence, one should set a negative matching point $x = x_m$ with sufficiently large $|x_m|$.

Thus, the zero iteration resonance energy E_0 can be calculated by solving the equation:

$$y_{\mathrm{WKB}}(x_{m0}, E_0) = P_0(x_{m0}) - 2Q_0(x_{m0})E_0, \tag{20}$$

where

$$P_0(t) = \psi_0^{-2}(t) \int_0^t \psi_0^2(s) \left[y_0^2(s) + 2V(s) \right] \mathrm{d}s, \tag{21}$$

$$Q_0(t) = \psi_0^{-2}(t) \int_0^t \psi_0^2(s)\,\mathrm{d}s, \tag{22}$$

and

$$\psi_0(s) = \exp\left[\int^s y_0(u)\,\mathrm{d}u \right]. \tag{23}$$

The problems of finding the matching points and the initial guess function $y_0(x)$ will be considered in the following sections.

The resonance energy E_1 in the first QLM iteration could be calculated by applying the first iteration equation:

$$y_{\mathrm{WKB}}(x_{m1}, E_1) = P_1(x_{m1}) - 2Q_1(x_{m1})E_1. \tag{24}$$

The functions $P_1(t)$ and $Q_1(t)$ are obtained with the help of equations (21)–(23) by replacing $y_0(x)$ by the function $y_1(x)$ obtained earlier according to equation (19). The next iterations could be calculated in a similar fashion.

4. Constructing the initial guess function

Let us consider the Schrödinger equation (2) for the quartic anharmonic potential (3) and introduce the new variable $\sigma = x^2$. The differential equation is now

$$\phi''(\sigma) + \frac{1}{2\sigma}\phi'(\sigma) - \left(\frac{k}{4} + \frac{\lambda\sigma}{2} - \frac{E}{2\sigma} \right) \phi(\sigma) = 0, \tag{25}$$

for $\phi(\sigma) = \psi(x)$. Using the asymptotic functions (10) and (11), one obtains the following expression at large $|x|$ (and hence, at large $\sigma = x^2$):

$$\psi(x) \sim \exp \int y(x)\,\mathrm{d}x \simeq \exp \int \left(-\frac{1}{x} \pm \mathrm{i}\sqrt{-2\lambda}x^2 \right) \mathrm{d}x. \tag{26}$$

Then, one has:

$$\frac{\mathrm{d}\phi(\sigma)}{\mathrm{d}\sigma} = \frac{1}{2x}\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} \simeq \frac{1}{2x}\left(-\frac{1}{x} \pm \mathrm{i}\sqrt{-2\lambda}x^2 \right)\psi(x) \equiv \left(-\frac{1}{2\sigma} \pm \mathrm{i}\sqrt{-\frac{\lambda\sigma}{2}} \right)\phi(\sigma), \tag{27}$$

whence

$$\frac{\phi'(\sigma)}{2\sigma} \simeq \left(-\frac{1}{4\sigma^2} \pm \mathrm{i}\sqrt{-\frac{\lambda}{8\sigma}} \right)\phi(\sigma). \tag{28}$$

Our key assumption now consists in neglecting the terms $E\phi(\sigma)/2\sigma$ and $\phi'(\sigma)/2\sigma$ in equation (25) at sufficiently large σ.

Equation (25) then reduces to

$$\phi''(\sigma) - \left(\frac{k}{4} + \frac{\lambda\sigma}{2} \right)\phi(\sigma) = 0, \tag{29}$$

with the general solution of the form:

$$\phi(\sigma) = C_1 \mathrm{A}i(z) + C_2 \mathrm{B}i(z). \tag{30}$$

Here the Airy functions $\mathrm{A}i(z)$ and $\mathrm{B}i(z)$ depend on the variable

$$z = \left(\frac{2}{\lambda} \right)^{2/3} \left(\frac{k}{4} + \frac{\lambda\sigma}{2} \right). \tag{31}$$

The corresponding logarithmic derivative has the form:

$$y(x, C) \equiv \frac{\mathrm{d}\phi(x^2)}{\mathrm{d}x} \left[\phi(x^2) \right]^{-1} = \left(\frac{2}{\lambda} \right)^{2/3} \lambda x \frac{\mathrm{A}i'(z) + C\mathrm{B}i'(z)}{\mathrm{A}i(z) + C\mathrm{B}i(z)}, \tag{32}$$

where $C = C_2/C_1$ is an arbitrary constant, whereas the prime denotes differentiation over the variable z.

Let us consider the question of how to set the value of the coefficient C in the latter equation. The asymptotic expansion for $\mathrm{A}i(z)$ is [22, 23]:

$$\mathrm{A}i(z) \simeq \tfrac{1}{2}\pi^{-1/2} z^{-1/4} \mathrm{e}^{-\zeta} \sum_{m=0}^{\infty} (-1)^m c_m \zeta^{-m}, \quad (|\arg(z)| < \pi), \tag{33}$$

where

$$\zeta = \tfrac{2}{3}z^{3/2}. \tag{34}$$

Here c_m is defined in [22, 23], however, its explicit form is not important for our consideration.

The asymptotic expansion for $\mathrm{Bi}(z)$ can be found in equation (46) of [23]

$$\mathrm{Bi}(z) \simeq \pi^{-1/2}z^{-1/4}\left[\mathrm{e}^{\zeta}\sum_{m=0}^{\infty}c_m\zeta^{-m} \pm \frac{\mathrm{i}}{2}\mathrm{e}^{-\zeta}\sum_{m=0}^{\infty}c_m(-\zeta)^{-m}\right], \quad \left(0 < \pm\arg(z) < \tfrac{2}{3}\pi\right). \tag{35}$$

Note that for negative λ and positive k equation (31) yields at sufficiently large positive σ:

$$\arg(z) = \arg\left[-(-1)^{2/3}\right] \equiv -\frac{\pi}{3}, \tag{36}$$

which obeys the asymptotic formulae (33) and (35). Substituting this value into the rhs of equation (34), one obtains:

$$\arg(\zeta) = -\frac{\pi}{2}. \tag{37}$$

This means that parameter ζ takes pure imaginary values. This in turn implies that the asymptotic expansions (33) and (35) represent oscillatory functions due to the factors $\exp(\zeta)$ or $\exp(-\zeta)$ with the imaginary ζ. The presence of such exponentials in numerator and in denominator causes the oscillatory behavior of the logarithmic derivative (32) in the asymptotic region. The correct asymptotic formulae (10) and (11) as well as the exact numerical calculations, however, exhibit non-oscillatory curves.

To resolve this contradiction one has to choose the coefficient C in such a way that the expressions in the denominator of equation (32) and, hence, in its numerator will be reduced to one-exponential expressions. In this case the oscillating exponentials in the numerator and denominator are cancelled and non-oscillatory behavior results. There are two ways to achieve this. The first one is to put $C = 0$ in equation (32). The second possibility is to set $C = -i$. As it is seen from equations (33)–(35), the latter choice enables us to cancel the expressions with the factor $\exp(-\zeta)$.

Using representations (33)–(35) it is easy to show that asymptotic behavior of the logarithmic derivative (32) is defined as follows:

$$y(x, 0) \simeq -\frac{1}{2x} \pm \mathrm{i}\sqrt{-2\lambda}x^2, \quad (x \to \pm\infty), \tag{38}$$

$$y(x, -i) \simeq -\frac{1}{2x} \mp \mathrm{i}\sqrt{-2\lambda}x^2, \quad (x \to \pm\infty). \tag{39}$$

Only equation (38) corresponding to the parameter $C = 0$ exibits the correct asymptotic behavior (within a factor 1/2 for the real part, which is a consequence of our previous assumption) given by equations (10) and (11), whereas $y(x, -i)$ shows the complex conjugate behavior.

Thus, we propose the initial guess of the form:

$$y_0(x) = \left(\frac{2}{\lambda}\right)^{2/3}\lambda x\frac{\mathrm{Ai}'[z(x)]}{\mathrm{Ai}[z(x)]}, \tag{40}$$

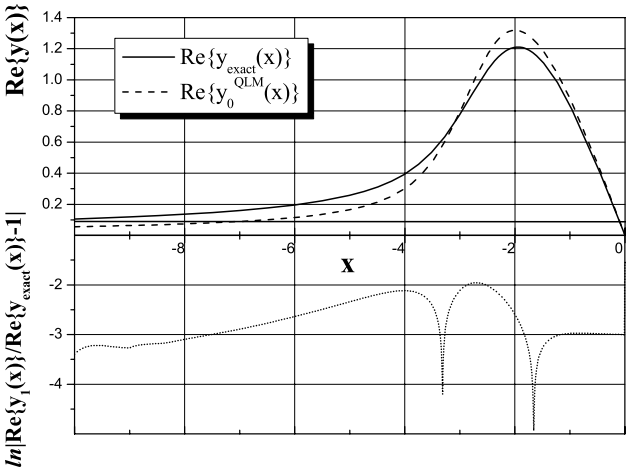

Figure 1. Real part of the logarithmic derivative function of the QAO with negative coupling constant $\lambda = -0.05$. The exact solution $\mathrm{Re}\{y_{\mathrm{exact}}(x)\}$ is depicted by the solid line. The initial guess function $\mathrm{Re}\{y_0(x)\}$ of the form (40) is represented by the dashed line. The logarithmic derivative of the first QLM iteration $\mathrm{Re}\{y_1^{\mathrm{QLM}}(x)\}$, calculated by equations (42)–(46), is shown in the form of its deviation (on the logarithmic scale) from the exact function depicted on the upper graph. This logarithmic deviation $\ln|\mathrm{Re}\{y_1(x)\}/\mathrm{Re}\{y_{\mathrm{exact}}(x)\} - 1|$ is represented by the dotted line on the lower graph.

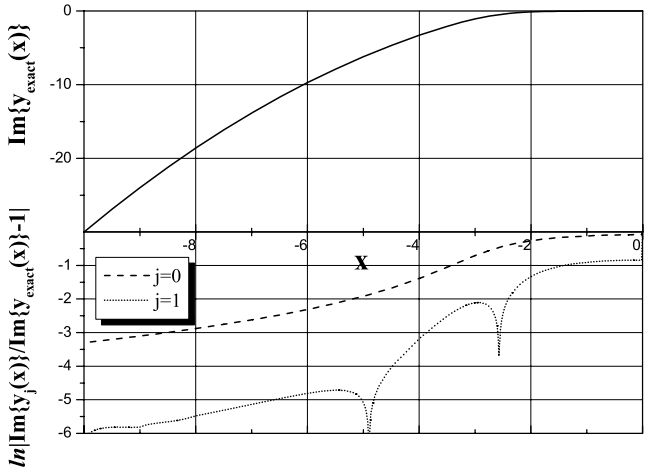

Figure 2. Imaginary part of the logarithmic derivative function of the QAO with negative coupling constant $\lambda = -0.05$. The exact solution $\mathrm{Im}\{y_{\mathrm{exact}}(x)\}$ is depicted by the solid line. The initial guess function $\mathrm{Im}\{y_0(x)\}$ and the logarithmic derivative of the first QLM iteration $\mathrm{Im}\{y_1^{\mathrm{QLM}}(x)\}$ are shown in the form of their deviations (on the logarithmic scale) from the exact function depicted on the upper graph. These logarithmic deviations $\ln|\mathrm{Im}\{y_j(x)\}/\mathrm{Im}\{y_{\mathrm{exact}}(x)\} - 1|$ are represented on the lower graph by the dashed and dotted lines for $j = 0$ and $j = 1$, respectively.

with

$$z(x) = \left(\frac{2}{\lambda}\right)^{2/3}\left(\frac{k}{4} + \frac{\lambda x^2}{2}\right). \tag{41}$$

Figures 1–4 demonstrate that this initial guess describes the exact numerically calculated logarithmic derivative (that is $\mathrm{Re}\{y(x)\}$ and $\mathrm{Im}\{y(x)\}$) with a reasonable accuracy at both small and intermediate values of $|x|$.

Substituting our initial guess (40) into the rhs of equation (19) one obtains the logarithmic derivative in

Table 1. QLM complex energies for the QAO.

λ/E	E_0	E_1	E_{exact}
−0.025	$0.479191–5.864\times10^{-6}i$	$0.479117–7.285\times10^{-6}i$	$0.479117–7.282\times10^{-6}i$
−0.05	0.450790–0.00286576*i*	0.450336–0.0033465*i*	0.450336–0.0033466*i*
−0.1	0.395866–0.043284*i*	0.397443–0.0447063*i*	0.397441–0.0447061*i*
−0.15	0.371073–0.0950959*i*	0.373767–0.0950571*i*	0.373767–0.0950567*i*
−0.25	0.359088–0.177705*i*	0.361457–0.175754*i*	0.361459–0.175755*i*
−0.375	0.363399–0.251785*i*	0.364996–0.248940*i*	0.364999–0.248940*i*

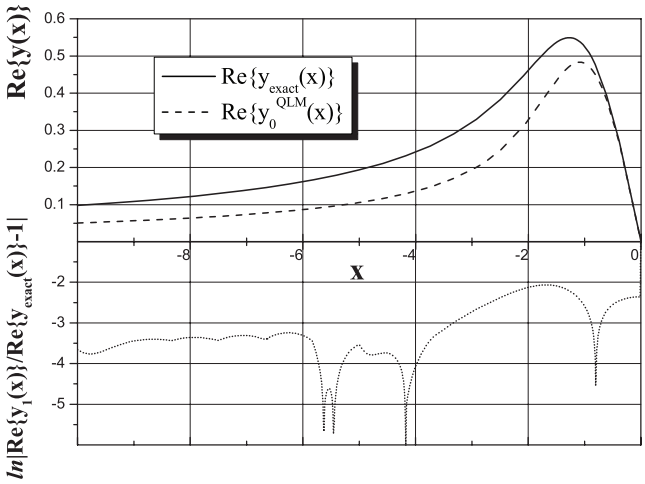

Figure 3. The same as in figure 1, but for the coupling constant $\lambda = 0.375$.

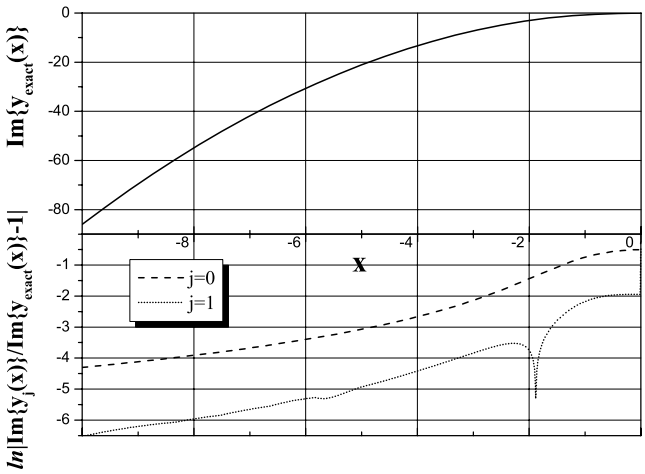

Figure 4. The same as in figure 2, but for the coupling constant $\lambda = 0.375$.

the form:

$$y_1(x, E_0) = P_0(x) - 2E_0 Q_0(x), \tag{42}$$

where

$$P_0(x) = \Phi_0^{-2}(x) \int_0^x \left[\left[\Phi_0'(s) \right]^2 + 2\Phi_0^2(s) V(s) \right] \mathrm{d}s, \tag{43}$$

$$Q_0(x) = \Phi_0^{-2}(x) \int_0^x \Phi_0^2(s)\, \mathrm{d}s, \tag{44}$$

with

$$\Phi_0(x) = \mathrm{Ai}\left[z(x)\right], \tag{45}$$

$$\Phi_0'(x) = \left(\frac{2}{\lambda}\right)^{2/3} \lambda x \mathrm{Ai}'\left[z(x)\right]. \tag{46}$$

The complex energy E_0 therefore can be calculated by solving the equation:

$$y_{\mathrm{WKB}}(x_{m0}, E_0) = y_1(x_{m0}, E_0). \tag{47}$$

The rhs of this equation is defined by equations (42)–(46), whereas the lhs is represented by equation (9).

To calculate the resonance energy E_1 of the next order in accuracy, one solves equation (24) with

$$P_1(x) = \int_0^x \Omega(x, s, E_0) \left[y_1^2(s, E_0) + 2V(s) \right] \mathrm{d}s, \tag{48}$$

$$Q_1(x) = \int_0^x \Omega(x, s, E_0)\, \mathrm{d}s, \tag{49}$$

where

$$\Omega(x, s, E_0) = \exp\left[2 \int_x^s y_1(t, E_0)\, \mathrm{d}t \right]. \tag{50}$$

5. Results and discussion

The results of the QLM calculations for the ground state resonance energies of QAO with the negative coupling constant λ and the parameter $k = 1$ are presented in table 1. For comparison we presented also the exact energies calculated in [13]. Note that the coupling constant $\tilde{\lambda}$ and the energies $\tilde{E}$ used in [13] correspond to 2λ and $2E$ in our notation, respectively. The complex QLM zero iteration energy E_0 was calculated by solving the algebraic transcendental equation (47) using equations (42)–(46). The first iteration energy E_1 was obtained by solving equation (24) with functions $P_1(x)$, $Q_1(x)$ and $y_1(x, E_0)$, defined by equations (48)–(50) and (42), respectively. It is seen from the data in table 1 that for E_0 we have an error only in the third decimal place for both the real and imaginary parts. E_1 has an error only in the sixth decimal place. We obtain slightly higher precision for small $|\lambda|$. All the results were obtained using the initial guess functions (40) and (45).

Let us discuss the specific question of the matching points mentioned above. According to equation (42) only the value of E_0 is required to calculate the logarithmic derivative $y_1(x, E_0)$. E_0 is calculated by solving equation (47) that includes the matching point x_{m0} as a parameter. In the upper graphs of figures 5 and 6 the real and imaginary parts of the energy E_0 are drawn as functions of the matching point x_m. We present only the case of $\lambda = 0.1$ as a typical example. One can see that both functions are oscillatory, with amplitudes that tend to diminish with increasing negative values of x_m. The amplitude of oscillation of ΔE_0 falls off very quickly, so that at $x_m < -7$ one has $\Delta\mathrm{Re}\{E_0\} < 10^{-5}$ and

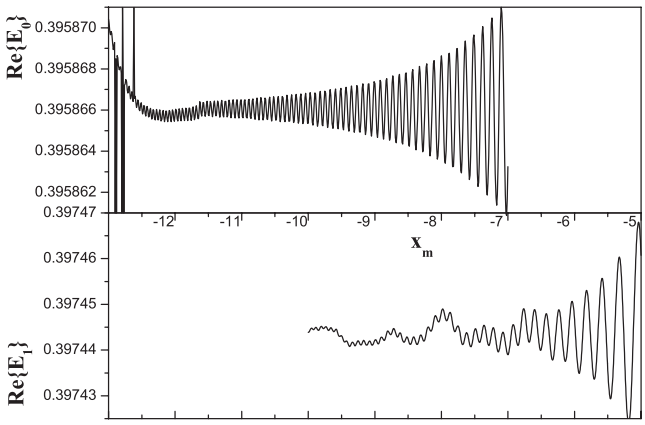

Figure 5. Real parts of the complex energies E_0 and E_1, calculated by equations (47) and (24), respectively. The energies are drawn as functions of the matching point x_m for $\lambda = 0.1$.

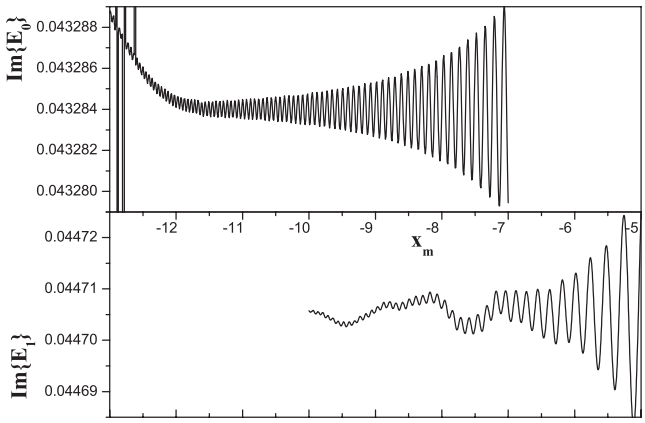

Figure 6. Imaginary parts of the complex energies E_0 and E_1, calculated by equations (47) and (24), respectively. The energies are drawn as functions of the matching point x_m for $\lambda = 0.1$.

$\Delta\mathrm{Im}\{E_0\} < 10^{-5}$. At negative (but sufficiently large) value of $x_m = x_{m0} \simeq -11.5$ one can observe a loss of a regular behavior of the plots. It is caused by the limited precision of computer calculations.

We propose two simple ways to determine E_0. The first is to set $E_0 = (E_0^{\max} + E_0^{\min})/2$, where $E_0^{\max}$ and $E_0^{\min}$ are extrema of E_0, which are next to $E_0(x_{m0})$ in the regular parts of the plots. The second way is to use the procedure of linear regression [24] to approximate the function $E_0(x_m)$ by a straight line in the regular region next to x_{m0}. We use the most common form of the linear regression based on the least squares fitting. Both approaches give the same results, presented in table 1.

In the lower graphs of figures 5 and 6 the real and imaginary parts of the resonance complex energy E_1 for $\lambda = 0.1$ are drawn as functions of the matching point x_m. The computations were performed by solving equation (24) involving x_m as a parameter. One obtains the plots of the oscillatory functions, which are identical in shape to the plots for E_0 discussed above. The only distinction is that the crucial point has a different value of $x_{m1} \simeq -6.5$. Therefore to calculate E_1 one can apply the same approach as was described above for E_0.

In figures 1–4 the real and imaginary parts of the logarithmic derivatives $y_0(x)$, $y_1(x)$, obtained from the analytic expression (42), and $y_{\mathrm{exact}}(x)$, obtained by direct numerical solution of the Riccati equation (12) with the QAO potential (3), are presented for two boundary values of $\lambda = -0.05$ and -0.375. The exact solutions $y_{\mathrm{exact}}(x)$ are depicted by solid lines. The real parts of the initial guess functions $y_0(x)$ are shown by dashed lines in figures 1 and 3.

To obtain the numerical solution we used the exact complex energies from [13]. A purely outgoing logarithmic derivative (9) was applied to start the procedure of solving the complex differential equation (12) at sufficiently large negative x.

Our approximate analytic forms of logarithmic derivatives $y_1(x)$ are very accurate. The differences between them and the exact numerical values cannot be revealed visually. Therefore we present only the relative logarithmic deviations from the exact functions $\ln|y_1(x)/y_{\mathrm{exact}}(x) - 1|$ instead of $y_1(x)$. Those deviations are depicted by a dotted line. The imaginary parts of our initial guess functions are accurate too and it is difficult to distinguish visually between them and the exact ones. Therefore, we present only the relative logarithmic deviations from the exact functions, $\ln|\mathrm{Im}\{y_0(x)\}/\mathrm{Im}\{y_{\mathrm{exact}}(x)\} - 1|$, instead of $\mathrm{Im}\{y_0(x)\}$ in figures 2 and 4. They are depicted by dashed lines.

One can see that the analytic representations of the first iteration logarithmic derivatives and the corresponding wavefunctions are rather accurate and that their precision increases with distance from the origin. This is caused by the method of generating the initial guess function since the corresponding differential equation (29) is accurate only at a sufficiently large distance from the origin.

In conclusion, the algebraic transcendental equation (47) and the integral expression (42) provide approximate but accurate analytic representations of both resonance energies and resonance wavefunctions which can be used for analytic estimates of the effects of the coupling constant variation on the positions and widths of the resonances. The higher iterations could serve for precise numerical computation of these quantities.

Acknowledgments

The research was supported by grant no. 2004106 from the United States–Israel Binational Science Foundation (BSF), Jerusalem, Israel.

References

[1] Gamow G 1928 *Z. Phys.* **51** 204
[2] Siegert A J F 1939 *Phys. Rev.* **56** 750
[3] Balslev E and Combes J C 1971 *Commun. Math. Phys.* **22** 280
[4] Bain R A, Bardsley J N, Junker B R and Sukumar C V 1974 *J. Phys. B: At. Mol. Opt. Phys.* **7** 2189
[5] Yaris R, Bendler J, Lovett R A, Bender C M and Fedders P A 1978 *Phys. Rev.* A **18** 1816
[6] Moiseyev N, Certain P R and Weinhold F 1978 *Mol. Phys.* **36** 1613
[7] Caliceti E, Graffi S and Maioli M 1980 *Commun. Math. Phys.* **75** 51
[8] Atabek O and Lefebvre R 1981 *Chem. Phys. Lett.* **84** 233
[9] Connor J N L and Smith A D 1983 *J. Chem. Phys.* **78** 6161

[10] Alvarez G 1988 *Phys. Rev.* A **37** 4079
Alvarez G 1989 *J. Phys. A: Math. Gen.* **22** 617
Alvarez G 1995 *J. Phys. A: Math. Gen.* **27** 4589
Alvarez G and Casares C 2000 *J. Phys. A: Math. Gen.* **33** 2499
Alvarez G and Casares C 2000 *J. Phys. A: Math. Gen.* **33** 5171
[11] Nicolaides C A, Gotsis H J, Chrysos M and Komninos Y 1990 *Chem. Phys. Lett.* **168** 570
[12] Gurvitz S A and Kalbermann G 1987 *Phys. Rev. Lett.* **59** 262
Gurvitz S A 1988 *Phys. Rev.* A **38** 1747
Gurvitz S A, Semmes P B, Nazarewicz W and Vertse T 2004 *Phys. Rev.* A **69** 042705
[13] Fernandez F M 2001 *Int. J. Quantum Chem.* **81** 268
[14] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
Bender C M and Wu T T 1973 *Phys. Rev.* D **7** 1620
[15] Simon B and Dicke A 1970 *Ann. Phys. (NY)* **58** 76
Loeffel J J, Martin A, Simon B and Wightman A S 1969 *Phys. Lett.* B **30** 656
Graffi S, Grecchi V and Simon B 1970 *Phys. Lett.* B **32** 631
[16] Mandelzweig V B 1999 *J. Math. Phys.* **40** 6266
Krivec R and Mandelzweig V B 2001 *Comput. Phys. Commun.* **138** 69
Mandelzweig V B and Tabakin F 2001 *Comput. Phys. Commun.* **141** 268
Krivec R and Mandelzweig V B 2003 *Comput. Phys. Commun.* **152** 165
Mandelzweig V B 2005 *Phys. At. Nucl.* **68** 1227
Mandelzweig V B 2006 *Ann. Phys.* **321** 2810
[17] Liverts E Z, Mandelzweig V B and Tabakin F 2006 *J. Math. Phys.* **47** 062109
[18] Liverts E Z and Mandelzweig V B 2007 *Ann. Phys.* **322** 2211
[19] Liverts E Z, Drukarev E G and Mandelzweig V B 2007 *Ann. Phys.* **322** 2958
[20] Liverts E Z and Mandelzweig V B 2008 *Phys. Scr.* **77** 025003
[21] Landau L D and Lifshitz E M 1991 *Quantum Mechanics: Non-relativistic Theory* (New York: Pergamon Press)
[22] Abramovitz M and Stegun I 1972 *Handbook of Mathematical Functions* (New York: Dover)
[23] Silverstone H J, Harris J G, Cizek J and Paldus J 1985 *Phys. Rev.* A **32** 1965
[24] Edwards A L 1976 *An Introduction to Linear Regression and Correlation* (San Francisco, CA: Freeman)