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Computer Physics Communications 174 (2006) 119–126
Computer Physics Communications
www.elsevier.com/locate/cpc

Quasilinearization method and WKB

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Received 27 October 2004; received in revised form 19 November 2004; accepted 3 December 2004

Available online 26 October 2005

Abstract

Solutions obtained by the quasilinearization method (QLM) are compared with the WKB solutions. While the WKB method generates an expansion in powers of $\hbar$, the quasilinearization method (QLM) approaches the solution of the nonlinear equation obtained by casting the Schrödinger equation into the Riccati form by approximating nonlinear terms by a sequence of linear ones. It does not rely on the existence of any kind of smallness parameter. It also, unlike the WKB, displays no unphysical turning point singularities. It is shown that both energies and wave functions obtained in the first QLM iteration are accurate to a few parts of the percent. Since the first QLM iterate is represented by the closed expression it allows to estimate analytically and precisely the role of different parameters, and influence of their variation on the properties of the quantum systems. The next iterates display very fast quadratic convergence so that accuracy of energies and wave functions obtained after a few iterations is extremely high, reaching 20 significant figures for the energy of the sixth iterate. It is therefore demonstrated that the QLM method could be preferable over the usual WKB method.

PACS: 03.65.Ca; 03.65.Ge; 03.65.Sq

Keywords: Quasilinearization; WKB; Nonlinear differential equations

1. Introduction

The quasilinearization method (QLM) was constructed as a generalization of the Newton–Raphson method [1,2] for the nonlinear differential equations to yield rapid quadratic and often monotonic convergence to the exact solution. It was developed originally in theory of linear programming by Bellman and Kalaba [3,4] to solve nonlinear ordinary and partial differential equations and their systems. In the original works of Bellman and Kalaba [3,4], however, the convergence of the method has been proven only under rather restrictive conditions of small intervals and bounded, nonsingular forces [10] which generally are not fulfilled in physical applications. This could explain an extremely sparse use of the technique in physics, where only a few examples of the references to it could be found [5–9]. Recently, however, it was shown [10] by one of the present authors (V.B.M.) that a different proof of the convergence can be provided which allows to extend the applicability of the method to realistic forces defined on infinite intervals with possible singularities at certain points. This proof was generalized and elaborated in the subsequent works [11–14].

In the first paper of the series [10], the analytic results of the quasilinearization approach were applied to the nonlinear Calogero equation [5] in the variable phase approach to quantum mechanics, and the results were compared with those of the perturbation theory and with the exact solutions. It was shown that the number of the exactly reproduced perturbation terms doubles with each subsequent QLM iteration, which, of course, is a direct consequence of a quadratic convergence.

The numerical calculation of higher QLM approximations to solutions of the Calogero equation with different singular and nonsingular, attractive and repulsive potentials performed in the work [12] has shown that already the first few iterations provide accurate and numerically stable answers for any values of the coupling constant and that the number of iterations necessary to reach a given precision increases only slowly with the coupling strength. It was verified that the method provides accurate and

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0010-4655/$ – see front matter
doi:10.1016/j.cpc.2004.12.017

stable answers even for super singular potentials for which each term of the perturbation theory diverges and the perturbation expansion consequently does not exist.

In the third paper of the series [13] the quasilinearization method was applied to other well-known typical nonlinear ordinary differential equations in physics, such as the Blasius, Duffing, Lane–Emden and Thomas–Fermi equations which have been and still are extensively studied in the literature. These equations, unlike the nonlinear Calogero equation [5] considered in Refs. [10,12], contain not only quadratic nonlinear terms but various other forms of nonlinearity and not only the first, but also higher derivatives. It was shown that again just a small number of the QLM iterations yield fast convergent and uniformly excellent and stable numerical results.

In the work [14] the quasilinearization method was applied to quantum mechanics by casting the Schrödinger equation in the nonlinear Riccati form and calculating the QLM approximations to bound state energies and wave functions for a variety of potentials, most of which are not treatable with the help of the perturbation theory or the $1/N$ expansion scheme. It was shown that the convergence of the QLM expansion for both energies and wave functions is very fast and that already the first few iterations yield extremely precise results. In addition it was verified that the higher QLM approximations, unlike those in $1/N$ expansion method, are not divergent at any order.

The present work is devoted to comparison of QLM and WKB. Indeed, the derivation of the WKB solution starts by casting the radial Schrödinger equation into nonlinear Riccati form and solving that equation by expansion in powers of $\hbar$. It is interesting instead to solve this nonlinear equation with the help of the quasilinearization technique and compare with the WKB results. Such a procedure was performed in works [7,8], where it was shown that the first QLM iteration reproduces the structure of the WKB series generating an infinite series of the WKB terms, but with different coefficients. Besides being a better approximation, the first QLM iteration is also expressible in a closed integral form. Similar conclusions are reached for higher QLM approximations and it can be shown [15] that the pth QLM iteration yields the correct structure of the infinite WKB series and reproduces 2^p terms of the expansion of the solution in powers of $\hbar$ exactly, as well as a similar number of terms approximately.

That the first QLM iteration already provides a much better approximation to the exact solution than the usual WKB is obvious, not only from comparison of terms of the QLM and WKB series [7,8,15], but also from the fact that the quantization condition in the first QLM iteration leads to exact energies for many potentials [15,17] such as for the Coulomb, harmonic oscillator, Pöschl–Teller, Hulthen, Hylleraas, Morse, Eckart and some other well-known physical potentials, which have a simple analytic structure. By comparison, the WKB approximation reproduces exact energies only in the case of the first two potentials.

The goal of this work is to point out that also for other potentials with more complicated analytical structure QLM iterates provide much better approximation than the usual WKB. If the initial QLM guess is properly chosen the wave function in all QLM iterations, unlike the WKB wave function, is free of unphysical turning point singularities. Since the first QLM iteration is given by an analytic expression [7,8,10–13], it allows one to analytically estimate the role of different parameters and the influence of their variation on different characteristics of a quantum system. The next iterates display very fast quadratic convergence so that accuracy of energies obtained after a few iterations is extremely high, reaching up to 20 significant figures for a sixth iterate as we show on the example of different widely used physical potentials.

The paper is arranged as follows: in Section 2 we present the main features of the quasilinearization approach to the solution of the Schrödinger equation, while in Section 3 we consider the application of the method to computations with the anharmonic oscillator, logarithmic, two-power (double-well), and Wood–Saxon potentials and to the two-body Dirac equation with static Coulomb potential. The final, Section 4 is devoted to the discussion of the results, convergence patterns, numerical stability, advantages of the method and its possible future applications.

2. Quasilinearization method

The usual WKB substitution

$$\chi(r) = C\exp\left(\lambda\int^{r} y(r')\,\mathrm{d}r'\right) \tag{1}$$

converts the Schrödinger equation to nonlinear Riccati form

$$\frac{\mathrm{d}y(z)}{\mathrm{d}z} + \left(k^2(z) + y^2(z)\right) = 0. \tag{2}$$

Here $k^2(z) = E - V - l(l+1)/z^2$, $\lambda^2 = 2m/\hbar^2$ and $z = \lambda r$.

The proper bound state boundary condition for potentials falling off at $z \simeq z_0 \simeq \infty$ is $y(z) = \text{const}$ at $z \geqslant z_0$. This means that $y'(z_0) = 0$, so that Eq. (2) at $z \simeq z_0$ reduces to $k(z_0)^2 + y^2(z_0) = 0$ or $y(z_0) = \pm ik(z_0)$. We choose here to define the boundary condition with the plus sign, so that $y(z_0) = ik(z_0)$.

The quasilinearization [7,10,13] of this equation gives a set of recurrence differential equations

$$\frac{\mathrm{d}y_p(z)}{\mathrm{d}z} = y_{p-1}^2(z) - 2y_p(z)y_{p-1}(z) - k^2(z) \tag{3}$$

with the boundary condition $y_p(z_0) = ik(z_0)$.

The analytic solution [7] of these equations expresses the pth iterate $y_p(z)$ in terms of the previous iterate:

$$y_p(z) = f_{p-1}(z) - \int_{z_0}^{z} \mathrm{d}s\,\frac{\mathrm{d}\,f_{p-1}(s)}{\mathrm{d}s}\exp\left[-2\int_{s}^{z} y_{p-1}(t)\,\mathrm{d}t\right], \tag{4}$$

$$f_{p-1}(z) = \frac{y_{p-1}^2(z) - k^2(z)}{2y_{p-1}(z)}.$$

Indeed, differentiation of both parts of Eq. (4) leads immediately to Eq. (3) which proves that $y_p(z)$ is a solution of this equation. The boundary condition is obviously satisfied automatically.

To utilize the recurrence relation (4) for wave function computation one has to pick up a proper initial guess. For the zeroth iterate $y_0(z)$ it seems natural to choose the zero WKB approximation that is to set $y_0(z) = ik(z)$, which in addition automatically satisfies the boundary condition. However, one has to be aware that this choice has unphysical turning point singularities. According to the existence theorem for linear differential equations [18], if $y_{p-1}(z)$ in Eq. (3) is a discontinuous function of z in a certain interval, then $y_p(z)$ or its derivatives may also be discontinuous functions in this interval, so consequently the turning point singularities of $y_0(z)$ may propagate to the next iterates. To avoid this we choose [16] the Langer WKB wave function [19] as the zero iteration. This function near the turning points a and b is given by the simple analytic expression[1]

$$\chi_i(r) = c_i \sqrt{\frac{S_i^{1/3}(r)}{|k(r)|}}\,\mathrm{Ai}\big[\mathrm{d}S_i^{1/3}(r)\big], \tag{5}$$

$$S_i(r) = \frac{3}{2}\lambda \left| \int_i^r \big|k(s)\big|\,\mathrm{d}s \right|.$$

Here Ai denotes the Airy function, $i = a, b$, $k^2(r) = 2m(E - V(r)) - (l + 1/2)^2/r^2$, d is -1 for $a < r < b$, and 1 for $r \leqslant a$, $r \geqslant b$, and $c_a = 1$, $c_b = (-1)^n$, where $n = 0, 1, 2, \ldots$ is the number of the bound state. $\chi_a(r)$ and $\chi_b(r)$ are continuous across the turning points and coincide with the usual WKB solution far from them. It is easy to check that $\chi_a(r)$ and $\chi_b(r)$ coincide at some point in the interval (a, b) between the turning points, and that their values, but not derivatives, can be matched at that point.

3. Examples

To show that the first QLM iteration gives very accurate results for wave functions and energies, as well as demonstrate very fast convergence of the next iterates let us consider five typical examples of potentials of rather different form used in atomic, nuclear and quark physics.

Let us start from the anharmonic oscillator $V(r) = \frac{1}{2}r^5$. This potential is typically used in different nuclear, quark and quantum field theory models. The exact energy of the ground state of this oscillator is 2.044 579 657 447 355 635 36 in atomic units with mass set to unity, $m = 1$. This result is obtained by us by a calculation using the Runge–Kutta method in quadruple precision. The WKB energy is different by 4.5% and equals 1.95159 in the same units, while the first-iteration QLM energy equals 2.04528 and differs from the exact energy only by 0.034%. The QLM energy coincides with the exact energy in all twenty digits after the sixth iteration.

For the first excited state the exact energy is 6.713 546 501 445 253 110 53, while the WKB and first-iteration QLM energies are 6.656623 and 6.713952 and are different from the exact energy by 0.84 and 0.006%, respectively. The similar picture exists for the second excited state where the exact energy is 12.767 866 541 180 535 228 88. The WKB and first-iteration QLM energies are 12.72396 and 12.76796 and are different from the exact energy by 0.34 and 0.0007%, respectively. Again, for both first and second excited states the QLM energies differ from the exact energies only in the twentieth digit after the sixth iteration.

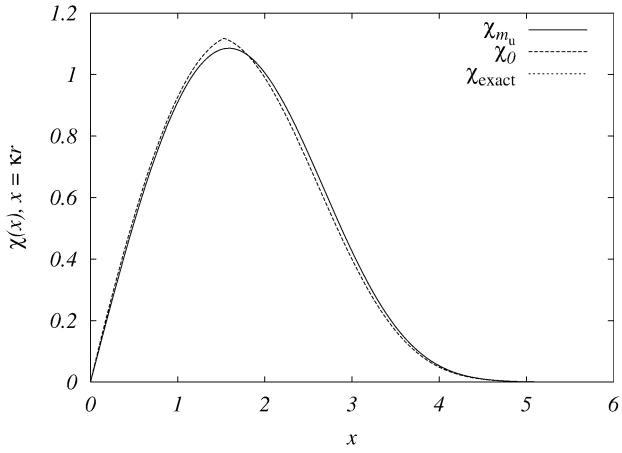

Fig. 1. Comparison of the Langer WKB solution χ_0 (dashed curve), the exact solution χ_{exact} (dotted curve) and the first QLM iterate χ_{m_u} (solid curve) for the ground state of the anharmonic oscillator $V(r) = \frac{1}{2}r^5$. The last two are indistinguishable on the plot. Here $x = \kappa r$, $\kappa^2 = 2mE/\hbar^2$.

The graphs corresponding to the Langer WKB solution, the exact solution and the first QLM iterate for the ground state are displayed in Fig. 1. One can see that while the Langer solution is noticeably different from the exact solution, the curve of the first QLM iteration is indistinguishable from the exact curve.

This could be followed more precisely by looking at Fig. 2 where the logarithm of the difference between the exact and WKB solutions and between the exact solution and the first QLM iteration are shown. One can see that the difference between the exact solution and the first QLM iteration is two orders of magnitude smaller than the difference between the exact and the WKB solutions, that is one QLM iteration increases the accuracy of the result by two orders of magnitude. Note that the dips on the graphs are artifacts of the logarithmic scale, since the logarithm of the absolute value of the difference of two solutions goes to minus infinity at points where the difference changes sign. The overall accuracy of the solution can be inferred only at x values not too close to the dips.

The accuracy of the WKB approximation increases for higher excitations. Therefore in the case of the excited state both the Langer WKB and QLM curves are indistinguishable from the exact one. Fig. 3 shows, however, that also in this case the difference between the exact solution and the first QLM iteration is by two orders of magnitude smaller than the difference between the exact and the WKB solutions.

Another interesting example is the modified Coulomb potential

$$V(r) = -\frac{1}{2\rho} + \frac{l(l+1) - \frac{1}{4}\alpha^2}{\rho^2} + \frac{\frac{3}{4}\alpha^2}{\rho^2(\rho + \alpha^2)^2}, \quad \rho = \alpha E r$$

[1] This form is based on a linear potential interpolation near turning points from which the Airy function arises.

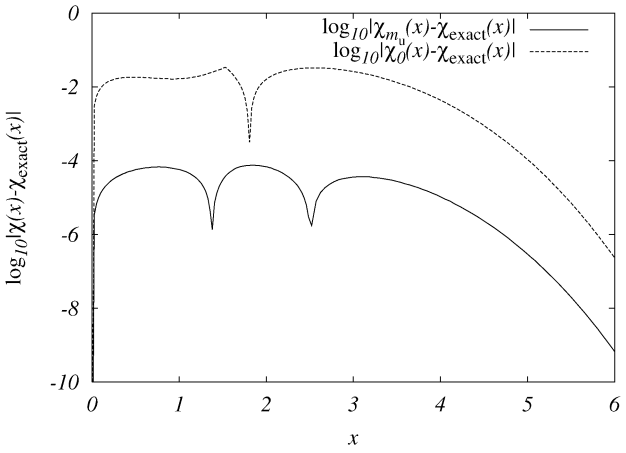

Fig. 2. Logarithm of the difference between the exact χ_{exact} and WKB solutions χ_0 (dashed curve) and between the exact solution and the first QLM iterate χ_{m_u} (solid curve) for the ground state of the anharmonic oscillator. The dips on the graphs are artifacts of the logarithmic scale, since the logarithm of the absolute value of the difference of two solutions goes to minus infinity at points where the difference changes sign. The overall accuracy of the solution can be inferred only at x values not too close to the dips.

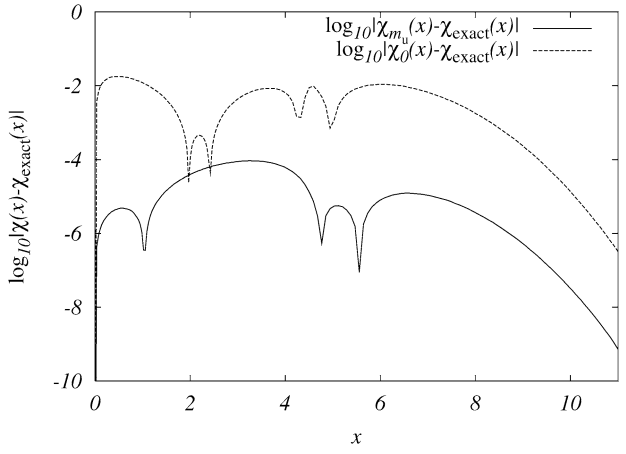

Fig. 3. As in Fig. 2, but for the excited state of the oscillator potential.

which is obtained when the equal masses two-body Dirac equation with the static Coulomb interaction is reduced to the Schrödinger equation [20,21]. The exact energy of the ground state with quantum numbers $(N, L, S, J) = (1, 0, 0, 0)$ is 0.999 993 340 148 538 880 1 in atomic units with double mass set to unity, $2M = 1$. This result was obtained in the work [21] by an elaborate computation using the finite element method and confirmed by ourselves using the Runge–Kutta method in quadruple precision. The WKB energy equals 0.999 986 680 and differs from the exact one by 6.6×10^{-4}. The first-iteration QLM energy equals 0.999 993 335 and differs from the exact one only by 5×10^{-7}. The QLM energy coincides with the exact one in all given digits after the sixth iteration.

The graph in Fig. 4 of the exact, WKB and QLM ground state wave functions is similar to Fig. 2.

The graph in Fig. 5 for their differences for this case is similar to Fig. 2 and shows that the difference between the exact wave function and the first QLM iteration is by two orders of magnitude smaller than the difference between the exact and the

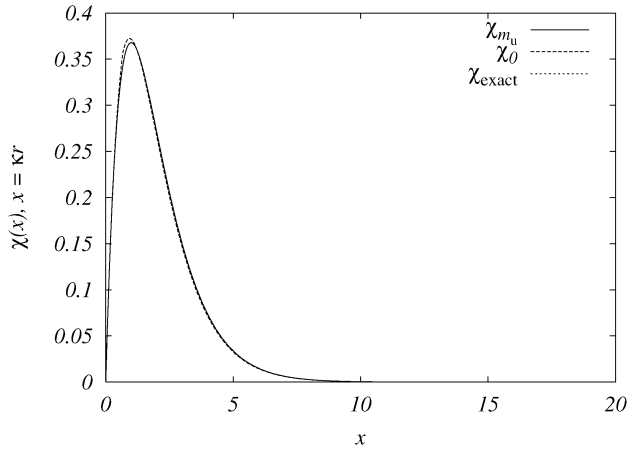

Fig. 4. As in Fig. 1, but for the ground state with quantum numbers $(N, L, S, J) = (0, 0, 0, 0)$ in the modified Coulomb potential $V(r) = -\frac{1}{2\rho} + (l(l+1) - \frac{1}{4}\alpha^2)/\rho^2 + \frac{3}{4}\alpha^2/\rho^2(\rho + \alpha^2)^2$, $\rho = \alpha E r$.

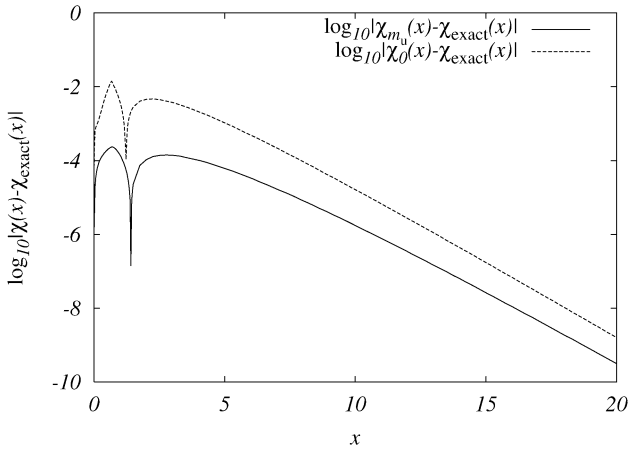

Fig. 5. As in Fig. 2, but for the ground state in the modified Coulomb potential.

WKB solutions. Thus also in this case just one QLM iteration increases the accuracy of the wave function by a remarkable two orders of magnitude.

The results for the ground and excited states with different quantum numbers (N, L, S, J) for the modified Coulomb potential are summed up in Table 1 and also in Figs. 6, 7, 8 where the differences between the exact wave function and the first QLM iteration and between the exact and the WKB solutions are displayed. We see, that though the accuracy of the WKB approximation increases for excited states and states with higher orbital momenta, also in these cases one QLM iteration increases the accuracy of the wave function by at least two orders of magnitude. In Table 1, E_{WKB} and $E^{(1)}_{\text{QLM}}$ are given to a limited number of digits, $E^{(1)}_{\text{QLM}}$ being slightly dependent on the discontinuity in the derivative of the Langer WKB solution at its joining point between the turning points. The high-precision results have at least 18 correct digits; E values tend to be more precise by 1 or 2 digits, therefore we list them to 20 or 21 digits. Since the computer arithmetic was quadruple precision (128-bit, about 30 decimal places), the differences in the last digits of E_{QLM} and E_{exact} reflect the different methods used.

Table 1
WKB, first iteration QLM, full QLM and exact binding energies. K is the number of QLM iterations, m is the (reduced) mass of the particle. The state label is nl (N, L, S, J for Breit–Coulomb). $D_1 = 10^2(1 - E_{\mathrm{WKB}}/E_{\mathrm{exact}})$, $D_2 = 10^2(1 - E^{(1)}_{\mathrm{QLM}}/E_{\mathrm{exact}})$. $x[y]$ denotes $x \times 10^y$. "+" marks the ground (symmetric) state of one-dimensional double-well potential; "−" marks regular states of two-power potential or the antisymmetric state of one-dimensional double-well potential

Potential	m	State	E_{WKB}	$E^{(1)}_{\mathrm{QLM}}$	E_{QLM}	K	E_{exact}	D_1	D_2
Breit–Coulomb	1	1 0 0 0	0.999986679987	0.999993335480	0.99999334014853888012	6	0.99999334014853888016	7[−4]	5[−7]
		2 0 0 0	0.999996670008	0.999998335239	0.99999833502466540218	7	0.99999833502466540223	2[−4]	−2[−8]
		1 1 0 1	0.999996670037	0.999998335831	0.99999833501727839123	44	0.99999833501727839122	2[−4]	−8[−8]
		2 1 0 1	0.999998520016	0.999999260060	0.99999926000774772931	47	0.99999926000774772931	7[−5]	−1[−8]
$\log r$	$\frac{1}{2}$	$1s$	1.05346726985	1.044738	1.04433226746060809298	5	1.04433226746060809380	−0.88	−0.039
		$2s$	1.850802588	1.8475	1.84744258030447816386	5	1.84744258030447816385	−0.18	−0.003
		$3s$	2.299218712	2.289659	2.28961571419653762102	5	2.28961571419653762102	−0.42	−0.002
$\frac{1}{2}r^5$	1	$1s$	1.9515942	2.045279	2.04457965744735563534	6	2.04457965744735563536	4.5	−0.03
		$2s$	6.656623	6.713952	6.71354650144525311020	6	6.71354650144525311053	0.85	−0.006
		$3s$	12.72396	12.76796	12.7678665411805352297	6	12.7678665411805352289	0.34	−0.001
$\frac{-24}{1+\exp\frac{r-1}{0.2}}$	1	$1s$	−17.61192	−17.5432	−17.5597967410317970585	5	−17.5597967410317970589	−0.30	0.095
		$2s$	−7.190505	−7.37920	−7.37854164337449079226	5	−7.37854164337449079262	2.5	−0.009
		$3s$	−0.029269	−0.105156	−0.10819568493119384889	6	−0.10819568493119384933	72.9	2.8
$\frac{g^2(r^2-a^2)^2}{2}$	1	$1s+$	0.484067[1]	0.483017[2]	0.48295865991331554844	6	0.48295865991331554820	−0.98	−0.009
		$1s-$	0.49734197	0.484218	0.48314820684089227025	6	0.48314820684089227025	−2.9	−0.22
		$2s-$	1.39372888	1.373747	1.37363583606219407956	6	1.37363583606219407958	−1.5	−0.008
		$3s-$	2.17217337	2.178319	2.17745782251542955262	6	2.17745782251542955243	0.24	−0.040

[1] Includes the tunneling correction to E.
[2] Initial WKB approximation includes tunneling correction to E.

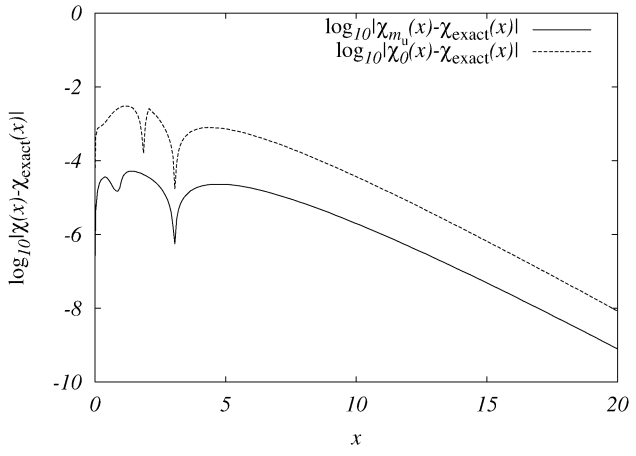

Fig. 6. As in Fig. 2, but for the excited state with quantum numbers $(N, L, S, J) = (2, 0, 0, 0)$ in the modified Coulomb potential.

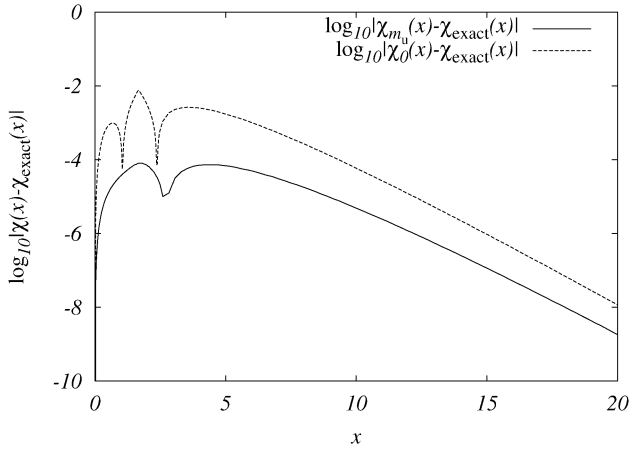

Fig. 7. As in Fig. 2, but for the excited state with quantum numbers $(N, L, S, J) = (1, 1, 0, 1)$ in the modified Coulomb potential.

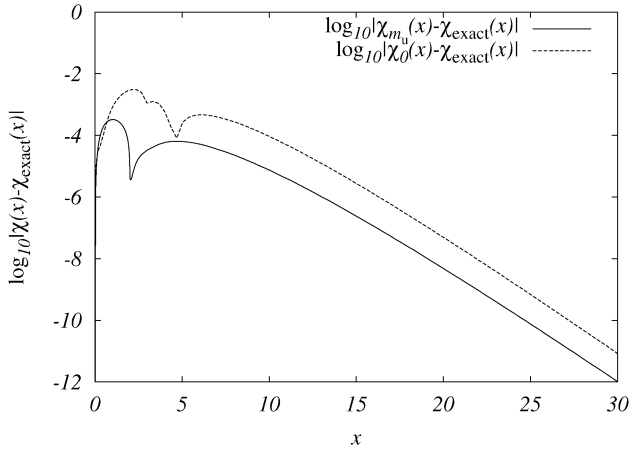

Fig. 8. As in Fig. 2, but for the excited state with quantum numbers $(N, L, S, J) = (2, 1, 0, 1)$ in the modified Coulomb potential.

The other examples considered in this paper are the logarithmic $V(r) = \log r$, Wood–Saxon $V = -V_0/(1 + \exp((r - R)/a))$ and the two-power (double-well) $V(r) = \frac{1}{2}g^2(r^2 - a^2)^2$ potentials, the results for which are summarized in Table 1. The graphs corresponding to different states of these potentials

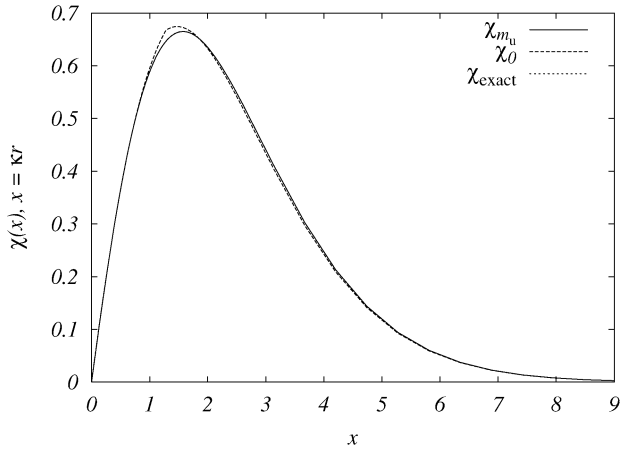

Fig. 9. As in Fig. 1, but for the ground state of the logarithmic potential $V = \log(r)$.

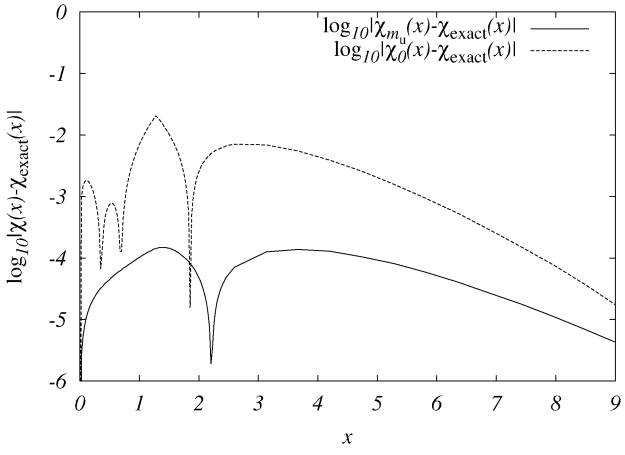

Fig. 10. As in Fig. 2, but for the ground state of the logarithmic potential.

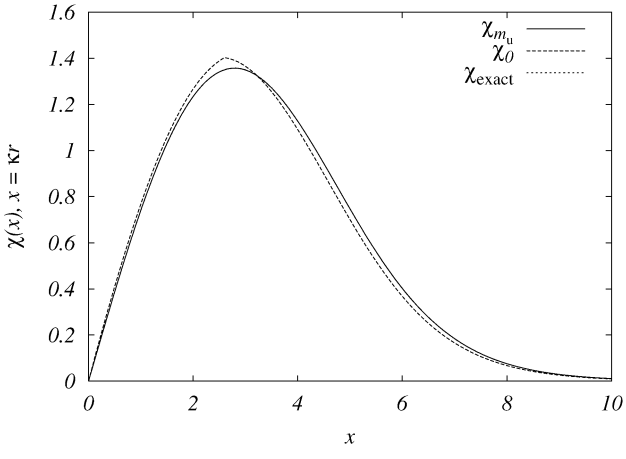

Fig. 11. As in Fig. 1, but for the ground state of the Wood–Saxon potential $V = -V_0/(1 + \exp((r - R)/a))$, with $V_0 = 24$, $R = 1$, $a = 0.2$.

are shown in Figs. 9–17. The first two potentials are used respectively for computations in quark and nuclear physics. The double-well potential, that is the quartic potential in one dimension with degenerate minima, is typically studied in quantum field theory and in the framework of the tunneling problem in quantum mechanics. Its perturbation series does not converge

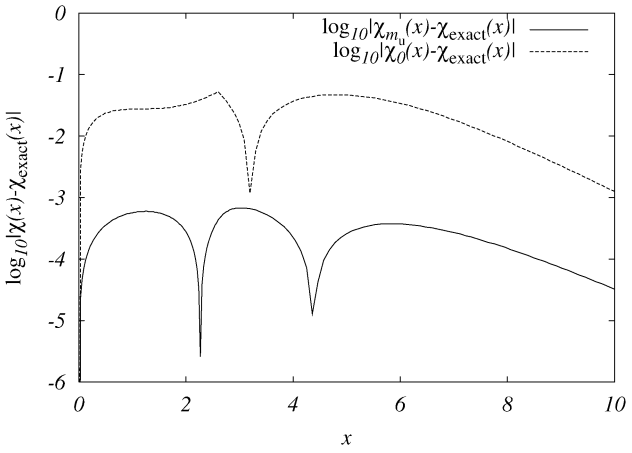

Fig. 12. As in Fig. 2, but for the ground state of the Wood–Saxon potential.

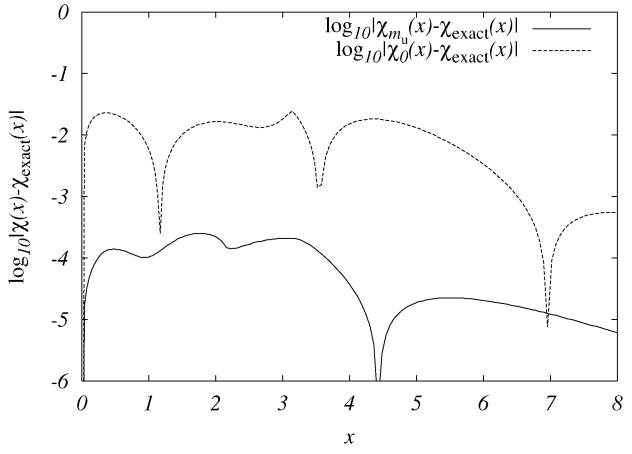

Fig. 13. As in Fig. 2, but for the first excited state of the Wood–Saxon potential.

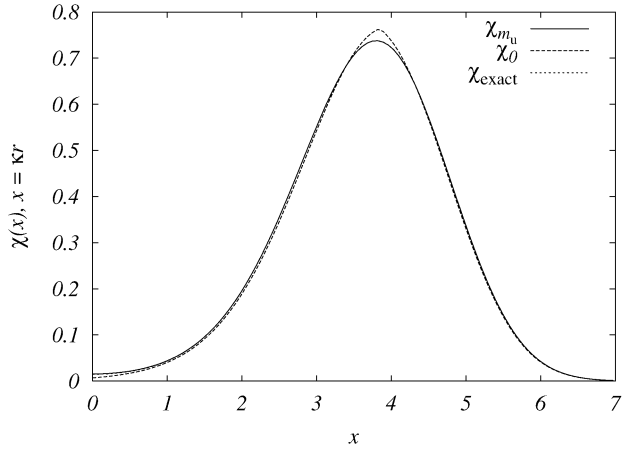

Fig. 14. As in Fig. 1, but for the ground (symmetric) state of the double-well potential $V = \frac{1}{2}g^2(r^2 - a^2)^2$, $g^2 = 1/4a^2$, $a = 4$ in one dimension.

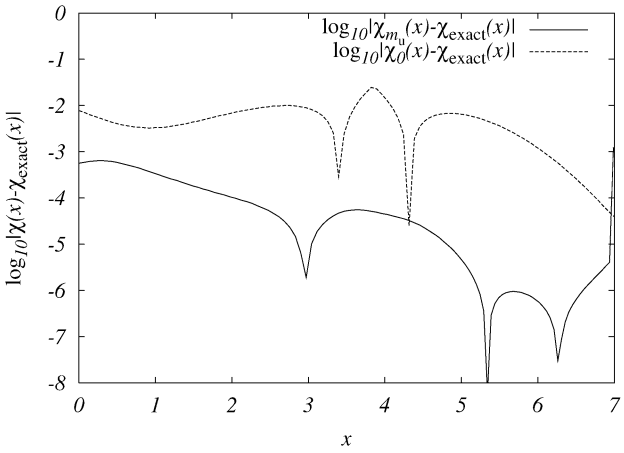

Fig. 15. As in Fig. 2, but for the state of Fig. 14.

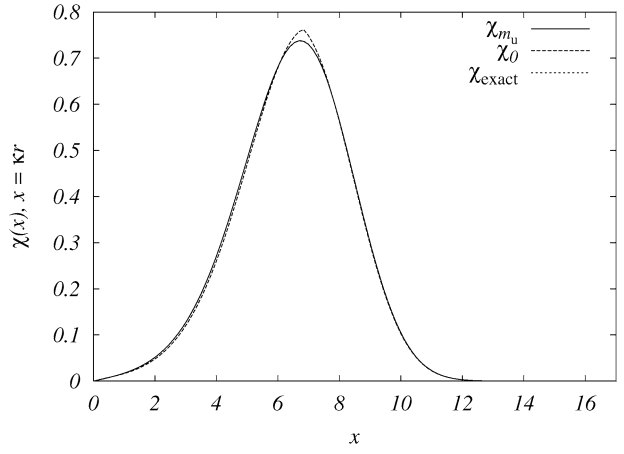

Fig. 16. As in Fig. 1, but for the ground state of the two-power potential $V = \frac{1}{2}g^2(r^2 - a^2)^2$, $g^2 = 1/4a^2$, $a = 4$, or for the first (antisymmetric) excited state of the corresponding double-well potential in one dimension.

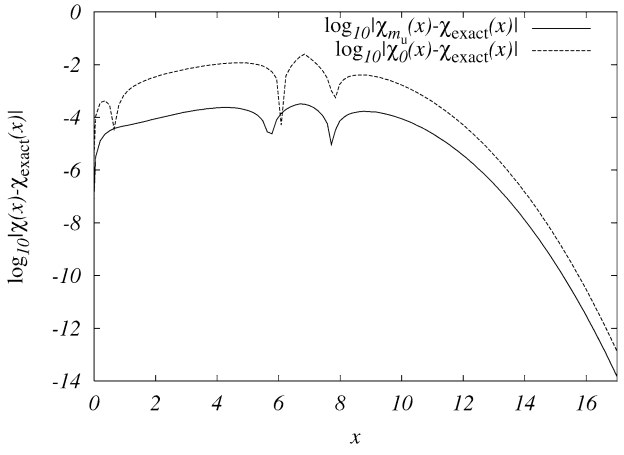

Fig. 17. As in Fig. 2, but for the state of Fig. 16.

and different alternative nonperturbative approaches are therefore explored since the description of tunneling between two minima should be necessarily nonperturbative (see, for example, Ref. [22] and the references therein).

In particular, in the paper [23] using the $1/N$ expansion method, the tunneling terms were not included for the symmetric (ground) state of the double-well potential in one dimension, giving the $1/N$ energy of 0.48305 compared to the exact energy, 0.48295... In addition, in our calculation it is easy to specify the boundary condition at $r = 0$ in this particular case (where $\chi(0) \neq 0$), so we can calculate on the interval $r \geqslant 0$ only: because we do the QLM iteration on the function

$u(\kappa r) = \arctan(-\kappa\chi(r)/\chi'(r))$, we have simply $u(0) = -\frac{\pi}{2}$. This can easily be seen by taking into account that $\chi(r)$ has an even-power Taylor expansion at $r = 0$. We use the tunneling term just to correct the energy of the initial WKB approximation, changing the usual WKB quantization condition to

$$\int_a^b k(r)\,\mathrm{d}r = \left(n + \frac{1}{2}\right)\pi - \frac{1}{2}\mathrm{e}^{-\int_{-a}^{a} K(r)\,\mathrm{d}r},$$

where the second term on the RHS is the tunneling term [24]; $k(r) = iK(r)$ and $n = 0, 1, 2, \ldots$ is the number of the bound state. The tunneling correction affects the 1st QLM iteration but of course not the full QLM calculation, where the boundary conditions completely specify the converged solution.

4. Conclusion

One can show [15,17] that the approximation by the first QLM iterate in Eq. (4) leads to exact energies for many well-known physical potentials such as the Coulomb, harmonic oscillator, Pöschl–Teller, Hulthen, Hylleraas, Morse, Eckart, etc. For other potentials which have more complicated analytical structure we show on examples of the anharmonic oscillator, logarithmic, two-power (double-well), and Wood–Saxon potentials and for the solution of the two-body Dirac equation with static Coulomb potential, that the use of the Langer WKB wave function as an initial guess already in the first QLM approximation gives energies and wave functions two orders of magnitude more accurate than the WKB results. Such a QLM solution, unlike the usual WKB solution, displays no unphysical turning point singularities. Since the first QLM iterate is given by an analytic expression (4) for $p = 1$ it allows one to estimate analytically the role of different parameters and their influence on properties of a quantum system with much higher precision than provided by the WKB approximation. In addition, it was shown that six QLM iterations are typically enough to obtain both the wave function and energy with the accuracy of twenty significant digits.

Acknowledgements

The research was supported by the Bilateral Cooperation Program at the Ministry of education, science and sport of Slovenia (R.K.) and by grant No. 2004106 from the United States–Israel Binational Science Foundation (BSF), Jerusalem, Israel (VBM).

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