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Physics Letters A 337 (2005) 354–359
PHYSICS LETTERS A
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# Quasilinearization method and summation of the WKB series

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Received 10 September 2004; received in revised form 26 January 2005; accepted 28 January 2005

Communicated by A.P. Fordy

**Abstract**

Solutions obtained by the quasilinearization method (QLM) are compared with the WKB solutions. Expansion of the $p$th QLM iterate in powers of $\hbar$ reproduces the structure of the WKB series generating an infinite number of the WKB terms with the first $2^p$ terms reproduced exactly. The QLM quantization condition leads to exact energies for the Pöschl–Teller, Hulthén, Hylleraas, Morse, Eckart potentials, etc. For other, more complicated potentials the first QLM iterate, given by the closed analytic expression, is extremely accurate. The iterates converge very fast. The sixth iterate of the energy for the anharmonic oscillator and for the two-body Coulomb–Dirac equation has an accuracy of 20 significant figures.


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

*Keywords:* Quasilinearization; WKB; Nonlinear differential equations

The quasilinearization method (QLM) and its iterations were constructed [1] as a generalization of the Newton–Raphson method [2] for the nonlinear differential equations to yield rapid quadratic and often monotonic convergence to the exact solution. It does not rely on the existence of any kind of smallness parameter. The derivation of the WKB solution starts by casting the 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 method (QLM) whose application to physical problems are discussed in works [3–6] and compare with the WKB results.

The goal of this work is to point out that QLM iterates which are expressible in a closed integral form provide better approximation than the usual WKB. We show that the $p$th QLM iterate when expanded in powers of $\hbar$ reproduces the structure of the WKB series generating an infinite number of the WKB terms

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0375-9601/$ – see front matter 
doi:10.1016/j.physleta.2005.01.072

with the first $2^p$ terms reproduced exactly. A similar number of the next terms are reproduced with approximately correct coefficients. We prove also that the exact quantization condition in any QLM approximation, including the first, leads to exact energies for many known physical potentials used in molecular and nuclear physics such as the Pöschl–Teller, Hulthén, Hylleraas, Morse, Eckart, etc. In the general case of arbitrary potentials that do not have a simple analytic structure, we illustrate that both the wave functions and energies are very well reproduced by the first QLM iterate and show significant improvement over those obtained by the usual WKB approximation. If the initial QLM guess is properly chosen, the wave function in the first QLM iteration, unlike the WKB wave function, is free of unphysical turning point singularities. Since the first QLM iteration is given by an analytic expression [3–6], 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 the sixth iterate as we show on the examples of the anharmonic oscillator and the two-body Dirac equation with the Coulomb potential.

The usual WKB substitution

$$\chi(r) = C\exp\left(\lambda\int^{r} y(r')\,dr'\right)$$

converts the radial Schrödinger equation to nonlinear Riccati form

$$\frac{dy(z)}{dz} + \left(k^2(z) + y^2(z)\right) = 0, \tag{1}$$

where $k^2(z) = E - V - l(l+1)/z^2$, $\lambda^2 = 2m/\hbar^2$, $z = \lambda r$. 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. (1) 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 [3,4,6] of this equation gives a set of recurrence differential equations

$$\frac{dy_p(z)}{dz} = y_{p-1}^2(z) - 2y_p(z)y_{p-1}(z) - k^2(z) \tag{2}$$

with the boundary condition $y_p(z_0) = ik(z_0)$. The analytic solution [6] of these equations expresses the $p$th iterate $y_p(z)$ in terms of the previous iterate:

$$y_p(z) = f_{p-1}(z) - \int_{z_0}^{z} ds\frac{df_{p-1}(s)}{ds}\exp\left[-2\int_{s}^{z} y_{p-1}(t)\,dt\right],$$

$$f_{p-1}(z) = \frac{y_{p-1}^2(z) - k^2(z)}{2y_{p-1}(z)}. \tag{3}$$

Indeed, differentiation of both parts of Eq. (3) leads immediately to Eq. (2) which proves that $y_p(z)$ is a solution of this equation. The boundary condition is obviously satisfied automatically.

The successive integrations by parts of Eq. (3) lead [6] to the series

$$y_p(z) = \sum_{n=0}^{\infty}\mathcal{L}_n^{(p)}(z) \tag{4}$$

with $\mathcal{L}_n^{(p)}(z)$ given by recursion relation

$$\mathcal{L}_n^{(p)}(z) = \frac{1}{2y_{p-1}(z)}\frac{d(-\mathcal{L}_{n-1}^{(p)}(z))}{dz},$$

$$\mathcal{L}_0^{(p)}(z) = f_{p-1}(z).$$

Since $d/dz = g\,d/dr$, $g = \lambda^{-1} = \hbar/\sqrt{2m}$, Eq. (4) represents the expansion of the $p$th QLM iterate in powers of $g$, that is in powers of $\hbar$, which one can compare with the WKB series. For the zeroth iterate $y_0(z)$ it seems natural to choose the zeroth 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 [7], if $y_{p-1}(z)$ in Eq. (2) 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.

Eq. (3) gives an especially simple expression [6] for the first QLM iterate

$$y_1(z) = ik(z) - i\int_{z_0}^{z} ds\,k'(s)\exp\left[-2i\int_{s}^{z} k(t)\,dt\right]$$

which thus is expressible in a closed integral form. This expression takes into account, though approximately, an infinite number of the WKB terms corresponding to higher powers of $\hbar$, as will be shown in the next section. In view of this it is a better approximation than the usual WKB.

To obtain the WKB series one has to expand the solution $y$ of the Riccati equation (1) in powers of $\hbar$. This is easy to do by looking for $y$ in the form of a series and equating terms of identical powers of $g$,

$$y = \sum_{m=0}^{\infty} g^m Y_m,$$

$$Y_m = -\frac{1}{2\,Y_0}\left(Y'_{m-1} + \sum_{k=1}^{m-1} Y_k\, Y_{m-k}\right). \tag{5}$$

The derivatives in this and subsequent expressions are in the variable $r$. The zeroth WKB approximation $Y_0$ is given by $Y_0 = ik$. The comparison of expansion of the first QLM iterate in powers of $\hbar$ and the WKB series was originally performed in [6]. There it was shown that the expansion reproduces exactly the first two terms and also gives correctly the structure of the WKB series up to the power $g^3$ considered in these works, generating series with proper WKB terms, but with different coefficients. Comparison of Eqs. (4) and (5) in the present work shows that this conclusion is true also if higher powers of $g$ are taken into account.

The computation of the expansion of the second QLM iterate $y_2$ in powers of $\hbar$ is done by reexpanding the term $1/(2y_1)$ in $\mathcal{L}_n^{(p)}(z)$ in the series in powers of $g$ and keeping the powers up to $g^7$ inclusively in this expression as well as in the sum in Eq. (4). This procedure performed with the help of MATHEMATICA [8] shows that expansion of $y_2$ reproduces exactly already the first four terms of the WKB series. It also gives the true structure of the next terms of the WKB series, generating series with proper WKB terms which have approximately correct coefficients. The expansion of $y_3$ is obtained in the similar fashion. It reproduces exactly the first eight terms of the WKB series, that is all the terms up to the power $g^7$ inclusively.

Summing up, we have proved that the expansion of the first, second and third QLM iterates reproduces exactly two, four and eight WKB terms, respectively. Since the zeroth QLM iterate $y_0$ was chosen to be equal to the zeroth WKB approximation $ik$, one can state that the $p$th QLM iterate contains $2^p$ exact terms. In addition, the expansion of each QLM iterate has the proper structure whose terms are identical to those of the WKB series but have only approximately correct coefficients.

The $2^p$ law is, of course, not accidental. The QLM iterates are quadratically convergent [1,3], that is the norm of the difference of the exact solution and the $p$th QLM iterate $\|y - y_p\|$ is proportional to the square of the norm of the differences of the exact solution and the $(p-1)$th QLM iterate:

$$\|y - y_p\| \sim \|y - y_{p-1}\|^2. \tag{6}$$

Here the norm $\|g\|$ of the function $g(x)$ is the maximum of the function $g(x)$ on the whole interval of values of $x$. Since $y_0$ contains just one correct WKB term of power $g^0$ and thus $\|y - y_0\|$ is proportional to $g$, one has to expect that $\|y - y_1\| \sim g^2$ and thus $y_1$ contains two correct WKB terms of powers $g^0$ and $g^1$. The difference $\|y - y_2\| \sim \|y - y_1\| \sim g^4$ so that $y_2$ contains four correct WKB terms of powers $g^0$, $g^1$, $g^2$ and $g^3$. Finally, the difference $\|y - y_3\|$ should be proportional to $g^8$, and therefore $y_3$ has to contain eight correct terms with powers between $g^0$ and $g^7$ inclusively. This explains the $2^p$ law.

The exact quantum-mechanical quantization condition for the energy [9,10] has the form:

$$J = \oint_C y(z)\,dz = i2\pi n. \tag{7}$$

Here $y(z)$ is the logarithmic derivative of the wave function, given by Eq. (1), $z = gr$, $n = 0, 1, 2, \ldots$, is the bound state number which counts the number of poles of $y(z)$; the integration is along a path $C$ in the complex plane encircling the segment of the $\Re z$ axis between the turning points.

The $p$th QLM iterate $y_p(z)$, as we have seen, contains, in addition to $2^p$ exact WKB terms of powers $g^0, g^1, \ldots, g^{2^p-1}$, also an infinite number of structurally correct WKB terms of higher powers of $g$ with approximate coefficients. One can expect therefore that the quantization condition (7) with $y(z)$ approximated by any QLM iterate $y_p(z)$, $p = 1, 2, \ldots$, including the first, gives more accurate energy than the usual WKB quantization condition which is obtained by substituting into exact quantization condition (7) the WKB expansion up to the first power of $g \sim \hbar$,

that is

$$y(z) = ik(z) - \frac{dk(z)/dz}{2k(z)},$$

and neglecting all higher powers of $g$ in the expansion. Indeed, we will prove now that Eq. (7) with $y(z)$ approximated by any QLM iterate leads to exact energies not only for the Coulomb and harmonic oscillator potentials as was shown earlier in Ref. [6], but for many other well-known physical potentials used in molecular and nuclear physics such as the Pöschl–Teller, Hulthén, Hylleraas, Morse, Eckart, etc. The WKB quantization condition yields the exact energy only for the first two potentials, but not for the rest of them.

Let us prove it on the example of the Hulthén potential

$$V(r) = -A\exp(-r/a)\big(1-\exp(-r/a)\big),$$
$$A>0, \quad 0<r<\infty,$$

which plays an important role in molecular and nuclear physics. To compute the energy levels in the quasilinear approximation we have to use the QLM equation (2) which after switching to the variable $t = \exp(-r/a)$, $0<t<1$, has the form

$$-\frac{t}{a}\frac{dy_p}{dt} = y_p^2 - 2y_p\,y_{p-1} + \epsilon - A\frac{t}{1-t}. \tag{8}$$

Here $\epsilon = -E$ and $E$ is the energy. For convenience of further computations we set here $2m/\hbar^2$ equal to unity. The quantization condition (7) in variable $t$ is given by

$$J_p = a\oint_C \frac{y_p(t)}{t}\,dt = i2\pi n, \quad p=1,2,\ldots.$$

At the singular point $t\sim 0$ of the integrand, Eq. (8) reduces to

$$-\frac{t}{a}\frac{dy_p}{dt} = y_p^2 - 2y_p y_{p-1} + \epsilon$$

whose solution is $y_p = c_p$, where $c_p$ is a constant satisfying the algebraic equation $c_p^2 - 2c_p c_{p-1} + \epsilon = 0$. Since at large $p$ we expect $y_{p-1}\to y_p\to y$, where $y$ is an exact solution at $t=0$, it means, in view of $c_p$ being a constant, that we should have $c_p = c_{p-1} = c$, that is, we are looking for a fixed point solution of this algebraic equation, which is $c_p = \sqrt{\epsilon}$. The positive sign before the root is chosen since the first term in expansion of $y_p(t)$ in the WKB terms is $ik(t)$. Thus

$$y_p(t) \simeq ik(t) = i\sqrt{-\epsilon + At/(1-t)},$$

that is, $y_p(0)\simeq +\sqrt{\epsilon}$.

In the same way one finds that the residues at other singular points $t=1$ and $t=\infty$ equal $1/a$ and $\sqrt{\epsilon+A}$, respectively. After taking into account that poles $t=0$ and $t=1$ are encircled in the opposite direction compared with the pole at infinity (which is encircled counterclockwise) and the reinstatement of the factor $2m/\hbar^2$ the exact quantization condition gives

$$\sqrt{2ma^2/\hbar^2}\left(-\sqrt{\epsilon}+\sqrt{\epsilon+A}\right) = n+1,$$
$$n=0,1,2,\ldots.$$

This expression coincides with the exact one for the Hulthén potential calculated in [11,12] and is different from the WKB quantization condition

$$\sqrt{2ma^2/\hbar^2}\left(-\sqrt{\epsilon}+\sqrt{\epsilon+A}\right) = n+\frac{1}{2}.$$

Similar computations show that the quantization condition (7) in any QLM approximation including the first leads to exact energies for all the potentials mentioned above and for other potentials with a simple singular structure.

For more complicated potentials numerical calculation is necessary. However, as we will see now, already the first QLM iterate, given by the closed analytic expression, is extremely accurate. For the zeroth iterate $y_0(z)$ one can choose the usual WKB approximation. However, this choice has unphysical turning point singularities. Consequently, if $y_p(z)$ in Eq. (2) is a discontinuous function of $z$ in a certain interval, then [7] $y_{p+1}(z)$ or its derivatives could also be discontinuous functions in this interval, so the turning point singularities of $y_0(z)$ will unfortunately propagate to the next iterate. To avoid this we choose the Langer WKB wave function [13] as the zeroth iteration. This function near the turning points $a$ and $b$ is given by the simple analytic expression

$$\chi_i(r) = c_i\sqrt{\frac{S_i^{1/3}(r)}{|k(r)|}}\,\mathrm{Ai}\big[dS_i^{1/3}(r)\big],$$
$$S_i(r) = \frac{3}{2}\lambda\left|\int_i^r |k(s)|\,ds\right|. \tag{9}$$

Here Ai denotes the Airy function, $i=a,b$,

$$k(r) = \frac{2m}{\hbar^2}\left[\big(E-V(r)\big) - \frac{(l+1/2)^2}{2mr^2}\right],$$

$d$ 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. It is easy to check that $\chi_a(r)$ and $\chi_b(r)$ coincide at some point at the interval $(a, b)$ between the turning points, are continuous across them and coincide with the usual WKB solutions far from them.

Let us consider a couple of examples. The exact energy of the ground state of the anharmonic oscillator $V(r) = r^4$ is 2.393 644 016 482 303 115 6 in atomic units with mass set to unity, $m = 1$. This result is obtained by us using the Runge–Kutta method and quadruple precision arithmetic. The WKB energy is different by 2.8% and equals 2.326 62, while the first-iteration QLM energy equals 2.394 75 and differs from the exact energy only by 0.046%. The QLM energy coincides with the exact energy in all twenty digits after the sixth iteration.

The graph in Fig. 1 displays the logarithm of the difference between the exact and WKB solutions and between the exact solution and the first QLM iteration. 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, just one QLM iteration increases the accuracy of the wave function by two orders of magnitude.[1]

The second example is the modified Coulomb potential

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

obtained when the equal-mass two-body Dirac equation with the static Coulomb interaction is reduced to the Schrödinger equation [14]. The exact energy of the $^1S_0$ ground state is 0.999 993 340 148 538 880 12 in atomic units with double mass set to unity, $2M = 1$. This result was obtained in the work [15] by an elaborate computation using the finite element method and verified by ourselves using the Runge–Kutta method in quadruple precision. WKB in this case predicts the

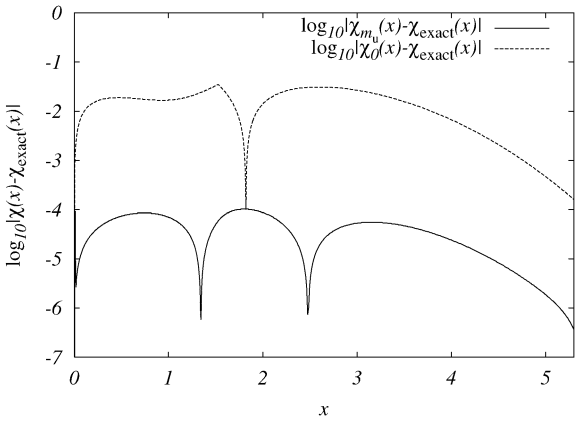


Fig. 1. Logarithm of the difference between the exact solution $\chi_{\text{exact}}$ and the WKB solution $\chi_0$ (dashed curve) and between $\chi_{\text{exact}}$ and the first QLM iterate $\chi_{m_u}$ (solid curve) for the ground state of the anharmonic oscillator.[1]

energy very accurately since the potential is very close to the Coulomb potential, for which WKB energy is precise. It equals 0.999 986 680 0 and differs from the exact one only by $6.66 \times 10^{-6}$. The first-iteration QLM energy equals 0.999 993 335 4 and differs from the exact energy by $5 \times 10^{-9}$, that is, it is more accurate than the WKB energy by three orders of magnitude. The QLM energy coincides with the exact one up to the twentieth digit after the sixth iteration.

The calculation shows that the difference between the exact wave function and the first QLM iteration is, as in previous example, by two orders of magnitude smaller than the difference between the exact and the WKB solutions. Thus also in this case one QLM iteration increases the accuracy of the wave function by a remarkable two orders of magnitude.

In conclusion, we have shown that the quasilinearization method (QLM) which approaches solution of the Riccati–Schrödinger equation by approximating the nonlinear terms by a sequence of the linear ones, and is not based on the existence of a small parameter, sums the WKB series. The expansion of the $p$th QLM iteration in powers of $\hbar$ reproduces the structure of the WKB series generating an infinite number of the WKB term with $2^p$ terms of the expansion reproduced exactly and a similar number approximately. As a result, one expects that the exact quantization condition with integrand replaced by any QLM iterate including the first gives more accurate energy than the WKB quantization condition which is obtained by substitut-

[1] The dips are artifacts of the logarithmic scale, as the logarithm of the absolute value of the difference of two solutions goes to $-\infty$ at points where the difference changes sign. The overall accuracy of the solution can therefore be inferred only at $x$ values not too close to the dips.

ing into Eq. (7) the WKB expansion up to the first power of $\hbar$ and neglecting all higher powers of $\hbar$. We show on examples of the Hulthén potential that it in fact, the QLM energy is exact already in the first iteration. Similarly, one can show that the approximation by the first QLM iterate in Eq. (7) leads to exact energies for many well-known physical potentials such as the Coulomb, harmonic oscillator, Pöschl–Teller, Hulthén, Hylleraas, Morse, Eckart, etc. For other potentials which have more complicated analytical structure we show on examples of the anharmonic oscillator and modified Coulomb potentials that the use of the Langer WKB solution as an initial guess already in the first QLM approximation gives energies and wave functions at least 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 a closed analytic expression 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 usually enough to obtain both the wave function and the energy with extreme accuracy of twenty significant figures.

## Acknowledgements

The research was supported by the Bilateral Cooperation Program at the Ministry of Education, Science and Sport of Slovenia (R.K.).

## References

[1] R. Kalaba, J. Math. Mech. 8 (1959) 519;
R.E. Bellman, R.E. Kalaba, Quasilinearization and Nonlinear Boundary-Value Problems, Elsevier, New York, 1965.
[2] S.D. Conte, C. de Boor, Elementary Numerical Analysis, McGraw–Hill, New York, 1981.
[3] V.B. Mandelzweig, J. Math. Phys. 40 (1999) 6266;
V.B. Mandelzweig, Few-Body Systems Suppl. 14 (2003) 185.
[4] V.B. Mandelzweig, F. Tabakin, Comput. Phys. Commun. 141 (2001) 268.
[5] R. Krivec, V.B. Mandelzweig, Comput. Phys. Commun. 138 (2001) 69;
R. Krivec, V.B. Mandelzweig, Comput. Phys. Commun. 152 (2003) 165.
[6] K. Raghunathan, R. Vasudevan, J. Phys. A 20 (1987) 839;
M. Jameel, J. Phys. A 21 (1988) 1719.
[7] E.L. Ince, Ordinary Differential Equations, Dover, New York, 1956.
[8] S. Wolfram, The MATHEMATICA Book, fourth ed., Wolfram Media/Cambridge Univ. Press, 1999.
[9] J.L. Dunham, Phys. Rev. 41 (1932) 713;
C.M. Bender, K. Olaussen, P.S. Wang, Phys. Rev. D 16 (1977) 1740.
[10] R.A. Leacock, M.J. Padgett, Phys. Rev. Lett. 50 (1983) 3;
R.A. Leacock, M.J. Padgett, Phys. Rev. D 28 (1983) 2491.
[11] S. Flügge, Practical Quantum Mechanics, Springer-Verlag, New York, 1971.
[12] A. Galindo, P. Pascual, Quantum Mechanics, vols. I, II, Springer-Verlag, Heidelberg, 1991.
[13] R.E. Langer, Phys. Rev. 51 (1937) 669.
[14] J. Malenfant, Phys. Rev. D 38 (1988) 3295.
[15] T.C. Scott, J. Shertzer, R.A. Moore, Phys. Rev. A 45 (1992) 4393.