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Quasilinear Approximation and WKB*

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Abstract. Quasilinear solutions of the radial Schrödinger equation for different potentials are compared with corresponding WKB solutions. For this study, the Schrödinger equation is first cast into a nonlinear Riccati form. While the WKB method generates an expansion in powers of $\hbar$, the quasi-linearization method (QLM) approaches the solution of the Riccati equation by approximating its nonlinear terms by a sequence of linear iterates. Although iterative, the QLM is not perturbative and does not rely on the existence of any kind of smallness parameters. If the initial QLM guess is properly chosen, the usual QLM solution, unlike the WKB, displays no unphysical turning-point singularities. The first QLM iteration is given by an analytic expression. This allows one to estimate analytically the role of different parameters, and the influence of their variation on the boundedness or unboundedness of a critically stable quantum system, with much more precision than provided by the WKB approximation, which often fails miserably for systems on the border of stability. It is therefore demonstrated that the QLM method is preferable over the usual WKB method.

1 Introduction and Brief History

The application of a very powerful approximation technique called the quasilinearization method (QLM), which was introduced years ago by Bellman and Kalaba [3] in the theory of linear programming, to various physics problems was discussed in a series of recent papers [1, 2]. The QLM approaches the solution of a nonlinear

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differential equation by approximating the nonlinear terms by a sequence of linear ones, and is not based on the existence of any smallness parameter. Indeed, although iterative, the QLM is not perturbative and it has very fast quadratic convergence. It has been shown [1, 2] that the QLM solution sums an infinite number of terms of the expansion in powers of the different parameters and therefore well approximates the exact solution in a wide region of the parameter values.

When the structure of a critically stable quantum system is analyzed, understanding the analytic behavior of the solution as a function of different physical parameters is often of decisive importance. In one-dimensional two-body problems, or in three-dimensional two-body problems with central potentials, such understanding is usually provided by the application of the WKB method, which supplies an approximate solution accurate up to some low (usually the first) power of $\hbar$.

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 the work [4], 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 all the higher QLM approximations and it can be shown [5] that the n-th QLM iteration yields the correct structure of the infinite WKB series and reproduces 2^n 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 [4, 5], but also from the fact that the quantization condition in the first QLM iteration leads to exact energies for many potentials [5]; namely, 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 the present work is to show that also in the general case of arbitrary potentials that do not have a simple analytic structure, both the wave functions and energies are very well reproduced by the first QLM iteration and show significant improvement over those obtained by the usual WKB approximation. In addition, we show that 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 [1, 2, 4], it allows one to analytically estimate the role of different parameters and the influence of their variation on boundedness or unboundedness of a critically stable quantum system with much more precision than obtained by the WKB approximation, which often fails miserably for systems on the border of stability. In addition, we show that five QLM iterations are usually enough to obtain both the wave function and energies with the extreme accuracy of ten significant figures.

2 Computation and the Results

The usual WKB substitution

$$\chi(r) = C \exp\left[\lambda \int^r Y(r')\, dr'\right] \tag{1}$$

converts the radial Schrödinger equation

$$\chi''(r) + \lambda^2 k^2 \chi(r) = 0 \tag{2}$$

to nonlinear Riccati form

$$y'(z) + (k^2 + y^2(z)) = 0. \tag{3}$$

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

The proper bound-state boundary condition for potentials falling off at $z \simeq z_0$ is $y(z) = \text{const}$ at $z \geq z_0$. The quasilinearization [1, 2, 4] of this equation gives a set of recurrence differential equations

$$y_p' = y_{p-1}^2 - 2y_p y_{p-1} - k^2. \tag{4}$$

The analytic solution [4] of these equations expresses the p-th iterate $y_p(z)$ in terms of the previous iterate,

$$\begin{aligned} y_p(z) &= f_{p-1}(z) - \int_{z_0}^{z} ds\, f_{p-1}'(s) \exp\left[-2\int_s^z y_{p-1}(t)\, dt\right], \\ f_{p-1}(z) &= \frac{y_{p-1}^2(z) - k^2(z)}{2y_{p-1}(z)}. \end{aligned} \tag{5}$$

Indeed, differentiation of both parts of Eq. (5) leads immediately to Eq. (4) which proves that $y_p(z)$ is a solution of this equation.

For the zeroth iterate $y_0(z)$, it seems natural to choose the WKB approximation. However, that choice has unphysical turning-point singularities. Consequently, if $y_p(z)$ in Eq. (4) is a discontinuous function of z in a certain interval, then [6] $y_{p+1}(z)$ 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 iterates. To avoid this, we choose the Langer [7] WKB wave function $\chi_{\mathrm{L}}(x)$ as the zero iteration, which near a turning point b is given by the simple analytic expression[1]

$$\chi_{\mathrm{L}}(x) = \sqrt{\frac{S^{1/3}(x)}{|k(x)|}}\, \mathrm{Ai}[S^{1/3}(x)], \tag{6}$$

$$S(x) = \frac{3}{2}\lambda \int_b^x |k(s)|\, ds, \tag{7}$$

where Ai denotes the Airy function. It is easy to check [7] that $\chi_{\mathrm{L}}(x)$ is continuous across the turning points and coincides with the usual WKB solution far from them.

Let us consider a couple of simple examples of how to apply this first iterate to the Riccati-equation problem.

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

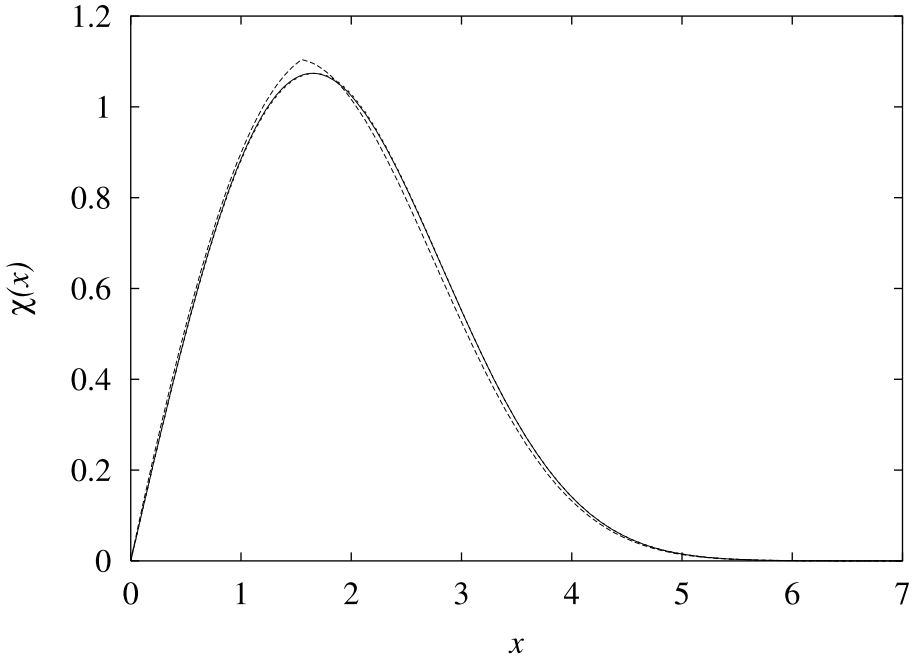

Fig. 1. Comparison of the Langer WKB solution χ_{L} (dashed curve), the exact solution χ_{exact} (dotted curve) and the first QLM iteration χ_1 (solid curve) for the ground state of the anharmonic oscillator. The last two are almost indistinguishable on the plot. Here $x = \kappa r$, $\kappa^2 = 2mE/\hbar^2$

2.1 Ground State of the Anharmonic Oscillator $V(r) = \frac{1}{2}(r^2 + r^4)$

The exact energy of this state is 2.324406352 in atomic units with mass $m = 1$. The WKB energy is different by 2.14% and equals 2.27460 in the same units, while the first-iteration QLM energy equals 2.32575 and differs from the exact energy only by 0.058%. The fifth-iteration QLM energy coincides with the exact energy in all ten digits.

The graphs corresponding to the Langer WKB solution, the exact solution, and the first QLM iteration 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 almost 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 just one QLM iteration increases the accuracy of the result by remarkably two orders of magnitude.

2.2 Second Excited State of the Linear Potential $V(r) = 2^{7/2}r$

The exact energy in this case is 9.352429642 in atomic units. The WKB energy is different by 0.49% and equals 9.39863 in the same units. The first-iteration QLM energy equals 9.3582123 and differs from the exact one only by 0.062%. The QLM

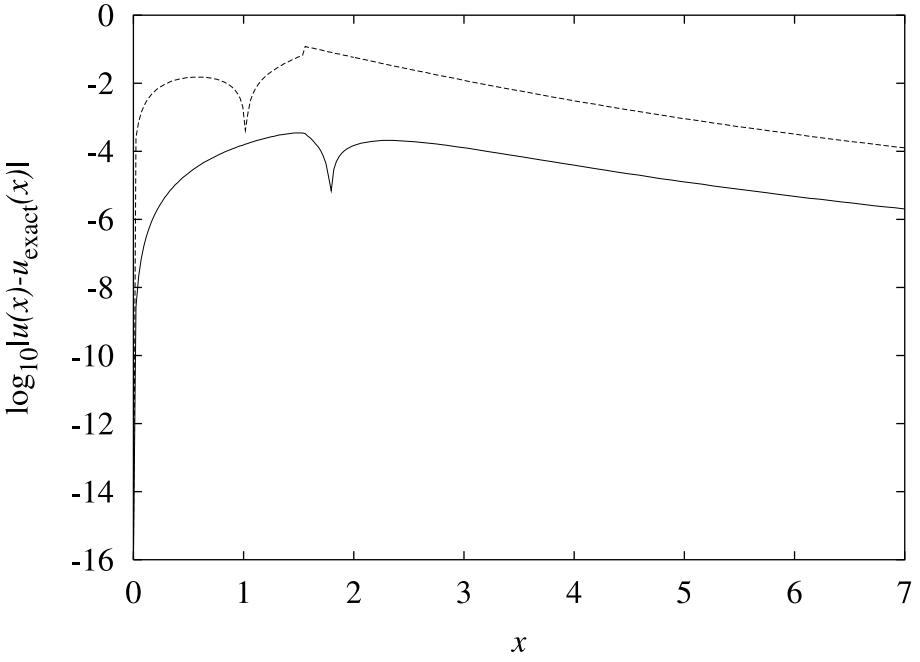

Fig. 2. Logarithm of the differences of the functions u_{exact} and u_{L} corresponding to the exact solution χ_{exact} and the WKB solution χ_{L} (dashed curve), and of u_{exact} and u_1 corresponding to the exact solution χ_{exact} and the first QLM iteration χ_1 (solid curve) for the ground state of the anharmonic oscillator. $u(x)$ is defined as $u(x) = -\arctan(\kappa\chi(r)/\chi'(r)) = -\arctan(E/y(\lambda r))$. QLM iteration is performed on the monotonic function $u(x)$, not on the singular function $y(\lambda r)$

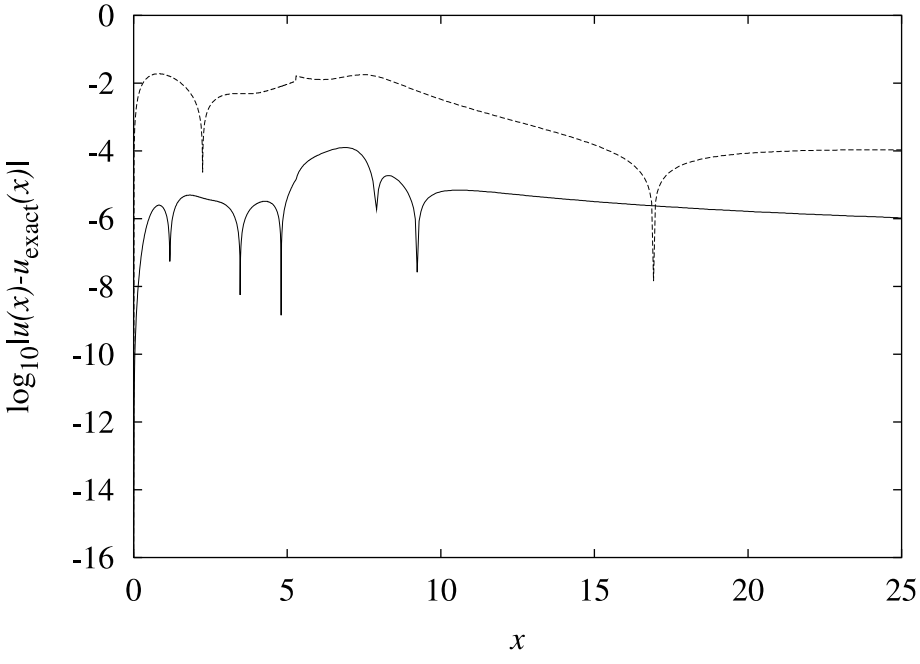

Fig. 3. As in Fig. 2, but for the second excited state of the linear potential

energy, as in the case of the anharmonic potential, coincides with the exact one after the fifth iteration in all ten digits.

The accuracy of the WKB approximation increases for higher excitations. Therefore in the case of the second excited state in the linear potential 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 two orders of magnitude smaller than the difference between the exact and WKB solutions.

3 Conclusion

The quasilinear solutions of the radial Schrödinger equation for different potentials are compared with the corresponding WKB solutions. It is shown by two typical examples that the use of the Langer WKB solution as 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. The first QLM iteration is given by an analytic expression. It allows one therefore to estimate analytically the role of different parameters and their influence on boundedness or unboundedness of a critically stable quantum system with much higher precision than provided by the WKB approximation, which often fails miserably for systems on the border of stability. In addition, it was shown that five QLM iterations are usually enough to obtain both the wave function and energy with extreme accuracy of ten significant figures.

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