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Quasilinearization approach to computations with singular potentials

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ABSTRACT

We pioneered the application of the quasilinearization method (QLM) to the numerical solution of the Schrödinger equation with singular potentials. The spiked harmonic oscillator $r^2 + \lambda r^{-\alpha}$ is chosen as the simplest example of such potential. The QLM has been suggested recently for solving the Schrödinger equation after conversion into the nonlinear 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.

We show that the energies of bound state levels in the spiked harmonic oscillator potential which are notoriously difficult to compute for small couplings λ, are easily calculated with the help of QLM for any λ and α with accuracy of twenty significant figures.

1. Introduction

Singular potentials have been and continue to be the subject of intensive theoretical study, due to the variety of their applications in different fields of physics. The most used example is the spiked harmonic oscillator potential

$$V(r) = r^2 + \frac{\lambda}{r^\alpha} \quad [\lambda > 0, \alpha \geqslant 0] \tag{1}$$

which derives its name from the graphical form which has a substantial peak near the origin due to the perturbative term $\lambda r^{-\alpha}$. This peak becomes more pronounced with increase of the coupling constant λ and especially with growth of power α which characterizes a degree of the singularity at the origin. The spiked oscillator has a practical importance since it corresponds to different interactions which occur in atomic, molecular, nuclear and particle physics. For $\alpha > 2$ it is also of relevance to the quantum field theory describing so-called supersingular interactions for which matrix elements of the perturbation in the nonperturbed harmonic oscillator quantum states diverge, so that every term in the perturbation series is infinite and the perturbation expansion does not exist [1].

Aside of the physical relevance the spiked harmonic oscillator has very interesting and nontrivial mathematical properties. Indeed, the singular term $\lambda r^{-\alpha}$ provides an infinite repulsive barrier near the origin and therefore could not be neglected even for very small λ. Because of this the singular term in potential could not be smoothly turned off with $\lambda \to 0$, the phenomenon first pointed out by Klauder [2–7]. On the other side, the harmonic oscillator r^2 term could not be neglected either, because its absence destroys the possibility of existence of the bound states. Therefore no dominance of one of those potentials could be established, which makes the construction of the perturbation theory a rather difficult proposition. This was first stressed by Detwiler and Klauder [1] who pointed out that the usual perturbation theory could not be used for $\alpha > \frac{5}{2}$. Later Aguilera-Navarro and Guardiola [8] confirmed that for $\alpha < \frac{5}{2}$ the ground state energy could be expanded in powers of λ while Harrel [9], using a specially constructed modified singular perturbation theory, was able to show that in the case of $\alpha < \frac{5}{2}$ for $\lambda \ll 1$ there exists a non-power series expansion containing, along with the powers of λ, also powers of $\ln\lambda$.

The works of Klauder and Harrel started the era of intensive study of the spiked harmonic oscillator resulting in many different approaches to the problem [10–34,36–40]. Variational computations [13,14] and strong coupling perturbation expansions [14] as well as large order perturbative expansions [17] were employed beside the different specially adjusted numerical procedures [30–34,36–40].

Recently the quasilinearization method (QLM) was suggested for solving the Schrödinger equation after conversion to the Riccati equation [41–46]. In the QLM the nonlinear differential equation is

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treated by approximating the nonlinear terms with 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. The method provides finite and reasonable results for both small and large values of the coupling constant and is able to handle even super singular potentials for which each term of the perturbation theory is infinite and the perturbation expansion does not exist [41,42].

It was shown [47] that the first QLM iteration generates closed analytic representations of the energies and the wave functions for an arbitrary potential. The subsequent iterates display very fast quadratic convergence so that the accuracy of both energies and wave functions obtained after a few iterations is extremely high, reaching up to 20 significant figures for the sixth iterate, as shown in Refs. [48,49] on the examples of different widely used physical potentials.

In view of the multitude of computations concerning different expansions or numerical solutions of the spiked oscillator problem it was very interesting and helpful to even approximately envision an analytic form of the spiked harmonic oscillator wave function. As we have mentioned above, QLM provides such a possibility. In works [50,51] the closed analytic presentations of ground and excited energies and of the corresponding wave functions in the spiked harmonic oscillator potential were obtained for different values of parameters α and λ which are accurate to about a few parts of the percent or even better in the region of variable r where wave functions are not extremely small.

The goal of this work is to calculate higher iterates in order to demonstrate that QLM is as good for singular potentials as for the smooth ones. Namely, we show in this work that the QLM computation of ground state energies for different values of α and λ of the spiked harmonic oscillator could be performed without any problems with extreme precision of twenty significant figures. Our computation includes also the region of small values of λ which are notoriously difficult to calculate due to the fact that the greatest reshaping of the potential and correspondingly of the wave functions for small couplings happens at very small values of radius near to the origin [34]. This region was not possible to compute with such an accuracy with any of the whole multitude of different numerical methods applied earlier.

2. Numerical computations

The Schrödinger equation for the spiked harmonic oscillator has the form

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

where $V(r)$ is given by Eq. (1). Throughout this paper we use the atomic unit system ($2m = e = \hbar = 1$). In the numerical approach we solve the corresponding first-order nonlinear equation

$$\frac{du(x)}{dx} = f\big(u(x), x\big), \quad u(0) = 0, \tag{3}$$

where $x = \kappa r$, $\kappa^2 = |E|$, and

$$\kappa \frac{\chi(r)}{\chi'(r)} = -\tan u(x), \tag{4}$$

where $\chi(r) = r\psi(r)$. In the differential representation of QLM, Eq. (3) results in the following iteration scheme

$$u'_{k+1}(x) = f(u_k, x) + \big(u_{k+1}(x) - u_k(x)\big) f_u(u_k, x),$$
$$u_{k+1}(0) = 0, \tag{5}$$

where $f_u(u, x) = \partial f(u, x)/\partial u$ is the functional derivative of the functional $f(u(x), x)$. For positive energies, f is given by [44]

$$f\big(u(x), x\big) = -1 + W(x)\sin^2 u(x), \tag{6}$$

where $W(x) = U(x/\kappa)\kappa^{-2}$, and $U(r) = V(r) + l(l+1)r^{-2}$.

The QLM iteration (5) is performed in several passes until desired precision is attained, as follows. First, the integration interval $[0, x_u]$ of the order of $x_u = 10$ is selected. A matching point x_m inside the classically allowed region and an approximate value of κ are fixed. A small number of integration points n on both the left-hand side and right-hand side of the matching point, of the order of $n = 100$, is specified. The QLM iteration is performed up to a selected number of iterations k_m of the order of $k_m = 5$. For each iteration the differential equation is integrated towards x_m starting at $x = 0$ and $x = x_u$. The convergence criterion is the difference between the left-hand side and right-hand side solutions $u_k(x)$ at the matching point. In the following passes we selectively increase n, x_u and k_m based on which of these parameters has affected most strongly the matching precision in the previous pass, until desired accuracy is achieved. We also repeat the entire process for at least two different values of x_m for each energy value.

Once the desired accuracy at the chosen κ is achieved, a zero search is performed within a small interval of κ, using the optimized parameters n, x_u and k_m.

Since the computation time increases between passes, the total time is a small multiple of the time required by the final pass. Finally, the zero search requires only of the order of 5 passes.

Each QLM iteration is solved in 128-bit precision arithmetic using the fourth-order Runge–Kutta method. The same points are used for all QLM iterations within the same pass, avoiding the need to interpolate the previous solution $u_k(x)$ in Eq. (5). This method is a compromise between accuracy and the number of points used. We need only to calculate one intermediate point between each pair of integration points. Tests showed that the selected nonuniform point density was more effective than low-order implicit methods.

As initial approximation we use the Langer WKB solution [48]. The calculation of this solution has been automated; it has a discontinuity but already the first QLM iteration is smooth [48]. It is clearly sufficient to calculate the Langer solution to a relatively small precision.

In order to increase the efficiency of numerical computation in what is essentially a two-scale problem, for $\alpha > 2$ we use a strongly nonuniform integration point distribution, where the point density near the origin is approximately inversely proportional to the first-order solution of Eq. (2) near the origin [50]:

$$\psi \approx \exp\big(-br^{-\beta}\big), \quad \beta = \frac{\alpha}{2} - 1, \quad b = \frac{\sqrt{\lambda}}{\beta} \tag{7}$$

and not, as one would expect, inversely proportional to, e.g., $u(x) \approx -(\kappa/\lambda)r^{\alpha/2}$. Eq. (7) is only used at those x near the origin for which the point separation is increasing; afterwards a power-law point distribution up to x_m is used. On the RHS, uniform point density is used.

Since the most difficult cases for calculations with small values of λ were reported to be grouped near the values of α around 2.5 [34] we started our computation using very a small value of $\lambda = 0.0001$ and "difficult" values of $\alpha = 2.5$, 3 and 3.5. The calculations have proceeded without any special complications. Their results with accuracy of 20 significant figures are given in Table 1 together with the results of previous, less precise calculations, made using a method of one parameter coordinate transformation suggested by Killingbeck et al. [34]

To be sure that $\lambda = 0.0001$ is not accidentally a special case of small λ and that other small values of λ can also be computed

Table 1
Ground state energies for $\lambda = 0.0001$ and different powers α. All values are guaranteed to be correct to 20 significant digits but rounded to 20 digits after decimal point

α	QLM							Killingbeck et al. [34]			
2.5	3.000	407	898	618	163	168	82	3.000	407	898	621
3.0	3.001	754	252	825	589	676	54	3.001	754	252	826
3.5	3.007	864	636	336	272	961	99	3.007	864	636	336

Table 2
As in Table 1 but for $\lambda = 0.001$

α	QLM							Buendía et al. [35]				
2.5	3.004	011	251	013	051	566	32	3.004	011	251	013	044
3.0	3.012	418	523	458	183	683	45					
3.5	3.033	848	550	516	771	486	08					

Table 3
As in Table 1, but for $\alpha = 2.5$ and different λ

λ	QLM							Buendía et al. [35]				
0.01	3.036	729	472	634	750	701	64	3.036	729	472	634	750
0.1	3.266	873	026	113	020	288	38	3.266	873	026	113	018
1	4.317	311	689	247	367	365	98	4.317	311	689	247	366
10	7.735	111	103	489	144	371	88	7.735	111	103	489	141
1000	44.955	484	788	095	629	904	00	44.955	484	788	095	62

without difficulties and with the same accuracy, we repeated our calculations using $\lambda = 0.001$ and the same values of α. The results are summed up in Table 2 together with the value obtained with the help of the analytic continuation method by Buendía et al. [35].

In order to show that QLM method could be used also for computations with larger values of λ, we give the results of calculations for $\alpha = 2.5$ and λ varied between 0.01 and 1000 in Table 3. Again, these results are compared with values obtained by the analytic continuation method by Buendía et al. [35].

3. Results and discussion

In conclusion, we pioneered here the application of the quasilinearization method (QLM) to the numerical solution of the Schrödinger equation with singular potentials. The spiked harmonic oscillator $r^2 + \lambda r^{-\alpha}$ was chosen as an example of such a potential.

We calculated, with the help of QLM, the energies of bound state levels for different values of coupling constant λ and the power α of this potential with accuracy of twenty significant figures and have shown that the energies even for very small λ values which are notoriously difficult to compute [34] are easily calculated in the quasilinearization approach.

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