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Unified QLM for regular and arbitrary singular potentials

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ABSTRACT

A parameterless numerical implementation of the Quasilinearization Method (QLM) is constructed and tested to 21–25 digits precision to give quadratically convergent energies E of the Klauder effect exhibiting spiked harmonic oscillator with the λ/r^α or $\exp(\lambda/r^\alpha)$ type spikes in a Riccati reformulation of the Schrödinger equation. The radial solution is uniformly quadratic convergent to the same precision as E, except in the small minorization interval where the self-correcting property of QLM assures geometric convergence like in the Picard algorithm to about 12–16 digits, sufficient not to affect the convergence of E, confirming what is expected on physical grounds. It was shown before that for regular potentials, immediate onset of quadratic convergence is guaranteed by the initial iteration of the WKB form, and that for quadratic convergence of E for power-type spikes it suffices to augment this by a nonlinear integration point distribution and by minorization of (negative) solution values. The form of the Riccati equation used allows the minorization function to easily be formally defined over the entire interval, without the need for a cutoff radius of application, and dependence on its scale factor is plateau-like and negligible.

1. Introduction

For decades [1] a general method of solution has been sought applicable to small and large values $\lambda,\ \alpha$ for the spiked harmonic oscillator (SHO) potential,

$$V = r^2 + \frac{\lambda}{r^\alpha}. \tag{1}$$

Potentials of this type appear in molecular, atomic, nuclear and particle physics, for example in scattering [3,4], As Klauder has shown [5–10], the effect of the spike does not vanish in the limit $\lambda \to 0$. Detwiler and Klauder [5] have also shown that its matrix elements diverge (supersingularity for $\alpha \geqslant 5/2$), and the WKB method cannot be used. Analytical and numerical approaches limited to small regions of the $\lambda,\ \alpha$ space have been used to calculate energies and wave functions of SHO starting with variational and large-coupling perturbative expansions by [1], followed by e.g. [11] and culminating with Ref. [12], which is an algebraic method for a finite sum of λ/r^α type spikes.

A purely numerical approach has rarely been pursued, e.g. in [13], and such approaches relied on the detailed form of the singular terms. However, from the viewpoint of QLM, a purely numerical approach is worth trying, as the "self-correcting' property of OLM iterations might maintain convergence near singularities. In the work [2], QLM [14] has been applied to the SHO using an "adaptive grid" and a minorization technique to regularize effects of numerical errors, resulting in E values with up to 28 digits precision for a large region of $\alpha,\ \lambda$ values. In the present work we modify, automatize algorithms

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and test the independence of our method of the form of V by applying it to a very singular infinite series version of the potential in Ref. [12], and analyze local convergence of the radial solution in comparison with earlier applications to different potentials.

2. The QLM approach

The QLM devised by Mandelzweig [15] is a generalization of an iterative method for solving nonlinear differential equations to arbitrary regular and singular potentials, able of quadratic and often monotonic convergence [16]. It is applied in quantum mechanics by rewriting the radial Schrödinger equation as a Riccati equation for a function expressed in terms of the logarithmic derivative $\phi(r)$ of the wave function. QLM is a resummation of WKB: the kth QLM iteration sums 2^k terms [17,18] of the WKB series. For exactly solvable potentials the first QLM iteration gives exact energies if a quantization condition is imposed [19]. Quadratic convergence starts once the norm of the difference of the current and previous iterations is small enough [15].

However, a practical numerical implementation of QLM requires (i) a method to control the onset of quadratic convergence, i.e., to guarantee its onset already at the first iteration, and (ii) a method to handle singular points preferably without changing the form of equations, i.e., without coordinate transformations.

Our numerical implementation for the radial Schrödinger equation [14,17,18,21], for easier handling of nodes in the radial solution $\chi(r)$, uses the (negative) form of solution:

$$u(x) = \arctan\left(-\frac{\kappa}{\phi(r)}\right) = \arctan\left(-\kappa\frac{\chi(r)}{\chi'(r)}\right), \tag{2}$$

where $x = \kappa r,\ \kappa = \sqrt{E}$ with $2m = 1$. In the resulting Riccati equation

$$u'(x) = -1 + W\sin^2 u(x) = q(x, u(x)), \quad E > 0, \tag{3}$$

$W(x) = 2mV(r)/\kappa^2$ for angular momentum $l = 0$. The QLM iteration equations in differential form [14,21] for $k = 1, 2, \ldots, M$ are

$$u_k'(x) = q(x, u_{k-1}(x)) + (u_k(x) - u_{k-1}(x))q_u(x, u_{k-1}(x)) = Q(x, u_{k-1}(x), u_k(x)), \tag{4}$$

or, in simplified notation,

$$Q(x, u_{k-1}, u_k) = -1 + W\sin^2 u_{k-1} + (u_k - u_{k-1})W\sin 2u_{k-1} \tag{5}$$

with q_u denoting the functional derivative $\partial q(x, u(x))/\partial u$.

For regular potentials, the numerical implementation has been completed in the work [18], where the Langer WKB solution [20] was found to assure immediate onset of quadratic convergence of the QLM iteration.

For power-type singular potentials (exhibiting the Klauder effect), numerical noise due to large $W(x)$ but small $u^2(x)$ in products of the type $W(x)u(x)^2$ in Eq. (5) near the singularity may preclude the onset of quadratic convergence just like a bad initial solution does, as follows. The Klauder effect amounts to the fact that $q(0, u(0)) = Q(0, u_{k-1}(0), u_k(0)) = 0$ in Eqs. (4) and (5). (For regular potentials, $q(0, u(0)) = Q(0, u_{k-1}(0), u_k(0)) = -1$.) We must ensure that numerically the terms of $Q(x, u_{k-1}, u_k)$ cancel out near the origin. The work [2] demonstrated that to guarantee immediate onset of quadratic convergence, it is sufficient to (i) construct a special "adaptive grid" point distribution not unlike the approach taken in the Finite Element Method, and (ii) simply confine (minorize) the numerical noise of $u(x) \leqslant 0$ near the origin into a finite interval provided by a small multiplier of the leading term of the solution near the origin. This works well as long as large values of $W(x)$ are representable in the computer sufficiently close to the singularities.

The goal of the present work is (a) to improve the automatic algorithm for point density (which was not entirely automatic in [2]), (b) to address the problem of computer representability of large $V(r)$ or $W(x)$ values near the singularities, and (c) to check for local deviations from quadratic convergence of $u(x)$ due to minorization and their effect on convergence of E. The aim is a unified QLM numerical implementation to give stable results for both regular and singular potentials without resorting for example to coordinate transformations which may not be suitable across the whole LHS subinterval in the matching procedure. To this end we chose the exponentially spiked harmonic oscillator potential (ESHO),

$$V = r^2 + \mu e^{\lambda r^{-\alpha}}, \tag{6}$$

which can be viewed as a series of power-law spike terms $(\lambda^k/k!)r^{-k\alpha},\ k = 1, \ldots, \infty$ like in Eq. (1), or a generalization of the finite-sum potential of Ref. [12], or representing a special case of nonlinear perturbation [22]. We expect ESHO will exceed all the difficulties of the SHO. Supersingular potentials of the form $\exp(\lambda r^{-\beta})r^{-m}$ were studied before in works on the so-called "peratization" method of regularization [4,23,24]. The potential Eq. (6) and the corresponding potential with the singularity at infinity are representatives of the class of potentials dealt with in [5].