QLM approach to possible Klauder effect in sinusoidal well [V2, 18/05/27]

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There has been some controversy in recent papers on the possible existence of the Klauder phenomenon in the square well potential with the sinusoidal bottom. We attempt a quasilinearization method (QLM) approach to this problem, in view of our past application of QLM to the calculation of supersingular potentials where the Klauder effect is clearly present.

I. INTRODUCTION

There has been controversy in recent papers [1, 2] regarding the existence of the Klauder phenomenon in the square well potential with the sinusoidal bottom. The Klauder phenomenon concerns the behavior of the solution as the coupling constant approaches zero and is well established in supersingular potentials [3–8].

One example of supersiongual potential exhibiting the Klauder phenomenon is the spiked harmonic oscillator

$$V = r^2 + \frac{\lambda}{r^\alpha} \qquad (1)$$

There is no perturbation series for this potential. Various specialized, combined analytical and numerical methods have been proposed, therefore numerical results in the literature tend to be limited to a single value of α, most commonly the critical value $\alpha = 5/2$. Aguilera et al. [9] combined difference approximation with Richardson extrapolation. The work Ref. [10] used analytic continuation, but for $\alpha > 2$, when the solution acquires an essential singularity, either the potential had to be approximated or the leading term of the solution used for some $r < R_c$. The specialized method of Ref. [11] aims to provide the solution at the origin in addition to energies, and lists converged values for $\alpha = 5/2$ and $0.001 < \lambda < 20$. The QLM (Quasilinearization Method) [12–23] has been applied, strictly numerically but with no restriction in principle on the ranges of α, λ, to the spiked oscillator problem for a few α, λ values [20], with precision exceeding that of the literature.

Quasilinearization transforms a nonlinear problem to a series of linear initial value problems, for which efficient algorithms exist. The quasilinearization iteration exhibits quadratic convergence. It is a generalization of the Bellman and Kalaba [24, 25] method developed within the theory of linear programming by as a generalization of the Newton-Raphson method [26, 27] and applied to different fields [28], but with no systematic research into convergence criteria resulting in restricted conditions of small intervals and bounded, nonsingular potentials.

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The necessary generalizations initiated in the work [12] resulted in extended proof of convergence for realistic potentials on infinite intervals and with singularities, on condition that quadratic convergence occur at some iteration. The works [17, 18] further provided the missing guarantee of occurrence of quadratic convergence, where quadratic convergence was shown to be guaranteed already at the first iteration if the Langer WKB solution was used as the initial QLM iterate. This enabled the development of an entirely numerical QLM implementation suitable for nonsingular as well as supersingular potentials [22, 23], exhibiting the Klauder phenomenon and where a perturbation series does not exist, without any variable substitution.

II. FORMULATION OF THE PROBLEM IN QLM

For a one-dimensional problem in coordinate z with potential $V(z)$ inifinite except on $[0, L]$, $L > 0$, the Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\chi''(z) + V(z)\chi(z) = E\chi(z), \ E < 0. \qquad (2)$$

In our case of a regular $V(z)$ any method will work, including the perturbation expansion or variational principle. However, we use QLM to gain additional insight.

The notation $\hbar = 1$, $\kappa^2 = 2m|E|$, $U(z) = 2mV(z)$, $x = \kappa z$ and the substitution involving the inverse logarithmic derivative of $\chi(z)$, $\phi(x) = \kappa\chi(z)/\chi'(z)$, lead to the Riccati equation

$$\phi'(x) = -1 + (1 + W(x))\phi^2(x), \qquad (3)$$

where $W(x) = U(x/\kappa)/\kappa^2$. The further substitution $\phi(x) = -\tan u(x)$ avoids poles at excited states

$$u'(x) = -1 + (2 + W(x))\sin^2 u(x). \qquad (4)$$

At $z = 0$ the solution behaves as

$$\chi(z) \underset{z\to 0}{\sim} z, \ u(x) \underset{x\to 0}{\sim} -x. \qquad (5)$$

The $(k+1)$-th QLM iteration $u_{k+1}(x)$ [12–14, 24, 25] of the solution of the first order nonlinear differential equation

$$u'(x) = f(u(x), x), \ u(0) = 0 \qquad (6)$$

is given by the linear term of the expansion in functional space

$$u'_{k+1}(x) = f(u_k, x) + (u_{k+1}(x) - u_k(x))f_u(u_k, x),$$
$$u_{k+1}(0) = 0, \qquad (7)$$

where $f_u(u, x) = \partial f(u, x)/\partial u$ is a functional derivative of $f(u(x), x)$. We solve the iteration using standard methods for ordinary differential equations (ODE). Alternatively, we could use the integral formulation

$$u_{k+1}(x) = \int_0^x ds(f(u_k(s), s) - f_u(u_k(s), s)u_k(s))$$
$$\times \exp \int_s^x dt f_u(u_k(t), t). \quad (8)$$

$u_k(x)$, $k = 0, 1, 2, ...$ converge uniformly and quadratically to $u(x)$ of Eq. (6) from the first interation provided the initial guess for the zeroth iteration is sufficiently good (in general, the Langer WKB function [18]). For strictly convex (concave) functionals $f(u(x), x)$, $u_{k+1}(x) - u_k(x)$ is strictly positive (negative), so convergence is monotonic from below (above) [12]. The QLM energy also satisfies the Rayleigh-Ritz variational principle [29], ensuring its quadratic convergence.

The method of solution is integration of Eq. (7) from both sides of the potential well with matching at $x = 0$.

The variant of the method used also avoids the interpolation of the functional values of the previous iteration [22, 23], by solving all iterations simultaneously in the form of a system of linear ODE [25]. This streamlines the numerics somewhat by relieving the self-correcting QLM algorithm of the numerical error of interpolation.

The potential is an infinite well with sinusoidal shape on $[0, L]$, for $k = 1, 2, 3, \ldots$,

$$V(z) = \lambda \cos\left(\frac{k\pi z}{L}\right) \qquad (9)$$

or

$$W(x) = \frac{\lambda}{\kappa^2} \cos\left(\frac{k\pi x}{\kappa L}\right). \qquad (10)$$

With κ approaching zero the width of the potential well in the x coordinate vanishes and the coupling diverges.

III. RESULTS

IV. DISCUSSION

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