Quasilinearization method and its verification on exactly solvable models in quantum mechanics

V. B. Mandelzweig[a)]
Physics Department, Hebrew University, Jerusalem 91904, Israel

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The proof of the convergence of the quasilinearization method of Bellman and Kalaba, whose origin lies in the theory of linear programming, is extended to large and infinite domains and to singular functionals in order to enable the application of the method to physical problems. This powerful method approximates solution of nonlinear differential equations by treating the nonlinear terms as a perturbation about the linear ones, and is not based, unlike perturbation theories, on existence of some kind of small parameter. The general properties of the method, particularly its uniform and quadratic convergence, which often also is monotonic, are analyzed and verified on exactly solvable models in quantum mechanics. Namely, application of the method to scattering length calculations in the variable phase method shows that each approximation of the method sums many orders of the perturbation theory and that the method reproduces properly the singular structure of the exact solutions. The method provides final and reasonable answers for infinite 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. [S0022-2488(99)01812-5]

I. INTRODUCTION

Most problems of physics are not solvable exactly and therefore should be tackled with the help of analytical or numerical approximation methods. In quantum mechanics and quantum field theory over the years many such methods were developed, from perturbation theories, Wentzel–Kramers–Brillouin (WKB) approach and Monte Carlo simulations to lattice computations, strong coupling approximation, 1/N expansion, and so on. The purpose of this paper is to apply to quantum mechanical problems an additional very powerful approximation technique called the quasilinearization method (QLM), whose origin lies in the theory of linear programming. The method, whose iterations are carefully constructed to yield rapid quadratic convergence and often monotonicity, was developed around 30 years ago by Bellman and Kalaba to solve a wide variety of nonlinear ordinary and partial differential equations or their systems arising in such different physics, engineering, and biology problems as orbit determination, detection of periodicities, radiative transfer, and cardiology.[1,2] The modern developments and applications of the method to different fields are given in Ref. 3. QLM, however, was never systematically studied or extensively applied in quantum physics though references to it could be found in well-known monographs[4,5] dealing with the variable phase approach to potential scattering as well as in a few scattered research papers.[6–9] This could be explained by the fact that convergence of the method has been proved only under rather restrictive conditions[1,2] which generally are not fulfilled in physical applications, such as, for example, a rather small domain of variables or forces which are finite everywhere in the domain (see the following). A goal of this work is to reformulate the proof of the convergence for more realistic physical conditions of infinite domains and forces which

[a)]Electronic-mail: victor@vms.huji.ac.il

could be singular at certain points of the domains. We also show how to deal with solutions which themselves could be infinite at certain values of variable such as, for example, scattering amplitudes at values corresponding to bound state energies, etc.

Since this is our first paper on the subject, in order to make presentation as simple and short as possible, we limit ourselves to the case of the first-order nonlinear ordinary differential equation in one variable. Physically this covers the quantum mechanics of one particle in a central field since in this case the Schrödinger equation for a wave function could be rewritten as the Ricatti equation for its logarithmic derivative.

Our proof of the convergence of the quasilinearization method for a general nonlinear ordinary or partial nth order differential equation in N-dimensional space could be formulated along the same lines and will be given in a subsequent article.

The paper is arranged as follows. In Sec. II we present the main ideas and conditions of convergence of the quasilinearization approach, formulated by Bellman and Kalaba[1,2] for the case of the first-order nonlinear ordinary differential equation in one variable, and modify their proof in order to meet the physical reality of infinite interval of the variable or the possibility of singular potentials. In order to highlight the power of the method in Sec. III we consider examples of different singular and nonsingular, attractive and repulsive potentials $V(r)$ for which the nonlinear first-order ordinary differential equation

$$\frac{da(r)}{dr} = -V(r)(r+a(r))^2, \quad a(0)=0, \tag{1.1}$$

for an S-wave scattering length $a_0 = a(\infty)$, obtained in variable phase approach,[4,5] can be solved exactly and compare the iterations obtained by the Bellman–Kalaba linearization method with exact solutions and with the usual perturbation theory. Our results, advantages of the method, and its possible future applications are discussed in Sec. IV.

II. THE QUASILINEARIZATION METHOD (QLM)

The aim of QLM is to obtain the solution $v(z)$ of a nonlinear first-order differential equation

$$\frac{dv(z)}{dz} = g(v(z),z) \tag{2.1}$$

with the boundary condition $v(a)=c$ as a limit of a sequence of linear differential equations. This goal is easily understandable in view of the fact that there is no useful technique of presenting the general solution of Eq. (2.1) in terms of a finite set of particular solutions as in a linear case where, as a result of the superposition property, the equation could be solved analytically or numerically in a convenient fashion. In addition, the sequence should be constructed in such a way as to obtain quadratic convergence and, if possible, monotonicity.

The shift of the coordinate $z = x + a$ and of the solution itself $u(x) = v(x+a) - c$ reduces Eq. (1) to the canonical form[10]

$$\frac{du(x)}{dx} = f(u(x),x), \quad u(0)=0, \tag{2.2}$$

where $f(u(x),x) \equiv g(u(x)+c, x+a)$.

The QLM prescription[1,2] determines the $n+1$ iterative approximation $u_{n+1}(x)$ to the solution of Eq. (2.2) as a solution of

$$u'_{n+1}(x) = f(u_n, x) + (u_{n+1}(x) - u_n(x)) f_u(u_n, x), \quad u_{n+1}(0)=0, \tag{2.3}$$

where the function $f_u(u,x)=\partial f(u,x)/\partial u$ is a functional derivative of a functional $f(u(x),x)$. If one defines m as an upper limit of a maximum of absolute values of the functional and its first and second functional derivatives

$$\max(|f(u(x),x)|,|f_u(u,x)|,|\tfrac{1}{2}f_{uu}(u,x)|)\leqslant m<\infty, \tag{2.4}$$

one can prove that the sequence of iterations $u_n(x)$, $n=1,2,\ldots$ converges *uniformly and quadratically* on the interval $[0,b]$ to solution $u(x)$ of Eq. (2.2) for bm sufficiently small. Indeed, introducing the metric $\|g\|$ of the function $g(x)$ as a maximum of the function on the interval $[0,b]$,

$$\|g\|=\max|g(x)|,0\leqslant x\leqslant b, \tag{2.5}$$

and introducing notations $\Delta u_{n+1}(x)=u(x)-u_n(x)$, $\delta u_{n+1}(x)=u_{n+1}(x)-u_n(x)$ one proves[1,2] the following inequalities:

$$\|\Delta u_{n+1}\|\leqslant k\|\Delta u_n\|^2, \tag{2.6}$$

$$\|\delta u_{n+1}\|\leqslant k\|\delta u_n\|^2, \tag{2.7}$$

$$k=\frac{bm}{1-bm}, \tag{2.8}$$

which establish the uniform quadratic convergence of sequence $u_n(x)$ on $[0,b]$ for sufficiently small bm. A simple induction of Eq. (2.7) shows[2] that $\delta u_{n+1}(x)$ for an arbitrary $l<n$ satisfies the inequality

$$\|\delta u_{n+1}\|\leqslant(k\|\delta u_{l+1}\|)^{2^{n-l}}/k, \tag{2.9}$$

or for $l=0$,

$$\|\delta u_{n+1}\|\leqslant(k\|\delta u_1\|)^{2^n}/k. \tag{2.10}$$

The convergence depends therefore upon the quantity $q_1=k\|u_1-u_0\|$, where zero iteration $u_0(x)$ satisfies the condition $u_0(0)=0$ and is chosen from physical and mathematical considerations. In view of Eq. (2.8) the convergence is reached if bm is sufficiently small. However, from Eq. (2.9) it follows that for the convergence it is sufficient that just one of the quantities $q_m=k\|\delta u_{m+1}\|$ will be small enough. Consequently, one can always hope[2] that even if the first convergent coefficient q_1 is large a well chosen initial approximation u_0 results in a smallness of at least one of the convergence coefficients q_m, $m>1$, which enables a rapid convergence of the iteration series for $n>m$.

One can prove in addition[1,2] that the convergence is monotonic from below (above), if functional $f(u(x),x)$ is strictly convex (concave), that is if the second functional derivative $f_{uu}(u,x)$ in interval $[0,b]$ exists and is strictly positive (negative).

The QLM treats the nonlinear terms as a perturbation about the linear ones[1,2] and is not based, unlike perturbation theories, on the existence of some kind of small parameter. In the proof of Bellman and Kalaba, a small parameter, bm, however, does appear sort of through the back door. The requirement of small bm is unfortunately too restrictive in most physical problems where m and b are often large or infinite, since x normally changes in an infinite domain and many potentials are infinite at some points in the domain. For example, in the case of the variable phase equation—Eq. (1.1), since most of the realistic forces, like Yukawa, Coulomb, van der Waals, or hard core potentials, are infinite at origin, a function

$$f(a(x),x)=-V(x)(x+a(x))^2 \tag{2.11}$$

or its first

$$f_a(a(x),x) = -2V(x)(x + a(x)) \tag{2.12}$$

or second

$$f_{aa}(a(x),x) = -2V(x) \tag{2.13}$$

functional derivatives, are infinite at the origin. This means $m = \infty$, which is a zero convergence interval. However it has been well known for a long time[4,5,11] that a first approximation of QLM gives finite and reasonable results even for super singular $1/r^n$, $n \geqslant 4$ potentials for which all the terms of the usual perturbation theory are strongly divergent. It indicates that the condition bm being small may be too restrictive and should be relaxed.

Our goal now is to modernize the proof of uniform quadratic convergence of QLM so the requirement of smallness of an interval for large m as well as the requirement of m being finite is removed. Let us subtract from both sides of Eq. (2.2) a term $h(w(x),x)u(x)$, where $w(x)$ and $h(w(x),x)$ are some arbitrary function and functional, respectively, which we chose later. We obtain

$$\frac{du(x)}{dx} - h(w(x),x)u(x) = f(u(x),x) - h(w(x),x)u(x), \quad u(0) = 0. \tag{2.14}$$

The integral form of Eq. (2.14) is

$$u(x) = \int_0^x ds(f(u(s),s) - h(w(s),s)u(s))\exp\int_s^x dth(w(t),t), \tag{2.15}$$

or, in case of nonzero boundary condition $u(0) = c$,

$$u(x) = c\exp\int_0^x dth(w(t),t) + \int_0^x ds(f(u(s),s) - h(w(s),s)u(s))\exp\int_s^x dth(w(t),t), \tag{2.16}$$

which can be checked easily by a simple differentiation.

We consider three different forms of function $w(x)$ and its functional $h(w(x),x)$:

$$h(w(x),x)) \equiv 0, \tag{2.17}$$

$$h(w(x),x) = f_w(w(x),x), \quad w(x) \equiv 0, \tag{2.18}$$

$$h(w(x),x) = f_w(w(x),x), \quad w(x) \equiv u(x). \tag{2.19}$$

We can now define the iteration scheme by setting the function $u(x)$ on the right equal to its nth approximation $u_n(x)$ and obtaining the $(n+1)$th approximation on the left-hand side. The zero approximation $u_0(x)$ is chosen from some mathematical or physical considerations and satisfies the boundary condition $u_0(0) = 0$. We get three different iteration schemes, corresponding to Eqs. (2.17)–(2.19), respectively:

$$u_{n+1}(x) = \int_0^x ds(f(u_n(s),s), \tag{2.20}$$

$$u_{n+1}(x) = \int_0^x ds(f(u_n(s),s) - f_u(0,s)u_n(s))\exp\int_s^x dtf_u(0,t), \tag{2.21}$$

and

$$u_{n+1}(x)=\int_0^x ds(f(u_n(s),s)-f_u(u_n(s),s)u_n(s))\exp\int_s^x dt f_u(u_n(t),t). \tag{2.22}$$

In case of nonzero boundary condition $u(0)=c$ the iteration sequence should be slightly modified. For example, in this case, according to Eq. (2.16), Eq. (2.22) has a somewhat different form, namely

$$u_{n+1}(x)=c\exp\int_0^x dt\, f_u(u_n(t),t)+\int_0^x ds(f(u_n(s),s)-f_u(u_n(s),s)u_n(s))\exp\int_s^x dt\, f_u(u_n(t),t). \tag{2.23}$$

Let us concentrate in the beginning on Eq. (2.22), which, being the solution of Eq. (2.3), displays the iteration sequence of the QLM. The subtraction of Eq. (2.3) for n and $n-1$ gives a similar differential equation for the difference $\delta u_{n+1}(x)=u_{n+1}(x)-u_n(x)$:

$$\delta u'_{n+1}(x)=f(u_n(x),x)-f(u_{n-1}(x),x)+\delta u_{n+1}(x)f_u(u_n(x),x)-\delta u_n(x)f_u(u_{n-1}(x),x),$$

$$\delta u_{n+1}(0)=0. \tag{2.24}$$

By use of the mean value theorem[12] one can write

$$f(u_n(x),x)=f(u_{n-1}(x),x)+\delta u_n(x)f_u(u_{n-1}(x),x)+\tfrac{1}{2}f_{uu}(\overline{u_n}(x),x)\,\delta u_n^2(x), \tag{2.25}$$

where $\overline{u_n}(x)$ lies between $u_n(x)$ and $u_{n-1}(x)$. As a result Eq. (2.24) could be written as

$$\delta u'_{n+1}(x)-\delta u_{n+1}(x)f_u(u_n(x),x)=\tfrac{1}{2}f_{uu}(\overline{u_n}(x))\,\delta u_n^2(x), \tag{2.26}$$

whose solution has a form

$$\delta u_{n+1}(x)=\frac{1}{2}\int_0^x ds\, f_{uu}(\overline{u_n}(s),s)\,\delta u_n^2(s)\exp\int_s^x dt\, f_u(u_n(t),t). \tag{2.27}$$

Obviously,

$$|\delta u_{n+1}(x)|\leqslant\frac{1}{2}\int_0^x ds|f_{uu}(\overline{u_n}(s),s)||\delta u_n(s)|^2\exp\int_s^x dt\, f_u(u_n(t),t)$$

$$\leqslant k_n(x)\cdot|\delta u_n(\bar{x})|^2\leqslant k_n(b)\cdot\|\delta u_n\|^2. \tag{2.28}$$

Here $\bar{x}$ is the point on the interval $[0,x]$ where $|\delta u_n(x)|$ is maximal,

$$k_n(x)=\frac{1}{2}\int_0^x ds|f_{uu}(\overline{u_n}(s),s)|\exp\int_s^x dt\, f_u(u_n(t),t), \tag{2.29}$$

and positiveness of the integrand in Eq. (2.29) as well as definition (2.5) are used. Since Eq. (2.28) is correct for any x in the interval $[0,b]$, it is correct also for a value of $x\in[0,b]$ for which $|\delta u_{n+1}(x)|$ reaches its maximal value. This gives

$$\|\delta u_{n+1}\|\leqslant k_n(b)\cdot\|\delta u_n\|^2. \tag{2.30}$$

Let us assume the boundness of the first two functional derivatives of $f(u(x),x))$, that is the existence of bounding functions $F(x)$ and $G(x)$ which for any u and x satisfy

$$f_u(u(x),x))\leqslant F(x), \quad |f_{uu}(u(x),x)|\leqslant G(x). \tag{2.31}$$

In this case $k_n(b) \leqslant k(b)$, where

$$k(b) = \frac{1}{2} \int_0^b ds\, G(s) \exp \int_s^b dt\, F(t), \tag{2.32}$$

and Eq. (2.30) could be written in the form

$$\| \delta u_{n+1} \| \leqslant k(b) \cdot \| \delta u_n \|^2, \tag{2.33}$$

which is identical to Eq. (2.7) but with $k = k(b)$ instead of k given by Eq. (2.8). We can reproduce the results of Bellman and Kalaba[1,2] by following their bounding restriction Eq. (2.4) and setting $F(x) = m$, $G(x) = 2m$. In this case the integrals in Eq. (2.32) could be easily calculated and give $k(b) = (1 - e^{-mb})/e^{-mb}$, which for small mb reduces to the expression for k given by Eq. (2.8). However, as we will see in different examples in Sec. III, $k(b)$ given by Eq. (2.32), unlike k given by Eq. (2.8), could be sufficiently small also for an infinite interval length b and for singular functions $G(x)$ and $F(x)$. This means that the quantity $q_1(b)$,

$$q_1(b) = k(b) \| u_1 - u_0 \|, \tag{2.34}$$

which is responsible for the convergence [see the discussion after Eq. (2.10)] could be less than unity and thus assure the convergence even in this case. As was pointed out there, the rapid convergence is actually enough that an initial guess for zero iteration is sufficiently good to ensure the smallness of just one of the convergence coefficients $q_m(b) = k(b) \| u_{m+1} - u_m \|$.

With the uniform quadratic convergence of the sequence $u_n(x)$ for the intervals $[0,b]$ in which at least one of the convergence coefficients $q_m(b) < 1$ now proven, one can conclude from Eq. (2.27), that in addition for strictly convex (concave) functionals $f(u(x),x)$ the difference $u_{n+1}(x) - u_n(x)$ is strictly positive (negative), which establishes the monotonicity of the convergence from below (above), respectively, on this interval.

If $F(x)$ is a sign-definite function and $G(x) = |F(x)|$, the integral in Eq. (2.32) could be taken explicitly and produces a simple expression for $k(b)$,

$$k(b) = \frac{1}{2} \left| \exp \int_0^b dt\, F(t) - 1 \right|. \tag{2.35}$$

The subtraction of Eq. (2.3) from Eq. (2.2) gives

$$\Delta u'_{n+1}(x) = f(u,x) - f(u_n(x),x) + \Delta u_{n+1}(x) f_u(u_n(x),x) - \Delta u_n(x) f_u(u_n(x),x),$$
$$\Delta u_{n+1}(0) = 0, \tag{2.36}$$

which is similar to Eq. (2.24)—the starting point for our derivation of Eq. (2.33). The derivation along the same lines, starting from Eq. (2.36), gives the analog of Eq. (2.6) with k changed to $k(b)$:

$$\| \Delta u_{n+1} \| \leqslant k(b) \cdot \| \Delta u_n \|^2. \tag{2.37}$$

Equation (2.31) again confirms the uniform quadratic convergence of the sequence u_n to a solution $u(x)$ of Eq. (2.2). One can show in exactly the same fashion as before that for strictly convex (concave) functionals $f(u(x),x)$ difference Δu_{n+1} is strictly positive (negative), proving in this case the monotonic convergence to a limiting function u from below (above), respectively.

In case the solution $u(x)$ and, respectively, its iterations $u_n(x)$ are going to infinity at some points on interval $[0,b]$, Eq. (2.22) could become meaningless. To deal with it, it is necessary to regularize Eq. (2.2), that is reformulate it in terms of a new function $v(x)$ which is finite, as, for example, to change to function $v(x)=1/u(x)$ for $|u(x)|>1$, the prescription which is used in the present work, or to set $u(x)=\tan v(x)$ as it was suggested in Refs. 13 and 14. The corresponding nonlinear equations for $v(x)$ have the form

$$\frac{dv(x)}{dx}=-v(x)^2 f\left(\frac{1}{v(x)},x\right), \quad v(0)=u(c), \quad |u(c)|=1, \tag{2.38}$$

and

$$\frac{dv(x)}{dx}=\cos^2 v(x) f(\tan v(x),x), \quad v(0)=0, \tag{2.39}$$

respectively.

Let us now turn our attention to the iteration sequences given by Eqs. (2.20) and (2.21). These successive approximation schemes were considered by Picard[15] and Calogero, Babikov, and Fluegge (CBF),[4,5,11] respectively. The quadratic convergence, reached in QLM, is based on a specific choice of function $w(x)$ and its functional $h(w(x),x)$ given by Eq. (2.19) which, in view of the mean value theorem of Eq. (2.25), assures cancellation of the first power of $\delta u_n(x)$ and $\Delta u_n(x)$ in recurrence relations of Eqs. (2.24) and (2.36), respectively. Such cancellation will not happen for the Picard and CBF choices of $w(x)$ and $h(w(x),x)$, given by Eqs. (2.17) and (2.18). One obtains, therefore, for these approximation schemes the usual inequality characteristic of the first-order convergence

$$\|\delta u_{n+1}\|<p\|\delta u_n\|, \tag{2.40}$$

where p is a correspondent convergence coefficient. This leads, instead of the very rapid 2^n-power type of convergence, displayed in Eqs. (2.33) and (2.37), to the much slower geometric convergence

$$\|\delta u_{n+1}\|<p^n\|\delta u_1\|. \tag{2.41}$$

III. QLM SCATTERING LENGTH CALCULATIONS AND THEIR COMPARISON WITH THE PERTURBATION THEORY AND EXACT SOLUTIONS

In Sec. II we proved that the QLM successive approximations to the exact solution $u(x)$ of Eq. (2.22) given by Eq. (2.2) converge quadratically and uniformly on interval $[0,b]$, where b is found from the requirement that one of the convergent coefficients $q_m(b)$ defined in a paragraph following Eq. (2.34) is less than unity. In addition for strictly convex (concave) functionals $f(u(x),x)$ the convergence to a limiting function u is monotonic from below (above), respectively.

In order to highlight the power of the method in this section we consider examples of different singular and nonsingular, attractive and repulsive potentials for which the nonlinear first-order ordinary differential equation for an S-wave scattering length, Eq. (1.1), obtained in variable phase approach[4,5] could be solved exactly. We will compare the iterations obtained by the Bellman–Kalaba quasilinearization method (QLM) with exact solutions and with the usual perturbation theory.

A. Square well potential

1. Repulsive square well

Let us start from the repulsive square well potential

$$V(r)=\frac{\lambda}{R^2}\Theta(R-r), \tag{3.1}$$

where $\Theta(R-r)$ is the Heavyside function and λ is a potential strength, which for now is assumed to be positive. The change of variables to the dimensionless variable $x=\sqrt{\lambda}(r/R)$ and dimensionless function $A(x)=\sqrt{\lambda}[a(xR/\sqrt{\lambda})]/R$ allows one to express Eq. (1.1) for $x\leqslant x_0$, $x_0=\sqrt{\lambda}$ in a form

$$\frac{dA(x)}{dx}=-(x+A(x))^2, \quad A(0)=0. \tag{3.2}$$

For $x>x_0$ $A(x)$ is a constant equal to the dimensionless scattering length $A_0=\sqrt{\lambda}(a_0/R)$, the scattering length itself being $a_0\equiv a(R)$. A further change of the function to $u(x)=x+A(x)$ gives a familiar equation for the hyperbolic tangent,

$$\frac{du(x)}{dx}=1-u^2(x), \quad u(0)=0. \tag{3.3}$$

The exact variable scattering length $a(r)$ for the repulsive square well potential is therefore

$$a(r)=\frac{R}{\sqrt{\lambda}}\tanh\left(\sqrt{\lambda}\frac{r}{R}\right)-r, \tag{3.4}$$

while the scattering length is given by

$$a_0=R\left(\frac{\tanh\sqrt{\lambda}}{\sqrt{\lambda}}-1\right)\equiv R\left(\frac{\tanh x_0}{x_0}-1\right). \tag{3.5}$$

Here we use the Calogero definition of the scattering length[4]

$$a_0=\lim_{k\to 0}\frac{\tan\delta(k)}{k}, \tag{3.6}$$

δ is a scattering phase, which is different in sign from the definition used in most publications.

Before considering the QLM, let us turn to the usual perturbation theory. Displaying explicitly the dependence of the potential on the coupling constant $V(r)=\lambda v(r)$ and expanding $a(r)$ in powers of λ, one obtains from Eq. (1.1):

$$\sum_{k=1}^{\infty}\lambda^k a_k'(r)=-\lambda v(r)\left(r+\sum_{n=1}^{\infty}\lambda^n a_n(r)\right)^2. \tag{3.7}$$

Comparisons of coefficients before the powers of λ gives the recurrence relation

$$a_k'(r)=-v(r)\left(r^2\delta_{k1}+2ra_{k-1}(r)+\sum_{n=1}^{k-2}a_{k-n-1}(r)\cdot a_n(r)\right), \quad k=1,2,3\ldots \tag{3.8}$$

The successive integrations of Eq. (3.8) produce the expansion $a(r)$ in the powers of the coupling constant. The first three terms of the perturbation expansion of the variable scattering length, for example, are

$$a_1(r)=-\int_0^r ds\, s^2 v(s),$$

$$a_2(r)=-\int_0^r ds\, 2sv(s)a_1(s), \tag{3.9}$$

$$a_3(r) = -\int_0^r ds\, v(s)(2sa_2(s) + a_1^2(s)),$$

and so on. For $u(x)$ this expansion gives

$$u(x) = x - \frac{1}{3}x^3 + \frac{2}{15}x^5 - \frac{17}{315}x^7 + \frac{62}{2835}x^9 - \frac{1382}{155\,925}x^{11} + \frac{21\,844}{6\,081\,075}x^{13} - \frac{929\,569}{638\,512\,875}x^{15} + \frac{6\,404\,582}{10\,854\,718\,875}x^{17} + O(x^{19}). \tag{3.10}$$

These series, of course, could also be obtained by using the power series expansion of tanh(x). The power expansion of scattering length is given by Eqs. (3.10) and (3.5), the latter can be written in the form $a_0 = R([u(x_0)/x_0] - 1)$.

Let us consider now the approximate QLM solutions of Eq. (3.3), choosing as a zero approximation a solution of this equation for a very small x: $u_0(x) = x$. The recurrence relation (2.22) now has the form

$$u_{n+1}(x) = \int_0^x ds(1 + u_n^2(s))\exp\left(-2\int_s^x dt\, u_n(t)\right), \tag{3.11}$$

while the nth approximation to the scattering length is given by

$$a_{0,n} = R\left(\frac{u_n(x_0)}{x_0} - 1\right). \tag{3.12}$$

The substitution of the zero iteration in Eq. (3.11) leads to a first-order approximation,

$$u_1(x) = -i\frac{\sqrt{\pi}}{4}\mathrm{erf}(ix)e^{-x^2} + \frac{x}{2}, \tag{3.13}$$

where erf(x) is the error function.[16] Expansion of (3.13) in power series enables a comparison with perturbation series (3.10),

$$u_1(x) = x - \frac{1}{3}x^3 + \frac{2}{15}x^5 - \frac{4}{105}x^7 + \frac{8}{945}x^9 + O(x^{11}), \tag{3.14}$$

which shows that the first approximation reproduces exactly three terms of the perturbation series, that is two more terms than was given correctly by the zero QLM approximation $u_0(x) = x$. This improvement of the representation of the perturbation series not by one, but by two powers of λ is, of course, precisely what one should expect from the quadratic convergence. In addition, the fourth term is also mostly correct being $-\frac{12}{315}$ vis-a-vis exact $-\frac{17}{315}$. The second iteration $u_2(x)$ could not be calculated analytically, but could be computed numerically or expressed by power series expansion with the help of symbolic computation program.[17] The latter gives

$$u_2(x) = x - \frac{1}{3}x^3 + \frac{2}{15}x^5 - \frac{17}{315}x^7 + \frac{62}{2835}x^9 - \frac{1382}{155\,925}x^{11} + \frac{21\,844}{6\,081\,075}x^{13} - \frac{918\,844}{638\,512\,875}x^{15} + \frac{39\,944}{70\,945\,875}x^{17} + O(x^{19}). \tag{3.15}$$

One can see that the second iteration of QLM reproduces correctly the first seven terms of the perturbation series, an improvement by 4 powers of λ compare with previous QLM approximation

$u_1(x)$. In addition, the eighth and ninth terms of the power series expansion of $u_2(x)$ are very close to their precise values in perturbation theory, being $-\frac{918\,844}{638\,512\,875}$ and, 5.63×10^{-4} vis-a-vis exact values $-\frac{929\,569}{638\,512\,875}$ and 5.90×10^{-4}, respectively.

Aside from the fact that already first QLM approximations sum many orders of the usual perturbation theory, the QLM iterations, unlike the perturbation series, have meaning also for a large or even infinite values of coupling constant. Indeed, for $\lambda\to\infty$ any term of the perturbation series is infinite. Even for a finite moderately large potential strength $\lambda\geqslant 2.5$ perturbation expansion (3.10) diverges since the power series expansion of the hyperbolic tangent of x_0 converges[16] only for $x_0<\pi/2$, that is for $\lambda<\pi^2/4$. On the other side, the QLM approximations to the scattering length are finite. The first QLM approximation to scattering length (3.13) in view of an asymptotic expression

$$\mathrm{erf}(z)\simeq\left(1-\frac{e^{-z^2}}{\sqrt{\pi}z}\right) \tag{3.16}$$

for $|z|\to\infty$[16] shows that the scattering length in this approximation equals $-R/2$, a reasonable approximation to exact value $a_0=-R$. The computation of the scattering length in the second QLM approximation gives again a finite and improved result $a_0=-\frac{3}{4}R$.

To tackle more rigorously the question of convergence of the iteration series for dimensionless scattering length $A_{0,n}=a_{0,n}/R$ given by Eqs. (3.11) and (3.12) to exact result $A_0=a_0/R$ let us turn to the convergence condition demanding the smallness of convergence coefficient (2.34), which in this case is given by

$$q_1(b)=k(b)\|a_{0,1}-a_{0,0}\|=k(b)\left\|\frac{u_1(x)-u_0(x)}{x}\right\|=k(b)\cdot\max_{0\leqslant x\leqslant b}\left|\frac{u_1(x)}{x}-1\right|. \tag{3.17}$$

To calculate $q_1(b)$ one first has to estimate $k(b)$ using, for example, Eq. (2.35). From Eq. (3.3) and the boundary condition there follows $u(-x)=-u(x)$. We can consider therefore only positive branch of the solution whose extremum is reached when $u'(x)=1-u^2(x)=0$, that is when $u(x)=1$. This means that $0\leqslant u(x)\leqslant 1$. Since the first and second functional derivatives of $f(u(x),x)=1-u^2(x)$ equal $-2u(x)$ and -2, respectively, one can set $F(x)=-2$ and $G(x)=|F(x)|=2$, which gives

$$k(b)=\tfrac{1}{2}|e^{-2b}-1|\leqslant\tfrac{1}{2}. \tag{3.18}$$

In view of the fact that, due to the properties[16] of the error function $|u_1(x)/x-1|\leqslant\frac{1}{2}$ for all positive x, one obtains that $q_1(b)\leqslant\frac{1}{4}$ for all values of b. Thus the convergence of QLM approximations Eq. (3.11), and therefore $a_{0,n}$, given by Eq. (3.12), to the exact scattering length a_0 in case of the repulsive square well is uniform and quadratic for all values of x_0, that is for all values of coupling constant λ.

2. Attractive square well

The same conclusions are correct also for the attractive square well potential the equations for which are obtained by changing λ to $-\lambda$. The equation for $u(x)$ now has a form

$$\frac{du(x)}{dx}=1+u^2(x),\quad u(0)=0. \tag{3.19}$$

Its solution is

$$u(x)=\tan x \tag{3.20}$$

and the scattering length is given by

$$a_0 = R\left(\frac{\tan\sqrt{\lambda}}{\sqrt{\lambda}} - 1\right) \equiv R\left(\frac{u(x_0)}{x_0} - 1\right). \tag{3.21}$$

The QLM subsequent approximations are obtained with the help of recursion equations

$$u_{n+1}(x) = \int_0^x ds(1-u_n^2(s))\exp\left(2\int_s^x dt\, u_n(t)\right). \tag{3.22}$$

Choosing the zero QLM approximation as before in form $u_0(x)=x$ leads to first QLM approximation,

$$u_1(x) = \frac{\sqrt{\pi}}{4}\operatorname{erf}(x)e^{x^2} + \frac{x}{2}. \tag{3.23}$$

Now there is, however, an additional difficulty, since exact scattering length $a_0(x_0)$ is a singular function of $x_0 = \sqrt{\lambda}$ and becomes infinite at values of the coupling constant corresponding to zero bound state energies $\lambda = ((2n+1)\ \pi/2)^2$. This finds reflection in the fact that $u_1(x_0)$ is increasing very fast for x_0 around $\pi/2$. To deal with it let us, in accordance with the discussion in Sec. II, regularize Eq. (3.19), that is to rewrite it for $|u(x)|>1$ in terms of a new function

$$v(x) = \frac{1}{u(x)}. \tag{3.24}$$

Defining c as a singular point where $u(c)=\infty$ one obtains, according to Eq. (2.38), the following nonlinear equation for $v(x)$:

$$\frac{dv(x)}{dx} = -(1+v(x)^2), \quad v(c) = \frac{1}{u(c)} = 0. \tag{3.25}$$

In view of Eq. (3.19) a solution of Eq. (3.25) is $v(x)=u(c-x)$. Equation (3.24) then gives

$$u(x) = \frac{1}{u(c-x)}. \tag{3.26}$$

Setting $x = c/2$ allows us to write

$$u^2\left(\frac{c}{2}\right) = 1 \tag{3.27}$$

for constant c. Since the solution of Eq. (3.19) should be an odd function of x,

$$u(-x) = -u(x), \tag{3.28}$$

it is enough to choose only a positive branch of Eq. (3.27), that is

$$u\left(\frac{c}{2}\right) = 1. \tag{3.29}$$

From Eqs. (3.26) and (3.28) follows the $2c$ periodicity of solution $u(x)$: $u(x+2c) = 1/u(c-(x+2c)) = -1/u(x+c) = -u(c-(c+x)) = u(x)$. Thus it is enough to find a solution only on the interval $(0,2c)$. We can now formulate the following result.

The nth QLM approximation $U_n(x)$ to the solution of Eq. (3.19) on the interval $[0,2c_n]$, which is able to properly describe a singularity, is given by

$$U_n(x)=u_n(x)\Theta\left(\frac{c_n}{2}-x\right)\Theta(x)+\frac{1}{u_n(c_n-x)}\Theta\left(x-\frac{c_n}{2}\right)\Theta\left(\frac{3c_n}{2}-x\right)$$
$$+u_n(x-2c_n)\Theta\left(x-\frac{3c_n}{2}\right)\Theta(2c_n-x), \tag{3.30}$$

where the nth QLM approximation $u_n(x)$ on interval $(0,c_n/2)$ is found with the help of recurrence relations Eq. (3.22) and the nth approximate value c_n of c is given by

$$u_n\left(\frac{c_n}{2}\right)=1. \tag{3.31}$$

Computation of $c_n/2$ shows that the differences between the exact value $c=\pi/2$ and approximate values c_n are very small already for the first and second QLM iterations, namely $(c_1-\pi/2)$ and $(c_2-\pi/2)$ are 0.005 29 and 0.000 001 32, the errors of 0.5% and 10^{-4}%, respectively. Since the nth QLM approximation, Eq. (3.30), has a pole at $x_0=c_n$, $\lambda=c_n^2$ gives a value of potential strength corresponding to a zero energy bound state. One sees that the QLM description of such state is extremely accurate already in the first and especially in the second approximations.

To prove the uniform quadratic convergence of the QLM iterations it is enough, in view of Eqs. (3.28) and (3.30) to consider $u_n(x)$ only on intervals $(0,c_n/2)$ which are very close to interval $(0,\pi/4)$. Since the first and second functional derivatives of the left-hand side of Eq. (3.19) are $2u(x)$ and 2, respectively, and $|u(x)|\leqslant 1$, one can chose $F(x)=G(x)=2$ and use Eq. (2.35), which produces a simple expression for $k(b)$,

$$k(b)=\tfrac{1}{2}(e^{2b}-1). \tag{3.32}$$

This leads to the following result for $q_1(b)$:

$$q_1(b)=\frac{1}{2}(e^{2b}-1)\left(\frac{\sqrt{\pi}}{4}\operatorname{erf}(b)e^{b^2}-\frac{b}{2}\right). \tag{3.33}$$

A simple computation shows that $0<q_1(b)<1$ for $0<b<0.92$, which proves the uniform quadratic convergence of the QLM iterations on even larger interval (0,0.92) than interval $(0,\pi/4)$ and thus the convergence of the sequence $U_n(x_0)$ to the exact solution $\tan x_0$ on the interval $(0,2c_n)$ $\approx(0,\pi)$. In view of its $2c_n\approx\pi$ periodicity the nth QLM approximation $U_n(x_0)$ converges therefore to the exact solution for all x_0, that is for all values of the coupling constant λ.

The extremely fast convergence of QLM approximations given by Eq. (3.30) is evident from the ratios of the first [Eq. (3.23)] and second [Eq. (3.22) for n=1] QLM iterations to the exact solution (3.20), which are shown in Figs. 1 and 2, respectively.

B. δ-function potential

In case of the δ-function potential

$$V(r)=\frac{\lambda}{R}\delta(r-R), \tag{3.34}$$

Eq. (1.1) for the scattering length has the form

$$A'(x)=\lambda(x-A(x))^2\delta(x-1)\equiv\lambda(1-A(x))^2\delta(x-1),\quad A(0)=0, \tag{3.35}$$

where $x=r/R$ and $A(x)=-a(r)/R$ are dimensionless variable and variable scattering length, respectively; note, that in Eq. (3.35) $A(x)$ could not be set equal $A(1)$, since $A(x)$ is discontinu-

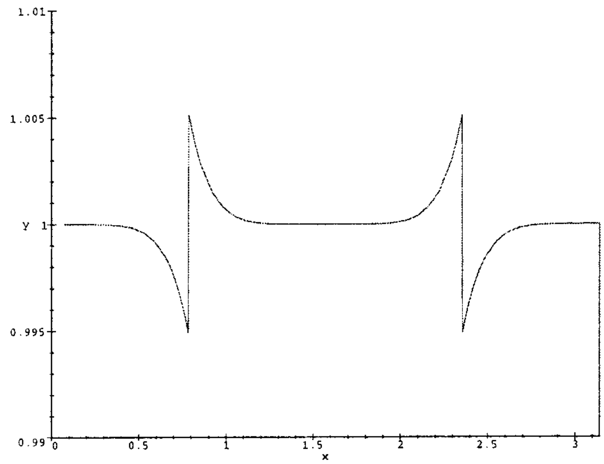

FIG. 1. The ratio of the first QLM iteration to the exact solution for the attractive square well as a function of the potential strength λ (axis x).

ous at $x=1$, its derivative being proportional to the δ-function. Introduction of a new function $y(x)=\lambda\Theta(x-1)$, $y(0)=0$, $y(\infty)=\lambda$ with a derivative $dy(x)=\lambda\,\delta(x-1)dx$ reduces Eq. (3.35) to the form

$$\frac{dA(y)}{dy}=(1-A(y))^2, \quad A(y)_{y=0}=0. \tag{3.36}$$

A solution of Eq. (3.36) is

$$A(y)=\frac{y}{1+y}. \tag{3.37}$$

An exact solution of Eq. (1.1) for the δ-potential thus is given by $a(r)=-RA(y)\equiv-R[\lambda\Theta(r-R)]/[1+\lambda\Theta(r-R)]$. The scattering length a_0 equals $a(r)_{r=\infty}\equiv-R\lambda/(1+\lambda)$. It is is singular at $\lambda=-1$, reflecting the existence of the zero energy bound state for the unit potential strength.

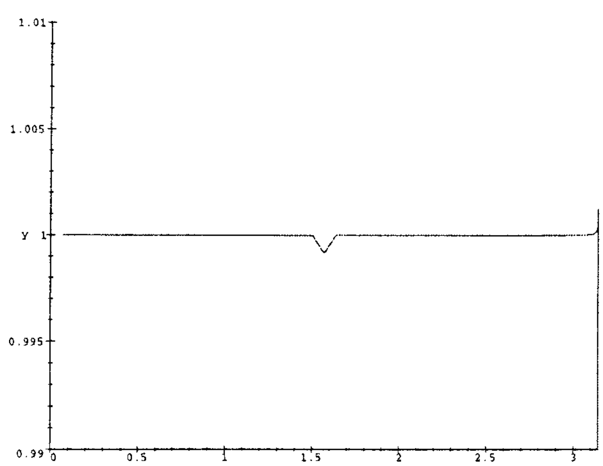

FIG. 2. Same as in Fig. 1, but for the second QLM approximation.

1. Repulsive δ-function potential

Let us now consider QLM approximations to the exact solution (3.37) in the case of the repulsive δ-function potential, $\lambda > 0$. According to Eq. (2.22) they are given by the following iteration sequence:

$$A_{n+1}(y)=\int_0^y ds(1-A_n^2(s))\exp\left(-2\int_s^y dt(1-A_n(t))\right), \tag{3.38}$$

since the functional derivative of the right-hand part of Eq. (3.36) equals $-2(1-A(y))$. The introduction of the nth approximation $u_n(y)=1-A_n(y)$ to a function $u(y)=1-A(y)=1/(1+y)$ helps to write recurrence relationship (3.38) in a simpler form:

$$u_{n+1}(y)=\exp\left(-2\int_0^y dt\, u_n(t)\right)+\int_0^y ds\, u_n^2(s))\exp\left(-2\int_s^y dt\, u_n(t)\right), \tag{3.39}$$

which coincides with the QLM iteration scheme (2.23) for Eq. (3.36), rewritten with the help of the function $u(x)=1-A(x)$ as

$$u'(x)=-u(x)^2, \quad u(0)=1, \tag{3.40}$$

Since for $x=\infty$ $y=\lambda$, $u_n(\lambda)$ gives the nth approximation to $u(\lambda)=1-A_0(\lambda)=1/(1+\lambda)$ where $A_0(\lambda)$ is the exact dimensionless scattering length.

Let us chose as a zero approximation $u_0(y)\equiv u(0)=1$. The substitution in Eq. (3.39) for $n=0$ gives

$$u_1(y)=\tfrac{1}{2}(1+e^{-2y}). \tag{3.41}$$

One can see that already the first approximation $u_1(\lambda)$ for $\lambda\to\infty$ is finite and equals $\frac{1}{2}$, which gives a value of $\frac{1}{2}$ for the approximate dimensionless scattering length vis-a-vis the exact value $A_0=1$. Each term in the perturbation series for $u(\lambda)$,

$$u(\lambda)=\sum_{m=0}^{\infty}(-\lambda)^m, \tag{3.42}$$

in this case is infinite while the perturbation expansion itself is divergent already for $|\lambda|\geqslant 1$. The comparison of perturbation expansion (3.42) with the perturbative expansion of the first QLM approximation (3.41),

$$u_1(\lambda)=\tfrac{1}{2}(1+e^{-2\lambda})=1-\lambda+\lambda^2-\tfrac{2}{3}\lambda^3+\tfrac{1}{3}\lambda^4-\tfrac{2}{15}\lambda^5+O(\lambda^6), \tag{3.43}$$

shows that in this approximation the perturbation series is correct up to the fourth term. The next, second approximation also could be calculated analytically with the help of symbolic computation program[17] and gives the rather cumbersome expression

$$u_2(\lambda)=-1/4\,\frac{-2\sqrt{e^{e^{-2\lambda}}}-e^{1/2-\lambda}+\sqrt{2\pi}\,\mathrm{erf}\left(\dfrac{e^{-\lambda}}{\sqrt{2}}\right)\sqrt{e^{e^{-2\lambda}}}e^{1/2}-e^{1/2+\lambda}-\sqrt{2\pi}\,\mathrm{erf}\left(\dfrac{1}{\sqrt{2}}\right)e^{1/2}\sqrt{e^{e^{-2\lambda}}}}{\sqrt{e^{e^{-2\lambda}}}e^{1/2(-e^{-2\lambda}+2\lambda+1)}}. \tag{3.44}$$

For $\lambda\rightarrow\infty$ the largest term both in the numerator and denominator is $e^{1/2+\lambda}$. Therefore $u_2(\infty)=\frac{1}{4}$, which corresponds to the second QLM approximation to A_0 being $\frac{3}{4}$, a significant improvement compared with the result, obtained in this limit in the first QLM approximation (3.41). The computation of the power series expansion yields

$$u_2(\lambda)=1-\lambda+\lambda^2-\lambda^3+\lambda^4-\lambda^5+\lambda^6-\frac{62}{63}\lambda^7+\frac{79}{84}\lambda^8-\frac{4931}{5670}\lambda^9+O(\lambda^{10}). \tag{3.45}$$

The perturbation series in the second QLM approximation is given correctly up to the seventh term, while the coefficients of the eighth and ninth terms are different only by $\frac{1}{63}$ and $\frac{5}{84}$, that is by 1.6% and 6%, respectively.

Analytic calculation of the third QLM approximation seems impossible but the power series expansion could be evaluated with the help of the same program,[17] which yields

$$\begin{aligned}u_3(\lambda)=&1-\lambda+\lambda^2-\lambda^3+\lambda^4-\lambda^5+\lambda^6-\lambda^7+\lambda^8-\lambda^9+\lambda^{10}-\lambda^{11}+\lambda^{12}-\lambda^{13}+\lambda^{14}\\&-\frac{59\,534}{59\,535}\lambda^{15}+\frac{1\,904\,891}{1\,905\,120}\lambda^{16}-\frac{12\,139\,457}{12\,145\,140}\lambda^{17}\\&+\frac{161\,721\,779}{161\,935\,200}\lambda^{18}-\frac{113\,880\,892\,943}{114\,225\,041\,700}\lambda^{19}+O(\lambda^{20}).\end{aligned} \tag{3.46}$$

In the third QLM approximation the first 15 terms of the perturbation series are given exactly while the next 5 terms have coefficients extremely close to being exact.

Summing up, the number of the terms given precisely in the zero, first, second, and third QLM approximations equals 1, 3, 7, and 15, increasing by 2, 2^2 and 2^3, respectively, that is according to geometric progression with $q=2$, exactly as one should expect from the quadratic law of the convergence. The number N_n of perturbation series terms reproduced exactly in the nth QLM approximation is therefore

$$N_n=\sum_{k=0}^{n} q^k=\frac{q^{n+1}-1}{q-1}=2^{n+1}-1 \tag{3.47}$$

and for larger n approximately doubles with n increasing by each unit. For example, the sixth QLM approximation reproduces exactly $2^7-1=127$ terms of the perturbation expansion, while the twelfth approximation reproduces already $2^{13}-1=8191$ terms, and so on.

The numerical computation of $u_3(\infty)$ gives 0.125, corresponding to $A_0=0.875$, a finite and gratifying result.

Comparison of the first three QLM approximations $u_n(\lambda)$, $n=1,2,3$ with exact solution $u(\lambda)=1/(1+\lambda)$ and its perturbation expansion (3.42) containing 15 terms (up to λ^{14}, inclusively) for the δ-function potential with the potential strength λ changing in the interval (0,10) is shown graphically in Fig. 3. One can see that each subsequent QLM approximation reproduces the exact solution better than the previous one up to infinite values of the coupling constant, while even the 15th-order perturbation theory is not able to describe the exact solution adequately beyond $\lambda=1$.

To prove the uniform quadratic convergence of QLM iterations let us note that the first and second functional derivatives of the left hand side of Eq. (3.40) are $-2u(x)$ and -2, respectively, exactly as in the case of the repulsive square well which was discussed earlier. The extremal value of $u(x)$, reached when $u'(x)=-u^2(x)=0$, is, obviously, zero, which, in view of boundary condition $u(0)=1$, means $0\leqslant u(x)\leqslant 1$. This allows one to choose the same functions $F(x)=-2$, $G(x)=2$ as for the repulsive square well, and consequently results in the same expression 3.18 for $k(b)$. Since it follows from Fig. 3 that the maximal difference between zero and first QLM approximations $\|u_1(x)-u_1(x)\|$ equals $\frac{1}{2}$, one obtains as before $q_1(b)\leqslant\frac{1}{4}$, which proves the uniform quadratic convergence of the QLM iterations for all values of b. This means that the

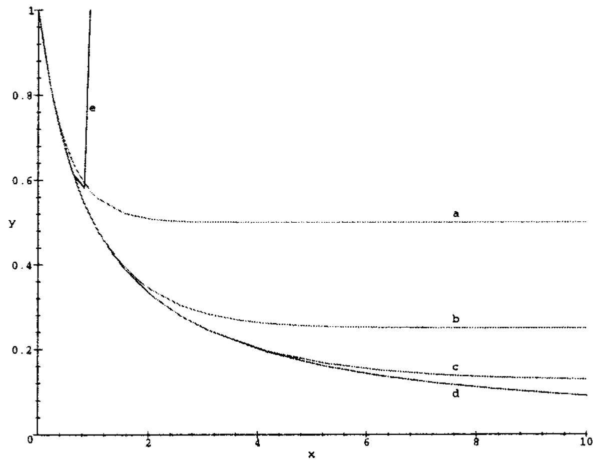

FIG. 3. Comparison of first three QLM approximations $u_n(\lambda), n=1,2,3$, curves a, b, and c, respectively, with exact solution $u(\lambda)=1/(1+\lambda)$, curve d, and its perturbation expansion (3.42), curve e, containing 15 terms (up to λ^{14}, inclusively), for the δ-function potential with the potential strength λ (axis x) changing in the interval (0,10).

convergence of subsequent QLM approximations to the exact scattering length for the repulsive δ-function potential is uniform and quadratic for all values of coupling constant λ, including very large and infinite ones.

2. Attractive δ-function potential

For negative λ the subsequent approximations $u_n(\lambda)$ start to increase very rapidly with $|\lambda|$ as one can see, for example, from analytic expressions (3.41) and (3.44). According to discussion before Eq. (2.38) we have to switch in this case in Eq. (3.40) to a new function $v(x)=1/u(x)$, which thus satisfies the trivial equation $v'(x)=1$ with a boundary condition $v(0)=1$. The QLM solution of this equation in the nth approximation, calculated from Eq. (2.23), is $v_n(x)=1+x$ or $u_n(x)=1/(1+x)$ for any n, which means that this form of the equation for the attractive δ-function potential generates an exact solution in any QLM approximation and there is no need for further investigation.

C. Inverse square potential

Let us consider now the inverse square potential

$$V(r)=\frac{\lambda}{r^2}\Theta(R-r), \tag{3.48}$$

where λ is the dimensionless coupling constant. As is well known,[18] this potential produces a fall to the center in case of $\lambda<-\frac{1}{4}$. For $r\leqslant R$, Eq. (1.1) for the scattering length could be written in the form

$$A'(x)=-\lambda\left(1+\frac{A(x)}{x}\right)^2, \quad A(0)=0, \tag{3.49}$$

where $x=r/R$ and $A(x)=a(r)/R$ are the dimensionless variable and variable scattering length, respectively; for $x>1$, $A(x)\equiv A(1)$ is a constant and represents the dimensionless scattering length A_0. Looking for a solution in the form $A(x)=x\alpha(x)$, we obtain for $\alpha(x)$,

$$\alpha'(x)=-\frac{1}{x}[\alpha(x)+\lambda(1+\alpha(x))^2. \tag{3.50}$$

Note, that in this equation boundary condition $\alpha(0)=0$ is not necessary: $\alpha(x)$ could be any function regular at $x=0$ so that condition $A(0)=0$ is satisfied. Setting $\alpha(x)=\text{constant}\equiv A_0$ gives an algebraic equation $A_0=-\lambda(1+A_0)^2$ whose solution is given by $A_0=-1-1/2\lambda\,(1\pm\sqrt{1+4\lambda})$. Since for $\lambda\to 0$ there should be no scattering only solution with the minus sign before the square root should be chosen, since only for this solution $A_0\to 0$ when $\lambda\to 0$. Setting for convenience $g=4\lambda$ we finally obtain

$$A_0=-1-\frac{2}{g}(1-\sqrt{1+g}). \tag{3.51}$$

The solution has a singularity, namely a branch point, at $g=-1$, that is at $\lambda=-\frac{1}{4}$. The singularity marks the beginning of interval $-\infty<\lambda<-\frac{1}{4}$ where a fall to the center takes place[18] and the expression for the scattering length becomes complex, its real and imaginary parts for $g<-1$ are given by

$$\operatorname{Re} A_0=-1-\frac{2}{g}, \quad \operatorname{Im} A_0=\frac{2}{g}\sqrt{-1-g}. \tag{3.52}$$

Note that in view of our definition (3.6) of the scattering length one has to chose $\operatorname{Im} A_0\geqslant 0$.[18] The perturbation series for the scattering length could be obtained by expansion of the square root in Eq. (3.51) in the power series which gives

$$\begin{aligned}
A_0=&-\frac{1}{4}\,g+\frac{1}{8}\,g^2-\frac{5}{64}\,g^3+\frac{7}{128}\,g^4-\frac{21}{512}\,g^5+\frac{33}{1024}\,g^6-\frac{429}{16\,384}\,g^7\\
&+\frac{715}{32\,768}\,g^8\frac{2431}{131\,072}\,g^9+\frac{4199}{262\,144}\,g^{10}-\frac{29\,393}{2\,097\,152}\,g^{11}+\frac{52\,003}{4\,194\,304}\,g^{12}\\
&-\frac{185\,725}{16\,777\,216}\,g^{13}+\frac{334\,305}{33\,554\,432}\,g^{14}-\frac{9\,694\,845}{1\,073\,741\,824}\,g^{15}+\frac{17\,678\,835}{2\,147\,483\,648}\,g^{16}\\
&-\frac{64\,822\,395}{8\,859\,934\,592}\,g^{17}+\frac{119\,409\,675}{17\,179\,869\,184}\,g^{18}-\frac{883\,631\,595}{137\,438\,953\,472}\,g^{19}\\
&+\frac{1\,641\,030\,105}{274\,877\,906\,944}\,g^{20}-\frac{6\,116\,566\,755}{1\,099\,511\,627\,776}\,g^{21}+\frac{11\,435\,320\,455}{2\,199\,023\,255\,552}\,g^{22}\\
&-\frac{171\,529\,806\,825}{35\,184\,372\,088\,832}\,g^{23}+\frac{322\,476\,036\,831}{70\,368\,744\,177\,664}\,g^{24}-\frac{1\,215\,486\,600\,363}{281\,474\,976\,710\,656}\,g^{25}\\
&+\frac{2\,295\,919\,134\,019}{562\,949\,953\,421\,312}\,g^{26}-\frac{17\,383\,387\,729\,001}{4\,503\,599\,627\,370\,496}\,g^{27}\\
&+\frac{32\,968\,493\,968\,795}{9\,007\,199\,254\,740\,992}\,g^{28}-\frac{125\,280\,277\,081\,421}{36\,028\,797\,018\,963\,968}\,g^{29}\\
&+\frac{238\,436\,656\,380\,769}{72\,057\,594\,037\,927\,936}\,g^{30}-\frac{14\,544\,636\,039\,226\,909}{4\,611\,686\,018\,427\,387\,904}\,g^{31}\\
&+\frac{27\,767\,032\,438\,524\,099}{9\,223\,372\,036\,854\,775\,808}\,g^{32}+O(g^{33}).
\end{aligned} \tag{3.53}$$

The expansion is convergent[16] for $|g|<1$, that is for $|\lambda|<\frac{1}{4}$.

Let us now turn our attention to QLM approximations and their convergence. The QLM iterations sequences are easiest to find by considering differential form 2.3 of Eq. (2.22) which could be written as

$$\alpha_{n+1}'(x) = -\frac{1}{x}\left[\frac{g}{4}(1-\alpha_n^2(x)) + \alpha_{n+1}(x)\left(1+\frac{g}{2}(1+\alpha_n(x))\right)\right]. \tag{3.54}$$

The assumption that $\alpha_n(x)$ are constant functions, $\alpha_n(x) \equiv c_n$, immediately establish the QLM recurrence relationship

$$c_{n+1} = -g\frac{1-c_n^2}{4+2g(1+c_n)}. \tag{3.55}$$

Note that since $c_{n+1} \rightarrow 0$ when $g \rightarrow 0$ each approximation to the scattering amplitude vanishes for $g=0$ as it should be since in the absence of the potential there is no scattering. The convergence of the QLM iteration sequence to the exact solution (3.51) is obvious. Indeed, for $n\rightarrow\infty$, Eq. (3.55) is

$$c_\infty = -g\frac{1-c_\infty^2}{4+2g(1+c_\infty)}, \tag{3.56}$$

whose solution vanishing for $g\rightarrow 0$ is given by the expression for A_0 in Eq. (3.51). The QLM approximation c_n to the dimensionless scattering length for an infinite n therefore indeed is $c_\infty \equiv A_0$ as we wanted to show.

The explicit calculation of the first few QLM approximations, starting from the usual initial guess $c_0=0$ gives

$$c_1 = -\frac{g}{4+2g}, \tag{3.57}$$

$$c_2 = -1/4\frac{(16+16g+3g^2)g}{(8+8g+g^2)(2+g)}, \tag{3.58}$$

$$c_3 = -1/8\frac{(4096+12\,288g+14\,080g^2+7680g^3+2016g^4+224g^5+7g^6)g}{(128+256g+160g^2+32g^3+g^4)(2+g)(8+8g+g^2)}. \tag{3.59}$$

These expressions, unlike that of the perturbation theory, give finite values also for $g>1$ or even for $g=\infty$, where the first, second, and third QLM approximations give $-\frac{1}{2}$, $-\frac{3}{4}$, $-\frac{7}{8}$ vis-a-vis the exact value $A_0=-1$; the fourth approximation, not given here because of its cumbersome form, results in $-\frac{15}{16}$, and so on. The convergence of these values is from above in agreement with the law of convergence for the concave functions proved in Sec. II, since the second functional derivative $-\lambda/x^2$ of the right-hand side of Eq. (3.49) is negative for the repulsive potential.

The expansion of the QLM approximations in the power series in the coupling constant shows as in previous examples that each QLM iteration sums exactly many perturbation series terms, whose number is given by Eq. (3.47). One obtains:

$$c_0 = 0, \tag{3.60}$$

$$c_1 = -\frac{1}{4}g + \frac{1}{8}g^2 - \frac{1}{16}g^3 + \frac{1}{32}g^4 - \frac{1}{64}g^5 + O(g^6), \tag{3.61}$$

$$c_2=-\frac{1}{4}g+\frac{1}{8}g^2-\frac{5}{64}g^3+\frac{7}{128}g^4-\frac{21}{512}g^5+\frac{33}{1024}g^6 -\frac{107}{4096}g^7+\frac{177}{8192}g^8-\frac{593}{32\,768}g^9+O(g^{10}), \tag{3.62}$$

$$c_3=-\frac{1}{4}g+\frac{1}{8}g^2-\frac{5}{64}g^3+\frac{7}{128}g^4-\frac{21}{512}g^5+\frac{33}{1024}g^6-\frac{429}{16\,384}g^7+\frac{715}{32\,768}g^8 -\frac{2431}{131\,072}g^9+\frac{4199}{262\,144}g^{10}-\frac{29\,393}{2\,097\,152}g^{11}+\frac{52\,003}{4\,194\,304}g^{12}-\frac{185\,725}{16\,777\,216}g^{13} +\frac{334\,305}{33\,554\,432}g^{14}-\frac{2\,423\,711}{268\,435\,456}g^{15}+\frac{4\,419\,705}{536\,870\,912}g^{16}-\frac{16\,205\,537}{2\,147\,483\,648}g^{17} +\frac{29\,852\,049}{4\,294\,967\,296}g^{18}-\frac{220\,900\,693}{34\,359\,738\,368}g^{19}+O(g^{20}), \tag{3.63}$$

$$c_4=-\frac{1}{4}g+\frac{1}{8}g^2-\frac{5}{64}g^3+\frac{7}{128}g^4-\frac{21}{512}g^5+\frac{33}{1024}g^6-\frac{429}{16\,384}g^7+\frac{715}{32\,768}g^8 -\frac{2431}{131\,072}g^9+\frac{4199}{262\,144}g^{10}-\frac{29\,393}{2\,097\,152}g^{11}+\frac{52\,003}{4\,194\,304}g^{12}\frac{185\,725}{16\,777\,216}g^{13} +\frac{334\,305}{33\,554\,432}g^{14}-\frac{9\,694\,845}{1\,073\,741\,824}g^{15}+\frac{17\,678\,835}{2\,147\,483\,648}g^{16}-\frac{64\,822\,395}{8\,589\,934\,592}g^{17} +\frac{119\,409\,675}{17\,179\,869\,184}g^{18}-\frac{883\,631\,595}{137\,438\,953\,472}g^{19}+\frac{1\,641\,030\,105}{274\,877\,906\,944}g^{20} -\frac{6\,116\,566\,755}{1\,099\,511\,627\,776}g^{21}+\frac{11\,435\,320\,455}{2\,199\,023\,255\,552}g^{22}-\frac{171\,529\,806\,825}{35\,184\,372\,088\,832}g^{23} +\frac{322\,476\,036\,831}{70\,368\,744\,177\,664}g^{24}-\frac{1\,215\,486\,600\,363}{281\,474\,976\,710\,656}g^{25}+\frac{2\,295\,919\,134\,019}{562\,949\,953\,421\,312}g^{26} -\frac{17\,383\,387\,729\,001}{4\,503\,599\,627\,370\,496}g^{27}+\frac{32\,968\,493\,968\,795}{9\,007\,199\,254\,740\,992}g^{28} -\frac{125\,280\,277\,081\,421}{36\,028\,797\,018\,963\,968}g^{29}+\frac{238\,436\,656\,380\,769}{72\,057\,594\,037\,927\,936}g^{30} -\frac{3\,636\,159\,009\,806\,727}{1\,152\,921\,504\,606\,846\,976}g^{31}+\frac{6\,941\,758\,109\,631\,017}{2\,305\,843\,009\,213\,693\,952}g^{32}+O(g^{33}). \tag{3.64}$$

Comparison of Eqs. (3.60)–(3.64) with Eq. (3.53) shows that the QLM iterations with $n=0,1,2,3,4$ reproduce exactly 1,3,7,15,31 terms of the perturbation series, respectively, in exact agreement with Eq. (3.47), while the next few terms have coefficients extremely close to being exact. The number of terms given precisely by the zero, first, second, third and fourth QLM approximations is increasing by 2, 2^2, 2^3 and 2^4, exactly as we saw earlier in the case of the δ-function potential and in precise agreement with the quadratic law of the convergence, proved in Sec. II. Due to simplicity of the algebraic recurrence relations (3.55) Eq. (3.47) for number N_n of the perturbation series terms given precisely by the nth QLM approximation could be checked for higher QLM approximations. For example, in Sec. III B on the example of the repulsive δ-potential we concluded that $N_6 = 127$. The simple calculation using a symbolic manipulation program[17] shows immediately that it is precisely the same for the inverse square potential. Indeed, the first seven nonzero terms of the expansion in powers of g of difference $A_0 - c_6$ between exact scattering length Eq. (3.51) and its sixth QLM approximation are

$$
\begin{aligned}
&-\frac{1}{28\,948\,022\,309\,329\,048\,855\,892\,746\,252\,171\,976\,963\,317\,496\,166\,410\,141\,009\,864\,396\,001\,978\,282\,409\,984}\,g^{127}\\
&+\frac{127}{57\,896\,044\,618\,658\,097\,711\,785\,492\,504\,343\,953\,926\,634\,992\,332\,820\,282\,019\,728\,792\,003\,956\,564\,819\,968}\,g^{128},\\
&-\frac{16319}{231\,584\,178\,474\,632\,390\,847\,141\,970\,017\,375\,815\,706\,539\,969\,331\,281\,128\,078\,915\,168\,015\,826\,259\,279\,872}\,g^{129},\\
&+\frac{707\,135}{463\,168\,356\,949\,264\,781\,694\,283\,940\,034\,751\,631\,413\,079\,938\,662\,562\,256\,157\,830\,336\,031\,652\,518\,559\,744}\,g^{130},\\
&-\frac{92\,988\,123}{3\,705\,346\,855\,594\,118\,253\,554\,271\,520\,278\,013\,051\,304\,639\,509\,300\,498\,049\,262\,642\,688\,253\,220\,148\,477\,952}\,g^{131},\\
&+\frac{2\,473\,622\,041}{7\,410\,693\,711\,188\,236\,507\,108\,543\,040\,556\,026\,102\,609\,279\,018\,600\,996\,098\,525\,285\,376\,506\,440\,296\,955\,904}\,g^{132},\\
&-\frac{110\,916\,205\,323}{29\,642\,774\,844\,752\,946\,028\,434\,172\,162\,224\,104\,410\,437\,116\,074\,403\,984\,394\,101\,141\,506\,025\,761\,187\,823\,616}\,g^{133},
\end{aligned}
\tag{3.65}
$$

exactly as one expects from Eq. (3.47). In addition, one can see that the next terms of the perturbation series are also reproduced extremely well, their difference with the precise terms being infinitesimally small. Namely, the coefficient of 127th power of g is about 3.45×10^{-76}, the coefficient of 128th power is about 2.19×10^{-74}, and so on.

For the attractive potential expressions (3.57)–(3.59) become singular, with the number of zeros of denominators increasing with each iteration. This, of course, is a reflection of the fact that the exact scattering length A_0 has a branch point at $g = -1$ and a cut line along the real axis between $g = -1$ and $g = -\infty$. When n is increasing, the poles are getting closer and closer to each other and fuse together at $n = \infty$, where, as we saw earlier, the exact amplitude and its singularity are reproduced.

To handle the singularities one can try, as we have discussed earlier, to consider instead of the function $\alpha(x)$ a new function $\beta(x)$ such that $\alpha(x) = 1/\beta(x)$. Substitution of Eq. (3.65) into Eq. (3.50) leads to

$$
\beta'(x) = \frac{1}{x}[\beta(x) + \lambda(1+\beta(x))^2, \tag{3.66}
$$

which is different from Eq. (3.50) only by the sign of the right-hand side. The QLM iterations sequence is found as before by considering differential form (2.3) of Eq. (2.22):

$$
\beta'_{n+1}(x) = \frac{1}{x}\left[\frac{g}{4}(1-\beta_n^2(x)) + \beta_{n+1}(x)\left(1+\frac{g}{2}(1+\beta_n(x))\right)\right], \tag{3.67}
$$

which leads under a previous assumption of β_n being a constant function, $\beta_n \equiv c_n$, to exactly the same QLM recurrence relations (3.55). Again, the convergence of the QLM series follows from the fact that at $n\to\infty$ we have the same Eq. (3.56), as before, with only distinction—since now the scattering amplitude in the limit $n = \infty$ is given by $1/\beta_\infty$, one should take a solution of this equation which is going to infinity at $g \to 0$ rather than to zero. Such solution is given by

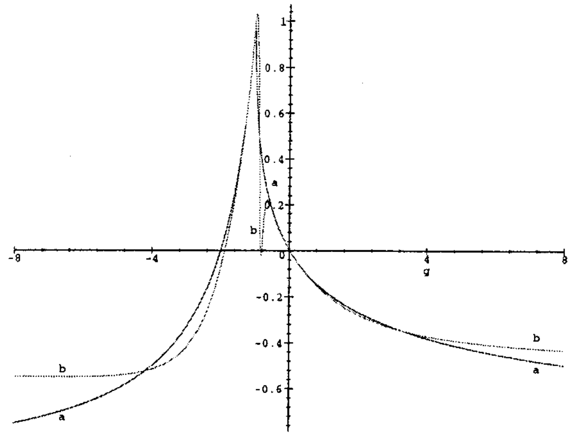

FIG. 4. Comparison of real parts of the exact scattering length (curve a) and of the second QLM approximation to it (curve b) for inverse square potential, $|g|\leqslant 8$.

$$\beta_\infty = -1 - \frac{2}{g}(1+\sqrt{1+g}). \tag{3.68}$$

The $n=\infty$ QLM approximation to the scattering length A_0 thus equals to

$$\frac{1}{\beta_\infty} = \frac{1}{-1-\frac{2}{g}(1+\sqrt{1+g})}$$
$$\equiv -1 - \frac{2}{g}(1-\sqrt{1+g}), \tag{3.69}$$

which indeed coincides exactly with expression (3.51) for A_0.

Since the change to $\beta_n(x) = 1/\alpha_n(x)$ does not give anything new, the only way to avoid the singularities in the case of attractive potential seems therefore to use the fact that the zero approximation could be an arbitrary, not necessarily real, number, and to choose c_0 as a complex number with a positive imaginary part of the same order as a real part. The necessity of choosing c_0 complex in the case of the attractive potential follows also from the fact that in this case the fall to the center happens. The inelastic cross section for zero energies, determined by the imaginary part of the S-wave scattering length,[18] could not therefore be zero; however, from recurrence relations (3.55) it is obvious that unless the initial guess c_0 is a complex number, all subsequent QLM approximations are real.

Comparison of real and imaginary parts of the scattering length with those calculated in the second and third QLM approximations for an arbitrary initial guess $\alpha_0 = 1+i$ and for coupling constant values $|\lambda|\leqslant 2$ ($|g|\leqslant 8$) is shown in Figs. 4–7. One can see that already for the second QLM iteration the agreement between the exact scattering length and the QLM approximation to it is quite good. It improves visibly for the next QLM iteration. For the fourth and next iterations the distinction between exact and approximate scattering length is difficult to see and therefore the correspondent graphs are not shown.

D. Inverse quartic potential

Our next and last example is the inverse quartic potential of radius ρ,

$$V(r) = \lambda \frac{R^2}{r^4}\Theta(\rho - r), \tag{3.70}$$

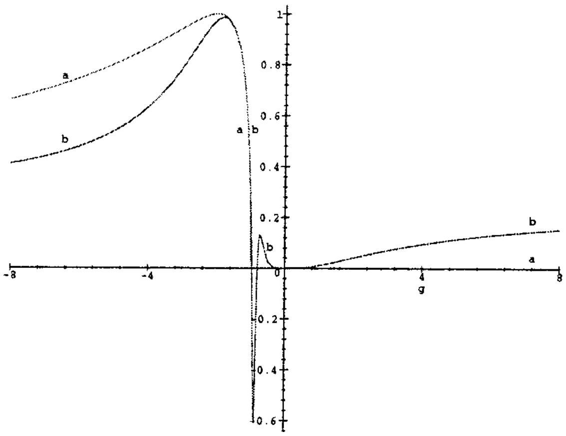

FIG. 5. Comparison of imaginary parts of the exact scattering length (curve a) and of the second QLM approximation to it (curve b) for inverse square potential, $|g| \leqslant 8$.

where λ is a dimensionless coupling constant. For $r \leqslant \rho$ the equation for a variable scattering length $a(r)$ is given by

$$\frac{da(r)}{dr} = -\lambda \frac{R^2}{r^4}(r + a(r))^2, \quad a(0) = 0, \tag{3.71}$$

while the scattering length a_0 equals $a(\rho)$. Introduction of the dimensionless function $\alpha(x) = a(r)/R\sqrt{\lambda}$ and of the dimensionless variable $x = r/R\sqrt{\lambda}$ reduces Eq. (3.71) to

$$\frac{d\alpha(x)}{dx} = -\frac{1}{x^4}(x + \alpha(x))^2, \quad \alpha(0) = 0, \tag{3.72}$$

whose solution is obviously given by

$$\alpha(x) = -\frac{x}{1+x}. \tag{3.73}$$

Since for $r = \rho$ $x = x_0 = \rho/R\sqrt{\lambda}$, and $\alpha(\rho/R\sqrt{\lambda}) = -\rho/(\rho + R\sqrt{\lambda})$, the dimensionless scattering length $A_0 = a_0/R$ is given by

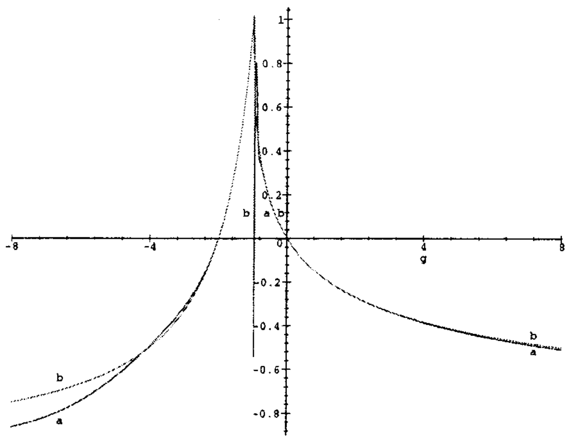

FIG. 6. Same as in Fig. 4, but in the third QLM approximation.

$$A_0 = \sqrt{\lambda}\,\alpha\left(\frac{\rho}{R\sqrt{\lambda}}\right) = -\frac{\rho\sqrt{\lambda}}{\rho + R\sqrt{\lambda}} \equiv -\frac{\rho}{R}\,\frac{y_0}{1+y_0}, \quad y_0 = \frac{1}{x_0} = \frac{R}{\rho}\sqrt{\lambda}, \tag{3.74}$$

which coincides with that found in Ref. 19 and also in Refs. 4, 11, and 14, where ρ is set to ∞. The solution has a singularity, namely a branch point, at $\lambda = 0$. The singularity marks the beginning of interval $-\infty < \lambda < 0$, where potential is attractive and a fall to the center takes place[18,20] and where the expression for the scattering length A_0 becomes complex. We consider therefore only repulsive potentials.

As always, let us start from the perturbation expansion (3.7), whose coefficients $a_n(r)$ are calculated from recurrence relations (3.8). In view of a strong singularity of the potential at the origin from Eq. (3.9) it follows, however, that first coefficient $a_1(r)$, and therefore all the others, are infinite. The perturbation expansion does not exist, which, of course, is a consequence of the branch point singularity of the scattering length directly at $\lambda = 0$.

There is, however, no problems with the QLM approximations to solution (3.73), whose iteration sequence in this case is given by

$$\alpha_{n+1}(x) = -\int_0^x \frac{ds}{s^4}[s^2 - \alpha_n^2(s)]\exp\left(-2\int_s^x \frac{dt}{t^4}(t + \alpha_n(t))\right). \tag{3.75}$$

Starting from the usual initial guess $\alpha_0(x) = 0$ one easily computes[4,11] the first iteration $\alpha_1(x) = -\exp(1/x^2 \int_0^x ds/s^2\, e^{-1/s^2})$, which substitution $s = 1/\sqrt{t}$ reduces to a form $\alpha_1(x) = -\frac{1}{2}\exp(1/x^2 \int_{1/x^2}^{\infty} dt/t^{1/2}\, e^{-t}) \equiv -\sqrt{\pi}/2\, e^{1/x^2}\,\mathrm{erfc}(1/x)$. The dimensionless scattering length in the first QLM approximation therefore is

$$A_{0,1} = \sqrt{\lambda}\,\alpha_1(x_0) = -\frac{\sqrt{\pi}}{2}\,\frac{\rho}{R}\, y_0 e^{y_0^2}\,\mathrm{erfc}(y_0), \tag{3.76}$$

where $\mathrm{erfc}(x) = 1 - \mathrm{erf}(x)$ is the complementary error function.[16] One can see that $A_{0,1}$, like A_0, is a function of y_0 and therefore has the same branch point singularity at $\lambda = 0$ as the exact scattering length.

To obtain a higher QLM approximation it is convenient to remove a fourth power of variable in the denominators of the integrals in Eq. (3.75). To do this, let us introduce a new variable $y = 1/x$ and a new function $\beta(x) = \alpha(1/x)$ with a boundary condition $\beta(\infty) = \alpha(0) = 0$. Equation (3.72) then has the form

$$\frac{d\beta(y)}{dy} = (1 + y\beta(y))^2, \quad \beta(\infty) = 0, \tag{3.77}$$

whose exact solution is given by

$$\beta(y) = -\frac{1}{(1+y)}, \tag{3.78}$$

while Eq. (3.75) is written as

$$\beta_{n+1}(y) = -\int_y^{\infty} ds[1 - s^2\beta_n^2(s)]\exp\left(2\int_s^y dt\,t(1 + \beta_n(t))\right). \tag{3.79}$$

The nth QLM approximation to $\alpha(x)$ is $\alpha_n(x) = \beta_n(1/x) \equiv \beta_n(y)$ so that $\alpha(x_0) \equiv \beta(y_0)$ and the initial guess could be chosen $\beta_0(x) \equiv \beta(\infty) = 0$. In the long ranged case $\rho = \infty$, $y_0 = 0$, and, since $\mathrm{erfc}(0) = 1$, $A_{0,1} = -\sqrt{\pi}/2\sqrt{\lambda} = -0.886\sqrt{\lambda}$, a very good approximation[11] to exact value $A_0 = -\sqrt{\lambda}$. The next QLM approximation, which can be computed numerically, results in $A_{0,2} = -0.988\sqrt{\lambda}$, a precision of 1.2%. For comparison, calculation of A_0 in the second CBF approxi-

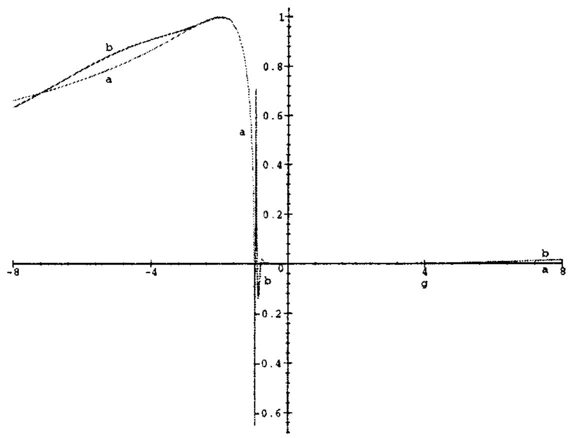

FIG. 7. Same as in Fig. 5, but in the third QLM approximation.

mation, Eq. (2.21), which in this case reduces to a simple minded linearization approach,[11] based on neglecting a nonlinear term, gives $A_{0,2} = -0.954\sqrt{\lambda}$, precision of only 4.6%. In the infinite coupling finite range case y_0 is very large and one can use asymptotic expression (3.16), which gives $A_{0,1} = -\frac{1}{2}\rho/R$, a reasonable first approximation to exact value $A_0 = -\rho/R$. In the next, second QLM approximation, the numerical computation yelds $A_{0,2} = -\frac{3}{4}\rho/R$, a significant improvement.

The uniform quadratic convergence of QLM sequence (3.75) is proved, according to Eq. (2.34), by showing that the first convergence coefficient $q_1(b)$ is less than unity. In our case, we have chosen $\alpha_0(x) \equiv 0$ and therefore $q_1(b) = k(b)\|\alpha_1(x)\| \leqslant k(b)$, since in view of the properties of the complimentary error function[16] $|\alpha_1(x)| \leqslant 1$ for all x.

To estimate $k(b)$ we have to know $G(x)$ and $F(x)$, which have to satisfy inequalities (2.31). Since the first and the second derivatives of the right-hand side of Eq. (3.72) are $-2/x^4(x + \alpha(x))$ and $-2/x^4$, respectively, and since the scattering length for the repulsive potential has no poles and should be finite, $\alpha(x) \leqslant M$ where M is some positive constant, and therefore one can choose $G(x) = F(x) \equiv F_1(x) = 2M/x^4$. For small $(x \leqslant \epsilon)$, where $\epsilon \ll 1$ is some small but finite number, looking for $\alpha(x)$ in the form $\alpha(x) \sim ax + bx^2$ and substituting in Eq. (3.72) gives $a = -1$, $b = 1$. The first functional derivative for small x therefore equals $-2/x^2$ and one can choose in this case negative boundary function $F(x) \equiv F_2(x) = -2/x^2$ and $G(x) = |F_2(x)|$.

Separating in Eq. (2.35) for $k(b)$ smaller and larger values of x gives

$$k(b) = \frac{1}{2}\left| C \exp \int_0^{\epsilon} dt\, F_2(t) - 1 \right|, \tag{3.80}$$

where $C = \exp \int_{\epsilon}^{b} dt\, F_1(t)$ is a finite constant even for infinite interval $b = \infty$. Since $\exp(\int_0^{\epsilon} dt F_2(t)) = \exp(-2\int_0^b dt\, 1/t^2) = \exp(2/t\,|_{+0}^{\epsilon}) = 0$, Eq. (3.80) gives $k(b) \equiv \frac{1}{2}$ und thus $q_1(b) \leqslant \frac{1}{2}$, which proves uniform quadratic convergence of QLM iteration sequence $\alpha_n(x_0)$, Eq. (3.75), on the whole interval $(0,\infty)$, that is for all values of coupling constant λ, including large and infinite ones.

IV. CONCLUSION

Summing up, we have reformulated the proof of the convergence of the quasilinearization method (QLM) of Bellman and Kalaba[1,2] by removing unnecessary restrictive conditions generally not fulfilled in physical applications, and have generalized the proof for large or infinite domains of variables and for functionals which are singular at some points in the domain. We also have shown how to deal with solutions which are infinite at certain values of variable such as, for example, scattering amplitudes at values corresponding to bound state energies, etc.

In order to make presentation as simple and short as possible, we have limited ourselves here to the case of the first-order nonlinear ordinary differential equation in one variable, which physically covers the quantum mechanics of one particle in a central field (in this case the Schrödinger equation for a wave function could be rewritten as the nonlinear Ricatti equation for its logarithmic derivative) though the same modernization of the Bellman and Kalaba proof[1,2] could be provided also for a general nonlinear ordinary or partial nth order differential equations in the N-dimensional space.

In order to highlight the power of the method in Sec. III we have considered examples of different singular and nonsingular, attractive and repulsive potentials $V(r)$ for which the nonlinear first-order ordinary differential equation (1.1) for the S-wave scattering length $a_0 = a(\infty)$ obtained in variable phase approach[4,5] could be solved exactly and have compared the iterations obtained by the Bellman–Kalaba linearization method with exact solutions and with the usual perturbation theory. The results could be summed up as follows.

(i) The sequence $u_n(x)$, $n=1,2,\ldots$ of QLM iterations, Eq. (2.22), converges *uniformly and quadratically* to solution $u(x)$ of Eq. (2.2). For the convergence on the interval $[0,b]$ is enough that an initial guess for zero iteration is sufficiently good to ensure the smallness of just one of convergence coefficients $q_m(b) = k(b)\|u_{m+1} - u_m\|$, where $k(b)$ is given by Eq. (2.32) or Eq. (2.35). In addition, for strictly convex (concave) functionals $f(u(x),x)$ difference $u_{n+1}(x) - u_n(x)$ is strictly positive (negative), which establishes *the monotonicity* of the convergence from below (above), respectively, on this interval.

(ii) The QLM treats the nonlinear terms as a perturbation about the linear ones[1,2] and is not based, unlike perturbation theories, on the existence of some kind of small parameter. As a result, it is able to handle, unlike the perturbation theory, large or even infinite values of the coupling constant.

(iii) Comparison of QLM with the perturbation theory shows that each QLM iteration reproduces and sums many orders of perturbation theory exactly and in addition many more orders approximately. Namely, in agreement with the quadratic pattern of the convergence, the number N_n of the terms of the perturbation series, reproduced exactly in the nth QLM approximations, equals $2^{n+1} - 1$, and approximately the same number of terms is reproduced approximately. The number of the exactly reproduced terms thus doubles with each subsequent QLM approximation, and reaches, for example, 127 terms in the sixth QLM approximation, 8191 terms in the twelfth QLM approximation and so on.

(iv) QLM handles without any problems not only singular potentials, like the inverse squared potential, for which the perturbation theory is divergent outside a narrow interval of the values of the coupling constant, but even super singular potentials, like reverse quartic potential, for which perturbation series are not existent at all, since their calculation leads to infinities in each order of the perturbation expansion.

(v) As we saw in all of our examples, QLM easily handles different singularities, like poles or branch point singularities, reproducing correct type of the singularity already in first iterations.

(vi) Although the analytic calculations of third and higher approximation in QLM, like in the usual perturbation theory, in most cases (excluding inverse square potential) seem impossible, the simplicity of the QLM iterational sequence Eq. (2.22) (which, unlike perturbation theory, containes no sums on intermediate energy states) assures nonproblematic numerical calculation of higher order iterations, while the extremely fast convergence of the method allows accurate estimate of the solution after relatively small number of iterations.

In view of all this, since most equations of physics, from classical mechanics to quantum field theory, are either not linear or could be transformed to a nonlinear form, the quasilinear method may turn out to be extremely useful and in many cases more advantageous than the perturbation theory or its different modifications, like expansion in inverse powers of the coupling constant, $1/N$ expansion, etc.

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