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Numerical investigation of quasilinearization method in quantum mechanics

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Abstract

The general properties of the quasilinearization method (QLM), particularly its fast convergence, monotonicity and numerical stability are analyzed and verified on the example of scattering length calculations in the variable phase approach to quantum mechanics. The method, whose mathematical basis in physics was discussed recently by one of the present authors (VBM), approximates the solution of a nonlinear differential equation by treating the nonlinear terms as a perturbation about the linear ones, and is not based, unlike perturbation theories, on the existence of some kind of a small parameter. Each approximation of the method sums many orders of the perturbation theory.

It is shown that already the first few iterations provide very accurate and numerically stable answers for small and intermediate values of the coupling constant. The number of iterations necessary to reach a given precision only moderately increases for its larger values. The method provides accurate and stable answers for any coupling strengths, including for super singular potentials for which each term of the perturbation theory diverges and the perturbation expansion does not exist even for a very small coupling.

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1. Introduction

The purpose of this paper is to verify the possibility of the application of a very powerful approximation technique called the quasilinearization method (QLM) in quantum physics. The method, whose iterations are constructed to yield rapid convergence and often monotonicity, was introduced years ago by Bellman and Kalaba [1,2] to solve nonlinear ordinary and partial differential equations or systems of these. It is a generalization of the Newton–Raphson method of finding roots of the scalar equation $f(x) = 0$ to nonlinear differential equations. The modern developments and applications of the method to different fields are given in a monograph [3]. QLM, however, was never systematically studied or extensively applied in quantum physics, although references to it could be found in well-known monographs [4,6] dealing with the variable phase approach to potential scattering, as well as in a few scattered research papers [7–10]. The reason is that the convergence of the method has been proven only under rather restrictive conditions [1,2], which generally are not fulfilled in physical applications. Recently, though, it was shown [11] by one of the present authors (VBM) that a different proof of the conver-

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gence could be provided so that the applicability of the method is extended to incorporate realistic physical conditions of forces defined on infinite intervals or singular at certain points there, etc.

The quasilinearization approach is applicable to a general nonlinear ordinary or partial nth order differential equation in N-dimensional space, and to complicated nonlinear two-point boundary conditions [1,2]. To reach convergence, the simple guess of the zeroth iteration being equal to zero or to one of the boundary conditions, is usually enough [12]. In order to make this initial presentation as simple and short as possible, however, 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 the wave function could be rewritten as the Riccati equation for its logarithmic derivative.

In the paper [11] the quasilinearization approach was compared with the results of the perturbation theory. It was found theoretically and on examples that the nth approximation of QLM sums exactly $2^n - 1$ terms of the perturbation theory. In addition, a similar number of terms is reproduced approximately. The number of the exactly reproduced perturbation terms thus doubles with each subsequent QLM approximation, and reaches, for example, 127 terms in the 6th QLM approximation, 8191 terms in the 12th QLM approximation, and so on.

The computational approach in the work [11] was, however, mostly analytical, and therefore one was able to compute only two to three QLM iterations, mainly for power potentials. Only in the case of the $1/r^2$ potential, the calculation of QLM iterations could be done analytically for any n. The goal of the present work is, by dropping the restriction of analytical computation, to calculate higher iterations as well as to extend the analysis to non-power potentials, in order to make better assessment of the applicability of the method and of the numerical stability and the convergence pattern of the QLM iterations.

The paper is arranged as follows: in Section 2 we present the main features of the quasilinearization approach. In Section 3 we use the method to obtain accurate solutions of the nonlinear first order ordinary differential equation

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

for the S-wave scattering length [1] $a_0 = a(\infty)$ in the variable phase approach [4–6] and compare the results of subsequent iterations with exact solutions for different singular and nonsingular, attractive and repulsive potentials $V(r)$. The results, convergence patterns, numerical stability, advantages of the method and its possible future applications are discussed in Section 4.

2. The quasilinearization method (QLM)

The aim of the QLM [1–3,11] is to obtain the solution of a nonlinear nth order ordinary or partial differential equation in N dimensions 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 such an equation in terms of a finite set of particular solutions as in 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.

As we discussed in the introduction, we limit ourselves here to the case of the first order nonlinear ordinary differential equation in one variable on the interval $[0, b]$ which could be, of course, infinite:

$$\frac{\mathrm{d}u(x)}{\mathrm{d}x} = f\big(u(x), x\big), \tag{2.1}$$

with the boundary condition $u(0) = 0$.

The QLM prescription [1,2,11] determines the $(n+1)$th iterative approximation $u_{n+1}(x)$ to the solution of Eq. (2.1) as a solution of the linear differential equation

[1] We use here the Calogero definitions [4] of the scattering length a_0 and of the potential $V(r)$,

$$a_0 = \lim_{k\to 0} \frac{\tan\delta(k)}{k}, \tag{1.2}$$

$$V(r) = 2mU(r), \tag{1.3}$$

where m is the reduced mass and $\delta(k)$ is the scattering phase. These definitions are different in sign and in dimension, respectively, from the definitions of the scattering length and of the potential $U(r)$ used in most publications.

$$u'_{n+1}(x) = f(u_n, x) + \big(u_{n+1}(x) - u_n(x)\big) f_u(u_n, x),$$
$$u_{n+1}(0) = 0, \tag{2.2}$$

where the function $f_u(u, x) = \partial f(u, x)/\partial u$ is a functional derivative of the functional $f(u(x), x)$. This equation could be explicitly integrated and written as the iteration sequence

$$u_{n+1}(x) = \int_0^x \mathrm{d}s \left(f(u_n(s), s) - f_u(u_n(s), s)u_n(s)\right) \times \exp \int_s^x \mathrm{d}t\, f_u\big(u_n(t), t\big). \tag{2.3}$$

The zeroth approximation $u_0(x)$ is chosen from mathematical or physical considerations and satisfies the boundary condition $u_0(0) = 0$.

Let us assume the boundedness 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

$$f_u\big(u(x), x\big) \leqslant F(x),$$
$$\big|f_{uu}(u(x), x)\big| \leqslant G(x). \tag{2.4}$$

In this case one can prove [11] that the equation for the error estimate could be written in the form

$$\|\Delta u_{n+1}\| \leqslant k \cdot \|\Delta u_n\|^2,$$
$$\|\delta u_{n+1}\| \leqslant k \cdot \|\delta u_n\|^2. \tag{2.5}$$

Here k is given by

$$k = \frac{1}{2} \int_0^b \mathrm{d}s\, G(s) \exp \int_s^b \mathrm{d}t\, F(t). \tag{2.6}$$

The notation $\|g\|$, introduced here and used throughout the paper, refers to a metric of some function $g(x)$ which is defined as the maximum of a function $g(x)$ on the interval $[0, b]$

$$\|g\| = \max_{0 \leqslant x \leqslant b} \big|g(x)\big|, \tag{2.7}$$

while $\Delta u_{n+1}(x)$ and $\delta u_{n+1}(x)$ are the difference between the exact solution and the nth iteration and between two subsequent iterations, respectively:

$$\Delta u_{n+1}(x) = u(x) - u_n(x),$$
$$\delta u_{n+1}(x) = u_{n+1}(x) - u_n(x). \tag{2.8}$$

Eq. (2.5) thus shows that the maxima of the absolute value of the difference of the $(n+1)$th and the nth iterations or of the exact solution and the nth iteration are less than a number k multiplied by the square of the maximum of the absolute value of the difference of the nth and the $(n-1)$th iterations or of the exact solution and the $(n-1)$th iteration, respectively.

If $F(x)$ is a sign-definite function and $G(x)$ can be chosen as the absolute value of $F(x)$, $G(x) = |F(x)|$, the integral in Eq. (2.6) can be taken explicitly and produces a simple expression for k

$$k = \frac{1}{2} \left| \exp \int_0^b \mathrm{d}t\, F(t) - 1 \right|. \tag{2.9}$$

A simple induction of Eq. (2.5) shows [2] that $\delta u_{n+1}(x)$ for an arbitrary $l < n$ satisfies the inequality

$$\|\delta u_{n+1}\| \leqslant \big(k\|\delta u_{l+1}\|\big)^{2^{n-l}}/k, \tag{2.10}$$

or, for $l = 0$,

$$\|\delta u_{n+1}\| \leqslant \big(k\|\delta u_1\|\big)^{2^n}/k. \tag{2.11}$$

The convergence depends therefore on the quantity $q_1 = k\|u_1 - u_0\|$, where the zeroth iteration $u_0(x)$ satisfies the condition $u_0(0) = 0$ and is chosen from physical and mathematical considerations. However, from Eq. (2.10) it follows that for the convergence it is sufficient that just one of the quantities $q_m = k\|\delta u_{m+1}\|$ is 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 the smallness of at least one of the convergence coefficients q_m, $m > 1$, which enables a rapid convergence of the iteration series for $n > m$.

It is important to stress that in view of the quadratic convergence of the QLM method displayed in Eq. (2.5) the difference $\|\Delta u_{n+1}\|$ between the exact solution and the QLM iteration always converges to zero if the difference δu_{n+1} between two subsequent QLM iterations becomes infinitesimally small. Indeed, the first impression is that if δu_{n+1} is very close to zero, it could mean, since $\delta u_{n+1} = \Delta u_n - \Delta u_{n+1}$, that $\Delta u_n = \Delta u_{n+1}$ or

$$Q_n = Q_{n+1}, \tag{2.12}$$

where $Q_n = k\|\Delta u_n\|$, when either of them is not small, that is that the iteration process "stagnates".

In view of the second of Eqs. (2.5) which could be written as $Q_{n+1} \leqslant Q_n^2$, Eq. (2.12) cannot be satisfied, however, unless both Q_{n+1} and Q_n are equal to zero, which proves that stagnation of the iteration process is impossible and convergence of $\|\delta u_{n+1}\|$ to zero automatically leads to convergence of the QLM iteration sequence to the exact solution.

One can show that for strictly convex (concave) functionals $f(u(x), x)$, where the second functional derivative $f_{uu}(u, x)$ of $f(u(x), x)$ is strictly positive (negative), the difference Δu_{n+1} (δu_{n+1}) is also strictly positive (negative), ensuring in this case the monotonic convergence to the exact solution u from below (above), respectively.

In the case that the solution $u(x)$ and respectively its iterations $u_n(x)$ are going to infinity at some points on the interval $[0, b]$, Eq. (2.3) could become meaningless. To deal with it it is necessary to regularize Eq. (2.1), that is, reformulate it in terms of a new function $v(x)$ which is finite. In this work we would use the prescription $u(x) = \tan v(x)$ as it was suggested in Refs. [5,11]. The corresponding nonlinear equation for $v(x)$ has the form

$$\frac{\mathrm{d}v(x)}{\mathrm{d}x} = \big(\cos v(x)\big)^2 f\big(\tan v(x), x\big), \quad v(0) = 0. \tag{2.13}$$

Based on this summary one can deduce the following important features of the quasilinearization method:

(i) The method approximates the 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 the existence of some kind of small parameter.

(ii) The iterations converge uniformly and quadratically to the exact solution. In the case when the second functional derivative of $f(u(x), x)$ has a definite sign, the convergence in addition is monotonic.

(iii) For the rapid convergence it is actually enough that an initial guess for the zeroth iteration is sufficiently good to ensure the smallness of just one of the quantities $q_m = k\|u_{m+1} - u_m\|$. The convergence is extremely fast: if, for example, q_1 is of the order of $\frac{1}{3}$, only 4 iterations are necessary to reach the accuracy of 8 digits, since $(\frac{1}{3})^{2^n}$ is of the order of $(\frac{1}{10})^{2^{n-1}}$.

(iv) The computation of each iteration involves the estimate of the same double integral given by Eq. (2.3). In the case of numerical integration using the trapezoidal rule, the values of $u_m(x)$ on the same set of integration points are utilized in each iteration, making the calculation of subsequent iterations time efficient, and, as we shall see in the next section, numerically stable.

3. QLM solution of variable phase equations and comparison with exact results

In order to investigate the applicability of the quasilinearization method in quantum mechanics, its convergence and numerical stability, we compare in this chapter the QLM iterations of Eq. (1.1) for potentials of different forms and strengths with the corresponding exact solutions. In the case of attractive potentials the scattering length has poles at the zero energy bound states. In this case we will use a different nonlinear differential equation,

$$\frac{\mathrm{d}\delta(r)}{\mathrm{d}r} = -V(r)\big(r\cos\delta(r) + \sin\delta(r)\big)^2, \quad \delta(0) = 0, \tag{3.1}$$

obtained from Eq. (1.1) using the prescription $a(r) = \tan\delta(r)$ (see Eq. (2.13) whose solution has no singularity).

3.1. Yukawa potential

Let us start from the Yukawa potential

$$V(r) = -g\frac{\mathrm{e}^{-r/R}}{r/R}. \tag{3.2}$$

Here and further in this paper g denotes the dimensionless coupling constant and R defines the radius of the force. Normally we will set $R = 1$, thus measuring distances in units of R. Since this potential is attractive for positive g and the scattering length therefore could have poles corresponding to zero energy bound states, we will here instead of the scattering length a_0 calculate the phase $\delta_0 = \arctan a_0$ using Eq. (3.1).

The simple QLM program, based on Eqs. (2.3) and (3.1), was created and was instructed to stop the iteration process when the maximum difference $\|\delta u_{n+1}\|$ between two subsequent iterations was less than a given error which in our case was chosen to be

Table 1
Comparison of QLM and exact phases δ_0 (defined as $\delta_0 = \arctan a_0$, where a_0 is the scattering length) for the Yukawa potential $V(r) = -g\mathrm{e}^{-r}/r$. The distance is measured in units of R, that is, R is set to unity. The exact results were obtained by integrating the Schrödinger equation at the energy $E = 0$. m_u is the minimum QLM iteration number required in order that the absolute value of difference between successive iterations be less than 10^{-5}. The resulting absolute value of the difference $\Delta = \Delta u_{m_u+1}$ between the final QLM approximation and the exact solution is displayed in the last column where square brackets denote the powers of 10

g	m_u	QLM	Exact	$\lvert\Delta\rvert$
−5.0	9	−1.0304583	−1.03045838	8[−8]
−4.0	8	−0.98595953	−0.9859595	3[−8]
−3.0	8	−0.92085518	−0.92085518	0
−2.0	7	−0.81370645	−0.813696	1[−5]
−1.0	5	−0.59790986	−0.5979102	3[−7]
1.0	4	1.1453493	1.145350	7[−7]
2.0	5	1.6965263	1.6965297	3[−6]
3.0	6	2.0100191	2.0100207	2[−6]
4.0	8	2.5357573	2.53576	3[−6]
5.0	12	3.9818256	3.981825	6[−7]
6.0	12	4.6016314	4.601635	4[−6]
7.0	16	4.8071005	4.8071024	2[−6]

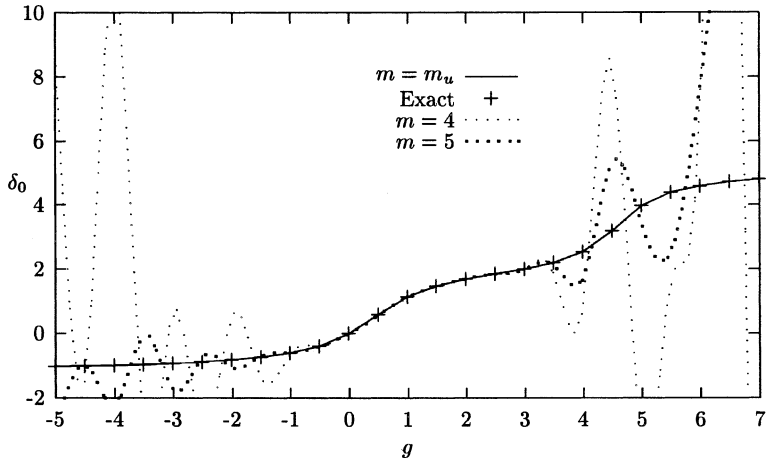

Fig. 1. Convergence of QLM iterations for the phase δ_0 of the Yukawa potential (Table 1) and comparison with the exact results.

10^{-5}. The starting, zeroth iteration was chosen to be identically equal to r. The integration was performed using the trapezoidal integration rule in order that the integration result on the left-hand side of Eq. (2.3) could be substituted at the same points in the integrand on the right-hand side of this equation for the next iteration. The results of the QLM computations are compared with exact results (found by extracting the scattering length from an accurate numerical solution of the Schrödinger equation at zero energy) in Table 1. The corresponding graphs for the first few iterations and for the last iteration as well as the exact solution are displayed in Fig. 1, while Fig. 2 shows the dependence of the number of iterations necessary to

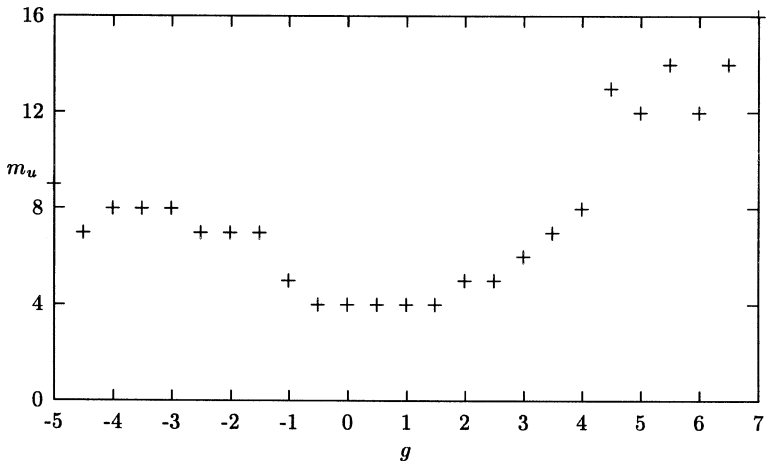

Fig. 2. Minimum QLM iteration number required in order that the absolute value of the difference between successive iterations be less than 10^{-5} for the potential of Fig. 1.

obtain five digit accuracy as a function of the coupling strength. One can see that if $\|\delta u_{n+1}\|$ is within the requested 10^{-5} accuracy the difference between the last iteration and the exact solution is also within the expected error. From Fig. 1 it follows that the largest deviations from the exact results for the first few QLM approximations occur at large absolute values of the coupling constant. Fig. 2 confirms this conclusion showing that the number of iterations necessary for the requested five digit accuracy is rather small for small and intermediate values of the coupling constant but increases for larger potential strengths. This is, of course, natural to expect since larger couplings, being coefficients before nonlinear terms, mean larger nonlinearity and require more quasilinear iterations to obtain the proper accuracy. Since the second functional derivative of the right-hand side of Eq. (3.1),

$$-V(r)\big((1-r^2)\sin 2\delta(r)+2\cos 2\delta(r)\big), \tag{3.3}$$

having no definite sign, is neither convex nor concave, the corresponding QLM iterations display no monotonicity. This could be seen from Fig. 1 where the curves corresponding to the fourth and fifth iterations oscillate around the exact solution and around each other so that the difference of these curves has no definite sign.

The kth zero energy bound state occurs when δ_0 equals $(2k+1)\pi/2$. In the interval g given in Table 1, two such states in the QLM approximation appear at values of g equal to 1.679808 and 6.44727, to be compared with the exact values of 1.679808 and 6.447261. These values were calculated as the zeros of the expression $\arctan a_0 - (2k+1)\pi/2$ where a_0 was considered a function of the coupling constant g. We see that the error of QLM in the calculation of the zero energy bound states is very small: less than 1×10^{-6}, and 1×10^{-5}, respectively.

3.2. Modified Pöschl–Teller potential

$$V(r) = -\frac{g(g-1)}{R^2\cosh^2 r/R}. \tag{3.4}$$

This potential is repulsive for $0 < g < 1$ and attractive for $g > 1$. The zero energy bound states occur [13] for g equal to an even integer. The results of exact and QLM computations performed as in the previous section are displayed in Table 2 and Figs. 3 and 4 and lead to exactly the same conclusions as in the case of the Yukawa potential. In the interval of g given in Table 2, two zero energy bound states in the QLM approximation appear at values of g equal to 1.9999991 and 4.0000028, to be compared with the exact values 2.0 and 4.0, an error of 9×10^{-7} and 2.8×10^{-6}, respectively. As in the case of the Yukawa potential we see that the bound states are reproduced extremely well in QLM computations. Since calculations, as in the previous section, were performed

Table 2
As in Table 1, but for the Pöschl–Teller potential $V(r) = -g(g-1)(\cosh r)^{-2}$ $(R = 1)$

g	m_u	QLM	Exact	$\lvert\Delta\rvert$
0.5	4	−0.18245004	−0.18244984	2[−7]
1.0	4	0.0	0.0	0
1.5	5	0.76347680	0.763476	7[−7]
2.0	4	1.5707972	1.570796	1[−6]
2.5	5	1.9081209	1.90812432	3[−6]
3.0	9	2.1587985	2.158799	2[−7]
3.5	16	3.0324501	3.0324505	4[−7]
4.0	16	4.7123861	4.712389	3[−6]
4.5	17	4.9879295	4.98793181	2[−6]
5.0	24	5.1599088	5.159909	2[−7]

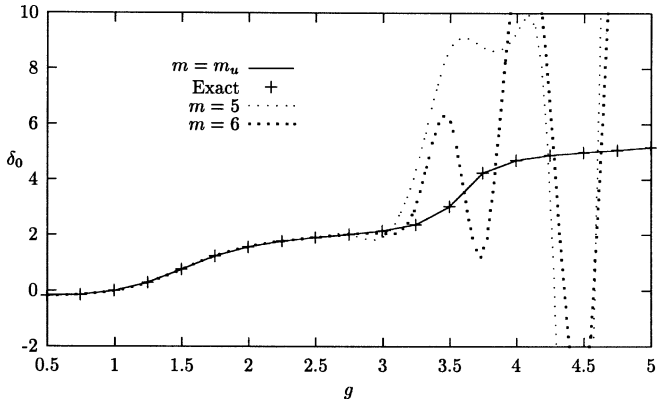

Fig. 3. As in Fig. 1, but for the Pöschl–Teller potential of Table 2.

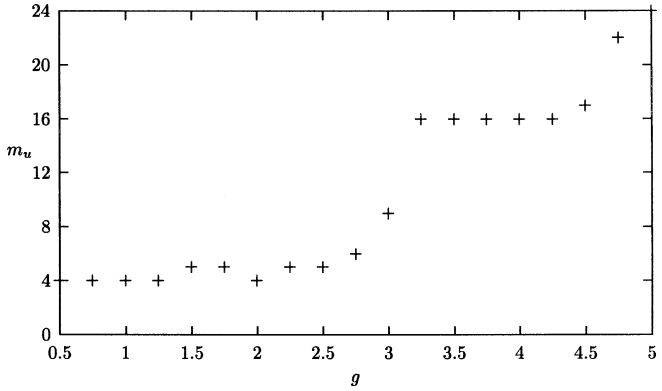

Fig. 4. Minimum QLM iteration number required in order that the absolute value of the difference between successive iterations be less than 10^{-5} for the potential of Fig. 3.

Table 3
As in Table 1, but for the scattering length a_0 for the Newton potential $V(r) = g(1 + p\mathrm{e}^{1/r})/r^4$ ($R = 1$). The choice $p = 0$ here reduces $V(r)$ to the special case $1/r^4$

g	m_u	QLM	Exact	$\lvert\Delta\rvert$
1.0	5	−0.99999987	−1.00000000	1[−7]
2.0	6	−1.41421510	−1.41421356	2[−6]
3.0	6	−1.73205380	−1.73205081	3[−6]
4.0	6	−2.00000120	−2.00000000	1[−6]
5.0	6	−2.23606960	−2.23606798	2[−6]
6.0	6	−2.44949190	−2.44948974	2[−6]
7.0	6	−2.64575400	−2.64575131	3[−6]
8.0	6	−2.82843040	−2.82842712	3[−6]
9.0	6	−3.00000100	−3.00000000	1[−6]
10.0	6	−3.16227880	−3.16227766	1[−6]

using Eq. (3.1), where the second functional derivative (3.3) of the right hand side has no definite sign, the QLM iterations converge nonmonotonically. This can be seen from Fig. 3 where the curves displaying the fifth and sixth QLM iterations are oscillating around the exact solution and around each other, so that the difference of these curves has no definite sign.

3.3. Newton supersingular potential

Our next and last example is the highly singular Newton potential [14]

$$V(r) = \frac{a^2}{(r/R)^4}\left(b^2 + c^2\mathrm{e}^{R/r}\right), \tag{3.5}$$

which in the canonical form, setting $(ab)^2 = g$, $(c/b)^2 = p$, $R = 1$ could be written as

$$V(r) = \frac{g}{r^4}\left(1 + p\mathrm{e}^{1/r}\right). \tag{3.6}$$

This potential contains a fourth order pole at the origin and for the nonzero p in addition an essential singularity there; g and p are inherently positive since the attractiveness of such a potential near the origin leads to the fall to the center [14,15].

The scattering length is given by the analytical expression

$$a_0 = -\frac{z}{2}\frac{H_\nu^{(1)'}(z)}{H_\nu^{(1)}(z)}, \tag{3.7}$$

where $\nu = 2\sqrt{g}$ and $z = 2\mathrm{i}\sqrt{gp}$. In the limit of the inverse quartic potential, when $p = 0$, this equation, using the property of the Hankel function at zero argument, $H_\nu^{(1)'}(z)/H_\nu^{(1)}(z) = -2\nu/z$, reduces to $a_0 = -\sqrt{g}$, a well known result [4,5,13]. Since for the repulsive potential no bound states are possible and the scattering length has no poles we now use Eqs. (1.1) and (2.3) to obtain the scattering length in the QLM approximation. Tables 3–5 contain our results for potential strengths g between 1 and 10 and for different values of p: $p = 0$ corresponds to pure inverse quartic potential, while $p = 1$ and $p = 10$ correspond to equal admixtures of the $1/r^4$ term and the term containing the essential singularity at the origin, and to the dominant contribution of the latter term, respectively. Since the patterns of convergence for different p are rather similar, we present the graphs only for one value of p. Namely, for $p = 1$ the first few iterations and the last iteration as well as the exact solution are displayed in Fig. 5, while Fig. 6 shows the dependence on the coupling strength of the number of iterations necessary to obtain five digit accuracy of the scattering length. We see that in this case this number always equals

Table 4
As in Table 3, but for $p = 1$

g	m_u	QLM	Exact	$\|\Delta\|$
1.0	6	−1.55117510	−1.55117440	7[−7]
2.0	6	−2.13431750	−2.13431460	3[−6]
3.0	6	−2.58243320	−2.58243170	2[−6]
4.0	6	−2.96048760	−2.96048510	2[−6]
5.0	6	−3.29370350	−3.29370260	9[−7]
6.0	6	−3.59504450	−3.59504330	1[−6]
7.0	6	−3.87221530	−3.87221380	2[−6]
8.0	6	−4.13024160	−4.13023970	2[−6]
9.0	6	−4.37261600	−4.37261370	2[−6]
10.0	6	−4.60188310	−4.60188040	3[−6]

Table 5
As in Table 3, but for $p = 10$

g	m_u	QLM	Exact	$\|\Delta\|$
1.0	6	−3.53935640	−3.53935320	3[−6]
2.0	6	−4.91444300	−4.91444030	3[−6]
3.0	6	−5.96917320	−5.96917180	1[−6]
4.0	6	−6.85821230	−6.85821020	2[−6]
5.0	6	−7.64140310	−7.64140000	3[−6]
6.0	6	−8.34941940	−8.34941840	1[−6]
7.0	6	−9.00048470	−9.00048340	1[−6]
8.0	6	−9.60646440	−9.60646280	2[−6]
9.0	6	−10.17560100	−10.17559900	2[−6]
10.0	6	−10.71389400	−10.71389200	2[−6]

6 and, due to the extreme singularity of the Newton potential, does not depend on the strength of the potential. One should stress, that unlike the QLM approach, which works perfectly well giving the accuracy of five significant figures with just six iterations even for large values of coupling constants, the perturbation treatment in this case is not possible at all even for a very small coupling. Indeed, in view of the strong singularity of the potential at the origin all the terms of the Born series for the scattering amplitude are divergent and the perturbation expansion does not exists for any coupling values [11], which is, of course, a direct consequence of the branch point singularity of the exact scattering length (3.7) at $g = 0$. Since we now use Eq. (1.1) where the second functional derivative on the right hand side,

$$-2V(r), \tag{3.8}$$

for the repulsive Newton potential is concave, the difference of subsequent QLM iterations should be strictly negative, ensuring the monotonic convergence to the exact solution from above. This, indeed, is what follows from Fig. 5, where the curve corresponding to the first iteration is lying above the curve correspond-

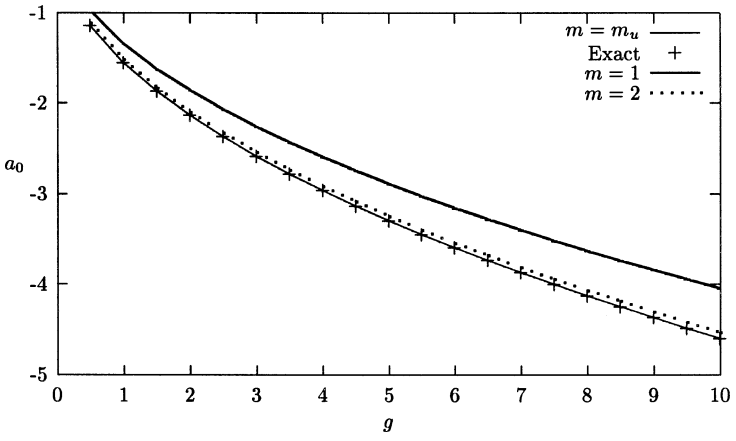

Fig. 5. As in Fig. 1, but for the scattering length a_0 for the Newton potential of Table 4 ($p = 1$).

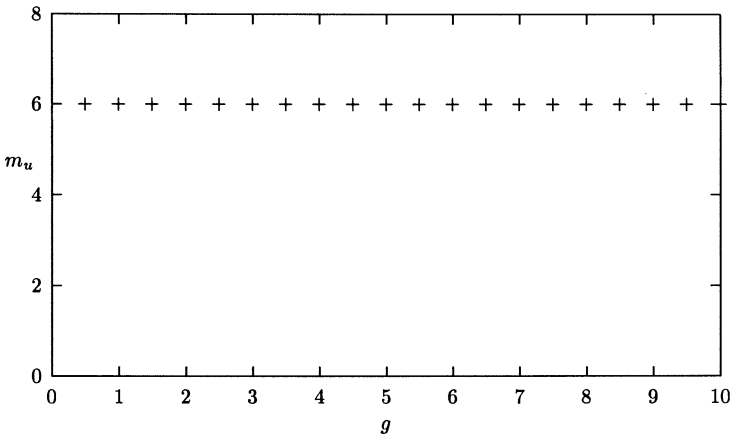

Fig. 6. Minimum QLM iteration number required in order that the absolute value of the difference between successive iterations be less than 10^{-5} for the potential of Fig. 5.

ing to the second iteration and both are lying above the exact solution as it should be.

4. Conclusion

Summing up, in order to analyze and highlight the power and features of the quasilinearization method (QLM), in this work we have made numerical computations on the nonlinear ordinary first order differential equations (1.1) and (3.1) for the S-wave scattering length $a_0 = a(\infty)$ and phase shifts δ_0, respectively, obtained in the variable phase approach [4–6]. We have considered different singular and nonsingular, attractive and repulsive potentials, namely Yukawa, Pöschl–Teller and Newton potentials, and have compared the results obtained by the quasilinearization method with the exact solutions.

Our conclusions can be formulated as follows:

(i) The QLM treats the nonlinear terms as a perturbation about the linear ones [1,2,11] and is not based, unlike perturbation theories, on the existence of some kind of small parameter. As a result, as we see on our examples, it is able to handle, unlike the perturbation theory, large values of the coupling constant.

(ii) Namely, we show that the method provides very accurate and numerically stable and fast convergent answers for any values of the coupling constant giving the accuracy of at least five significant figures required in this work. Already the first few iterations provide precise answers for small and intermediate values of the coupling constant. The number of iterations necessary to reach a given precision only moderately increases for larger values of the coupling constants.

(iii) In the case when the second functional derivative $f_{uu}(u(x), x)$ on the right-hand side of Eq. (2.1) has a definite sign, the convergence of the QLM sequence to the exact solution is monotonic from below or above depending on $f_{uu}(u(x), x)$ being convex or concave.

(iv) The method provides very accurate and numerically stable answers also for any potential strength in the case of super singular potentials for which each term of the perturbation theory is infinite and the perturbation treatment is not possible even for a very small coupling.

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 quasilinearization 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, the $1/N$ expansion, etc.

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