PHYSICAL REVIEW E, VOLUME 64, 056701

Numerically complemented analytic method for solving the time-independent one-dimensional Schrödinger equation

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(Received 7 May 2001; published 12 October 2001)

A general method of solving the one-dimensional Schrödinger equation is developed. The first step is to construct an exactly solvable reference potential of several smoothly joined Morse-type components, which should be a good approximation to a given potential. The exact solutions for that reference Hamiltonian are then combined with a nonperturbative approach [R. G. Gordon, J. Chem. Phys. **51**, 14 (1969)], which enables us to numerically solve the energy eigenvalue problem for the original potential to any desired accuracy. A full description of the analytical procedures is given and examples of both exact and numerical solutions, are presented.

DOI: 10.1103/PhysRevE.64.056701 PACS number(s): 02.60.Lj, 02.60.Jh, 03.65.Ge, 31.15.−p

I. INTRODUCTION

Seventy-five years after the birth of wave mechanics [1] the Schrödinger's famous equation still remains a subject for numerous studies, aiming at extending its field of applications and at developing more efficient solution methods. Concerning confining one-dimensional quantum systems, such a long-standing interest might seem surprising. Indeed, the relevant Schrödinger equation can always be solved numerically, which nowadays seems elementary, in view of the immensely increased computational power. However, even in this simplest case, the success of applying any direct numerical integration method depends on the quality of initial guesses for the boundary conditions and energy eigenvalues. These kinds of difficulties have stimulated development of more sophisticated integration approaches, e.g., embedded exponentially-fitted Runge-Kutta [2] and dissipative Numerov-type [3] methods, as well as interesting techniques, such as a relaxational approach [4] based on the Henyey algorithm [5], an adaptive basis set using a hierarchical finite element method [6], and an approach based on microgenetic algorithm [7], which is a variation of a global optimization strategy proposed by Holland [8].

Inevitably, to apply any numerical or other approximate method of solving the Schrödinger equation, one needs to fix the interaction potential for the system. Unfortunately, as proved long ago [9], even the complete knowledge of the discrete energy spectrum complemented with full scattering information is insufficient to ascertain a confining potential uniquely. On the other hand, one hardly could calculate an *ab initio* potential, which would be reliable in the whole physical domain. Thus, the regrettable conclusion is that one's knowledge of the real interaction potential for almost any quantum system to study is more or less incomplete.

As a kind of counterweight to this principle ambiguity, there has always been a remarkable interest in studying exactly solvable Schrödinger equations. At this point, we have to specify that traditionally the term ''exactly solvable'' has been used in a well-defined mathematical sense, meaning that eigenvalues and eigenfunctions of the Hamiltonian under consideration may be expressed in an explicit and closed form [10]. In this sense, the exact solubility has been found for only a very limited number of potentials, most of them being classified already by Infeld and Hull [11] on the basis of the Schrödinger factorization method [12], which in turn appeared to be a rediscovery of the formalism stated nearly 120 years ago by Darboux [13].

An important innovation for classifying the exactly solvable potentials was the concept of supersymmetry (SUSY) shape invariance introduced by Gendenshtein [14]. His simple and elegant method of solving the quantum-mechanical eigenvalue problem, however, was shown to be equivalent to the factorization method [15]. Another procedure for generating families of isospectral Hamiltonians has been devised by Abraham and Moses [16]. It is based on the Gel'fand-Levitan equation [17] and is, in general, inequivalent [18] to the Darboux construction. In recent years, a method of constructing nonshape-invariant so-called conditionally exactly solvable potentials has been developed [10], and several more attempts for the unified treatment of all known cases have been reported [19,20], along with a systematic search for other classes of solvable potentials.

Most works in this field concern exact solubility in the above-specified mathematical sense. For practical purposes, however, one may prefer a slightly modified definition, accepting a Hamiltonian as exactly solvable, if one can, in principle, calculate its eigenvalues and eigenfunctions with arbitrary accuracy [21], not necessarily in explicit form. In this sense, any potential giving a piecewise analytic solution of the Schrödinger equation in the whole physical domain would be exactly solvable. The latter definition also has a stronger impact on relevant numerical studies, because to some extent, any potential can be approximated by a substitute that enables a piecewise analytic solution. This kind of ''reference potential'' method was proposed over 30 years ago by Gordon [22] with an emphasis on the piecewise linear approximation of the initial potential. For any linear interval, the two independent solutions of the Schrödinger equation can be written in terms of the well-known Airy functions Ai(x) and Bi(x), nowadays available as standard functions in most math-oriented programming environments, such as MAPLE. This way Gordon elaborated an efficient numerical method. However, the real essence of his work was the deri-

1063-651X/2001/64(5)/056701(12)/$20.00

vation of a closed pair of coupled first-order differential equations, exactly equivalent to the original Schrödinger equation, but far more convenient for the numerical solution. We will make use of these equations in this paper.

Recently, the author proposed a similar approach based on several smoothly joined Morse-type potentials [23], which leads to an analytic solution in terms of the confluent hypergeometric functions, also well-studied mathematically. Compared with the linear fit, the main advantage of this approximation is the small number of analytically different components that are needed to get a good fit with the original potential (which may be of rather different shape) in a reasonably wide distance range [24]. In this paper, using the same approach, we demonstrate how easily one can solve the mentioned pair of Gordon equations to any desired accuracy, and thus, the whole energy eigenvalue problem for the original potential, provided the two linearly independent exact solutions for the reference potential are known.

The paper is organized as follows. In Sec. II, we describe the constructing of smooth Morse-type reference potentials, and the needed analytic procedures for an exact solution of the related Schrödinger equations. In Sec. III, a complete analytic solution of the Schrödinger equation for a smooth three-Morse-component potential is given. In Sec. IV, we specify Gordon equations relevant to the case, and present direct examples of their solution, in comparison with corresponding exact solutions. A possible extension of the method to many-body systems is discussed in Sec. V. Finally, some concluding remarks are presented in Sec. VI.

II. SOLUTION OF THE SCHRÖDINGER EQUATION FOR MORSE-TYPE REFERENCE POTENTIALS

A. Model

Let us consider the time-independent one-dimensional Schrödinger equation

$$\frac{d^2\Psi(R)}{dR^2}+\frac{2m}{\hbar^2}[E-U(R)]\Psi(R)=0, \tag{1}$$

where E is energy and m, the reduced masss. We will assume $U(R)$ to be an arbitrary *effective* radial potential (i.e., it may include centrifugal energy, proportional to R^{-2}) permitting a *physical* solution, meaning that $\Psi(R)\to 0$ as $R\to 0$ [25]. Throughout this paper, we will examine only bound states of $U(R)$, and therefore, for the true eigenstates, $\Psi(R)\to 0$ with $R\to\infty$ as well. In addition, we will assume that $U(R)$ has at least one minimum point (R_1).

The next step is to construct an exactly solvable substitute to the original potential. According to the general idea of the approach [23], the reference potential consists of several smoothly joined components, all having the well-known analytic form of the Morse potential [26]

$$U_k(R)=V_k+D_k[e^{-\alpha_k(R-R_k)}-1]^2,\quad k=0,1,2,\ldots\ . \tag{2}$$

Here, k is a subscript to distinguish different components, and in contrast to the classical Morse case, the parameters D_k and α_k can be negative. The number of components is arbitrary, but let us fix $k=0$ for a so-called pseudo-Morse potential, whose main peculiarity is that the parameters D_0 and α_0 are not independent, but $D_0=\hbar^2\alpha_0^2/(8m)$. It means that such a tiny potential well (if considered separately) is just of the limit depth when there is no discrete energy spectrum any more [27].

The region $X_1\leqslant R\leqslant X_2$ $(k=1)$ around the minimum point R_1 is fitted by an ordinary Morse potential, while the approximation in the long-distance region depends on the shape of the original potential. Let us assume that it approaches a finite limit as $R\to\infty$. Then the region $R\geqslant X_2$ $(k=2)$ is fitted by a ‘‘reversed’’ Morse potential, with a parameter D_2 being negative.

The latter approximation probably needs to be commented. Indeed, by introducing such a reversed potential one actually prescribes a maximum (at R_2) to the reference potential, which seems unjustified. However, even if there is no hump on the original potential curve, one may choose an arbitrarily large value for R_2 to create a tiny hump (the absolute value of D_2 being very small) in the far long-distance region of the reference potential. This artificial trick has an almost negligible effect on the solutions of the Schrödinger equation, but has proved very useful for the unified treatment.

Now, having fixed the number and the analytic form of the components, their parameters can be determined from an appropriate least squares’ fit to the original potential. In principle, one may introduce some boundary conditions at X_1, X_2, etc. To be more specific, we will require continuity of the reference potential and its first derivative at these boundary points. From the ‘‘pure’’ quantum-mechanical point of view there is no need for any further constraints regarding the reference potential. On the other hand, by requiring its smoothness at the boundary points, we will essentially decrease the number of independent paramaters, and the remaining ones can therefore be determined more easily. In addition, the smooth reference potential is more ‘‘physical’’ and can often be used simply as an exactly solvable substitute to the original potential, without any need for the additional numerical procedures, which we describe in Sec. IV. However, the smooth merging of Morse-type functions is not always possible. In such cases one may, of course, give up with the ‘‘voluntary’’ requirement of the derivative’s continuity or use linear fitting in a tiny ‘‘critical’’ range. Further treatment concerns reference potentials that entirely consist of smoothly joined Morse-type components.

Naturally, there are no restrictions for introducing much more than just three exactly solvable components, to achieve a better fit with the original potential. For example, one could introduce additional pseudo-Morse components $(k=-1,-2,-3,\ldots,)$, but with an eye to the efficacy of the method, it is recommended to keep the number of components as low as possible. Therefore, in this paper we will examine reference potentials having no more than three constituents in total, including no more than one (if any) pseudo-Morse component $(k=0)$, used for the small-distance region $0\leqslant R\leqslant X_1$.

TABLE I. The quantities related to Eq. (4).

	$R\leqslant X_1$	$X_1\leqslant R\leqslant X_2$ $E\leqslant V_1+D_1$	$X_1\leqslant R\leqslant X_2$ $E\geqslant V_1+D_1$	$R\geqslant X_2$ $E\leqslant V_2+D_2$
b	1/2	a_1	a_1	ia_2
c	$i\beta_0$	μ_1	$i\beta_1$	μ_2
x	y_0	y_1	y_1	iy_2

B. General solution scheme

Let us briefly recall the solution scheme for Morse-type potentials. First, one introduces dimensionless variables $y_k=2a_k\exp[-\alpha_k(R-R_k)]$, where the subscripts $k=0,1,2$ have the same meaning as specified in the previous subsection, and $a_k=\sqrt{2mD_k}/(\hbar\alpha_k)$. The relevant Schrödinger equations then read

$$\frac{d^2\Psi(y_k)}{dy_k^2}+\frac{1}{y_k}\frac{d\Psi(y_k)}{dy_k}+\left[-\frac{\mu_k^2}{y_k^2}\pm\left(\frac{a_k}{y_k}-\frac{1}{4}\right)\right]\Psi(y_k)=0, \tag{3}$$

where the plus sign in square brackets corresponds to the subscripts $k=0$ and $k=1$, and minus–to $k=2$. The quntities μ_k^2 are defined as follows: $\mu_k^2=(a_k^2/D_k)\cdot(V_k+D_k-E)$. Note that $D_2<0, a_0=1/2$ and μ_0 is a pure imaginary quantity for any bound state of the reference potential, since always $E>V_0+D_0$.

Next, using a transformation $\Psi\sim\exp(-x/2)x^cG(b,c;x)$, one converts Eq. (3) into the confluent hypergeometric form

$$x\frac{d^2G(b,c;x)}{dx^2}+(2c+1-x)\frac{dG(b,c;x)}{dx}+(b-c-1/2)G(b,c;x)=0, \tag{4}$$

with the parameters b,c, and the dimensionless coordinate x, which for different energy and distance regions are specified in Table I ($\beta_k\equiv|\mu_k|$):

The fundamental solution of Eq. (3) may be always built up of the special solutions $G_1\equiv\Psi(-b+c+1/2,2c+1;x)$ and $G_2\equiv\exp(x)\Psi(b+c+1/2,2c+1;-x)$ [28], containing special functions introduced by Tricomi [29], which for sufficiently large x, can be evaluated from the asymptotic series

$$\Psi(a,c;x)=x^{-a}\sum_{n=0}^{N}\frac{(a)_n(a-c+1)_n}{n!(-x)^n}, \tag{5}$$

where $(a)_n\equiv\Gamma(a+n)/\Gamma(a)=a(a+1)(a+2)\cdots(a+n-1)$ is the Pochhammer symbol, and N must not be too large. This simple formula may not work for smaller x, directing one to a more complicated but universal expansion [28]

$$\Psi(a,c;x)=\frac{\Gamma(1-c)}{\Gamma(a+1-c)}\Phi(a,c;x)+\frac{\Gamma(c-1)}{\Gamma(a)}x^{1-c}\times\Phi(a+1-c,2-c;x), \tag{6}$$

where the symbols

$$\Phi(a,c;x)=1+\frac{a}{c}\frac{x}{1!}+\frac{a(a+1)}{c(c+1)}\frac{x^2}{2!}+\cdots \tag{7}$$

denote the well-known confluent hypergeometric functions. Equivalently, the general solution of Eq. (4) can be directly constructed from $F_1\equiv\Phi(-b+c+1/2,2c+1;x)$ and $F_2\equiv x^{-2c}\Phi(-b-c+1/2,-2c+1;x)$.

C. Solutions for a two-Morse-component potential

In Sec. IV, to illustrate the solution of Gordon equations, we will make use of a reference potential, which consists of only two components: an ordinary Morse potential ($k=1$), and a reversed potential ($k=2$), smoothly joined at a boundary point X_2. The most convenient unified form of the two linearly independent solutions of Eq. (3) for this case is as follows:

$$\Psi_{k1}=\exp(-x_k/2)x_k^{\mu_k}\Phi(-b_k+\mu_k+1/2,2\mu_k+1;x_k), \tag{8}$$

$$\Psi_{k2}=\exp(-x_k/2)x_k^{-\mu_k}\Phi(-b_k-\mu_k+1/2,-2\mu_k+1;x_k),\quad k=1,2. \tag{9}$$

Note that, according to Table I, $b_1=a_1, b_2=ia_2, x_1=y_1, x_2=iy_2$, and $\mu_1=i\beta_1$ is a pure imaginary quantity in the energy range $E\geqslant V_1+D_1$. Naturally, when looking for the true bound states (which is not our goal in this section), one has to choose the correct linear combination of Eqs. (8) and (9), which means, for example, that Ψ_{22} should be omitted due to its unphysical asymptotic behavior as $R\to\infty$.

We will also need explicit expressions for the derivatives of Eqs. (8) and (9) in the range $R\leqslant X_2$, which read

$$\frac{d\Psi_{11}}{dR}=\alpha_1e^{-y_1/2}y_1^{\mu_1}\{[(y_1+1)/2-a_1]F(\mu_1)+(a_1-\mu_1-1/2)F^{+}(\mu_1)\}, \tag{10}$$

$$\frac{d\Psi_{12}}{dR}=\alpha_1e^{-y_1/2}y_1^{-\mu_1}\{[(y_1+1)/2-a_1]F(-\mu_1)+(a_1+\mu_1-1/2)F^{+}(-\mu_1)\}, \tag{11}$$

with $F(\mu_1)\equiv\Phi(-a_1+\mu_1+1/2,2\mu_1+1;y_1)$ and $F^{+}(\mu_1)\equiv\Phi(-a_1+\mu_1+3/2,2\mu_1+1;y_1)$.

III. EXACTLY SOLVABLE THREE-COMPONENT REFERENCE POTENTIAL

Our main analytic goal in this paper is the exact solution of the energy eigenvalue problem for the three-component smooth Morse-type reference potential, as specified above. In this case, the physical domain is divided into three analytically different subregions $(0,X_1),(X_1,X_2)$, and (X_2,∞), described in terms of pseudo-Morse, ordinary, and reversed Morse potential, respectively. Concerning true bound states, we have to take account of the general boundary conditions

$\Psi(R)\to 0$ as $R\to 0$ or $R\to\infty$. Since there are two equivalent possibilities of constructing the physical solution (see Sec. II B), we can always choose just that one that better suits our purposes.

The wave function's logarithmic derivative, which plays so important a role in SUSY quantum mechanics, here forms the basis for ascertaining the true eigenstates. Indeed, for any energy E within the scope, one can formally find two independent solutions of the Schrödinger equation, vanishing as $R\to 0$ or $R\to\infty$, respectively. From continuity requirements one therefore gets two estimations for the logarithmic derivative of the physical solution at any reference point $R\in(0,\infty)$. Naturally, these two independent estimations of the same quantity can only coincide for the true energy eigenvalues $E=E_n$. Consequently, the demand of continuity of the wave function's logarithmic derivative at an arbitrary reference point represents a universal quantization rule for multicomponent confining potentials. Having found the true eigenvalues, one then fixes the relevant normalization factors from demand of continuity of the wave function at the boundary points X_1 and X_2.

We will often exploit a very useful Tricomi expansion of the confluent hypergeometric functions through the Bessel functions [30], whose quantum-mechanical content becomes transparent in terms of the following S functions [23], used throughout this paper

$$S(a,\mu;x)\equiv e^{-x/2}\Phi(-a+\mu+1/2,2\mu+1;x)=\sum_{n=0}^{\infty}B_n, \tag{12}$$

where $B_0=1$, $B_1=-ax/(2\mu+1)$, $B_n=x(-aB_{n-1}+xB_{n-2}/4)/[n(2\mu+n)]$, $n=2,3,\ldots$.

A. Solution in the small-distance range $0\leqslant R\leqslant X_1$ ($k=0$)

In this region the special solution of Eq. (4) $G_2\to\infty$ as $R\to 0$ (i.e., $x\to\infty$), and should therefore be omitted. Thus, substituting $y_0=\exp(-\alpha(R-R_0))$ and making use of Eqs. (6) and (12), one immediately gets the right solution

$$\Psi_0=N_0C_0(y_0)\cos[\varphi_0+D_0(y_0)-\alpha_0\beta_0R], \tag{13}$$

where N_0 is the normalization factor,

$$\begin{aligned}C_0(y_0)e^{iD_0(y_0)}&\equiv S(1/2,i\beta_0;y_0)\\&=1-\frac{y_0/4}{\beta_0+1/2}+\frac{(y_0/4)^2}{(\beta_0+1/2)1!}\left(1-\frac{y_0/4}{\beta_0+3/2}\right)\\&\quad+\frac{(y_0/4)^4}{(\beta_0+1/2)(\beta_0+3/2)2!}\left(1-\frac{y_0/4}{\beta_0+5/2}\right)\\&\quad+\cdots,\end{aligned} \tag{14}$$

and the phase shift can be calculated from an exact formula (see [24] for details)

$$\begin{aligned}\varphi_0&\equiv\alpha_0\beta_0R_0-\arg[\Gamma(2i\beta_0)/\Gamma(i\beta_0)]\\&=\beta_0\left[\alpha_0R_0+1-\ln 2-\frac{1}{2}\ln(1+4\beta_0^2)\right]\\&\quad+\frac{1}{2}\int_0^{\infty}\left(\coth t-\frac{1}{t}\right)e^{-t}\sin(2\beta_0t)\frac{dt}{t}.\end{aligned} \tag{15}$$

The integral in Eq. (15) can be, in principle, calculated analytically, but is more conveniently evaluated numerically, using the expansion

$$\begin{aligned}I(\omega)&\equiv\int_0^{\infty}\left(\coth t-\frac{1}{t}\right)e^{-t}\sin(\omega t)\frac{dt}{t}\\&=\int_0^{T}e^{-t}\sin\left(\pi\frac{t}{T}\right)f(t)dt,\end{aligned} \tag{16}$$

with $T=\pi/\omega$ and

$$\begin{aligned}f(t)&=\frac{\coth t-1/t}{t}-e^{-T}\frac{\coth(t+T)-1/(t+T)}{t+T}\\&\quad+e^{-2T}\frac{\coth(t+2T)-1/(t+2T)}{t+2T}-\cdots.\end{aligned}$$

The wave function's logarithmic derivative then becomes

$$\frac{\Psi_0'}{\Psi_0}=\alpha_0\left\{\frac{y_0}{2}+\beta_0\frac{C_{00}(y_0)}{C_0(y_0)}\frac{\sin[\varphi_0+D_{00}(y_0)-\alpha_0\beta_0R]}{\cos[\varphi_0+D_0(y_0)-\alpha_0\beta_0R]}\right\}, \tag{17}$$

where $C_{00}(y_0)e^{iD_{00}(y_0)}\equiv S(1/2,i\beta_0;-y_0)$, in accordance with Eq. (12) and the general relation [28]

$$\begin{aligned}&\exp(-y_0/2)\Phi(i\beta_0+1,2i\beta_0+1;y_0)\\&\quad=\exp(y_0/2)\Phi(i\beta_0,2i\beta_0+1;-y_0).\end{aligned} \tag{18}$$

B. Solutions for central $X_1\leqslant R\leqslant X_2$ ($k=1$) and long-distance $R\geqslant X_2$ ($k=2$) regions

In the range $R\geqslant X_2$, the solution Ψ_{22} given by Eq. (9) tends to infinity as $R\to\infty$, and should be omitted. In accordance with Eqs. (8) and (12), one then immediately gets the solution

$$\Psi_2=N_2y_2^{\mu_2}S(ia_2,\mu_2;iy_2), \tag{19}$$

where N_2 is a normalization factor. The relevant logarithmic derivative becomes

$$\begin{aligned}\frac{\Psi_2'}{\Psi_2}=\alpha_2&\left\{\frac{S(ia_2,\mu_2+1;iy_2)}{S(ia_2,\mu_2;iy_2)}\frac{y_2^2}{8(\mu_2+1)}\left[1+\frac{a_2^2}{(\mu_2+1/2)^2}\right]\right.\\&\left.-\mu_2-\frac{a_2y_2}{2\mu_2+1}\right\}.\end{aligned} \tag{20}$$

In the central region $X_1\leqslant R\leqslant X_2$ where an ordinary Morse approximation is used, one has to examine the general solution built up of Eqs. (8) and (9), while according to Table I, the two energy regions $E \leqslant V_1 + D_1$ and $E \geqslant V_1 + D_1$ should be treated separately.

The case $E \geqslant V_1 + D_1$, when special solutions from Eqs. (8) and (9) become complex conjugate to each other, is more simple for the analysis (naturally, there are no real bound states in this range, if $V_1 + D_1 > V_2 + D_2$, which is typical to potentials with pronounced humps [31]). As the energy eigenfunction for any nondegenerate state should be real (apart from inessential phase factor) [27], the general solution and its logarithmic derivative read [23]

$$\Psi_> = N_1 C_1(y_1) \cos[\varphi_1 + D_1(y_1) - \alpha_1 \beta_1 R], E \geqslant V_1 + D_1, \tag{21}$$

$$\begin{aligned} \frac{1}{\alpha_1} \frac{\Psi'_>}{\Psi_>} &= (a_1 - 1/2) \frac{C_{11}(y_1) \cos[\varphi_1 + D_{11}(y_1) - \alpha_1 \beta_1 R]}{C_1(y_1) \cos[\varphi_1 + D_1(y_1) - \alpha_1 \beta_1 R]} \\ &\quad + \beta_1 \frac{C_{11}(y_1) \sin[\varphi_1 + D_{11}(y_1) - \alpha_1 \beta_1 R]}{C_1(y_1) \cos[\varphi_1 + D_1(y_1) - \alpha_1 \beta_1 R]} \\ &\quad + \frac{y_1 + 1}{2} - a_1, \end{aligned} \tag{22}$$

where $C_1(y_1) e^{iD_1(y_1)} \equiv S(a_1, i\beta_1; y_1)$, $C_{11}(y_1) e^{iD_{11}(y_1)} \equiv S(a_1 - 1, i\beta_1; y_1)$, while the constants N_1 and φ_1 should be determined from the boundary conditions at X_1 and X_2. Thus, from condition $\Psi'_0(E, X_1)/\Psi_0(E, X_1) = \Psi'_>(E, X_1)/\Psi_>(E, X_1)$ one easily gets the relation between the phase constants φ_0 and φ_1. Then, using Eq. (22), one calculates the logarithmic derivative $\Psi'_>(E, X_2)/\Psi_>(E, X_2)$ and compares it with the estimation for $\Psi'_2(E, X_2)/\Psi_2(E, X_2)$ obtained from Eq. (20). As explained above, these two independent estimations of the same quantity can only coincide for the true energy eigenvalues $E = E_n$.

In the range $E \leqslant V_1 + D_1$, the most convenient form for the solution is

$$\Psi_< = N_1^{(+)} y_1^{\mu_1} S(a_1, \mu_1; y_1) + N_1^{(-)} y_1^{-\mu_1} S(a_1, -\mu_1; y_1), \quad E \leqslant V_1 + D_1, \tag{23}$$

where $N_1^{(+)}$ and $N_1^{(-)}$ are some real constants to be determined from the boundary conditions. Correspondingly, the wave function's logarithmic derivative reads

$$\begin{aligned} \frac{1}{\alpha_1} \frac{\Psi'_<}{\Psi_<} &= (a_1 - 1/2) \frac{N_1 y_1^{\mu_1} S(a_1 - 1, \mu_1; y_1) + y_1^{-\mu_1} S(a_1 - 1, -\mu_1; y_1)}{N_1 y_1^{\mu_1} S(a_1, \mu_1; y_1) + y_1^{-\mu_1} S(a_1, -\mu_1; y_1)} \\ &\quad - \mu_1 \frac{N_1 y_1^{\mu_1} S(a_1 - 1, \mu_1; y_1) - y_1^{-\mu_1} S(a_1 - 1, -\mu_1; y_1)}{N_1 y_1^{\mu_1} S(a_1, \mu_1; y_1) + y_1^{-\mu_1} S(a_1, -\mu_1; y_1)} + \frac{y_1 + 1}{2} - a_1, \end{aligned} \tag{24}$$

where $N_1 \equiv N_1^{(+)}/N_1^{(-)}$. Using Eq. (24) and requiring, as usual, continuity of the logarithmic derivative, one comes to the following quantization equation:

$$\begin{aligned} &\frac{[F_{01} S(a_1, -\mu_1; y_{11}) - B_1 S(a_1 - 1, -\mu_1; y_{11})] \exp(y_{11}/2 + 2\mu_1 \alpha_1 X_1)}{F_{01} \Phi(-A_1, 2\mu_1 + 1; y_{11}) - A_1 \Phi(-A_1 + 1, 2\mu_1 + 1; y_{11})} \\ &\quad = \frac{[F_{12} S(a_1, -\mu_1; y_{12}) - B_1 S(a_1 - 1, -\mu_1; y_{12})] \exp(y_{12}/2 + 2\mu_1 \alpha_1 X_2)}{F_{12} \Phi(-A_1, 2\mu_1 + 1; y_{12}) - A_1 \Phi(-A_1 + 1, 2\mu_1 + 1; y_{12})}, \end{aligned} \tag{25}$$

where $y_{11} \equiv y_1(X_1), y_{12} \equiv y_1(X_2), F_{01} \equiv \Psi'_0(X_1)/[\alpha_1 \Psi_0(X_1)] + a_1 - (y_{11} + 1)/2$, $F_{12} \equiv \Psi'_2(X_2)/[\alpha_1 \Psi_2(X_2)] + a_1 - (y_{12} + 1)/2$, $A_1 \equiv a_1 - 1/2 - \mu_1$, and $B_1 \equiv a_1 - 1/2 + \mu_1$.

Slightly rearranging and taking the logarithm of Eq. (25), the quantization condition can be written in a more compact form

$$F(E) \equiv \ln \left| \frac{T_1(E)}{T_2(E)} \right| - \frac{y_{11} - y_{12}}{2} + 2\mu_1 \alpha_1 (X_2 - X_1) = 0, \tag{26}$$

where

$$\begin{aligned} T_1(E) &= A_1 F_{12} \Phi_{11}^+ S_{12} - F_{01} F_{12} \Phi_{11} S_{12} - A_1 B_1 \Phi_{11}^+ S_{12}^+ \\ &\quad + B_1 F_{01} \Phi_{11} S_{12}^+, \end{aligned} \tag{27}$$

$$\begin{aligned} T_2(E) &= A_1 F_{01} \Phi_{12}^+ S_{11} - F_{01} F_{12} \Phi_{12} S_{11} - A_1 B_1 \Phi_{12}^+ S_{11}^+ \\ &\quad + B_1 F_{12} \Phi_{12} S_{11}^+, \end{aligned} \tag{28}$$

in terms of the functions $\Phi_{1k} \equiv \Phi(-A_1, 2\mu_1 + 1; y_{1k}), \Phi_{1k}^+ \equiv \Phi(-A_1 + 1, 2\mu_1 + 1; y_{1k}), S_{1k} \equiv S(a_1, -\mu_1; y_{1k})$, and $S_{1k}^+ \equiv S(a_1 - 1, -\mu_1; y_{1k})$ for $k = 1,2$.

Thus, according to Eq. (26), the energy eigenvalues in the range $E \leqslant V_1 + D_1$ may be determined as the zeros of the function $F(E)$. Note that $T_1(E)/T_2(E) > 0$ for any physical solution, i.e., in this sense, Eqs. (25) and (26) are equivalent. However, Eq. (26) contains some additional solutions, which should be ruled out by the zero-searching algorithm. First, there may be such unphysical zeros E_n for which

$T_1(E_n)/T_2(E_n)<0$. Second, it can be shown that $F(E)\rightarrow 0$ as $\mu_1 \rightarrow \mu_N \equiv N-1/2$, where N is a positive integer. These kinds of solutions are also unphysical. Indeed, according to the well-elaborated theory of confluent hypergeometric equations [28], the special solutions F_1 and F_2 of Eq. (4) are not linearly independent, if $2\mu_1+1=N$, which means that in this case the general solution should be written in terms of the Tricomi functions G_1 and G_2 (see Sec. II B). Since one of them (G_2) will contain a logarithm of a negative argument, there is no way to construct a general solution for the relevant Schrödinger Eq. (3), which would be real. Consequently, any solution of Eq. (26) with $2\mu_1+1=N$ should be excluded. To this end one may, for example, search for a zero in an energy range fixed by neighboring μ_N values: $E_N=V_1+D_1(1-(N-1)^2/4a_1^2)$ and $E_{N+1}=V_1+D_1(1-N^2/4a_1^2)$. Now, if one finds a zero E_n within the range (E_{N+1},E_N), and $T_1(E_n)/T_2(E_n)>0$, this will definitely be a true energy eigenvalue.

C. Examples of exact solution

We have calculated the whole spectrum of bound states for a smooth three-Morse-component potential whose parameters were specified elsewhere [31]. The continuity of the potential and its first derivative at the boundary points $X_1=2.95$ Å and $X_2=5.08$ Å has been demanded, and an additional condition $U(X_0)=U_0$ ($X_0=2.7$ Å, $U_0=3$ eV) has been used to fix the pseudo-Morse component. This potential, which is shown in Fig. 1, is realistic for the excimer Xe_2^* in 0_u^+ state, but here it is used as a model potential to test the elaborated method of solving the Schrödinger equation.

A set of energy eigenvalues for the two- and three-component potentials (pseudo-Morse constituent being absent in the first case) are presented in Table II. Note that although the three-component levels are slightly ''lifted up'' by the pseudo-Morse potential wall, their total number remains unchanged ($n_{\max}=90$). Some typical illustrations related to the zero-searching procedure of $F(E)$ are presented in Fig. 2, while Fig. 3 demonstrates the shape of the relevant normalized energy eigenfunctions.

IV. SOLUTION OF THE ENERGY EIGENVALUE PROBLEM FOR THE ORIGINAL POTENTIAL

A. Gordon method

Suppose we have constructed an exactly solvable reference potential $U_0(R)$, a good approximation to the original potential $U(R)$ in some limited distance range. Correspondingly, the exact solutions of the Schrödinger equation for $U_0(R)$ provide reasonable estimations to those for $U(R)$, as well. In this section, however, we try to improve these estimations to a desired degree of accuracy.

Let $A_0(R)$ and $B_0(R)$ be two linearly independent exact solutions of the reference Schrödinger equation for a given energy E, which, in general, is not any true eigenvalue. The basic idea of the Gordon method [22] is to express the general solution $\Psi(R)$ of Eq. (1) in terms of the special solutions for $U_0(R)$:

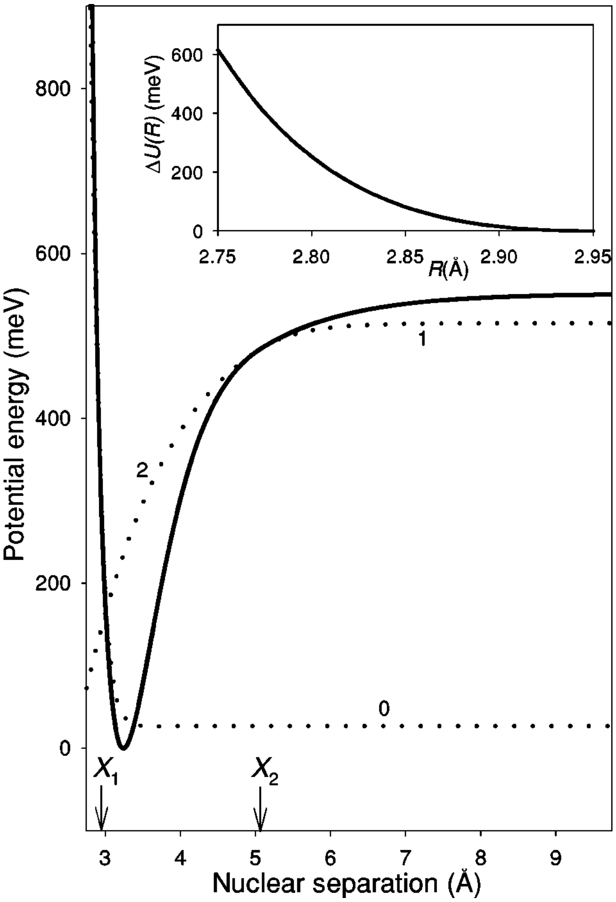

FIG. 1. Three-component model potential analyzed in this paper. Pseudo-Morse (0) and ordinary Morse (1) potentials are smoothly joined at $X_1=2.95$ Å, while a smooth ''transition'' to reversed Morse potential (2) occurs at $X_2=5.08$ Å. Dotted lines show the components' behavior outside their range of applicability. Although invisible in the scale of the figure, the pseudo-Morse potential has a minimum at $R_0=3.7028$ Å. The difference between three- and two-component potentials is brought forth in the inset.

$$\Psi(R)=a(R)A(R)+b(R)B(R), \tag{29}$$

where $A(R)=a_0A_0(R)$, $B(R)=b_0B_0(R)$, and the constants a_0 and b_0 were introduced to ensure just the right linear combination of the reference solutions in Eq. (29). Gordon demonstrated that the wave function's derivative can also be expressed in terms of the functions $a(R)$ and $b(R)$

$$\Psi'(R)=a(R)A'(R)+b(R)B'(R). \tag{30}$$

The essence of the method is the pair of equations for the expansion coefficients

$$a'(R)=-\frac{2m}{\hbar^2}W^{-1}B(R)[U(R)-U_0(R)][A(R)a(R)+B(R)b(R)], \tag{31}$$

TABLE II. Exact positions of the upper vibrational levels ($n=52$–90) for the specified two- and three-component models. All energies [in (meV)] are calculated relative to the bottom of the potential well.

n	2 Morse	3 Morse	*n*	2 Morse	3 Morse	*n*	2 Morse	3 Morse
52	492.454	492.773	65	525.885	526.127	78	544.100	544.238
53	495.756	496.071	66	527.750	527.985	79	545.010	545.139
54	498.911	499.221	67	529.531	529.758	80	545.856	545.976
55	501.927	502.232	68	531.229	531.449	81	546.639	546.751
56	504.816	505.116	69	532.847	533.059	82	547.360	547.464
57	507.581	507.875	70	534.387	534.591	83	548.021	548.116
58	510.231	510.519	71	535.851	536.047	84	548.621	548.707
59	512.768	513.051	72	537.243	537.429	85	549.162	549.239
60	515.199	515.476	73	538.557	538.737	86	549.643	549.711
61	517.528	517.798	74	539.803	539.974	87	550.065	550.124
62	519.757	520.021	75	540.978	541.141	88	550.427	550.478
63	521.891	522.148	76	542.086	542.240	89	550.730	550.771
64	523.933	524.183	77	543.126	543.272	90	550.971	551.002

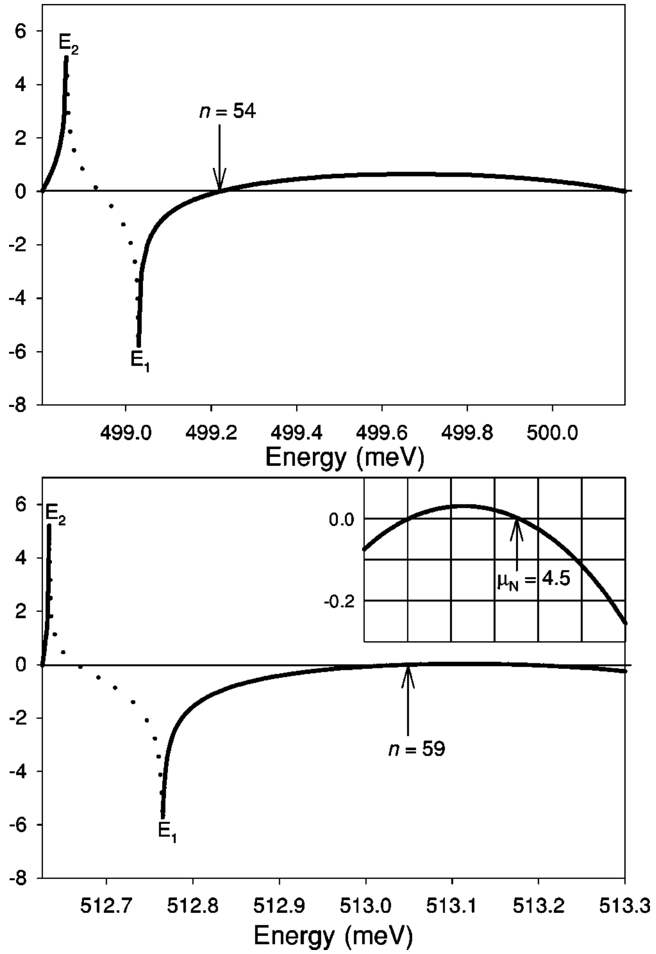

FIG. 2. Energy dependence of the quantization function $F(E)$ for the levels $n=54$ and 59 whose exact positions are shown by arrows. Discontinuity points E_1 and E_2 are related to the zeros of Eqs. (27) and (28), respectively, while the dotted lines denote unphysical regions where $T_1(E)/T_2(E)<0$. The energy range in the upper graph is fixed by $\mu_N=12$ and $\mu_N=11.5$, and the starting point of the lower graph corresponds to $\mu_N=5$.

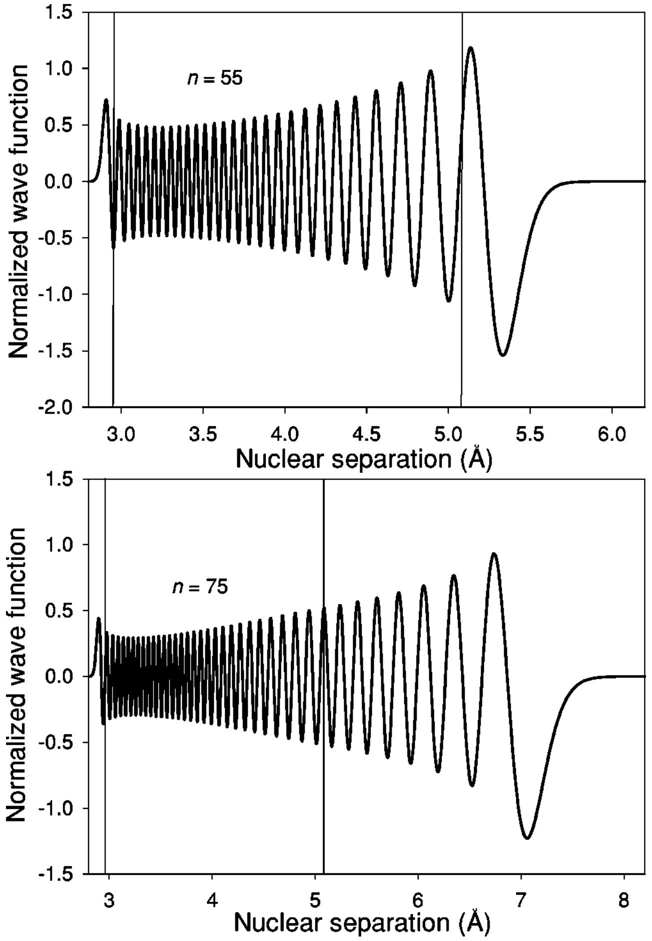

FIG. 3. Normalized wave functions of the eigenstates $n=55$ and 75 for the three-component model potential. Thin vertical lines in both graphs separate the three analytically different regions for the model potential used: $R \leqslant 2.95$ Å, $R \in (2.95$ Å$, 5.08$ Å$)$, and $R \geqslant 5.08$ Å.

$$b'(R)=\frac{2m}{\hbar^2}W^{-1}A(R)[U(R)-U_0(R)][A(R)a(R)+B(R)b(R)], \tag{32}$$

where $W=a_0b_0W_0$ and $W_0\equiv A_0(R)B_0'(R)-A_0'(R)B_0(R)$ is the Wronskian of the reference solutions $A_0(R)$ and $B_0(R)$, independent of *R*, as needed.

Equations (31) and (32) are mathematically equivalent to Eq. (1), but far more convenient in the sense of ease of numerical solution. Indeed, compared with the rapidly oscillating solutions of the original Schrödinger equation, the expansion coefficients $a(R)$ and $b(R)$ are slowly varying functions, since their derivatives are proportional to the difference of two close potentials. Naturally, the functional form of $a(R)$ and $b(R)$ related to analytically different parts of the reference potential is also different. Correlation between these different pairs of coefficients is determined by the continuity conditions of the wave function and its derivative at the boundary points, in accordance with Eqs. (29) and (30).

To solve Eqs. (31) and (32) we have to fix appropriate initial conditions. Suppose we have determined the farthest left-side extremum point R_L of the wave function (a completely analogous approach can be related to the wave function's farthest right-side extremum point R_R). Then, according to Eq. (30)

$$\frac{a_0}{b_0}=-\frac{b_1}{a_1}\frac{B_0'(R_L)}{A_0'(R_L)}, \tag{33}$$

where $a_1\equiv a(R_L)$ and $b_1\equiv b(R_L)$. Now, let us define dimensionless functions $y(R)\equiv a(R)/a_1, z(R)\equiv b(R)/b_1$, to get transformed Gordon equations

$$y'(R)=-\frac{\Delta U(R)}{W_0}\frac{B_0(R)}{B_0'(R_L)}[B_0'(R_L)A_0(R)y(R)-A_0'(R_L)B_0(R)z(R)], \tag{34}$$

$$z'(R)=-\frac{\Delta U(R)}{W_0}\cdot\frac{A_0(R)}{A_0'(R_L)}[B_0'(R_L)A_0(R)y(R)-A_0'(R_L)B_0(R)z(R)], \tag{35}$$

with $\Delta U(R)=U(R)-U_0(R)$ and the initial conditions $y(R_L)=1, z(R_L)=1$.

Fortunately, the farthest extremum points can be ascertained easily and accurately for any given energy *E*. Indeed, one may choose a trial value R_1 for R_L and fix arbitrarily $\Psi_1\equiv\Psi(R_1)$. Then, using the condition $\Psi'(R_1)=0$ and choosing a suitably small step Δ, one applies, for example, the Numerov method to calculate $\Psi_0\equiv\Psi(R_0)$ at the neighboring nodal point $R_0=R_1+\Delta$:

$$\Psi_0=\frac{1+(\Delta^2)/12(5w_1-3\varepsilon-2w_2)-(5\Delta^4)/72(\varepsilon-w_1)(\varepsilon-w_2)}{1+(\Delta^2)/8(2\varepsilon-w_0-w_2)+(\Delta^4)/72(\varepsilon-w_0)(\varepsilon-w_2)}\Psi_1, \tag{36}$$

where $\varepsilon\equiv(2mE)/\hbar^2$ and $w_k\equiv[2mU(R_k)]/\hbar^2$ with $R_k=R_0-k\Delta$. Thereafter, one uses the Numerov method in its traditional form (see, e.g., [32]) to get

$$\Psi_{k+1}\equiv\Psi(R_{k+1})=\frac{2\Psi_k-\Psi_{k-1}+(\Delta^2)/12[10(w_k-\varepsilon)\Psi_k+(w_{k-1}-\varepsilon)\Psi_{k-1}]}{1-(\Delta^2)/12(w_{k+1}-\varepsilon)},\quad k=1,2,\ldots . \tag{37}$$

The proposed method is convenient and sensitive for determining the solution with correct asymptotic behavior, i.e., vanishing as $R\rightarrow 0$. Indeed, the solutions with ''wrong'' trial value for R_L will rapidly tend to infinity as $R\rightarrow 0$ (see Fig. 4). An analogous procedure may be applied for locating the farthest right-side extremum point R_R for the wave function, vanishing as $R\rightarrow\infty$.

The solution of the energy eigenvalue problem for the original potential $U(R)$ now becomes straightforward. For any trial value of *E*, one first locates the extremum points R_L and R_R for the two solutions, which are asymptotically correct at one end of the physical domain. Thereafter, one solves numerically the pair of Gordon Eqs. (34) and (35) (and their analogues adjusted to R_R), to get two independent estimations for the wave function's logarithmic derivative at an arbitrary reference point $R\in(R_L,R_R)$. As explained in Sec. III, these two estimations can only coincide for the true eigenvalues $E=E_n$. Examples to the described procedures will be given in the next section.

To complete the analysis of the general form of Gordon equations, let us examine the case when the special solutions for the reference potential are complex conjugates, i.e., $A^*(R)=B(R)$. With reference to the real physical solution in the form of Eq. (29), it then follows that $A_0^*(R)=B_0(R)$ and $a_0^*(R)=b_0(R)$. Defining $x(R)\equiv y(R)B_0'(R_L)$, one may unify Eqs. (34) and (35)

$$x'(R)=-\frac{\Delta U(R)B_0(R)}{W_0}[A_0(R)x(R)-A_0^*(R)x^*(R)]. \tag{38}$$

Thus, introducing a complex function $x(R)\equiv X(R)|B_0'(R_L)|\exp[i\varphi(R)]$, putting $A_0(R)\equiv|A_0(R)|$

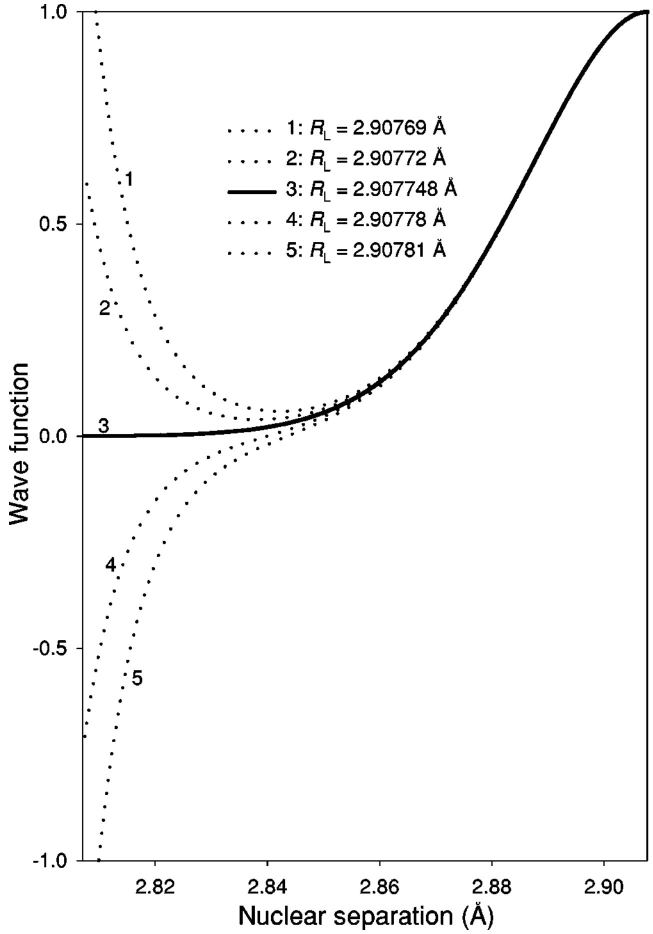

FIG. 4. Demonstration of locating the farthest left-side extremum point R_L of the wave function for $E=500$ meV. The solution of Eq. (1) vanishing as $R\rightarrow 0$ is shown by solid line, while the dotted lines represent calculated wave functions resulting from ''wrong'' trial values for R_L.

$\times\exp[i\delta(R)]$, and taking into account that W_0 becomes a pure imaginary quantity, $W_0 \equiv iW_{00}$, one comes to another transformed pair of Gordon equations

$$X'(R) = -\frac{\Delta U(R)|A_0(R)|^2}{W_{00}}\sin\{2[\delta(R)+\varphi(R)]\}X(R), \tag{39}$$

$$\varphi'(R) = \frac{2\Delta U(R)|A_0(R)|^2}{W_{00}}\sin^2[\delta(R)+\varphi(R)], \tag{40}$$

with the initial conditions $X(R_L)=1$ and $\varphi(R_L) = \arg[B_0'(R_L)]$.

B. Examples of numerical solution

To illustrate the general method described in the previous section, we will return to the model specified in Sec. III C. Namely, losing for a moment the remembrance of its exact solubility, we will consider the three-Morse potential as an ''original,'' which is approximated by a two-Morse substituent. This way we can easily compare the exact solutions for the three-component ''original'' with those obtained from the two-component ''reference'' solutions by applying the Gordon method. Since $\Delta U(R)=0$ as $R \geqslant X_1$, there is no need to search for the right-side extremum point R_R (provided $R_R > X_2$). Indeed, the wave function's logarithmic derivative for the whole range $R \geqslant X_2$ is given by Eq. (20).

To concern both general pairs of Gordon equations, i.e., Eqs. (34)–(35) and Eqs. (39)–(40), we will examine the same solutions for the eigenstates $n=55$ and 75, which are shown in Fig. 3. First, we consider the energy region $E \leqslant V_1 + D_1$. In this case, the special solutions and their derivatives for the reference potential are given by Eqs. (8)–(9) and Eqs. (10)–(11), respectively. Let us fix $A_0(R)=\Psi_{11}$ and $B_0(R)=\Psi_{12}$. The Wronskian then becomes (taking R arbitrarily)

$$W_0 = \alpha_1 \exp(-y_1)[(a_1+\mu_1-1/2)F(\mu_1)F^+(-\mu_1) - (a_1-\mu_1-1/2)F(-\mu_1)F^+(\mu_1)]. \tag{41}$$

Now one can solve the Gordon equations (34)–(35), starting from the initial conditions $y(R_L)=1, z(R_L)=1$. The standard fourth-order Runge-Kutta method is well suited for this purpose, as $y(R)$ and $z(R)$ are slowly varying functions. Naturally, the solutions $y(R)=y(X_1)$ and $z(R)=z(X_1)$ become constants in the range $R \geqslant X_1$. According to Eqs. (29)–(30) and general continuity requirements, one gets

$$\frac{a_0 a(X_1)A_0'(X_2)+b_0 b(X_1)B_0'(X_2)}{a_0 a(X_1)A_0(X_2)+b_0 b(X_1)B_0(X_2)} = F_{22}, \tag{42}$$

where $F_{22} \equiv \Psi_2'(E,X_2)/\Psi_2(E,X_2)$ is obtained from Eq. (20). Finally, using Eq. (33), one comes to the following quantization condition:

$$\frac{y(X_1)}{z(X_1)} = -C_0\frac{A_0'(R_L)}{B_0'(R_L)}, \tag{43}$$

where

$$C_0 \equiv \frac{a_0 a(X_1)}{b_0 b(X_1)} = -\frac{B_0'(X_2)-B_0(X_2)F_{22}}{A_0'(X_2)-A_0(X_2)F_{22}}. \tag{44}$$

The results for the eigenstate $n=55$ are shown in Fig. 5. Only the range $R \leqslant X_1$ is depicted where the two- and three-component potentials actually differ. One can see that $y(R)$ and $z(R)$ are indeed slowly varying functions, and the numerically calculated wave function $\Psi \sim B_0'(R_L)A_0(R)y(R) - A_0'(R_L)B_0(R)z(R)$ practically coincides with the relevant exact solution.

Now, let us consider the energy range $V_1+D_1 < E \leqslant V_2 + D_2$, where $A_0(R)$ and $B_0(R)$ become complex conjugates. Here, the treatment is based on Eqs. (39)–(40) and, according to Eqs. (43)–(44), the quantization condition becomes

$$\varphi(X_1) = -\arg[A_0'(X_2)-A_0(X_2)F_{22}] = -(\beta_0 - \alpha_1\beta_1 X_2 + \arg f). \tag{45}$$

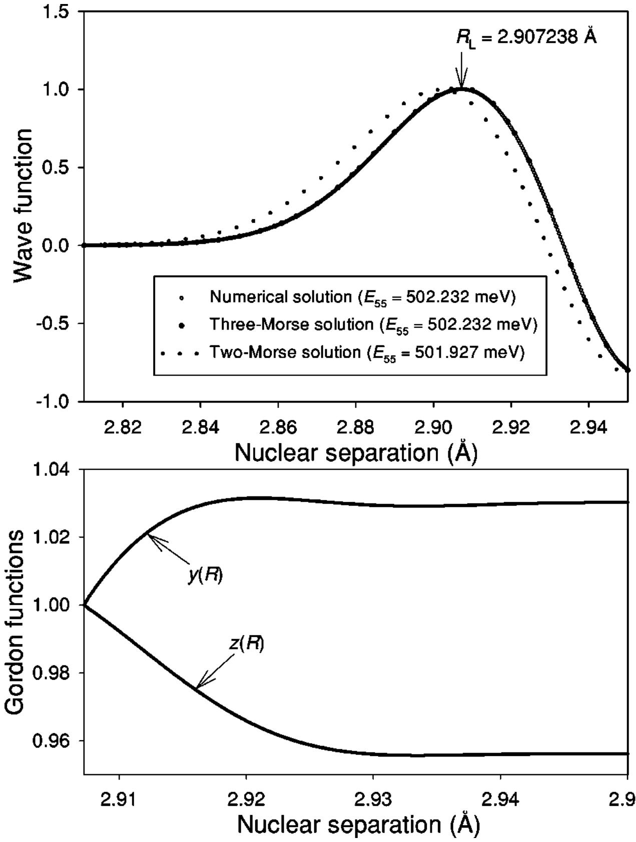

FIG. 5. Comparison between the exact three-component eigenfunction for the level $n=55$ and the numerical solution of Gordon equations (34)–(35) for the two-component reference potential, whose relevant exact solution is shown by a dotted line. Numerov method has been used for the range $R \leqslant R_L$. The lower graph demonstrates the coordinate dependencies of the Gordon functions $y(R)$ and $z(R)$.

The phase shift β_0 can be calculated from the following exact formula [24]:

$$\beta_0=\beta_1[1+\ln(4a_1)+\alpha_1 R_1-0.5\ln(1+16\beta_1^2)] + I(4\beta_1)/4-\frac{\pi+\arg[H(\mu_1)]}{2}, \tag{46}$$

where

$$H(\mu_1)=\sum_{n=0}^{\infty}\frac{(-2a_1+2\mu_1)_n(-4\mu_1)_n}{2^n n!(-a_1-\mu_1+1/2)_n} \times\left[\sum_{n=0}^{\infty}\frac{(4\mu_1)_n}{2^n(2\mu_1+1)_n}\right]^2, \tag{47}$$

$I(4\beta_1)$ is given by Eq. (16), and other quantities are defined in Sec. II (note that $\mu_1=i\beta_1$ is a pure imaginary parameter here). Further, using Eqs. (8)–(11) and (42), one gets

$$f=\left[\alpha_1\left(\frac{y_{12}+1}{2}-a_1\right)-F_{22}\right]\mathrm{Re}\,S_1+\alpha_1[(a_1-1/2)\mathrm{Re}\,S_2 +\beta_1\mathrm{Im}\,S_2]+i\left\{\left[\alpha_1\left(\frac{y_{12}+1}{2}-a_1\right)-F_{22}\right]\mathrm{Im}\,S_1 +\alpha_1[(a_1-1/2)\mathrm{Im}\,S_2-\beta_1\mathrm{Re}\,S_2]\right\}, \tag{48}$$

where $S_1\equiv S(a_1, i\beta_1; y_{12})$ and $S_2\equiv S(a_1-1, i\beta_1; y_{12})$ are calculated at $y_{12}=y_1(X_2)$, using Eq. (12).

A convenient form for the wave function is

$$\Psi(R)=\frac{C(R)X(R)\sin[\delta(R)+\varphi(R)]}{C(R_L)\sin[\delta(R_L)+\varphi(R_L)]}, \tag{49}$$

with $C(R)=|S_1(R)|$ and $\delta(R)=\beta_0-\alpha_1\beta_1 R+\arg S_1(R)$. Finally, the initial condition for $\varphi(R)$ becomes

$$\varphi(R_L)=\arg[B_0'(R_L)]=\beta_0-\alpha_1\beta_1 R_L+\arg f_0, \tag{50}$$

where

$$f_0=\left(\frac{y_{10}+1}{2}-a_1\right)\mathrm{Re}\,S_{10}+(a_1-1/2)\mathrm{Re}\,S_{20}+\beta_1\mathrm{Im}\,S_{20} +i\left[\left(\frac{y_{10}+1}{2}-a_1\right)\mathrm{Im}\,S_{10}+(a_1-1/2)\mathrm{Im}\,S_{20} -\beta_1\mathrm{Re}\,S_{20}\right], \tag{51}$$

$S_{10}=S_1(y_{10})$, $S_{20}=S_2(y_{10})$, and $y_{10}\equiv y_1(R_L)$.

A comparison between calculated wave functions for the eigenstate $n=75$ is seen in Fig. 6. Again, the numerical result by the Gordon method practically coincides with the exact solution, thus confirming the validity of the approach.

V. MULTIDIMENSIONAL CASE

An accurate solution of the two-body problem forms a natural basis for an adequate description of the properties of simple quantum systems, such as diatomic molecules. In addition, two-body methods can be sometimes applied to study rather complicated phenomena in solids, e.g., hot luminescence of strong vibrational excitations (self-trapped excitons) in rare-gas crystals [33]. In most cases of practical interest, however, one has to deal with complex many-body systems when an exact solution of the quantum-mechanical problem is not possible even in principle. Fortunately, remarkable progress has been achieved in recent years in developing special many-body techniques, but their use would be out of the scope of this paper. Instead, once again being guided by Gordon's work [22], let us examine how and to what extent our concept might be adjusted to a multidimensional case.

Direct generalization is easily obtained if the wave function can be expanded as

$$\Psi=\sum_{n=1}^{N}\Psi_n(R)\Phi_n(Q), \tag{52}$$

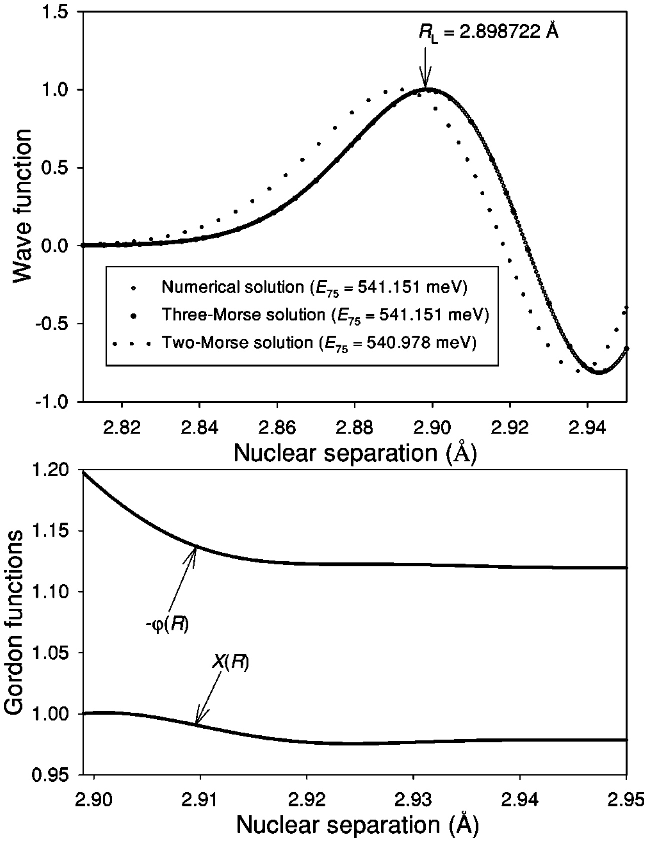

FIG. 6. Exact three-component eigenfunction for the level $n=75$ in comparison with the numerical solution of Gordon equations (39)–(40) for the two-component reference potential, whose relevant exact solution is shown by a dotted line. The coordinate dependencies of the Gordon functions $X(R)$ and $\varphi(R)$ [note that $-\varphi(R)$ is depicted] are seen in the lower graph.

where R is a specially separated coordinate in which the wave function shows its most oscillatory behavior (an analogue of the radial coordinate in one-dimensional problem), and Q stands for the collection of all other coordinates in the multidimensional problem. Correspondingly, $\Phi_n(Q)$ represent some ''global'' basis functions, which should form a sufficiently complete set and are considered orthonormal over the domain of interest

$$\int \Phi_m(Q)\Phi_n(Q)dQ=\delta_{mn}. \tag{53}$$

Using Eqs. (52)–(53), one comes to a set of coupled differential equations

$$\sum_{n=1}^{N}[\delta_{mn}(d^2/dR^2+\varepsilon)-V_{mn}(R)]\Psi_n(R)=0,$$

$$m=1,2,\ldots,N, \tag{54}$$

where $V_{mn}(R)$ is the reduced matrix element of the Hamiltonian (leaving out the kinetic-energy term in R)

$$V_{mn}(R)=\frac{2m}{\hbar^2}\int \Phi_m(Q)H(R,Q)\Phi_n(Q)dQ. \tag{55}$$

Thus, assuming the ''radial'' functions $\Psi_n(R)$ to be components of an N-dimensional vector function, Eq. (54) represents an analogue of Eq. (1) in matrix notation. Next, according to the general idea of the approach, we have to choose an appropriate reference potential matrix to approximate $V_{mn}(R)$. The most convenient choice for this purpose would be a diagonal matrix. Indeed, in this case, we get N uncoupled reference Schrödinger equations, each of the same form as in the one-dimensional case, and each can be solved separately. Further, to make any use of the analytical tools described in Secs. II and III, the diagonal elements $V_{nn}^{(0)}(R)$ ($n=1,2,\ldots,N$) of the reference potential matrix should ensure exact solubility of the relevant one-dimensional Schrödinger equations. Naturally, the diagonal form of the reference matrix is only justified if the actual Hamiltonian itself would be as nearly diagonal as possible. Such a desirable form of $V_{mn}(R)$ may be achieved with the help of an appropriate unitary transformation of the initial basis functions $\Phi_n(Q)$.

Provided one can overcome the described technical difficulties to the desired extent, the solution of the multidimensional eigenvalue problem is a simple generalization of the one-dimensional scheme. First, one finds the two linearly independent solution vectors for the reference Hamiltonian. Threafter, one locates the extremum points $R_L^{(n)}$ and $R_R^{(n)}$ for all components $\Psi_n(R)$, using matrix analogues of Eqs. (36)–(37). For example, Eq. (37) transforms as follows:

$$\left[1-\frac{\Delta^2}{12}(w_{k+1}-\varepsilon)\right]\Psi_{k+1}$$

$$=\left[2+\frac{5\Delta^2}{6}(w_k-\varepsilon)\right]\Psi_k-\left[1-\frac{\Delta^2}{12}(w_{k-1}-\varepsilon)\right]\Psi_{k-1},$$

$$k=1,2,\ldots\ . \tag{56}$$

Here, Ψ_k represents an N-dimensional vector function and w_k is an $N\times N$ matrix. Thus, given the vectors Ψ_{k-1} and Ψ_k at R_{k-1} and R_k, respectively (note that R_k also represents a vector with components $R_k^{(1)},R_k^{(2)},\ldots,R_k^{(N)}$), one solves a system of linear equations to find the next vector $\Psi_{k+1}(R_{k+1})$ in succession. This way, moving step by step into the classically forbidden region, one can gradually locate the true solution vector whose components should vanish at both ends of the physical domain. Then, having fixed all the extremum points $R_L^{(n)}$ and $R_R^{(n)}$, one can solve matrix Gordon equations to get the expansion coefficients $a_n(R)$ and $b_n(R)$ ($n=1,2,\ldots,N$) in the matrix analogue of Eq. (29), and therefore, the wave function's ''radial'' components $\Psi_n(R)$ in the range $R\in(R_L^{(n)},R_R^{(n)})$.

The overall analytical-numerical procedure looks arduous but still manageable. However, one has to bear in mind that the described simple extension of the one-dimensional method becomes meaningless if one cannot actually fix any ''radial'' coordinate for the real multidimensional system.

Then one should use special multidimensional tools, such as the Monte Carlo Green's function method (see [32], Chap. 11, for a good introductory overview).

VI. CONCLUSION

In this paper, our aim is to elaborate a possibly universal and accurate method of solving the energy eigenvalue problem for simple one-dimensional quantum systems. For this purpose, a unified analytical-numerical approach has been developed. First, one constructs an appropriate reference potential consisting of several smoothly joined Morse-type components, and finds the exact solutions of the relevant Schrödinger equations. These solutions are then used to apply a nonperturbative approach proposed by Gordon [22], which enables us to calculate the energy eigenvalues and eigenfunctions for the original potential. The overall success of the method mainly depends on the quality of the preparatory analytical work. Indeed, the numerical method of finding the slowly varying expansion coefficients in Eq. (29) is easily realizable and effective, if the reference potential is a sufficiently good approximation to the original one.

Involving Morse-type potentials as the constituents of reference potentials is not at all incidental for our concept. There are not so many multicomponent potentials whose two linearly independent exact solutions of the relevant Schrödinger equations could be easily found in the whole physical domain. One such possibility, the piecewise linear approximation, has been used by Gordon himself. Another easily realizable option, which can take advantage of the well-elaborated theory of confluent hypergeometric equations, is the piecewise Morse approach described in this paper. We have studied a confining three-component model potential, which might often be just the optimal choice for two-body systems. Naturally, one can construct a potential of much more Morse components to study both the scattering and/or the bound states of a given potential. However, there should always be a reasonable balance between the analytical and numerical efforts when aiming at developing a really efficient solution method.

ACKNOWLEDGMENTS

This work has been supported by Grant Nos. 4032 and 4508 from the Estonian Science Foundation. The author is grateful to Dr. Vladimir Sovkov from St. Petersburg State University for useful suggestions regarding the conceptual basis of the elaborated method.

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