Smooth amplitude-phase formulation of the Schrödinger equation based on the Ermakov invariant

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The amplitude-phase formulation of the one-dimensional Schrödinger equation is investigated within the context of Ermakov systems. The boundary conditions for amplitude functions corresponding to bound states are given in terms of the Ermakov invariant and a related constant, which also monitors the behavior of the accumulated phase function. A procedure leading to the numerical construction of smooth, nonoscillating amplitude and phase functions is proposed, and illustrated in the case of the harmonic oscillator and the centrifugal Coulomb potential. The use of this procedure as a tool to define radial basis functions for bound channels within the framework of scattering theory is discussed.

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I. INTRODUCTION

Systems composed of two coupled nonlinear differential equations for the functions u and ρ of the type

$$\partial_x^2 u(x)+k^2(x)u(x)=\frac{1}{\rho u^2(x)}Y[\rho(x)/u(x)], \tag{1}$$

$$\partial_x^2 \rho(x)+k^2(x)\rho(x)=\frac{1}{u\rho^2(x)}Z[u(x)/\rho(x)], \tag{2}$$

where Y and Z are arbitrary functions of their arguments, are known as Ermakov systems. The main characteristic of such a system follows from the existence of an exact invariant I,

$$I=\frac{1}{2}|u\partial_x\rho-\rho\partial_x u|^2+\int^{\rho/u}Y(\zeta)d\zeta+\int^{u/\rho}Z(\zeta)d\zeta, \tag{3}$$

through which $u(x)$ and $\rho(x)$ may be linked using a nonlinear superposition principle (see Sec. II). In what follows, we shall only be concerned by uncoupled systems, i.e., $Y(\zeta)=0$ and $Z(\zeta)=a\zeta$ where a is a constant. Although Ermakov was the first to investigate those systems back in 1880, intensive studies have only been undertaken since the late 1960's, culminating in the celebrated papers of Reid and Ray [1,2]. These studies were sparked by the countless number of applications Eqs. (1) and (2) have in various domains of physics, ranging from the time-dependent harmonic oscillator to soliton theory and fluid dynamics. The structure of generalized Ermakov systems are still a current topic of research, particularly concerning extensions to many dimensions [3], and the existence of a second invariant (Ref. [4], and references therein).

The amplitude-phase formulation of quantum mechanics is obtained by writing a general solution of the one-dimensional time-independent Schrödinger equation

$$\partial_x^2 u(x)+k^2(x)u(x)=0 \tag{4}$$

with $k^2(x)=2(E-V(x))$, under the form

$$u(x)=\alpha(x)[c_1\sin\phi(x)+c_2\cos\phi(x)], \tag{5}$$

where c_1 and c_2 are complex constants. It can be checked that the function $\alpha(x)$ obeys the second-order nonlinear equation

$$\partial_x^2\alpha(x)+k^2(x)\alpha(x)=\frac{a^2}{\alpha^3(x)} \tag{6}$$

and that $\partial_x\phi=a/\alpha^2$, a being a constant (see Sec. IIIA). $\alpha(x)$ is known as the amplitude function and $\phi(x)$ as the phase. This transformation, sometimes known as the Milne transform [5], was employed in different manners and different contexts (for a brief review, see Sec. 5.10 of Ref. [6]). The main use of amplitude-phase formalisms lies not as an alternative to find the eigenfunctions of the Schrödinger equation (though this was implemented in [7]), but in scattering theory, where in addition to the potential $V(x)$ of Eq. (4), there is a short-range potential inducing phase shifts. As known, the wave function of such a problem is given in each channel by a superposition of regular and irregular solutions of Eq. (4). The amplitude-phase method enters as a tool to construct a basis of regular and irregular solutions, through which the scattering parameters are then defined.

In particular, Greene, Rau, and Fano proposed an amplitude-phase method to treat the dynamics of an electron moving in the arbitrary field of an ionic core [8], typically suited to determine the spectra of Rydberg atoms. This treatment was undertaken within the framework of multichannel quantum defect theory (MQDT), a scattering theory-based formalism describing both bound-state and autoionizing spectra, characterized by the explicit inclusion of closed (negative electron energy) collision channels. It was shown in Ref. [8] how the MQDT (i.e., electron-ion scattering) parameters, and their behavior as a function of the energy, could be determined in a quite general manner by employing an amplitude-phase formulation. Since then, amplitude-phase-implemented MQDT has been successfully applied to a varied number of problems in atomic and molecular physics. The nature of the one-dimensional Schrödinger equation to be put in amplitude-phase form depends both on the geometry of the problem and on the choice of the long-range potential V. The spherical radius is obviously the most commonly encountered variable for the amplitude and phase

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functions, employed both for atoms (numerous examples can be found in Ref. [9]) and molecules (e.g., Ref. [10] for H_2) with one or two outer electrons. However, amplitude-phase techniques have also been used with other variables, such as the hyperspherical radius to treat He [11], the elliptical radius in polar molecules [12], or the internuclear coordinate in atom-atom scattering [13].

Despite all these developments, the determination of the amplitude α is still a delicate task for bound states in a potential well. For reasons that will become apparent in Sec. III, the amplitude function is tractable only if it does not present an oscillatory behavior in the radial variable [then the oscillatory behavior of the wave function as given by Eq. (5) is only due to the sine and cosine of the phase]. However, for a given Schrödinger equation, there exists an infinite number of real amplitude functions, corresponding to different boundary conditions. And these solutions generally oscillate, except for very specific choices of boundary conditions. To our knowledge, a general method that would lead to such a choice has not yet been proposed. Most works followed the suggestion initially made in Ref. [7], namely, to use classical boundary conditions for α at the potential minimum $x_{\min}$:

$$\alpha(E,x_{\min})=k^{-1/2}(x_{\min},E), \tag{7a}$$

$$\partial_x\alpha(E,x_{\min})=0, \tag{7b}$$

where k is the classical momentum (in units of $\hbar$) and E the energy of the particle in the well. But this choice is not always possible, and when it is, it does not always lead to a satisfactory behavior for the amplitude function: corrections to this method have consequently been proposed by different authors [14–16]. A related problem concerns the energy dependence of the phase function (more precisely of the accumulated phase function, to be defined below): one of the main advantages of MQDT over standard scattering theory relies on obtaining collision parameters smooth in energy—avoiding the singularities that usually appear at resonance energies—which makes possible the use of interpolation procedures. This feature is crucially dependent on the energy behavior of the phase function, which is highly oscillatory for arbitrary boundary conditions.

The aim of this paper is twofold. First, to establish an explicit link between Ermakov systems and the amplitude-phase approach. To this end, some results concerning uncoupled Ermakov systems and the principle of nonlinear superposition will be briefly reviewed in Sec. II. The other objective, reported in Sec. III, is to present results aimed toward the practical implementation of amplitude-phase techniques for bound states or bound channels. From a general standpoint, the principle of nonlinear superposition sheds new light on the amplitude-phase approach by clarifying the choices of boundary conditions for $\alpha(x)$ and of the energy dependence for $\phi(x)$; in particular, a procedure aimed at obtaining a smooth radial behavior for the amplitude function, using the Ermakov invariant I, will be presented. This procedure will be illustrated and discussed in Sec. IV for the harmonic oscillator potential and for the Coulomb field. It will be seen that our procedure which yields smooth amplitude functions in both of these paradigmatic cases, does not depend to a large extent on the properties of the potential (as the convexity of the potential or the type of minimum). For completeness, we point out that the interest for smooth amplitude-phase functions is not limited to MQDT analysis. In particular, Milne's transform has been used in trajectory representations of quantum mechanics, see Ref. [17] and especially Ref. [18], where it is suggested (and illustrated in the case of the harmonic oscillator) that the smoothness of the amplitude function plays a role in the interpretation of Born's probabilistic postulate.

II. UNCOUPLED ERMAKOV SYSTEMS

An uncoupled Ermakov system is a special case (actually the simplest one) of the system given above by Eqs. (1) and (2). It consists of the following pair of differential equations:

$$\partial_x^2 u(x)+k^2(x)u(x)=0, \tag{8}$$

$$\partial_x^2\alpha(x)+k^2(x)\alpha(x)=\frac{a^2}{\alpha^3(x)}, \tag{9}$$

where a^2 is real constant. It may be shown that $u(x)$ and $\alpha(x)$ are related by a transformation function $t=\alpha/u$. If the equation for t is solved, then one may obtain the general solution for one of the equations (8) or (9) from the knowledge of a particular solution of the other: this is a brief statement of the so-called nonlinear superposition principle. For details, the reader is referred to Refs. [2] and [19]; we only summarize the following results, useful in view of Sec. III below.

(i) It may be shown that the quantity

$$I=\frac{1}{2}\left[a^2\left|\frac{u}{\alpha}\right|^2+|u\partial_x\alpha-\alpha\partial_x u|^2\right] \tag{10}$$

is invariant (independent of x), or more precisely, that it defines a class of invariants. From now on, a^2 will be set equal to unity without any loss of generality (since a^2 can be absorbed into α by redefining $\alpha\rightarrow\alpha/a^{1/2}$).

(ii) If $u_1(x)$ is a particular real solution of Eq. (8), then the general solution of Eq. (9) is given by

$$\alpha(x)=u_1(x)\left[\frac{1}{2I}+2I\left(c-\int\frac{dx}{u_1^2(x')}\right)^2\right]^{1/2}, \tag{11}$$

where c is a real constant.

(iii) By choosing a second real solution $u_2(x)$ of Eq. (8), independent from $u_1(x)$ and labeling their Wronskian $W\equiv\mathcal{W}[u_1,u_2]=(\partial_x u_1)u_2-u_1(\partial_x u_2)$, the general solution of Eq. (9) takes the form

$$\alpha(x)=\left[\left(\frac{1}{2I}+2Ic^2\right)u_1^2(x)+\frac{2I}{W^2}u_2^2(x)-\frac{4Ic}{W}u_1(x)u_2(x)\right]^{1/2}. \tag{12}$$

Real solutions of Eq. (9) are thus positively defined quadratic forms, and it follows that $\alpha(x)$ does not vanish. A particular solution $\alpha(x)$ is obtained by choosing particular values for the two constants I and c [this is equivalent to setting particular boundary conditions for Eq. (9)].

(iv) Let us introduce another solution $g(x)$ of Eq. (8) and put

$$g(x;I,c)=2I\left(\frac{u_2(x)}{W}-cu_1(x)\right), \tag{13}$$

so that the Wronskian of u_1 and g becomes

$$\mathcal{W}[u_1,g]=2I. \tag{14}$$

Then we have

$$\alpha(x)=\left[\frac{1}{2I}[u_1^2(x)+g^2(x;I,c)]\right]^{1/2}, \tag{15}$$

which although similar to, is not the canonical form of the quadratic form.

III. AMPLITUDE-PHASE FORMULATION

We now specialize the formulas given above to the amplitude-phase formulation of the Schrödinger equation. Atomic units will be used throughout.

A. Milne transform and scattering basis functions

Clearly, by setting $k^2\equiv 2(E-V)$, Eq. (8) above is nothing but the time-independent Schrödinger equation. Let $u(x)$ be a general solution of Eq. (8), and search for u under the form given by Eq. (5). Then by a straightforward substitution, we are led to the two equations

$$\partial_x^2\alpha(x)+k^2(x)\alpha(x)=\alpha(x)[\partial_x\phi(x)]^2, \tag{16}$$

$$\alpha^2(x)=\frac{a}{\partial_x\phi}. \tag{17}$$

Here a is the same constant that appears in Eq. (9), which will be set equal to 1. Note also the identity $\mathcal{W}[\alpha\sin\phi,\alpha\cos\phi]=a$. Inserting Eq. (17) into Eq. (16) yields the (nonlinear) equation for α, which is simply Eq. (9). Therefore, the equation for α forms with the Schrödinger equation an uncoupled Ermakov pair.

Because Milne's transform maintains the WKB structure, α is called the amplitude and ϕ the phase. Recall that in the WKB approximation, the phase is the classical Jacobi principal function and the amplitude squared is the inverse of the classical momentum, which is a smooth function, so that the WKB wave functions oscillate in a well-defined envelope. This is not the case here: α diverges exponentially beyond the turning points but has a generally highly oscillatory behavior between the turning points of the potential, where u_1 and u_2 oscillate. This is problematic from a computational point of view, because within scattering theory, such as MQDT, a basis of the Schrödinger equation is constructed from the amplitude and phase functions. Let $V(x)$ define a potential well on an interval $[s_1,s_2]$ (typically $s_{1,2}=\pm\infty$ or 0). Two basis functions of the Schrödinger equation (8) lagging $\pi/2$ out of phase may be defined by

$$f=b\alpha(x)\sin\phi(x), \tag{18a}$$

$$g=b\alpha(x)\cos\phi(x), \tag{18b}$$

where b is a constant. It is usually required that $\phi(s_1)=0$, so f is regular at s_1. A general solution of Eq. (8) may then be written as a superposition of the basis functions

$$\begin{aligned}u(x,E)&=\cos\delta(E)f(x,E)+\sin\delta(E)g(x,E)\\&=b\alpha(x,E)\sin[\phi(x,E)+\delta(E)].\end{aligned} \tag{19}$$

$u(x,E)$ physically represents the radial wave function (for x larger than a cutoff radius r) of a particle in the long-range potential V that scatters off an additional short-range potential. $\delta(E)$ appears an effective phase shift in the given collision channel and generally depends on the energy. [$\delta(E)$ takes into account both the scattering phase-shift due to the short-range potential and the long-range boundary conditions in the potential V. Only in the case of single-channel scattering does δ represent a scattering phase shift, see, e.g., Ref. [22], where δ is denoted $\pi\bar{\mu}$].

It is now apparent that the radial behavior and the energy dependence of the amplitude and phase functions directly determine those of the radial basis functions f and g. Furthermore, quantities such as phase-shifts or scattering matrices are defined in terms of these functions through a procedure based on a Lippmann-Schwinger equation type [20] or R-matrix type [9] structure, where f is the nonperturbed solution. If α oscillates, f and g can still be formally defined through Eqs. (18a),(18b), but their pathological behavior will have as a counterpart an odd behavior of, say, the phase shifts, which renders the problem numerically intractable. For example, the wave function (19) represents physical states if u converges at s_2, that is for energies such that $\phi(s_2,E)+\delta(E)=n\pi$, where n is an integer. Clearly, a highly oscillatory energy dependence of $\phi(s_2,E)$ will translate into $\delta(E)$, i.e., in the energy dependence of the short-range and long-range dynamical parameters, making less reliable or even impossible the use of interpolation procedures.

α can be obtained by direct integration of the nonlinear Eq. (9). Alternatively it is also possible to obtain the amplitude from two arbitrary independent solutions of the Schrödinger equation, relying on the connection between solutions of Eqs. (8) and (9) given in the context of Ermakov systems. The goal is then to set the free parameters c and I [Eq. (12)] so as to yield smooth amplitude and phase functions, which in turn determine f and g through Eqs. (18a),(18b). We shall adopt this last approach in what follows.

B. General solution for α and ϕ

Let $V(x)$ define a potential well with singularities at the points $x=s_1$ and s_2 (typically $s_{1,2}=\pm\infty$ or 0). The general solution for the amplitude function is given by Eq. (12),

$$\alpha(x)=\left[\left(\frac{1}{2I}+2Ic^2\right)u_1^2(x)+\frac{2I}{W^2}u_2^2(x)-\frac{4Ic}{W}u_1(x)u_2(x)\right]^{1/2}. \quad (20)$$

The equation for the phase, Eq. (17), is readily integrated to give

$$\phi(x)=\arctan\left[\left(\frac{1}{2I}+2Ic^2\right)W\frac{u_1(x)}{u_2(x)}-2Ic\right]+d, \quad (21)$$

where d is the integration constant. We also introduce the parameter β defined by

$$\beta\equiv\phi(s_2)-\phi(s_1). \quad (22)$$

β is usually known as the accumulated phase function (since it gives the value of the accumulated phase at a given energy), or alternatively as the quantum number function (since β/π counts the number of half-cycles of the wave function between s_1 and s_2).

To be more specific, we choose from now on the independent solutions u_1 and u_2 to be respectively regular at s_1 and s_2. This choice is advantageous for the discussion that follows, and also in practical applications, as u_1 (u_2) is obtained by outward (inward) numerical integration of Eq. (8). We also set the integration constant of Eq. (21) to $d=\arctan(2Ic)$, so that $\phi(s_1)=0$. Comparison of Eq. (15) with Eqs. (18a),(18b) thus leads to the identification of f with u_1 and of b^2 with $2I$. Of course, this identification is only up to a multiplicative constant κ, that for simplicity will not be explicit here; note however that α and ϕ are left unchanged by the transformations $u_1\rightarrow\kappa u_1$, $W\rightarrow\kappa W$, $I\rightarrow\kappa^2 I$, $c\rightarrow c/\kappa^2$.

Note that $I=b^2/2$ only holds when $u=f$ or $u=g$ is inserted into the invariant Eq. (10). A general solution $u(x)$ of Eq. (8), $u=c_1f+c_2g$, gives for the invariant

$$I=\frac{b^2}{2}(|c_1|^2+|c_2|^2), \quad (23)$$

so if we put $|c_1|^2+|c_2|^2=1$, then $I=b^2/2$ holds for any solution of Eq. (8). This is the case in particular for the scattering wave function (19). We shall assume these choices to hold hereafter.

α and ϕ explicitly depend on the boundary conditions, i.e., on the parameters c and I. However, as observed in Ref. [21], β is independent of these parameters when $E=E_0$, E_0 denoting the eigenvalues of the Schrödinger equation. For these energies, u_1 is square integrable [$u_1(s_1)=u_1(s_2)=0$, and u_2 is thus irregular at s_1 and s_2], so that by Eqs. (21) and (22),

$$\beta(E=E_0)=n\pi, \quad (24)$$

the integer multiple (n) of π being obtained by counting the zeros of u_2. But when $E\neq E_0$, we see that β does depend on the boundary conditions, since a direct calculation shows that

$$\beta(E\neq E_0)=\arctan(2Ic)+\frac{(2n+1)}{2}\pi. \quad (25)$$

C. Smooth energy dependence and normalization

We now discuss how the energy dependence of the convergence and of the normalization of the scattering wave function given by Eq. (19) depends on the parameters c and I. Square-integrable (L^2) functions are only properly defined at the eigenvalues E_0 of Eq. (8). By normalizing through the well-known trick combining the continuity equation for the probability density and l'Hopital's rule (e.g., Sec. 5.7 of Ref. [6]), we have

$$\int_{s_1}^{s_2}f^2(x,E_0)dx=I\partial_E\beta(E_0)=I\pi\partial_E n, \quad (26)$$

where the last equality is obtained by using Eq. (25). Since $\partial_E\beta(E_0)$ is energy dependent (and has the dimensions of the inverse of the energy), I must also be energy dependent in order to normalize the functions to unity. Alternatively, I may be taken as energy independent, in which case the normalization is inversely proportional to the energy. The functions are said to be energy normalized (or normalized per unit energy increment) when $I=1/\pi$, given that $\partial_E n\simeq[E_0(n+1)-E_0(n)]^{-1}$. This choice is usually made in scattering theory, since it is the analog for bound states of the Dirac-delta normalization of continuum wave functions.

As known, $\partial_E\beta$ also fixes the (improper) normalization of non L^2 functions that converge at s_2 but diverge at s_1. This is the case for the wave function (19),

$$u(x,E)=\sqrt{2I}\alpha(x,E)\sin[\phi(x,E)+\delta(E)] \quad (27)$$

provided that $\beta(E)+\delta(E)=n\pi$. Its normalization is given by $I\partial_E[\beta(E)+\delta(E)]$ which with an energy independent invariant and by assuming $\partial_E\delta(E)$ negligible yields [Eq. (25)]

$$\int_r^{s_2}u^2(x,E)dx=I\frac{\partial_E c}{\frac{1}{2I}+2Ic^2}. \quad (28)$$

The normalization is thus conditioned by the energy dependence of the accumulated phase function β. This is why obtaining a nonoscillating dependence of β as a function of the energy has been a major goal of much work regarding the use of amplitude-phase procedure in generalized quantum defect theory [14,16]. The point is that for the L^2 solutions of Eq. (8), we have $\beta=n\pi$, but when $E\neq E_0$, $\beta(E)$ oscillates around the line $\beta=\pi n^*$ (n^*real) joining those points where $\beta=n\pi$ (an example is given in Fig. 1). As seen from Eq. (25), the value of $\beta(E\neq E_0)$ depends on the choice of c. The same goes for the normalization, that is well defined when $E=E_0$ but arbitrary elsewhere, depending on c and its energy dependence.

Now, from the relations given above, it is possible to set $c(E)$ so as to extend the expressions for β and for the normalization from $E=E_0$ to energy values $E\neq E_0$. Let $E_0=\xi(n)$, n being an integer counting the zeros of f, and ξ a

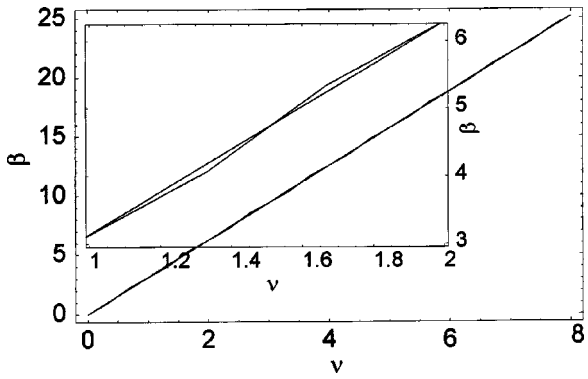

FIG. 1. The accumulated phase β is given as a function of the principal quantum number ν (in a.u.) for WKB boundary conditions (oscillating function) and for optimized boundary conditions (straight line, see text). The inset gives a magnification for $\nu=1-2$.

known function relating E_0 and n [e.g., for a Coulomb problem, $\xi(n)=-1/2(n+l)^2$]. The same functional relation holds for $E\neq E_0$, namely, $E=\xi(n^*)$, n^* real. If we require $u(E\neq E_0)$ to be normalized in an analogous manner as $f(E=E_0)$ then from Eqs. (26) and (28) we have

$$\partial_E c=\pi\partial_E n^*\left(\frac{1}{2I}+2Ic^2\right), \tag{29}$$

that is readily solved to give $c(n^*)=\tan(\pi n^*+\mathrm{cst})$. The constant is found by substituting $c(n^*)$ into the expression for the accumulated phase Eq. (25) and using the boundary condition $\beta(n^*\to n)=n\pi$, from which it follows that

$$2Ic(n^*)=-\cot\pi n^* \tag{30}$$

and with this choice $\beta(n^*)=\pi n^*$: the normalization (28) and the accumulated phase are then nonoscillating functions of n^* (and E). As a side product, we also obtain the following important result: the only solution $u[x,E=\xi(n^*)]$ given by Eq. (27) convergent at s_2 *and* normalized as f is the one for which the relations $2Ic(n^*)=-\cot\pi n^*$, $\beta(n^*)=\pi n^*$, and thus $\cot\delta=-\cot\pi n^*$ hold. This point will be further discussed in the illustrations given below.

D. Smooth amplitude function

We look here for the adequate parameters leading to a smooth amplitude function in the radial variable. We work with energy-normalized basis functions so I is fixed, and there is accordingly a single parameter c which may be varied. We will use a local condition on the derivatives of α to find a value of c yielding a nonoscillating amplitude. More precisely, since $\alpha(x)\to+\infty$ when $x\to s_1$ and s_2, there is at least one value x_0 such that $\partial_x\alpha(x_0)=0$. x_0 must lie between the classical turning points. This may be seen by writing Eq. (9) as

$$-\frac{1}{2}\langle\phi;x\rangle=\frac{\partial_x^2\alpha}{\alpha}=\alpha^{-4}-k^2, \tag{31}$$

where $\langle\phi;x\rangle\equiv\partial_x^3\phi/\partial_x\phi-\frac{3}{2}(\partial_x^2\phi/\partial_x\phi)^2$ is the Schwartzian derivative of the phase. It is easy to show that if $\langle\phi;x\rangle<0$ on an interval, then $\partial_x\phi$ cannot have a positive local minimum on this interval [23]. In the present case, this means that the amplitude cannot have a local maximum, and that its second derivative $\partial_x^2\alpha$ is positive. Thus if $\langle\phi;x\rangle$ is negative on an interval, α does not oscillate in this interval.

Now, beyond the turning points, the inequality $\langle\phi;x\rangle<0$ is always satisfied. We aim at constructing an amplitude function such that $\langle\phi;x\rangle$ is negative also between the turning points. Actually, since $\langle\phi;x\rangle<0$ is a sufficient but not necessary condition to have a nonoscillating α, we will only require $\langle\phi;x\rangle<0$ to hold locally on an interval. Denote by $F(x,E)$ the function

$$F(x,E)=k^{-2}(x,E)-\alpha^4(x,E), \tag{32}$$

which is positive if $\langle\phi;x\rangle<0$ holds. Let x_m denote a local minimum of F, so that the three conditions

$$F(x_m,E)>0, \tag{33a}$$

$$\partial_x F(x_m,E)=0, \tag{33b}$$

$$\partial_x^2 F(x_m,E)>0 \tag{33c}$$

are satisfied. The second of these conditions yields a relation between α and $\partial_x\alpha$, namely,

$$\partial_x\alpha(x_m)=\frac{\partial_x V(x_m)}{2k^4(x_m)\alpha^3(x_m)}, \tag{34}$$

which is inserted into the third condition. Setting $\theta\equiv\alpha^4(x_m)$, this gives

$$4k^2(x_m)\theta^2+2\left[\frac{\partial_x^2 V(x_m)}{k^4(x_m)}+\frac{4[\partial_x V(x_m)]^2}{k^6(x_m)}-2\right]\times\theta-\frac{3[\partial_x V(x_m)]^2}{k^8(x_m)}>0 \tag{35}$$

whose real roots are simply obtained, thereby setting bounds for the value of $\alpha(x_m)$. Next, insert Eq. (34) into the invariant, Eq. (10), setting $u=f$ and $I=b^2/2$. This leads to

$$\chi^4\left[\frac{f(x_m)\partial_x f(x_m)}{2k^4(x_m)}\right]^2+\chi^2\left[f^2(x_m)-\frac{\partial_x V(x_m)}{k^4(x_m)}f(x_m)\partial_x f(x_m)\right]-2I\chi+[\partial_x f(x_m)]^2=0 \tag{36}$$

with $\chi\equiv\alpha^{-2}(x_m)$,, which may be algebraically or numerically solved in χ. The real roots of this equation give the values of $\alpha(x_m)$ compatible with Eq. (33b). If one of these values fits with the other two conditions, Eq. (33a) and the inequality (35), then x_m is a local minimum of F. At first, an arbitrary value of x_m, lying between the turning points, is chosen. If the abovementioned conditions are not met, another x_m must be chosen, though x_m may be judiciously picked by examining the properties of the potential $V(x)$ (see

the examples given in Sec. IV). It seems reasonable, however, to choose x_m near the maximum of k, to put a stronger constraint on Eq. (33a). Once a suitable value of $\alpha(x_m)$ has been obtained, the amplitude function is found by calculating the corresponding value of the parameter c, which is done by means of the nonlinear superposition principle Eqs. (11) or (12),

$$c=\pm\left[\frac{1}{2I}\left(\frac{\alpha^2(x_m)}{f^2(x_m)}-\frac{1}{2I}\right)\right]^{1/2}+\frac{1}{W}\frac{u_2(x_m)}{f(x_m)}. \tag{37}$$

We thereby also obtain the phase function $\phi(x)$ as well as the basis function $g(x)$ via Eq. (13).

Note that if $\langle\phi;x\rangle<0$ is verified on the entire interval $[s_1,s_2]$, then α will not oscillate by virtue of the sign of the Schwartzian derivative. But it is generally sufficient for $\langle\phi;x\rangle<0$ to hold only locally around x_m, the reason being that since the Schwartzian derivative is negative both beyond the turning points and at x_m (between the turning points), it is expected at most to be mildly positive on finite intervals between the turning points. In other words, when $\langle\phi;x\rangle<0$ only holds locally, $\partial_x\alpha$ is allowed to oscillate mildly, but these oscillations do not change its sign.

IV. ILLUSTRATIONS

To illustrate the formulas given above and discuss further certain aspects of the procedure, we consider herein the harmonic oscillator and the Coulomb potential with a centrifugal barrier.

A. Harmonic oscillator

In atomic units and setting the frequency ω to 1, the amplitude equation for the linear harmonic oscillator is given by Eq. (9) with $k^2(x,E)=2(E-x^2/2)=2n^*+1-x^2$, and we introduce the effective quantum number $\nu=n^*$ by $E=\nu+1/2$. Here, the singularities are $s_1=-\infty$ and $s_2=+\infty$. We choose u_1 regular at s_1, u_2 regular at s_2, and normalize the eigenfunctions ($E=E_0$) of the Schrödinger Eq. (8) to unity (which is in this case equivalent to energy normalization apart the dimensional constant $\hbar\omega$). The invariant is accordingly set to $I=\mathcal{W}[f,g]/2=1/\pi$, implying by Eq. (26) $\partial_E\beta(E=E_0)=\partial_\nu\beta(\nu=n)=\pi$, where n is the integer counting the zeros of u_2.

Observe first that for an arbitrary value of c, the amplitude function displays strong oscillations, whereas a smooth behavior may be obtained by using an optimized value of c, keeping all other parameters constant, including the nonlinearity parameter a of Eq. (9) which has been set to unity: this disagrees with Figs. 2 and 3 of Ref. [18], where, for the harmonic oscillator, it was suggested the amplitude oscillates for $a\ll 1$ and is smooth for $a\simeq 1$ (it was furthermore given as an illustration of a general assumption regarding the behavior of α as a function of a).

Of course, the choice leading to a smooth amplitude function is not unique. We picked $x_m=0$: it can be checked that the conditions (33a)–(33c) are verified irrespective of the energy, and we take advantage of the simplification $\partial_x\alpha(x_m=0)=0$. The adequate root of Eq. (36) gives the value of $\alpha(x_m)$ that is injected in Eq. (37) to get c. Note that despite some similarity, we are not using here classical boundary conditions, as these would be given [Eqs. (7a),(7b)] by $\alpha(0,\nu)=(2\nu+1)^{-1/2}$ and $\partial_x\alpha(0,\nu)=0$. Actually, it can be seen that our boundary conditions tend toward the classical boundary conditions in the limit of high quantum numbers. In the particular case of the harmonic oscillator, these two choices of boundary conditions lead to nonoscillating amplitude functions in the radial variable. Nevertheless, with classical boundary conditions, the invariant cannot be chosen since it is given [Eq. (10)] by

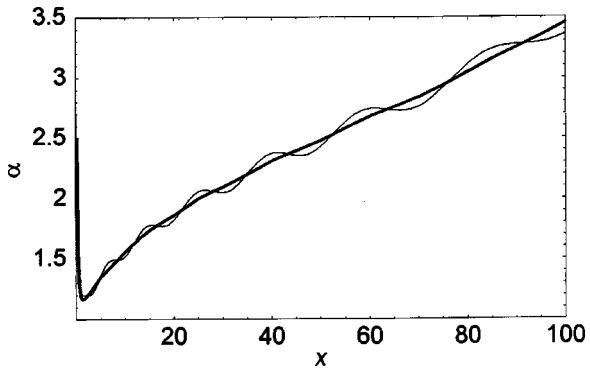

FIG. 2. WKB boundary conditions (thin line) and smooth (thick line) amplitude functions for an $l=1$ Coulomb centrifugal potential plotted for $\nu=8.77$. Units in a.u.

$$I(E)=\frac{1}{2}\left[u_1^2(x_m,E)k(E,x_m)+\frac{[\partial_x u_1(x,E)]^2}{k(E,x_m)}\right], \tag{38}$$

which as indicated, is energy dependent. Another difference concerns the energy dependence of the accumulated phase function β. As Korsch and Laurent [7], who used classical boundary conditions to generate α had remarked, their function $\beta(\nu)$ [denoted $N(E)$ in their work] presents oscillations about the line joining the eigenvalues of the Schrödinger equation [which, following Eq. (24) has the form $y=\pi\nu$]. Our initial conditions however yield $\beta(\nu)=\pi\nu$, as can be seen on Fig. 1. This is not a coincidence, since it can be checked that implementing our procedure with the choice $x_m=0$ leads to

$$c=-\frac{\pi}{2}\cot\pi\nu. \tag{39}$$

From Eq. (30) it is seen that this is precisely the value c must have if one compels β to the linear behavior $\beta=\pi\nu$. Note nonetheless that in general, when our procedure is successfully applied, smooth amplitude functions are obtained, but $\beta(\nu)$ does oscillate about $\pi\nu$, unless the condition (30) is enforced.

B. Centrifugal Coulomb potential

The amplitude equation for the radial variable in a unit charge Coulomb potential with a centrifugal barrier of magnitude l is given by Eq. (9) with $k^2(x,E,l)=2[E-l(l$

$+1)/(2x^2)-1/x]=-1/(n^*+l)^2-l(l+1)/x^2-1/(2x)$, and we introduced the effective quantum number by setting $\nu=n^*+l$, so $E=-1/(2\nu^2)$ for negative energies (and ν is an integer, $n+l$, when $E=E_0$ is an eigenvalue). The argument goes much as in the case of the harmonic oscillator except that here $s_1=0$ and $s_2=+\infty$, so u_1 (u_2) are obtained by inward (outward) integration from 0 (∞). The eigenfunctions of the Schrödinger equation are normalized to the energy by taking $I=1/\pi$ as energy independent: we then have $I\partial_E\beta(E=E_0)=(n+l)^3$.

Unlike the harmonic oscillator, classical boundary conditions at the potential minimum do not give a smooth amplitude function, as illustrated in Fig. 2 for $l=1$ (thin line), though the oscillations are rather moderate as compared to the ones obtained with arbitrary boundary conditions. On the other hand, the procedure described in Sec. III D yields a smooth behavior (thick line). Here we took $x_m=3$ and checked this behavior holds irrespective of the energy. Again, many other choices are possible. Of course, the accumulated phase $\beta(\nu)$ generally shows oscillations around the line $y=\pi n^*$. These oscillations are expected to be small if the amplitude function is smooth (for example with $x_m=3$ and $l=1$, the oscillations are about two orders of magnitude smaller than with the classical boundary conditions, which are in turn quite smaller than those obtained with arbitrary boundary conditions). These oscillations may be removed, following the analysis of Sec. III C, by setting [Eq. (30)] $c=-\pi\cot\pi(\nu-l)/2$ thereby constructing numerical functions for which the accumulated phase fulfills

$$\beta=\pi n^*=\pi(\nu-l). \tag{40}$$

It is interesting to note that these relations hold for the Coulomb functions described analytically by Seaton (denoted s and c in Ref. [24]) and which are known to yield nonoscillating amplitude functions. The scattering solutions (19) constructed with s and c (replacing f and g) are normalized to ν^3 and converge at infinity for $\nu=n-\delta/\pi$. In this sense, the relations given in Sec. III C generalize the remarkable properties of the Coulomb analytic functions to arbitrary long-range potentials. We also applied our procedure to the case $l=0$, where the potential displays no minimum; smooth amplitude functions were obtained at any energy by allowing an energy dependence of x_m.

V. DISCUSSION AND CONCLUSION

The failure of classical boundary conditions in practical implementations of amplitude-phase methods for the centrifugal Coulomb potential (moreover, for $l=0$, it is not clear where to take the classical boundary conditions) led to the development of alternative schemes, first to handle numerically studies of excited and autoionizing states of Rydberg atoms and molecules, and also in view of further generalizing quantum defect theory to an arbitrary long-range field. Yoo and Greene [14] had proposed to use boundary conditions for α at positive energies, where the amplitude function is well defined, then extrapolate to negative energies the energy dependence of $\alpha(E,x_m)$ and $\partial_x\alpha(E,x_m)$, where their x_m lies near the potential minimum. This method hinges on the fact that for small values of x, energy-normalized functions are independent of the energy, because the behavior of those functions is dominated by the singularity at s_1 of the centrifugal Coulomb potential. Although the method yielded excellent results and was repeatedly used in many applications, including in cold atom-atom scattering [13], it is not clear how it can be straightforwardly generalized to an arbitrary potential (for example, to a potential without singularities). Furthermore, although removing the oscillations in the energy dependence of β was one of the goals of the method, these oscillations are not controlled at the onset, but are examined *a posteriori*.

In a recent work Texier and Jungen [16] found that these oscillations could substantially be reduced by modifying in the classical boundary conditions, given by Eqs. (7a) and (7b): (i) $k(x,E,l)$, which is replaced by the second order WKB expansion of the quantum momentum $\partial_x\phi$ and (ii) $x_{\min}$ which is replaced by x_m, where x_m is chosen in order to minimize this second order correction $\partial_x\phi^{(2)}_{\mathrm{WKB}}-k$. The method results in important reductions of the oscillations of β for $\nu\gtrsim l+2$ and $l\neq 0$ (it becomes ineffective at low energies because the WKB expansion blows up at both turning points), but requires the potentials to have negative curvature (i.e., $\partial_x^2V<0$, which is not the case for the harmonic oscillator).

These authors also make a provision to determine well-behaved amplitude and phase functions in an energy range below the minimal eigenvalue of Eq. (8) ($\nu<l+1$ in the Coulomb case). Accumulated phase functions for those very low energies have proved to be necessary in problems where core states having different energies are considered (for example, Sec. II of Ref. [25] discusses how only an appropriate energy dependence of β for $\nu<l+1$ leads to a tractable energy dependence of the electronic quantum defects for triplet H_2). The procedure described in Sec. III D can also be employed in this case. Note in particular that for energies below the potential minimum ($\nu<[l(l+1)]^{1/2}$), the Schwartzian derivative $\langle\phi;x\rangle$ is, by Eq. (31), always negative, so α can never oscillate, and the desired behavior for β can be chosen.

This is one of the advantages of the method given in Sec. III: specific amplitude and phase functions are given in terms of two parameters that monitor the behavior of these functions both in the radial (x) and energy (E) variables in a transparent manner. It is not *a priori* dependent on the properties of the potential V, as long as it is possible to obtain two independent solutions of the Schrödinger equation (by inward and outward numerical integration). However, while the E dependence of the accumulated phase function is controlled in a straightforward way (Sec. III C) the x smoothness of the amplitude function is determined indirectly by a local condition: a nonoscillating amplitude is always obtained when the Schwartzian derivative is negative on the entire interval $[s_1,s_2]$, but it is most often sufficient for this condition to hold locally at x_m, because it constrains the behavior of α, as discussed in Sec. III D. This is a possible drawback of the method: depending on the potential properties, it

may be easy to determine analytically how to choose x_m (e.g., for the harmonic oscillator for which the conditions (33a)–(33c) taken for $x_m=0$ yield a negative Schwartzian derivative on $[s_1,s_2]$), whereas in other cases (e.g., numerical or model potential) a numerical exploration may result necessary. The asymmetry in the treatment of the energy and radial variables is due to the fact that there is a unique value of c yielding a nonoscillating behavior for β, whereas there are infinitely many values of c yielding, at a specified energy, nonoscillating amplitude functions: taking the second derivative of Eq. (20), it is seen that any value of c enclosed between $c_\pm(x)$, given by

$$c_\pm(x)=\frac{1}{W}\frac{u_2(x)}{f(x)}\pm\frac{1}{2If(x)}\sqrt{\frac{2I}{k(x)}-f^2(x)} \qquad (41)$$

and where x spans the entire interval between the turning points, gives rise to a nonoscillating amplitude function [a nonoscillating amplitude is also obtained if c crosses $c_\pm(x)$ a pair number of times without changing the sign of $\partial_x\alpha$ more than once].

The exact relationship between the accumulated phase function smooth in energy, i.e., with $c(n^*)=-\cot\pi n^*/2I$, and the radial properties of the amplitude function remains to be investigated. In both cases examined here, the Coulomb potential and the harmonic oscillator, the resulting amplitude function turned out to be oscillation free. Current work indicates that the peculiar properties of the choice $\beta=\pi n^*$ are best brought to light by examining the semiclassical limit, which may be done by setting up a semiclassical Ermakov system. Full details will be given elsewhere.

Anyhow, the results above suggest that techniques based on the properties of Ermakov systems should be useful in the context of the amplitude-phase formulation of the Schrödinger equation. In addition to possible improvements in numerical calculations of wave functions in scattering problems, the connection discussed in this article helps in clarifying the meaning of the amplitude-phase formalism of the wave function. Moreover, further links with current mathematical work on Ermakov systems could be fruitful in extensions of the formalism, for example to many dimensions.

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