Siegert-state expansion for nonstationary systems: Coupled equations in the one-channel case

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Expansion of the solution to the time-dependent Schrödinger equation for a one-channel nonstationary system in terms of Siegert states is discussed. A discrete set of coupled pseudodifferential equations defining time evolution of the coefficients in the expansion is derived, and physical observables (probabilities of transitions to discrete states and the spectrum of ejected particles) are expressed in terms of these coefficients. In contrast to other time-dependent close-coupling methods in atomic and molecular physics, the present approach treats the continuum with no approximation. A price for that is a more involved mathematical structure of the resulting coupled equations. The approach is implemented in terms of Siegert pseudostates and illustrated by calculations for a model time-dependent rectangular potential.

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I. INTRODUCTION

The quantum-mechanical scattering theory is traditionally formulated in terms of *physical states* (PS)—the eigenfunctions of the Hamiltonian satisfying physical asymptotic boundary conditions. The set of PS consists of discrete and continuous parts corresponding to bound and scattering states, respectively. Bound state eigenfunctions decay in the asymptotic region, while scattering states are given there by a superposition of incoming and outgoing waves. It is well-known that the discrete spectrum is much easier to deal with than the continuum, both in formal theory and calculations. Meanwhile, the approach based on PS is not the only one possible. In 1939 Siegert introduced [1] another set of states that now bare his name. *Siegert states* (SS) are also eigenfunctions of the Hamiltonian, but satisfy different asymptotic boundary conditions, namely, they have only incoming or outgoing waves in the asymptotic region. The corresponding eigenvalues give positions of the poles of the scattering matrix. The set of SS is purely discrete, which is an important advantage over the PS. At the same time, the two sets can be uniquely expressed in terms of each other. Therefore one could wish to reformulate scattering theory in terms of SS, and hence to get rid of the continuum. A noble goal indeed, but not easy to reach.

The difficulties originate from rather unusual orthogonality and completeness properties of the SS. The clarification of these basic issues, that for PS are covered even in elementary textbooks on quantum mechanics, for SS took much efforts of many researchers. Discussions of SS can be found in some advanced treatises [2–5] (where they are sometimes called by different names), but this is normally considered as an "exotic" of no practical use. The situation has changed after a new approach based on *Siegert pseudostates* (SPS) was proposed and demonstrated in [6]. This approach has opened a way to implement the power of SS in practical calculations. So far, the theory of SPS has been thoroughly developed only for s-wave scattering in one-channel [7] and two-channel [8] cases; further developments are in progress. In the time-independent framework, the efficiency of this approach was demonstrated by calculations of scattering and resonances in realistic three-body Coulomb systems [6,9,10] and some model problems [7,8,11–13], molecular dissociative photoionization and recombination [14,15], and electromagnetic resonances in inhomogeneous plasma [16]. In the time-dependent framework, the applications of SPS were pioneered in [17,18] and continued in [19] by studies of wave packet propagation in stationary (i.e., when the Hamiltonian does not depend on time) systems.

In this paper we make a further step in promoting SS and SPS for time-dependent problems, the former as a powerful tool in formal theory, and the latter as a means to implement this power in calculations. We discuss an expansion of the solution to the time-dependent Schrödinger equation (TDSE) for nonstationary (i.e., when the Hamiltonian does generally depend on time) systems in terms of SS. This problem should be viewed in the context of the results available in the time-dependent framework from earlier studies. Individual SS, corresponding to sharp resonances in scattering, have been long used in the analysis of the decay of unstable systems, see [2–5] and references therein, e.g., [20]. One of the first attempts to expand the solution to the TDSE in terms of SS was undertaken in [21]. However, apart from a discrete sum over SS the result contained an integral term because the completeness properties of the SS were not properly taken into account. The problem was resolved in [22] where an expansion for the time-dependent retarded Green's function in terms of SS was obtained by the Fourier transformation of the SS expansion for the stationary outgoing wave Green's function derived in [23]. A similar expansion in terms of SPS was obtained and illustrated by calculations in [19]. These results enable one to find the solution to the TDSE in the inner region, i.e., within the range of action of the potential. The SS expansion of the wave function in the outer region was obtained in [24,25]. Importantly, all these studies dealt with stationary systems.

We consider s-wave scattering in the one-channel case, as in [19,22,25], but with a time-dependent potential. Also as in [19,22,25], the potential is assumed to vanish beyond a finite radius $r=a$; for realistic potentials, this means that one has to reach convergence of the results as $a\to\infty$, see [7]. We analyze two initial value problems that are of main interest for physical applications: perturbation of a bound state prepared at $t=-\infty$ (problem I), and evolution of a wave packet prepared at $t=0$ (problem II). The corresponding solutions to the

TDSE can be expanded in terms of an appropriate set of SS. For each of the two problems, we derive coupled equations defining time evolution of the coefficients. These equations are the central result of the work. In contrast to various time-dependent close-coupling methods widely used in atomic physics, that are designed to deal with nonstationary Hamiltonians having purely discrete spectrum, but are often applied in situations where this is not the case, simply by neglecting the continuum or mimicking it by some pseudostates, our approach treats the continuum *with no approximation*. A price for that is a more involved mathematical structure of the coupled equations, which in the present case are pseudodifferential. The solutions to these equations, i.e., the coefficients in the SS expansion, completely define the wave function, both in the inner and outer regions. However, they do not have that simple physical meaning as the coefficients in the expansion in terms of PS. If the potential becomes independent of time for $t\to\infty$, we express the observables (probabilities of transitions to discrete states and the spectrum of ejected particles) in terms of these coefficients. We show how to implement this approach in terms of SPS. The results are illustrated by calculations for a time-dependent rectangular potential.

II. BASIC EQUATIONS

In this section we formulate two problems to be treated in the following discussion, simultaneously introducing our notation.

A. Hamiltonians

We consider a nonstationary system described by the TDSE (a system of units in which all the quantities involved in the analysis are dimensionless and $\hbar=m=1$ is used throughout the paper)

$$\left[i\frac{\partial}{\partial t}-H(t)\right]\psi(r,t)=0, \tag{1}$$

where

$$H(t)=-\frac{1}{2}\frac{\partial^2}{\partial r^2}+V(r,t), \tag{2}$$

and it is assumed that the potential has a finite range, i.e.,

$$V(r,t)\big|_{r\geqslant a}=0. \tag{3}$$

Equation (1) will be considered in the interval $0\leqslant r<\infty$ with the boundary condition

$$\psi(0,t)=0. \tag{4}$$

We also introduce an auxiliary stationary Hamiltonian

$$H=-\frac{1}{2}\frac{\partial^2}{\partial r^2}+V(r), \tag{5}$$

again assuming that

$$V(r)\big|_{r\geqslant a}=0. \tag{6}$$

It will be convenient to present $H(t)$ in the form

$$H(t)=H+U(r,t),\quad U(r,t)=V(r,t)-V(r), \tag{7}$$

where $U(r,t)$ also vanishes at $r\geqslant a$. The time-dependent potential $V(r,t)$ is a given function, while $V(r)$ may be chosen to some extent arbitrarily and will be defined for each problem separately.

B. Green's functions

The stationary outgoing wave Green's function for the time-independent Hamiltonian H is defined by

$$(E-H)G(r,r';k)=\delta(r-r'), \tag{8a}$$

$$G(0,r';k)=0, \tag{8b}$$

$$\left(\frac{\partial}{\partial r}-ik\right)G(r,r';k)\bigg|_{r\to\infty}=0. \tag{8c}$$

In this paper, E and k always denote energy and momentum related to each other by

$$E=\frac{1}{2}k^2,\quad k=\sqrt{2E}, \tag{9}$$

where the branch of the square root function for which $\mathrm{Im}\,k>0$ on the physical sheet of E is meant. Taking into account Eq. (6), condition (8c) actually applies at $r\geqslant a$ $(r>r')$ for $r'<a$ $(r'\geqslant a)$. The corresponding time-dependent retarded Green's function is defined by

$$\left[i\frac{\partial}{\partial t}-H\right]G(r,r';t)=\delta(t)\delta(r-r'), \tag{10a}$$

$$G(0,r';t)=0, \tag{10b}$$

$$G(r,r';t)\big|_{t<0}=0. \tag{10c}$$

These functions are related by the Fourier transformation,

$$G(r,r';t)=\int_{-\infty}^{\infty}G(r,r';k)e^{-iEt}\frac{dE}{2\pi}, \tag{11}$$

where, as usual in the scattering theory [2], it is understood that the integration path lies on the physical sheet infinitesimally above the real axis. One can similarly define the retarded Green's function for the full time-dependent Hamiltonian $H(t)$,

$$\left[i\frac{\partial}{\partial t}-H(t)\right]G(r,r';t,t')=\delta(t-t')\delta(r-r'), \tag{12a}$$

$$G(0,r';t,t')=0, \tag{12b}$$

$$G(r,r';t,t')\big|_{t<t'}=0. \tag{12c}$$

Alternatively, this function can be defined by the integral equation

$$G(r,r';t,t')=G(r,r';t-t')+\int_{-\infty}^{\infty}dt''\int_0^a dr''G(r,r'';t-t'')\times U(r'',t'')G(r'',r';t'',t'). \tag{13}$$

C. Initial conditions

To complete mathematical formulation of the problem, in addition to Eq. (1) and the boundary condition (4) we have to specify the initial conditions. We shall consider two types of initial conditions corresponding to two different physical problems.

1. Problem I: Perturbation of a bound state

Suppose that $V(r,t)$ becomes independent of time for $t\to-\infty$. In this case we define $V(r)$ by

$$V(r) = V(r,t)|_{t\to-\infty}, \tag{14}$$

hence $U(r,t)|_{t\to-\infty}=0$. In other words, the system was stationary in the infinite past, having the Hamiltonian H, and then a time-dependent potential $U(r,t)$ is switched on, continuously, starting from $t=-\infty$, or abruptly, at some finite moment. We assume that $U(r,t)$ vanishes sufficiently rapidly as $t\to-\infty$, so that the solution discussed below exists. Let H have a bound state with the energy $E_0<0$ and wave function $\phi_0(r)$ satisfying

$$(H-E_0)\phi_0(r)=0, \tag{15a}$$

$$\phi_0(0)=\phi_0(\infty)=0. \tag{15b}$$

Taking into account Eq. (6) we have

$$\phi_0(r)|_{r\geqslant a}=\phi_0(a)e^{ik_0(r-a)}, \quad k_0=i\sqrt{-2E_0}. \tag{15c}$$

Note that E_0 and k_0 are also related by Eqs. (9). Consider Eq. (1) in the time interval $-\infty<t<\infty$ with the initial condition

$$\psi(r,t)|_{t\to-\infty}=e^{-iE_0t}\phi_0(r). \tag{16}$$

This problem describes perturbation (one should not be confused by this term, it does not imply the use of perturbation theory) of a bound state of the initial stationary system caused by the time-dependent potential $U(r,t)$. Its solution will be denoted by $\psi_I(r,t)$. Using Eqs. (10) and (15), this function can be alternatively defined by the integral equation

$$\psi_I(r,t)=e^{-iE_0t}\phi_0(r)+\int_{-\infty}^{\infty}dt'\int_0^a dr'G(r,r';t-t') \times U(r',t')\psi_I(r',t'). \tag{17}$$

2. Problem II: Evolution of a wave packet

Consider Eq. (1) in the time interval $0\leqslant t<\infty$ with the initial condition

$$\psi(r,0)=\chi(r), \tag{18}$$

where $\chi(r)$ satisfies

$$\chi(0)=\chi(r)|_{r\geqslant a}=0, \tag{19}$$

and we assume that

$$\int_0^a|\chi(r)|^2=1. \tag{20}$$

This problem describes evolution of a wave packet, initially confined in the interval $0\leqslant r\leqslant a$, governed by the time-dependent Hamiltonian $H(t)$. In this case we define $V(r)$ by

$$V(r)=V(r,0), \tag{21}$$

hence $U(r,0)=0$. Using standard approach [2], we extend the interval of time under consideration in the initial value problem (1) and (18) to $-\infty<t<\infty$, assuming that $\psi(r,t)$ vanishes for $t<0$. Thus defined function satisfies

$$\left[i\frac{\partial}{\partial t}-H(t)\right]\psi(r,t)=i\delta(t)\chi(r), \tag{22a}$$

$$\psi(r,t)|_{t<0}=0. \tag{22b}$$

The solution to this problem will be denoted by $\psi_{II}(r,t)$. Using Eqs. (12) and (22) we obtain

$$\psi_{II}(r,t)=i\int_0^a G(r,r';t,0)\chi(r')dr'. \tag{23}$$

Substituting here Eq. (13), this function can be alternatively defined by the integral equation

$$\psi_{II}(r,t)=i\int_0^a G(r,r';t)\chi(r')dr'+\int_{-\infty}^{\infty}dt'\int_0^a dr'G(r,r';t-t') \times U(r',t')\psi_{II}(r',t'). \tag{24}$$

III. OUTGOING WAVE SOLUTIONS

It turns out that for a certain class of the solutions to Eq. (1) that have only outgoing waves in the outer region $r\geqslant a$ and hence will be called outgoing wave solutions, the derivative $\partial\psi(r,t)/\partial r$ at $r=a$ can be expressed in terms of $\psi(a,t')$ for $t'\leqslant t$. Using this relation, in this section we transform Eq. (1) to a form suitable for expansion in terms of SS.

A. Outgoing wave boundary condition in the time domain

Let us introduce the function and derivative value operators at $r=a$,

$$\mathcal{F}=\delta(r-a), \quad \mathcal{D}=\delta(r-a)\frac{d}{dr}. \tag{25}$$

The $\mathcal{D}$ is proportional to the Bloch operator [26]. Following Bloch, we also introduce hermitized Hamiltonians,

$$\tilde{H}(t)=H(t)+\frac{1}{2}\mathcal{D}, \quad \tilde{H}=H+\frac{1}{2}\mathcal{D}. \tag{26}$$

Finally, we introduce a pseudodifferential [27] operator $\hat{\lambda}_t$ whose action on a function

$$f(t)=\int_{-\infty}^{\infty}f(E)e^{-iEt}\frac{dE}{2\pi} \tag{27}$$

is defined by

$$\hat{\lambda}_t f(t)=\int_{-\infty}^{\infty}ikf(E)e^{-iEt}\frac{dE}{2\pi}. \tag{28}$$

Taking into account Eqs. (9), $\hat{\lambda}_t$ is related to the time derivative by

$$i\frac{\partial}{\partial t} = -\frac{\hat{\lambda}_t^2}{2}, \quad -i\hat{\lambda}_t = \sqrt{2i\frac{\partial}{\partial t}}. \tag{29}$$

The operator $\hat{\lambda}_t$ plays the key role in the following consideration. More detailed discussion of this operator and some of its properties is given in Appendix A.

We now turn to the derivation of the desired relation. First we consider a stationary system with the Hamiltonian H. In this case, the relation of interest in the energy domain follows immediately from Eqs. (6) and (8c),

$$\mathcal{D}G(r,r';k) = ik\mathcal{F}G(r,r';k), \quad r' < a. \tag{30}$$

Using this and Eq. (11), we obtain the same relation in the time domain,

$$\mathcal{D}G(r,r';t) = \mathcal{F}\hat{\lambda}_t G(r,r';t), \quad r' < a. \tag{31}$$

Using this and Eq. (13), we obtain a similar relation for the nonstationary system with the Hamiltonian $H(t)$,

$$\mathcal{D}G(r,r';t,t') = \mathcal{F}\hat{\lambda}_t G(r,r';t,t'), \quad r' < a. \tag{32}$$

As is clear from the derivation, Eqs. (31) and (32) express the outgoing wave boundary condition (30) in the time domain. Remarkably that in the time domain this condition holds for stationary as well as nonstationary cases, provided that the potential vanishes at $r \geqslant a$.

B. Matrix form of the time-dependent Schrödinger equation for outgoing wave solutions

Equations (31) and (32) lead to similar relations for the solutions $\psi_I(r,t)$ and $\psi_{II}(r,t)$. From Eqs. (15c), (17), (31), and (A10) we obtain

$$\mathcal{D}\psi_I(r,t) = \mathcal{F}\hat{\lambda}_t\psi_I(r,t). \tag{33}$$

Then Eq. (1) for $\psi_I(r,t)$ can be presented in the form

$$\left[\hat{\lambda}_t - \begin{pmatrix} 0 & 1 \\ -2\tilde{H}(t) & \mathcal{F} \end{pmatrix}\right]\begin{pmatrix} \psi_I(r,t) \\ \tilde{\psi}_I(r,t) \end{pmatrix} = 0. \tag{34}$$

Indeed, eliminating from this equation $\tilde{\psi}_I(r,t) = \hat{\lambda}_t\psi_I(r,t)$ one restores Eq. (1). Similarly, from Eqs. (23) and (32) we have

$$\mathcal{D}\psi_{II}(r,t) = \mathcal{F}\hat{\lambda}_t\psi_{II}(r,t). \tag{35}$$

Then Eq. (22a) for $\psi_{II}(r,t)$ becomes

$$\left[\hat{\lambda}_t - \begin{pmatrix} 0 & 1 \\ -2\tilde{H}(t) & \mathcal{F} \end{pmatrix}\right]\begin{pmatrix} \psi_{II}(r,t) \\ \tilde{\psi}_{II}(r,t) \end{pmatrix} = -2i\delta(t)\begin{pmatrix} 0 \\ \chi(r) \end{pmatrix}, \tag{36}$$

where $\tilde{\psi}_{II}(r,t) = \hat{\lambda}_t\psi_{II}(r,t)$.

We shall consider Eqs. (34) and (36) as matrix equations for two unknown functions, ψ and $\tilde{\psi}$. Rewriting the TDSE in such a matrix form is a rather dramatic step whose consequences must be recognized. First, the introduction of a two-component wave function is associated with doubling the dimension of the original Hilbert space. By convention, we use the same notation for both components indicating the second (lower) one by a tilde. Second, the pseudodifferential operator $\hat{\lambda}_t$ is nonlocal in time, although the dynamics described by Eqs. (34) and (36) remains causal since $\hat{\lambda}_t f(t)$ depends only on $f(t')$ for $t' \leqslant t$, see Eq. (A5). In spite of these apparent complications the matrix form of the TDSE has an important advantage: it opens a way to expand the solution in terms of SS.

C. Discussion

The key element in arriving at Eqs. (34) and (36) is provided by Eqs. (33) and (35). These equations amount to the boundary condition

$$\left.\frac{\partial\psi(r,t)}{\partial r}\right|_{r=a} = \hat{\lambda}_t\psi(a,t). \tag{37}$$

Here and in the following, we omit the subscript in equations that apply to both solutions $\psi_I(r,t)$ and $\psi_{II}(r,t)$, when this may not lead to confusion. Condition (37) expresses the derivatives of $\psi_I(r,t)$ and $\psi_{II}(r,t)$ at $r=a$ in terms of their values at the same point at preceding moments, see Eq. (A5). It is clear that this condition holds for a more general class of the solutions to Eq. (1). For example, any linear combination of the bound states of H can be substituted into the initial condition (16) for $\psi_I(r,t)$ without changing Eq. (33). The class of the solutions to Eq. (1) satisfying Eq. (37) could be identified by appropriate initial conditions. We shall not discuss the most general form of such initial conditions, restricting our consideration to two particular cases defined by Eqs. (16) and (18). However, it is worthwhile to clarify the physical meaning of Eq. (37). From Eqs. (3) and (29) we have

$$i\frac{\partial}{\partial t} - H(t) = \frac{1}{2}\left(\frac{\partial}{\partial r} - \hat{\lambda}_t\right)\left(\frac{\partial}{\partial r} + \hat{\lambda}_t\right), \quad r \geqslant a. \tag{38}$$

Thus a general solution to Eq. (1) can be represented by a sum of two terms,

$$\psi(r,t) = \psi_+(r,t) + \psi_-(r,t), \tag{39}$$

where functions $\psi_\pm(r,t)$ satisfy

$$\frac{\partial\psi_\pm(r,t)}{\partial r} = \pm\hat{\lambda}_t\psi_\pm(r,t), \quad r \geqslant a. \tag{40}$$

The validity of this representation can be confirmed also in a different way. Substituting into Eq. (1) the Fourier transformation of $\psi(r,t)$ in time and requiring the equation to hold for $r \geqslant a$, one finds that a general solution in the outer region must have the form

$$\psi(r,t) = \int_{-\infty}^{\infty}[C_+(E)e^{ikr} + C_-(E)e^{-ikr}]e^{-iEt}\frac{dE}{2\pi}, \quad r \geqslant a, \tag{41}$$

where $C_\pm(E)$ are arbitrary functions. The two terms here, that obviously correspond to the two terms in Eq. (39), represent outgoing (we recall that this term in the scattering theory

commonly denotes truly outgoing and exponentially decaying) and incoming (which similarly includes truly incoming and exponentially growing) waves, respectively. Condition (37) means that only the first terms in Eqs. (39) and (41) are present. Thus the solutions to Eq. (1) satisfying Eq. (37) have only outgoing waves in the outer region.

IV. EXPANSION IN TERMS OF SIEGERT STATES

The outgoing wave solutions to Eq. (1) can be expanded in terms of SS defined by the stationary Hamiltonian H. The coefficients in the expansion are functions of time only, the dependence on the coordinate r is represented by the SS eigenfunctions. In this section we derive equations defining these coefficients for the solutions $\psi_I(r,t)$ and $\psi_{II}(r,t)$. Thus a partial differential equation (1) will be reduced to a discrete set of coupled equations in one (time) variable. At first sight, such an approach follows a scheme common to other time-dependent close-coupling methods. However, there is an essential difference: the continuum will be treated with no approximation for the expense of pseudodifferential character of the resulting coupled equations.

A. Siegert states

SS for the stationary Hamiltonian (5) are defined by [1]

$$(H-E)\phi(r)=0, \tag{42a}$$

$$\phi(0)=0, \tag{42b}$$

$$\left(\frac{d}{dr}-ik\right)\phi(r)\bigg|_{r=a}=0, \tag{42c}$$

where E and k are related by Eqs. (9). The solutions to Eq. (42a) satisfying simultaneously both boundary conditions (42b) and (42c) exist only for a discrete set of generally complex energies E and momenta k, so this is an eigenvalue problem. The eigenvalues and eigenfunctions will be denoted by k_n, $E_n=k_n^2/2$, and $\phi_n(r)$. Let us summarize basic results of the theory of SS needed for the following discussion; many more subtle relations, details of the derivation, and extensive bibliography can be found in [7]. In fact, we give here a concise introduction to the theory from a new standpoint.

The eigenvalue k enters into Eqs. (42) nonlinearly. However, this nonlinearity can be removed by introducing a two-component wave function. This important idea was anticipated in [28]; it was turned into a fruitful approach in [7]. Using operators (25), the boundary condition (42c) reads

$$\mathcal{D}\phi_n(r)=ik_n\mathcal{F}\phi_n(r). \tag{43}$$

Thus we can rewrite Eq. (42a) in a matrix form similar to Eqs. (34) and (36),

$$\left[\begin{pmatrix}0 & 1\\ -2\tilde{H} & \mathcal{F}\end{pmatrix}-ik_n\right]\begin{pmatrix}\phi_n(r)\\ \tilde{\phi}_n(r)\end{pmatrix}=0. \tag{44}$$

Multiplying this equation from the left by a weight matrix

$$\begin{pmatrix}-\mathcal{F} & 1\\ 1 & 0\end{pmatrix}, \tag{45}$$

we transform it to a symmetric form,

$$\left[\begin{pmatrix}-2\tilde{H} & 0\\ 0 & 1\end{pmatrix}-ik_n\begin{pmatrix}-\mathcal{F} & 1\\ 1 & 0\end{pmatrix}\right]\begin{pmatrix}\phi_n(r)\\ \tilde{\phi}_n(r)\end{pmatrix}=0. \tag{46}$$

The solutions to this eigenvalue problem are orthogonal with respect to the inner product

$$\int_0^a (\phi_n(r)\ \tilde{\phi}_n(r))\begin{pmatrix}-\mathcal{F} & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\phi_m(r)\\ \tilde{\phi}_m(r)\end{pmatrix}dr=2ik_n\delta_{nm}, \tag{47}$$

where the first factor in the integrand is a two-component row. This amounts to the following orthonormalization condition for the eigenfunctions $\phi_n(r)$ [29–31]

$$\int_0^a \phi_n(r)\phi_m(r)dr+i\frac{\phi_n(a)\phi_m(a)}{k_n+k_m}=\delta_{nm}. \tag{48}$$

Let $\mathcal{H}$ be the space of functions square integrable in the interval $0\leqslant r\leqslant a$, and $\mathcal{H}^2=\mathcal{H}\otimes\mathcal{H}$. The solutions to Eqs. (42) and (46) belong to $\mathcal{H}$ and $\mathcal{H}^2$, respectively. Introducing some primitive basis in $\mathcal{H}$ and reformulating the problem in an algebraic form (see [7] and Sec. VII), it can be shown that the solutions to Eq. (46) form a complete set in $\mathcal{H}^2$, i.e.,

$$\sum_n \frac{1}{2ik_n}\begin{pmatrix}\phi_n(r)\\ \tilde{\phi}_n(r)\end{pmatrix}(\phi_n(r')\ \tilde{\phi}_n(r'))=\delta(r-r')\begin{pmatrix}0 & 1\\ 1 & \mathcal{F}\end{pmatrix}, \tag{49}$$

where the matrix on the right-hand side is the inverse of the weight matrix (45). This amounts to the following completeness relations for the eigenfunctions $\phi_n(r)$ [7,32]:

$$\sum_n \frac{1}{ik_n}\phi_n(r)\phi_n(r')=0, \tag{50a}$$

$$\sum_n \phi_n(r)\phi_n(r')=2\delta(r-r'), \tag{50b}$$

$$\sum_n ik_n\phi_n(r)\phi_n(r')=2\delta(r-a)\delta(r'-a), \tag{50c}$$

where both r and r' lie within the interval $[0,a]$. Thus while the two-component solutions to Eq. (46) form a "normal" complete set in the space of doubled dimension $\mathcal{H}^2$, with standard orthogonality (47) and completeness (49) properties dictated by the weight matrix (45), the solutions to Eqs. (42) form an overcomplete set in the original Hilbert space $\mathcal{H}$, satisfying rather unusual relations (48) and (50).

An important question is: Given a function $\psi(r)\in\mathcal{H}$, how to expand it in terms of SS eigenfunctions $\phi_n(r)$? As follows from the above discussion, this question does not have a unique answer. To define the expansion coefficients uniquely, one has to introduce another function $\tilde{\psi}(r)$ and consider a two-component vector $(\psi(r)\tilde{\psi}(r))^T$. This vector belongs to $\mathcal{H}^2$, and hence can be uniquely expanded in terms of the solutions to Eq. (46),

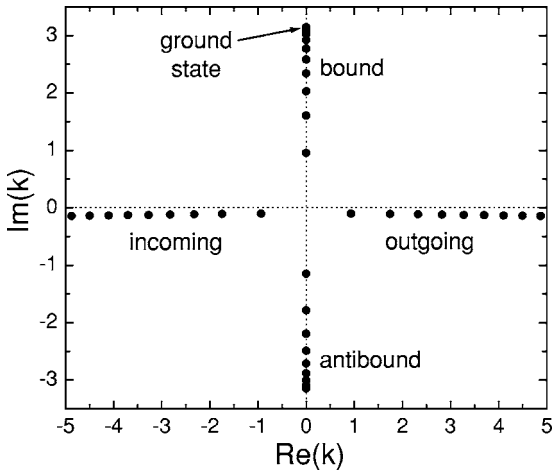

FIG. 1. SS momentum eigenvalues k_n for a rectangular potential (103) with $V_0=-5$ and $a=10$.

$$\begin{pmatrix} \psi(r) \\ \tilde{\psi}(r) \end{pmatrix} = \sum_n a_n \begin{pmatrix} \phi_n(r) \\ \tilde{\phi}_n(r) \end{pmatrix}. \tag{51}$$

Multiplying this expansion from the left by

$$(\phi_n(r)\ \tilde{\phi}_n(r)) \begin{pmatrix} -\mathcal{F} & 1 \\ 1 & 0 \end{pmatrix} \tag{52}$$

and integrating over $r \in [0,a]$ using Eq. (47), we find the coefficients

$$a_n = \frac{1}{2ik_n} \left(ik_n \int_0^a \phi_n(r)\psi(r)dr - \phi_n(a)\psi(a) + \int_0^a \phi_n(r)\tilde{\psi}(r)dr \right). \tag{53}$$

These coefficients depend on both functions $\psi(r)$ and $\tilde{\psi}(r)$, which again shows that the second component $\tilde{\psi}(r)$ is needed to define them uniquely. Substituting Eq. (53) back into Eq. (51) and using Eqs. (50) one obtains the expected identity.

SS can be divided into four groups, according to the position of the momentum eigenvalue k_n in the complex plane: bound ($\mathrm{Re}\, k_n=0$, $\mathrm{Im}\, k_n>0$), antibound ($\mathrm{Re}\, k_n=0$, $\mathrm{Im}\, k_n<0$), incoming ($\mathrm{Re}\, k_n>0$, $\mathrm{Im}\, k_n<0$), and outgoing ($\mathrm{Re}\, k_n<0$, $\mathrm{Im}\, k_n<0$), see Fig. 1. The eigenfunctions $\phi_n(r)$ for bound and antibound states are real; the incoming and outgoing states appear in pairs: k_n, E_n, $\phi_n(r)$ and $-k_n^*$, E_n^*, $\phi_n^*(r)$. The set of SS is in one-to-one correspondence with the set of PS for the same Hamiltonian H. The bound states of H are given by the bound SS. Taking into account Eq. (6), in this case Eq. (48) reduces to the ordinary orthonormalization condition for bound states. Let $\{b\}$ denote the set of subscripts n corresponding to bound SS. We shall assume that the bound state in the initial condition (16) for problem I is given by the SS with $n=0 \in \{b\}$. All the other SS serve to represent the continuum. Namely, the scattering states of H can be expanded in terms of SS [7,29],

$$\varphi(r,k) = ike^{-ika} \sum_n \frac{\phi_n(r)\phi_n(a)}{k_n(k-k_n)}, \quad 0 \leqslant r \leqslant a, \tag{54a}$$

$$= e^{-ikr} - S(k)e^{ikr}, \quad r \geqslant a, \tag{54b}$$

where the scattering matrix $S(k)$ is given by [7]

$$S(k) = e^{-2ika} \left[1 - ik \sum_n \frac{[\phi_n(a)]^2}{k_n(k-k_n)} \right]. \tag{55}$$

To derive Eq. (54a), one has to take $ik\varphi(r,k)$ as the second component in Eq. (51), a fact which has not been recognized previously. The stationary outgoing wave Green's function defined by Eqs. (8) also can be expanded in terms of SS [23],

$$G(r,r';k) = \sum_n \frac{\phi_n(r)\phi_n(r')}{k_n(k-k_n)}, \quad 0 \leqslant r,r' \leqslant a. \tag{56}$$

Note a difference in sign here as compared to [7], which comes from a difference in the defining equation. Substituting Eq. (56) into Eq. (11) and using Eq. (A13), we obtain the SS expansion for the time-dependent retarded Green's function defined by Eqs. (10),

$$G(r,r';t) = \sum_n \frac{i}{k_n} g(t;k_n)\phi_n(r)\phi_n(r'), \quad 0 \leqslant r,r' \leqslant a, \tag{57}$$

where $g(t;k)$ is the retarded Green's function for the operator $\hat{\lambda}_t - ik$, see Appendix A. Using Eqs. (50a) and (A14), one can rewrite Eq. (57) in the equivalent form [19,22]

$$G(r,r';t) = -\frac{i}{2}\theta(t) \sum_n w(-e^{i\pi/4}k_n\sqrt{t/2})\phi_n(r)\phi_n(r'), \quad 0 \leqslant r,r' \leqslant a, \tag{58}$$

where $w(z)$ is the Faddeeva function, see Appendix B.

B. Expansion in the inner region: Coupled equations for the coefficients

SS form a complete set in $\mathcal{H}^2$, therefore the solutions to Eqs. (34) and (36) in the inner region can be sought in the form

$$\begin{pmatrix} \psi(r,t) \\ \tilde{\psi}(r,t) \end{pmatrix} = \sum_n a_n(t) \begin{pmatrix} \phi_n(r) \\ \tilde{\phi}_n(r) \end{pmatrix}, \quad 0 \leqslant r \leqslant a. \tag{59}$$

Let $a_n^I(t)$ and $a_n^{II}(t)$ be the coefficients in this expansion for the solutions $\psi_I(r,t)$ and $\psi_{II}(r,t)$, respectively. Introduce notation

$$U_{nm}(t) = \int_0^a \phi_n(r)U(r,t)\phi_m(r)dr, \tag{60}$$

$$\chi_n = \int_0^a \phi_n(r)\chi(r)dr. \tag{61}$$

Substituting Eq. (59) into Eq. (34), multiplying from the left by expression (52), integrating over $r \in [0,a]$ using Eq. (47),

and taking into account the initial condition (16), we obtain a set of coupled equations defining $a_n^I(t)$,

$$ik_n(\hat{\lambda}_t - ik_n)a_n^I(t) + \sum_m U_{nm}(t)a_m^I(t) = 0, \tag{62a}$$

$$a_n^I(t)|_{t\to-\infty} = \delta_{n0}e^{-iE_0t}. \tag{62b}$$

Similarly, from Eqs. (36) and (22b) we obtain equations defining $a_n^{II}(t)$,

$$ik_n(\hat{\lambda}_t - ik_n)a_n^{II}(t) + \sum_m U_{nm}(t)a_m^{II}(t) = -i\delta(t)\chi_n, \tag{63a}$$

$$a_n^{II}(t)|_{t<0} = 0. \tag{63b}$$

The evolution in time in these equations is driven by the operator $\hat{\lambda}_t$, so these are pseudodifferential equations. Solving them, one finds $\psi_I(r,t)$ and $\psi_{II}(r,t)$ in the inner region.

C. Wave function in the outer region

We now find solutions $\psi_I(r,t)$ and $\psi_{II}(r,t)$ in the outer region. The derivation below applies to any outgoing wave solution to Eq. (1), so we omit the subscript. As follows from Eq. (59), in the inner region such a solution is given by

$$\psi(r,t) = \sum_n a_n(t)\phi_n(r), \quad 0 \leqslant r \leqslant a. \tag{64}$$

In the outer region we have from Eq. (41)

$$\psi(r,t) = \int_{-\infty}^{\infty} C_+(E)e^{ikr-iEt}\frac{dE}{2\pi}, \quad r \geqslant a. \tag{65}$$

Requiring continuity of $\psi(r,t)$ at $r=a$, we obtain

$$C_+(E) = e^{-ika}\int_{-\infty}^{\infty}\psi(a,t)e^{iEt}dt. \tag{66}$$

Thus

$$\psi(r,t) = \frac{e^{-3i\pi/4}}{\sqrt{2\pi}}(\hat{\lambda}_t, \partial/\partial r)\int_{-\infty}^{t}\exp\left[i\frac{(r-a)^2}{2(t-t')}\right]\frac{\psi(a,t')}{(t-t')^{1/2}}dt',$$

$$r \geqslant a, \tag{67}$$

where notation $(\hat{\lambda}_t, \partial/\partial r)$ stands for any of the two operators. This equation expresses $\psi(r,t)$ for $r \geqslant a$ in terms of $\psi(a,t)$ which, in turn, is given in terms of $a_n(t)$ by Eq. (64). Thus coefficients $a_n(t)$ completely define the solution $\psi(r,t)$ for all values of $r \in [0,\infty)$. Note that function (67) manifestly satisfies the outgoing wave boundary condition (37). Equation (67) generalizes a result obtained in [25] to the nonstationary case, see also Sec. VI A.

D. Integral form of the coupled equations

Using the retarded Green's function $g(t;k)$ for the operator $\hat{\lambda}_t - ik$, see Appendix A, we can rewrite Eqs. (62) and (63) in an integral form,

$$a_n^I(t) = \delta_{n0}e^{-iE_0t} + \frac{i}{k_n}\sum_m\int_{-\infty}^{t} g(t-t';k_n)U_{nm}(t')a_m^I(t')dt', \tag{68}$$

and

$$a_n^{II}(t) = -\frac{\chi_n}{k_n}g(t;k_n) + \frac{i}{k_n}\sum_m\int_0^t g(t-t';k_n)U_{nm}(t')a_m^{II}(t')dt'. \tag{69}$$

These are inhomogeneous Volterra equations of the second kind; they incorporate the initial conditions. These equations are more convenient for deriving some general properties of the solutions (see the next section) as well as for numerical calculations. Some other forms of the coupled equations are given in Appendix C.

One might think that Eqs. (68) and (69) could be easily obtained from Eqs. (17) and (24) by substituting there expansions (57) and (64) and omitting the summation over n, as if $\phi_n(r)$ were linearly independent. Even though such an approach indeed leads to Eqs. (68) and (69), it cannot be justified because $\phi_n(r)$ are linearly *dependent*. On the contrary, the derivation given above is rigorous and free from ambiguities. It operates with a two-component wave function, see Eq. (59), which is required for the expansion in terms of SS to be uniquely defined, see a discussion around Eqs. (51)–(53).

V. OBSERVABLES

In physical applications, the situation when the potential $V(r,t)$ becomes independent of time for $t\to\infty$ is of main interest. For simplicity, we assume that $V(r,\infty)=V(r,-\infty)=V(r)$, in problem I, and $V(r,\infty)=V(r,0)=V(r)$, in problem II, hence in both cases

$$U(r,t)|_{t\to\infty} = 0, \tag{70}$$

see Eqs. (7), (14), and (21). A more general situation when the limit of $U(r,t)$ for $t\to\infty$ exists, but is not equal to zero, can be treated similarly, but requires first to discuss an expansion of one set of SS in terms of the other defined by a different Hamiltonian; we leave this for the future. The problem is to calculate the observables, i.e., the probabilities to find the system in discrete states and the spectrum of ejected particles as $t\to\infty$. In this section we express these quantities in terms of the coefficients $a_n(t)$ in the SS expansion (59).

A. Reexpansion of the solution in terms of the physical states

The PS defined by the stationary Hamiltonian H form a complete set in the space of functions square integrable in the semiaxis $r \in [0,\infty)$, a fact which is expressed by

$$\sum_{n\in\{b\}} \phi_n(r)\phi_n(r') + \int_0^\infty \varphi^*(r,k)\varphi(r',k)\frac{dk}{2\pi} = \delta(r-r'). \tag{71}$$

Let $\psi(r,t)$ be an outgoing wave solution to Eq. (1) given by Eqs. (64) and (67). This function can be expanded in terms of the PS,

$$\psi(r,t) = \sum_{n\in\{b\}} C_n(t)\phi_n(r) + \int_0^\infty C(k,t)\varphi(r,k)\frac{dk}{2\pi}. \tag{72}$$

Using Eqs. (48), (54), and (64)–(66), we obtain

$$C_n(t) = \int_0^\infty \phi_n(r)\psi(r,t)dr = \sum_m a_m(t)\left[\delta_{nm} - i\frac{\phi_n(a)\phi_m(a)}{k_n+k_m}\right] - \phi_n(a)\int_{-\infty}^\infty g(t-t';-k_n)\psi(a,t')dt', \tag{73}$$

and

$$C(k,t) = \int_0^\infty \varphi^*(r,k)\psi(r,t)dr = ike^{ika}\sum_{n,m}\frac{\phi_n(a)a_m(t)}{k_n(k_n+k)} \times\left[\delta_{nm} - i\frac{\phi_n(a)\phi_m(a)}{k_n+k_m}\right] - \int_{-\infty}^\infty [e^{ika}g(t-t';-k) - S^*(k)e^{-ika}g(t-t';k)]\psi(a,t')dt'. \tag{74}$$

These formulas express the coefficients in the PS expansion (72) in terms of the coefficients in the SS expansion (59) [we recall that $\psi(a,t)$ is given in terms of $a_n(t)$ by Eq. (64)].

B. Large time asymptotics of the SS coefficients

From Eqs. (68), (69), and (A15) we find

$$a_n(t)\big|_{t\to\infty} = \begin{cases} a_n e^{-iE_n t}, & n\in\{b\}, \\ O(t^{-3/2}), & n\notin\{b\}, \end{cases} \tag{75}$$

where the constants a_n for problems I and II are given by

$$a_n^I = \delta_{n0} - i\sum_m \int_{-\infty}^\infty e^{iE_n t}U_{nm}(t)a_m^I(t)dt, \tag{76}$$

and

$$a_n^{II} = \chi_n - i\sum_m \int_0^\infty e^{iE_n t}U_{nm}(t)a_m^{II}(t)dt. \tag{77}$$

It is assumed that $U_{nm}(t)$ vanishes sufficiently rapidly as $t\to\infty$, see Eqs. (60) and (70), so that the integrals in these formulas exist.

C. Large time asymptotics of the PS coefficients

Using Eqs. (50a), (55), (75), (A15), and (A16), we obtain

$$C_n(t)\big|_{t\to\infty} = C_n e^{-iE_n t}, \tag{78a}$$

$$C(k,t)\big|_{t\to\infty} = C(k)e^{-iEt}, \tag{78b}$$

where

$$C_n = a_n, \tag{79}$$

and

$$C(k) = -kS^*(k)e^{-ika}\int_{-\infty}^\infty \psi(a,t)e^{iEt}dt = -kS^*(k)e^{-ika}\sum_n a_n(E)\phi_n(a). \tag{80}$$

Here a_n are defined by Eqs. (75)–(77), and $a_n(E)$ is the Fourier transform of $a_n(t)$,

$$a_n(E) = \int_{-\infty}^\infty a_n(t)e^{iEt}dt. \tag{81}$$

Using Eqs. (68) and (69), we obtain for problem I

$$a_n^I(E) = 2\pi\delta_{n0}\delta(E-E_0) + \frac{1}{k_n(k-k_n)}\sum_m \int_{-\infty}^\infty e^{iEt}U_{nm}(t)a_m^I(t)dt, \tag{82}$$

and for problem II

$$a_n^{II}(E) = \frac{1}{k_n(k-k_n)}\left[i\chi_n + \sum_m \int_0^\infty e^{iEt}U_{nm}(t)a_m^{II}(t)dt\right]. \tag{83}$$

These expressions have an advantage over Eq. (81) for computing $a_n(E)$ since the integrals in them contain a rapidly decaying factor $U_{nm}(t)$. Note that $E\geqslant 0$ in Eq. (80), so one can omit the first term in Eq. (82) when substituting into Eq. (80).

D. Final formulas

Let us summarize final formulas for the observables in terms of the coefficients $a_n(t)$ to be used in the calculations. The probability to find the system in a discrete state $n\in\{b\}$ at $t\to\infty$ is

$$P_n \equiv |C_n|^2 = |\delta_{n0} - iA_n(E_n)|^2, \quad \text{problem I} \tag{84a}$$

$$= |\chi_n - iA_n(E_n)|^2, \quad \text{problem II}, \tag{84b}$$

and the spectrum of ejected particles is

$$P(k) \equiv |C(k)|^2 = k^2\left|\sum_n \frac{A_n(E)}{k_n(k-k_n)}\phi_n(a)\right|^2, \quad \text{problem I} \tag{85a}$$

$$= k^2\left|\sum_n \frac{i\chi_n + A_n(E)}{k_n(k-k_n)}\phi_n(a)\right|^2, \quad \text{problem II}, \tag{85b}$$

where

$$A_n(E) = \sum_m \int_{-\infty}^\infty e^{iEt}U_{nm}(t)a_m(t)dt. \tag{86}$$

Both solutions $\psi_I(r,t)$ and $\psi_{II}(r,t)$ are normalized to unity, so we have

$$\int_0^\infty |\psi(r,t)|^2 dr = \sum_{n\in\{b\}} P_n + \int_0^\infty P(k)\frac{dk}{2\pi} = 1. \qquad (87)$$

VI. SOME LIMITING SITUATIONS ALLOWING ANALYTICAL TREATMENT

To test consistency of the formulation, let us discuss briefly some limiting situations allowing analytical treatment, when the present approach must yield well-known results.

A. Stationary case

In the stationary case the potential does not depend on time, $V(r,t)=V(r)$, hence $U(r,t)=0$. For problem I, we have from Eq. (68)

$$a_n^I(t) = \delta_{n0} e^{-iE_0 t}. \qquad (88)$$

Substituting this into Eqs. (64) and (67), we obtain the expected trivial result

$$\psi_I(r,t) = \phi_0(r) e^{-iE_0 t}, \quad 0 \leqslant r < \infty. \qquad (89)$$

For problem II, we have from Eq. (69)

$$a_n^{II}(t) = -\frac{\chi_n}{k_n} g(t;k_n). \qquad (90)$$

Substituting this into Eqs. (64) and (67), we find

$$\psi_{II}(r,t) = -\sum_n \frac{\chi_n}{k_n} g(t;k_n)\phi_n(r), \quad 0 \leqslant r \leqslant a \qquad (91a)$$

$$= \sum_{n\in\{b\}} \chi_n \phi_n(a) e^{ik_n(r-a)-iE_n t} + \sum_n \chi_n \phi_n(a) M(r-a,k_n,t), \quad r \geqslant a, \qquad (91b)$$

where $M(x,k,t)$ is the Moshinsky function, see Appendix B. Using Eqs. (50a) and (A14), one can rewrite Eq. (91a) in the form

$$\psi_{II}(r,t) = \frac{1}{2}\theta(t)\sum_n \chi_n w(-e^{i\pi/4} k_n \sqrt{t/2})\phi_n(r), \quad 0 \leqslant r \leqslant a, \qquad (92)$$

which coincides with a result obtained in [19]. On the other hand, Eq. (91b) agrees with a result obtained in [25].

B. Sudden approximation

Let the time dependent potential $U(r,t)$ be localized in time in an interval of duration T. Consider the limit $T\to 0$ without making any assumption regarding the strength of $U(r,t)$. For simplicity, we discuss only problem I, problem II can be dealt with similarly. In this case Green's function $g(t;k)$ in Eq. (68) can be replaced by the first term in Eq. (A14). Thus one obtains

$$P_n \approx \left| \int_0^\infty \phi_n(r) e^{-iS(r)} \phi_0(r) dr \right|^2, \qquad (93a)$$

$$P(k) \approx \left| \int_0^\infty \varphi^*(r,k) e^{-iS(r)} \phi_0(r) dr \right|^2, \qquad (93b)$$

where

$$S(r) = \int_{-\infty}^\infty U(r,t) dt. \qquad (94)$$

This agrees with the results of sudden approximation [33].

C. Perturbation theory

Let the strength of $U(r,t)$ be characterized by U_0. Consider the limit $U_0\to 0$, again restricting our discussion to problem I. In the leading order, substituting the first term in Eq. (68) into Eqs. (84a) and (85a), using Eq. (54a) and the fact that $\varphi^*(r,k)=-S^*(k)\varphi(r,k)$, one obtains

$$P_0 \approx 1, \qquad (95a)$$

$$P_{n\neq 0} \approx \left| \int_{-\infty}^\infty e^{i(E_n-E_0)t} U_{n0}(t) dt \right|^2, \qquad (95b)$$

$$P(k) \approx \left| \int_{-\infty}^\infty e^{i(E-E_0)t} U_0(k,t) dt \right|^2, \qquad (95c)$$

where

$$U_0(k,t) = \int_0^a \varphi^*(r,k) U(r,t) \phi_0(r) dr, \qquad (96)$$

and we recall that $U(r,t)|_{r\geqslant a}=0$. This agrees with standard results of the time-dependent perturbation theory [34].

VII. SIEGERT PSEUDOSTATES

The formal theory developed above can be implemented in terms of SPS. Let us recall the definition [7]. We employ some finite primitive basis,

$$\pi_i(r), \quad i = 1,2,\ldots N, \qquad (97)$$

which is assumed to be orthonormal in the interval $0\leqslant r \leqslant a$,

$$\int_0^a \pi_i(r)\pi_j(r) dr = \delta_{ij}, \qquad (98)$$

and becomes complete in $\mathcal{H}$ as $N\to\infty$, i.e.,

$$\sum_{i=1}^\infty \pi_i(r)\pi_i(r') = \delta(r-r'). \qquad (99)$$

In order to satisfy the boundary condition (42b) we assume that $\pi_i(0)=0$, but no restriction on the behaviour of $\pi_i(r)$ near $r=a$ is imposed, except that dictated by the condition of square integrability. Such basis can be constructed, e.g., from the Legendre polynomials, see Appendix C in [7]; finite elements have been used in [12,19]. The solutions to Eqs. (42) can be sought in the form

$$\phi_n(r) = \sum_{i=1}^{N} c_i^{(n)} \pi_i(r). \tag{100}$$

Substituting this expansion into Eq. (42a), multiplying from the left by $\pi_i(r)$, integrating over $r \in [0,a]$, and using the boundary condition (42c), one obtains [7]

$$\left[\begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -2\tilde{\mathbf{H}} & \mathbf{F} \end{pmatrix} - ik_n \right] \begin{pmatrix} \mathbf{c}^{(n)} \\ \tilde{\mathbf{c}}^{(n)} \end{pmatrix} = 0, \tag{101}$$

where $\mathbf{0}$ and $\mathbf{I}$ are zero and unit matrices, the elements of $\tilde{\mathbf{H}}$ and $\mathbf{F}$ are given by

$$\tilde{H}_{ij} = \int_0^a \pi_i(r) \tilde{H} \pi_j(r) dr = \frac{1}{2} \int_0^a \frac{d\pi_i(r)}{dr} \frac{d\pi_j(r)}{dr} dr + \int_0^a \pi_i(r) V(r) \pi_j(r) dr, \tag{102a}$$

$$F_{ij} = \int_0^a \pi_i(r) \mathcal{F} \pi_j(r) dr = \pi_i(a) \pi_j(a), \tag{102b}$$

and $\mathbf{c}^{(n)}$ is the vector of coefficients in Eq. (100). Equation (101) is an algebraic eigenvalue problem. By definition [7], SPS are the solutions to this equation. In other words, SPS are a finite basis representation of the SS discussed in Sec. IV A.

For a given dimension N of the basis (97) there are $2N$ SPS, this number being the dimension of the matrix in Eq. (101). The most important property of SPS, which makes them more than a mere computational tool, is that for any finite N they exactly satisfy finite basis representations of the orthogonality (48) and completeness (50) relations for SS [7]. These fundamental relations have been essentially used in the derivation of the basic results of the theory of SS, Eqs. (54)–(57), as well as present expressions for the observables, Eqs. (84) and (85). The fact that they remain valid for SPS means that *SPS formulation gives a finite N extension of the theory of SS*, as was emphasized in [7,8]. Therefore all the equations given above in terms of SS remain valid in terms of SPS, with the understanding that summations in them must run over $n=1,\ldots,2N$. To obtain physically meaningful results one has to reach convergence as $N \to \infty$.

VIII. ILLUSTRATIVE EXAMPLES

The coupled equations derived above are not what one is well familiar with in atomic and molecular theory. Unfortunately, nice theoretical constructions often turn out to be useless in practice because of difficulties in their implementation, the devil is in the details. The purpose of this section is to demonstrate the principle feasibility of the present approach and provide numerical illustrations of its internal consistency. To this end, we consider only a simplest model: problem I for a time-dependent rectangular potential. The time-independent part of the potential is defined by

$$V(r) = \begin{cases} V_0, & r < a \\ 0, & r \geqslant a, \end{cases} \tag{103}$$

where $V_0 = -5$ and $a = 10$, as in [19]. For the time-dependent part we take

$$U(r,t) = \begin{cases} U_0 \sin^2(\pi t/T), & r < a \text{ and } 0 \leqslant t \leqslant T \\ 0, & \text{otherwise}, \end{cases} \tag{104}$$

which can be viewed as a pulse of strength U_0 and duration T. Potential (103) supports 10 bound states, see Fig. 1. We take the ground state as the state 0 in the initial condition (16), with $E_0 \approx -4.954$. The results reported below were obtained by solving Eq. (68). The observables were calculated using Eqs. (84a), (85a), and (86). Our numerical procedure is discussed in Appendix D. The results are converged within the scale of the figures with respect to all parameters of the numerical scheme.

Of primary interest is the spectrum of ejected particles $P(k)$—a characteristic that naturally follows from the present approach, but is not easily obtainable by other methods. We start with sudden and perturbative regimes. As follows from Eqs. (93b) and (95c), in these cases $P(k)$ is given by

$$P_{SA}(k) = 4 \sin^2(U_0 T/4) f(k) \tag{105}$$

and

$$P_{PT}(k) = \frac{1}{4} (U_0 T)^2 g(x) f(k), \tag{106}$$

respectively, where the common factor $f(k)$ has a meaning of an effective matrix element squared for the present interaction,

$$f(k) = \left| \int_0^a \varphi^*(r,k) \phi_0(r) dr \right|^2, \tag{107}$$

and $g(x)$ comes from the integration in t,

$$g(x) = \left[\frac{8\pi^2 \sin(x/2)}{x(x^2 - 4\pi^2)} \right]^2, \quad x = (E - E_0)T. \tag{108}$$

Note that $g(0)=1$, so Eq. (105) for $U_0 \to 0$ coincides with Eq. (106) for $T \to 0$, as one would expect. A departure of the exact results from sudden approximation (105) as T grows is illustrated in Fig. 2. For the validity of sudden approximation the parameter x defined in Eq. (108) must be small, which agrees with the numerical results. For higher energies of ejected particles the departure occurs at smaller T. For the present model, function $f(k)$ defining the spectrum $P(k)$ in the sudden regime has pronounced oscillating structure with maxima at the positions of the outgoing SS momentum eigenvalues k_n, in accord with Eq. (54a). For potentials having infinite range, the distribution of the outgoing SPS eigenvalues becomes denser as the cutoff radius a grows [7], so the oscillations will be smoothed out, but true physical features, such as shape resonances, if any, will remain. A departure of the exact results from perturbation theory (106) for a fixed T and growing U_0 is illustrated in Fig. 3. The value of U_0 for which a considerable departure occurs is about five times

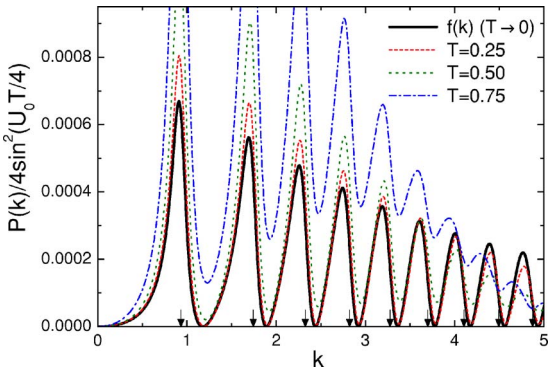

FIG. 2. (Color online) Spectra of ejected particles for $U_0=10$ and several values of T in the sudden regime. The solid line shows the results of sudden approximation, Eq. (105). Arrows indicate positions of the outgoing SS momentum eigenvalues k_n, see Fig. 1.

smaller than the depth of the unperturbed potential (103). The spectrum $P(k)$ in the perturbative regime is determined by a product of two oscillating functions, $g(x)$ and $f(k)$, which results in a rather complicated structure with nonmonotonic behavior of heights of the maxima.

We now consider a strong long pulse, i.e., a situation far beyond the above approximate treatments. The spectra for $U_0=-2V_0=10$ and two values of T are shown in Fig. 4. These spectra look quite different from those shown in Figs. 2 and 3. A further increase of T leads to an increase of the frequency of the oscillations with a little effect on the envelope (after devision by T). These results can be interpreted using adiabatic approximation [35]. The total potential $V(r,t)$ in the present model with $U_0=-2V_0$ has a rectangular shape with height $V_0(t)=V_0\cos(2\pi t/T)$, $0\leqslant t\leqslant T$. In the adiabatic regime, the initial state adiabatically follows the variation of $V_0(t)$, hence the corresponding SS momentum and energy eigenvalues become functions of time, $k_0(t)$ and $E_0(t)$. Let us trace the evolution of $k_0(t)$ in the momentum plane. It starts from the position of the ground state in Fig. 1 at $t=0$. As time grows, this eigenvalue moves down along the imaginary axis. At some moment close to $T/4$, when $V_0(t)\approx 0$, it crosses the real axis, which corresponds to promoting the adiabatic state to the continuum. At some further moment it

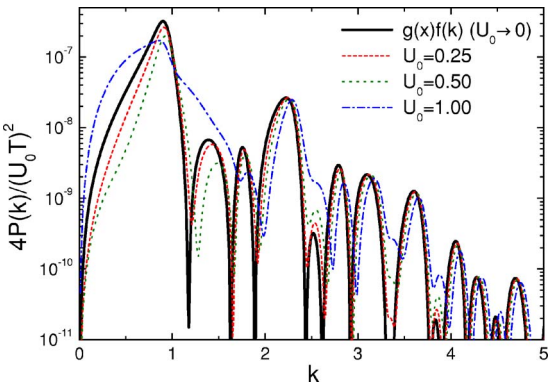

FIG. 3. (Color online) Spectra of ejected particles for $T=3$ and several values of U_0 in the perturbative regime. The solid line shows the results of perturbation theory, Eq. (106).

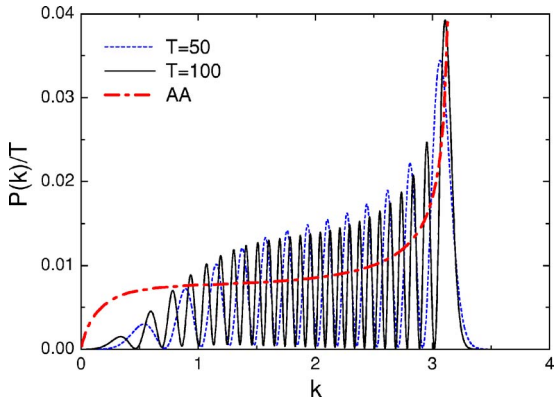

FIG. 4. (Color online) Spectra of ejected particles for two strong long pulses with $U_0=10$. The dash-dotted line shows the envelope in the adiabatic approximation, Eq. (109).

leaves the imaginary axis and then moves to the right and down in the forth quadrant. The motion stops at $t=T/2$, when function $V_0(t)$ reaches its maximum, and then is repeated in inverse direction as time varies from $T/2$ to T. During the time when the state is embedded into the continuum, its energy is complex and can be presented in the form $E_0(t)=\mathcal{E}(t)-i\Gamma(t)/2$. The dependence of the parameters $\mathcal{E}$ and Γ on the height V_0 of the potential (103) for positive values of V_0 is shown in Fig. 5; this implicitly defines their dependence on t. As follows from the figure, except for very small values of V_0 we have $\Gamma(t)\ll\mathcal{E}(t)$, so decay of the adiabatic state on its route through the continuum occurs slowly. Moreover, to a very good approximation $\mathcal{E}(t)\approx V_0(t)$. Under these conditions the spectrum of ejected particles in the adiabatic approximation is given by [35]

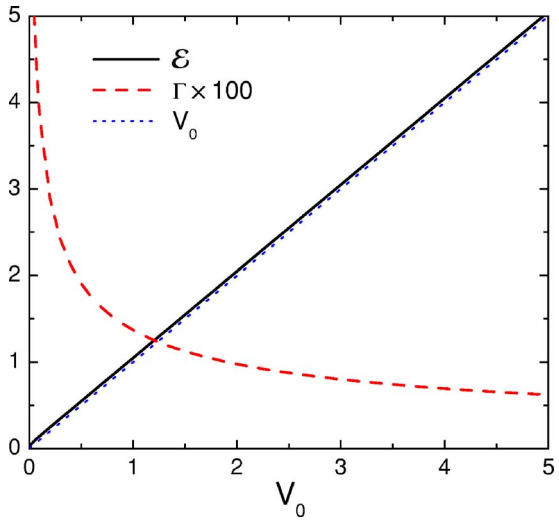

FIG. 5. (Color online) The adiabatic SS eigenvalue $E_0=\mathcal{E}-i\Gamma/2$ for the potential (103) as a function of V_0 for $a=10$. For $V_0=-5$, this eigenvalue corresponds to the ground state shown in Fig. 1, i.e., to the initial state for the present model.

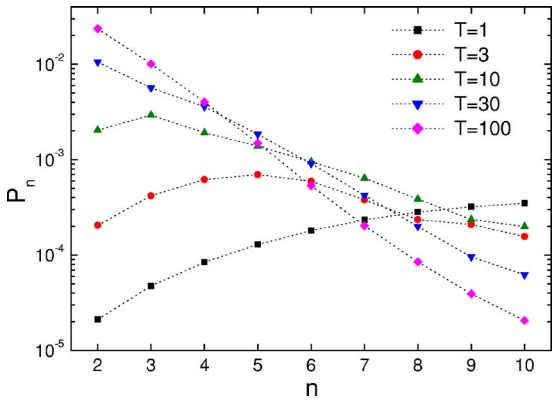

FIG. 6. (Color online) Probabilities of excitation by a strong pulse with $U_0=10$ for several values of T. The integer n enumerates bound states, with $n=1$ corresponding to the initial (ground) state. The connecting lines are to guide the eye only.

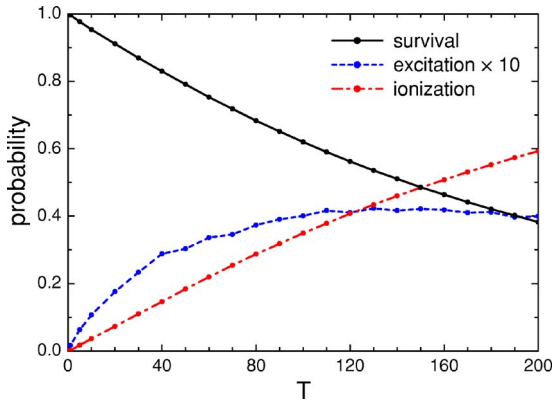

FIG. 7. (Color online) Total survival, excitation, and ionization probabilities for a strong pulse with $U_0=10$ as functions of T. The lines simply connect the calculated points.

$$P_{AA}(k) \approx 2 \times 2\pi k\Gamma(E)\frac{dt(E)}{dE} = \begin{cases} \dfrac{2k\Gamma(E)T}{\sqrt{V_0^2 - E^2}}, & 0 \leqslant E < |V_0| \\ 0, & E > |V_0|, \end{cases} \tag{109}$$

where function $t(E)$ is implicitly defined by equation $E=V_0(t)$ and $\Gamma(E)=\Gamma[t(E)]$. In the present model equation $E=V_0(t)$ has two solutions, in the raising and lowering parts of the pulse, so there are two moments contributing coherently to the spectrum at the given energy. This fact is taken into account by the first factor 2 in Eq. (109), hence this equation gives only an envelope of $P(k)$. For brevity, we do not discuss here the interference effects that account for rapid oscillations of the spectra shown in Fig. 4. The results obtained from Eq. (109) are shown by the dash-dotted line in Fig. 4. The adiabatic approximation explains the proportionality of $P(k)$ to the duration of the pulse T and the cutoff of the spectrum at $E=\max[V_0(t)]=|V_0|=5$ (this corresponds to $k\approx 3.16$). It also correctly reproduces the shape of the envelope of $P(k)$, although there is a difference by a factor of 1.5 in the magnitude. More rigorous development of the adiabatic approximation within the present approach will be the subject of a subsequent paper.

The present approach also yields the probabilities of excitation to discrete states, P_n. Some illustrative results are shown in Fig. 6. For short (long) pulses P_n monotonically grows (decays) with the degree of excitation. For intermediate values of T the probability P_n has a maximum at intermediate values of n.

Figure 7 shows results for total survival (P_1), excitation ($\Sigma_{n=2}^{10}P_n$), and ionization [the integral term in Eq. (87)] probabilities as functions of T. Inelastic transitions are dominated by ionization whose probability in the interval of T considered is approximately proportional to T, in accord with Eq. (109). Slight bending of the ionization curve at larger values of T indicates the onset of saturation of this linear growth. Small hardly visible irregularities in the excitation curve are true oscillations, not a numerical error. These results confirm that the unitarity condition, Eq. (87), is preserved by our numerical scheme within the specified accuracy.

IX. CONCLUSIONS

The main result of this work is a set of coupled equations describing time evolution of the coefficients in the expansion of the solution to the TDSE in terms of SS. These equations are given in pseudodifferential, Eqs. (62) and (63), and integral, Eqs. (68) and (69), forms for two initial value problems of main interest for physical applications. Another result is expressions for the observables, probabilities of transitions to discrete states (84) and the spectrum of ejected particles (85), in terms of the solutions to the coupled equations. These results provide a foundation for a consistent theory of transitions to the continuum in the time-dependent framework. They are implemented in terms of SPS and illustrated by calculations for a model time-dependent rectangular potential.

Despite the great simplicity of the problem considered (s-wave scattering in a time-dependent potential) the approach developed under certain approximations can be extended to realistic three-dimensional problems, as it was the case with the stationary theory given in [7,8], see its applications in Refs. [6,9,10,14,15]. Applications of the present approach to more realistic physical situations are in progress and will be reported elsewhere.

The expansion considered above can be called *diabatic* representation, because the SS basis does not depend on time. Of great interest for applications, as well as from a purely theoretical viewpoint, is to switch to the *adiabatic* representation and develop an adiabatic approximation. This should yield a theory of nonadiabatic transitions to the continuum generalizing the well-known results by Landau, Stueckelberg, and Dykhne for nonadiabatic transitions between discrete states, see [34]. The coupled equations derived in this paper provide a solid mathematical ground for such a development.

Finally, the following comment is in order here. When this paper was almost completed, I became aware of a mathematical literature that has close relation to the present sub-

ject, but which is not widely known in the physical community. This concerns two key technical elements used in arriving at Eqs. (62) and (63). The first is the pseudodifferential operator $\hat{\lambda}_t$. A relation between this operator and the fractional derivative of order 1/2 is discussed in Appendix A, see Eq. (A19). There are books [36–38] and even a special journal, see Ref. [39], dedicated to fractional calculus. I hope that further development of the present approach will benefit from the results available in this branch of mathematics. The second is the outgoing wave boundary condition (37). This condition was first derived in underwater acoustics [40], and then independently rederived by several authors in the field of quantum mechanics [41–43] and optics [44]. Its accurate numerical implementation has posed a separate problem that has been addressed in [45–49]. The results of these studies provide a mathematically consistent and numerically efficient alternative to the method of absorbing potentials [50] and deserve wider recognition among AMO physicists. The present derivation of Eq. (37) only slightly differs from, e.g., that given in [42]; however, for consistency of presentation I retained it in the text. But the present way of implementing Eq. (37) by means of SPS opens a new perspective for the use of this boundary condition in practical calculations.

ACKNOWLEDGMENTS

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APPENDIX A: THE OPERATOR $\hat{\lambda}_t$

The operator $\hat{\lambda}_t$ is defined by Eq. (28). Let us calculate [recall Eqs. (9)]

$$\hat{\lambda}_t \delta(t) = \int_{-\infty}^{\infty} ike^{-iEt} \frac{dE}{2\pi}. \tag{A1}$$

Using the integrals

$$\int_0^{\infty} e^{\pm ik^2 t/2} dk = \sqrt{\frac{\pi}{2}} \frac{e^{\pm i\pi/4}}{(t \pm i0)^{1/2}}, \tag{A2}$$

we obtain

$$\hat{\lambda}_t \delta(t) = \frac{2e^{3i\pi/4}}{\sqrt{2\pi}} \frac{d}{dt}\left[\frac{\theta(t)}{t^{1/2}}\right]. \tag{A3}$$

Using this result and identity

$$f(t) = \int_{-\infty}^{\infty} \delta(t-t') f(t') dt', \tag{A4}$$

we find

$$\hat{\lambda}_t f(t) = \frac{2e^{3i\pi/4}}{\sqrt{2\pi}} \frac{d}{dt} \int_{-\infty}^{t} \frac{f(t')}{(t-t')^{1/2}} dt', \tag{A5}$$

which may serve as an alternative definition of $\hat{\lambda}_t$. Solving this Abelian equation [51] (that is, multiplying both sides by $(t''-t)^{-1/2}$ and integrating over the interval $-\infty < t \leqslant t''$), one can express $f(t)$ in terms of $\hat{\lambda}_t f(t)$,

$$f(t) = \frac{e^{-3i\pi/4}}{\sqrt{2\pi}} \int_{-\infty}^{t} \frac{\hat{\lambda}_{t'} f(t')}{(t-t')^{1/2}} dt'. \tag{A6}$$

Thus Eqs. (A5) and (A6) define an invertable integral transformation. In the following, we assume that

$$f(t)/|t|^{1/2}|_{t\to-\infty} = 0, \tag{A7}$$

which is the case for both solutions $\psi_I(r,t)$ and $\psi_{II}(r,t)$ discussed in the paper. Then, integrating by parts, Eq. (A5) can be presented in the form

$$\hat{\lambda}_t f(t) = \frac{2e^{3i\pi/4}}{\sqrt{2\pi}} \int_{-\infty}^{t} \frac{df(t')}{dt'} \frac{dt'}{(t-t')^{1/2}}. \tag{A8}$$

In this case

$$\hat{\lambda}_t \left[\frac{df(t)}{dt}\right] = \frac{d}{dt}[\hat{\lambda}_t f(t)], \tag{A9}$$

i.e., $\hat{\lambda}_t$ commutes with the derivative in time.

Consider some elementary equations involving the operator $\hat{\lambda}_t$. From Eq. (A5) we obtain

$$(\hat{\lambda}_t - ik)e^{-iEt} = 0, \quad \mathrm{Im}\, E \geqslant 0, \tag{A10}$$

and

$$\hat{\lambda}_t \left[\frac{e^{-3i\pi/4}\theta(t)}{\sqrt{2\pi t}}\right] = \delta(t). \tag{A11}$$

Let us introduce the retarded Green's function for the operator $\hat{\lambda}_t - ik$,

$$(\hat{\lambda}_t - ik) g(t;k) = \delta(t), \quad g(t;k)|_{t<0} = 0. \tag{A12}$$

Solving this equation by the Fourier transformation one finds

$$g(t;q) = -i \int_{-\infty}^{\infty} \frac{e^{-iEt}}{k-q} \frac{dE}{2\pi}. \tag{A13}$$

Using Eqs. (A11) and (B9), the solution can be expressed in terms of the Faddeeva function (see Appendix B),

$$g(t;k) = \theta(t)\left[\frac{e^{-3i\pi/4}}{\sqrt{2\pi t}} - \frac{k}{2} w(-e^{i\pi/4} k\sqrt{t/2})\right]. \tag{A14}$$

The asymptotic behavior of this function for large real t is given by [52,53]

$$g(t;k)|_{t\to\infty} = -ke^{-iEt} + \frac{e^{-i\pi/4}}{k^2\sqrt{2\pi t^3}} + O(t^{-5/2}),$$
$$0 \leqslant \arg k \leqslant \pi/2 \tag{A15a}$$

$$= \frac{e^{-i\pi/4}}{k^2\sqrt{2\pi t^3}} + O(t^{-5/2}),$$
$$\pi/2 < \arg k < 2\pi. \tag{A15b}$$

We also have a useful relation [52,53]

$$g(t;-k) = g(t;k) + ke^{-iEt}\theta(t). \tag{A16}$$

Using this function and Eq. (A10), a general solution to

$$(\hat{\lambda}_t - ik)a(t) = r(t), \tag{A17}$$

where the right-hand side $r(t)$ is a known function, is given by

$$a(t) = Ce^{-iEt} + \int_{-\infty}^{\infty} g(t-t';k)r(t')dt', \tag{A18}$$

where C is an arbitrary constant.

If $f(t)$ is a casual function, i.e., $f(t)|_{t<0}=0$, as is the case for the solution $\psi_{II}(r,t)$, then we have from Eq. (A5)

$$\hat{\lambda}_t = \sqrt{2}e^{3i\pi/4}{}_0D_t^{1/2}, \tag{A19}$$

where ${}_0D_t^{1/2}$ is the Riemann-Liouville fractional derivative of order $1/2$ defined by [54]

$${}_0D_t^{1/2}f(t) = \frac{1}{\sqrt{\pi}}\frac{d}{dt}\int_0^t \frac{f(t')}{(t-t')^{1/2}}dt'. \tag{A20}$$

Equation (A19) agrees with Eqs. (29), if by $\sqrt{\partial/\partial t}$ one understands ${}_0D_t^{1/2}$. This equation establishes a link between the operator $\hat{\lambda}_t$ and fractional calculus [36–38].

APPENDIX B: THE FADDEEVA FUNCTION $w(z)$

This function is implicitly defined by the differential equation

$$\frac{dw(z)}{dz} = -2zw(z) + \frac{2i}{\sqrt{\pi}}, \quad w(0) = 1. \tag{B1}$$

Solving this equation, one explicitly obtains [55]

$$w(z) = e^{-z^2}\,\mathrm{erfc}(-iz). \tag{B2}$$

As follows from Eq. (B1), $w(z)$ is an entire function, i.e., its expansion [53]

$$w(z) = \sum_{n=0}^{\infty} \frac{(iz)^n}{\Gamma(n/2+1)} \tag{B3}$$

converges everywhere in the complex plane. The Mittag-Leffler function $E_\alpha(z)$ is defined by [52]

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n+1)}. \tag{B4}$$

Thus we obtain a relation

$$w(z) = E_{1/2}(iz). \tag{B5}$$

The Moshinsky function $M(x,k,t)$ is defined by [56]

$$M(x,k,t) = i\int_{-\infty}^{\infty} \frac{e^{iqx-iq^2t/2}}{q-k+i\epsilon}\frac{dq}{2\pi} \tag{B6a}$$

$$= \frac{1}{2}e^{ikx-iEt}\,\mathrm{erfc}\left(e^{-i\pi/4}\frac{x-kt}{\sqrt{2t}}\right) \tag{B6b}$$

and can be expressed in terms of $w(z)$,

$$M(x,k,t) = \frac{1}{2}\exp\left(i\frac{x^2}{2t}\right)w\left(e^{i\pi/4}\frac{x-kt}{\sqrt{2t}}\right). \tag{B7}$$

Among these three functions, the Faddeeva function has an advantage in practical calculations since a very accurate and fast algorithm to generate $w(z)$ for an arbitrary complex z has been developed recently [57].

From Eq. (B1) for an arbitrary constant α we obtain

$$\int_0^t \frac{w(\alpha\sqrt{t'})}{(t-t')^{1/2}}dt' = \frac{i\sqrt{\pi}}{\alpha}[1-w(\alpha\sqrt{t})]. \tag{B8}$$

Using this relation we find

$$\hat{\lambda}_t[\theta(t)w(\alpha\sqrt{t})] = \sqrt{2}e^{i\pi/4}\theta(t)\left[\frac{i}{\sqrt{\pi t}} - \alpha w(\alpha\sqrt{t})\right]. \tag{B9}$$

APPENDIX C: SOME OTHER FORMS OF THE COUPLED EQUATIONS

It is not clear at the moment which form of the coupled equations discussed in Secs. IV B and IV D will eventually turn out to be most convenient for calculations; an efficient numerical algorithm most suitable for this kind of equations is still to be found. So we believe that it is useful to give here some other forms of these equations. For brevity, we consider only problem I, problem II can be dealt with similarly. Acting on Eq. (62a) from the left by $\hat{\lambda}_t + ik_n$ we obtain a mixed differential/pseudodifferential representation,

$$\left(i\frac{d}{dt} - E_n\right)a_n^I(t) = -\frac{i}{2k_n}(\hat{\lambda}_t + ik_n)\sum_m U_{nm}(t)a_m^I(t). \tag{C1}$$

The left-hand side here looks typical for close-coupling methods, but the right-hand side contains a nonlocal operator $\hat{\lambda}_t$. Using Eqs. (62) and (A6), we obtain another integral representation,

$$a_n^I(t) = \frac{e^{-i\pi/4}}{\sqrt{2\pi}}\int_{-\infty}^{t}\left[k_n a_n^I(t') + \frac{1}{k_n}\sum_m U_{nm}(t')a_m^I(t')\right]\frac{dt'}{(t-t')^{1/2}}. \tag{C2}$$

This is a homogeneous Volterra equation of the second kind. It may have an advantage over Eq. (68) since it does not require one to generate a nontrivial function $g(t;k)$. The initial conditions for these equations are given by Eq. (62b).

APPENDIX D: NUMERICAL PROCEDURE

The primitive basis (97) was constructed from the Legendre polynomials and SPS were obtained by solving Eq. (101), as described in [7]. The integral form (68) of the coupled equations was chosen for the numerical solution. For a given dimension N of the basis (97) there are $2N$ SPS, and hence $2N$ coupled equations (68). To solve such a system of Volterra equations, in the present calculations we used the simplest method described in [58]. The time interval $0 \leqslant t \leqslant T$ was divided into M equidistant steps: $t_i = ih$, $i = 0,1,\ldots,M$, $h = T/M$. Green's function $g(t;k)$ in the inte-

gral term in Eq. (68) diverges as $t \to 0$, see Eq. (A14), so the method of [58] requires slight modification. We used the following quadrature for integration in time

$$\int_0^{t_i} \frac{f(t')}{(t_i - t')^{1/2}} dt' \approx \sqrt{h} \sum_{j=0}^{i} \omega_j^{(i)} f(t_j), \tag{D1}$$

where $f(t)$ is a smooth function, $i = 1, 2, \ldots, M$, and the weights $\omega_j^{(i)}$ are given by

$$\omega_0^{(i)} = \sqrt{i} - \sqrt{i-1}, \tag{D2a}$$

$$\omega_j^{(i)} = \sqrt{i-j+1} - \sqrt{i-j-1}, \quad j = 1, \ldots, i-1, \tag{D2b}$$

$$\omega_i^{(i)} = 1. \tag{D2c}$$

This quadrature is obtained from the trapezoidal rule for integration in $\tau = (t_i - t')^{1/2}$. The calculation time for solving Eq. (68) scales as NM^2. This procedure yields the values of $a_n^I(t_i)$, which are then substituted into Eq. (86) to calculate the observables (84a) and (85a). The parameters N and M differently effect the accuracy of the results. For a given N, there is some boundary value of the momentum, let us denote it by $\bar{k}_N$, that separates converged SPS eigenvalues k_n from the basis dependent ones, see [7]. Then the spectrum $P(k)$ calculated using Eq. (85a) is converged only for $k < \bar{k}_N$. In the present calculations we used $N = 50$, which was sufficient to obtain a converged spectrum up to $k = 10$. The value of M controls the accuracy of solving Eq. (68). We found that in calculations with a fixed time step h the error almost linearly grows with the length of time interval T. The present calculations were done with $h = 0.001$; in this case the error is beyond the scale of the figures even for the largest $T = 200$ considered. The overall accuracy of the numerical scheme was tested by how well the unitarity condition (87) is fulfilled; the error never exceeded 1%.

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