Nonstationary multistate Coulomb and multistate exponential models for nonadiabatic transitions

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The nonstationary Schrödinger equation is considered in a finite basis of states. The model Hamiltonian matrix corresponds to a single diabatic potential curve with a Coulombic $\sim 1/t$ time dependence. An arbitrary number of other diabatic potential curves are flat, i.e., time independent and have arbitrary energies. Related states are coupled by constant interactions with the Coulomb state. The resulting nonstationary Schrödinger equation is solved by the method of contour integral. Probabilities of transitions to any other state are obtained as $t\to\infty$ in a simple analytical form for the case when the Coulomb state is populated initially (at instant of time $t\to+0$). The formulas apply both to the cases when a horizontal diabatic potential curve is crossed by the Coulomb one and to a noncrossing situation. In the limit of weak coupling, the transition probabilities are interpreted in terms of a sequence of pairwise Landau-Zener-type transitions. Mapping of the Coulomb model onto an exactly solvable exponential multistate model is established. For the special two-state case, the well-known Nikitin model is recovered.

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I. INTRODUCTION

Solving the Schrödinger equation in a finite basis set of states is of importance in various applications of quantum mechanics, and, in particular, in atomic collision theory. When an exact analytical solution can be achieved, then transitions between several closely coupled states (channels) with a full account for nonadiabatic effects are described. The solutions may then be used as dynamic models or as reference (etalon) problems for developing various approximations, such as advanced semiclassical and adiabatic schemes.

The models can be subdivided into nonstationary and stationary ones, originating from the time-dependent and time-independent Schrödinger equation, respectively. Another classification principle groups models into two-state and multistate ones. The difficulties in analysis increase in transition from nonstationary to stationary models and from two-state to multistate models. The multistate models can be solved exactly in only a few cases. Each such solution contributes to our understanding of nonadiabatic dynamics in complicated systems.

Demkov and Osherov [1–6] applied contour integral methods to solve a particular multistate model both in stationary and nonstationary formulations. This Demkov-Osherov model generalizes the well-known two-state Landau-Zener model [7–10] to the multistate case via a special choice of Hamiltonian matrix with linear dependence on time t. The other exactly solvable multistate generalization of the Landau-Zener model is the bow-tie model [11] and its recent generalization suggested by Demkov and Ostrovsky [12,13]. Here, the exact solution was also achieved by using the contour integral method. All these multistate models contain an infinite number of parameters.

Demkov [3] and Demkov and Osherov [1] made an important remark that if one replaces the time variable t by $1/t$ in the Demkov-Osherov Hamiltonian, then the model (referred to as the *Coulomb model* below) is also solvable by the contour integral method. However, the solution was never actually implemented. The probable reason for this lies in the difficulty of interpreting the $1/t$ singularity in the Hamiltonian in physical terms. One of the key points in the present study is the observation that the situation of interest to physics corresponds to the initial (at time $t\to+0$) population of the Coulomb potential curve. In this approach, the singularity lies at the edge of the time interval under consideration and does not create problems. We obtain in a simple analytical form the probabilities of transitions to any other state as $t\to\infty$.

Some aspects of the *two-state* Coulomb problem were considered before. Recently, Osherov and Ushakov [14] derived an exact solution of the *stationary* two-state Coulomb model. Tantawi *et al.*[15] provided an exact solution of the nonstationary two-state Coulomb model and approximate solution of the multistate nonstationary model. Much earlier, Child [17] and Bandrauk [18] studied Coulomb model in a different formulation. The coupling between diabatic states was presumed not to be a constant, as in the Landau-Zener model and in the present model, but time dependent, namely $\sim 1/t$. Child used the WKB approximation, whereas Bandrauk solved exactly the two-state model problem by reducing it to Whittaker's equation. An extension of this form of the Coulomb model the to multistate case meets difficulties.

Contrary to previous authors, we obtain in this paper exact analytical results for the nonstationary Coulomb model with an arbitrary number of states. Section II contains a exact formulation of the model in the basis of diabatic states and Sec. III describes some essential properties of the adiabatic basis. Further solution of the model in terms of contour integral is developed (Sec. IV) and its asymptotic behavior is discussed (Sec. V). For the semiaxis ($0<t<\infty$) problem, the solutions are fully specified and the transition probabilities are extracted and physically interpreted (Sec. VI). In the case of the two-state model, our results are compared with those of previous works (Sec. VI E). The related multistate expo-

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nential model is introduced in Sec. VII. In the two-state case, it is shown to be identical to the well-known Nikitin model (Sec. VII B). Section VIII contains the concluding discussion.

II. MODEL FORMULATION: DIABATIC BASIS

The wave function $|\Psi\rangle$ is expanded over the basis of *diabatic* channel states $|\alpha\rangle$ ($\alpha=0,1,2,\ldots N-1$) as

$$|\Psi(t)\rangle=\sum_{\alpha}\psi_{\alpha}(t)|\alpha\rangle. \tag{2.1}$$

The coefficients $\psi_\alpha(t)$ in this expansion are functions of time t. They are subject to a set of coupled equations obtained by substituting $|\Psi\rangle$ into the nonstationary Schrödinger equation $[H(t)-id/(dt)]|\Psi\rangle=0$ with the Coulomb model Hamiltonian $H(t)$:

$$\left(-i\frac{d}{dt}-\frac{Z}{vt}+D_0\right)\psi_0(t)+\sum_j V_j\psi_j(t)=0, \tag{2.2a}$$

$$\left(-i\frac{d}{dt}+D_j\right)\psi_j(t)+V_j^*\psi_0(t)=0, \tag{2.2b}$$

where V_j is the t-independent coupling between the 0th and jth channels, v is velocity parameter, and parameter Z is interpreted as charge. Hereafter, a latin index, say j, runs over all channel labels, except 0. A greek index, say α, acquires all values including 0. A convenient way to label states is to ascribe positive (negative) integer indices j to the states with parameters $D_j>0$ ($D_j<0$) in a way such that larger $|j|$ correspond to larger $|D_j|$, i.e.,

$$\cdots<D_{-3}<D_{-2}<D_{-1}<D_0<D_1<D_2<D_3<\cdots. \tag{2.3}$$

The set of equations (2.2) presents an exact formulation of our nonstationary multistate Coulomb model, thereby defining its Hamiltonian $H(t)$. Explicitly, the Hamiltonian matrix $\mathbf{H}(R)$, $R=vt$, is described by the nonzero elements

$$H_{jj'}(R)=D_j\delta_{jj'}, \quad H_{j0}(R)=H_{0j}^*(R)=V_j,$$

$$H_{00}(R)=-\frac{Z}{R}+D_0. \tag{2.4}$$

The *diabatic* potential curves $U_\alpha(R)$ are diagonal elements of the Hamiltonian matrix in the chosen basis, i.e.,

$$U_0(R)=-\frac{Z}{R}+D_0, \quad U_j(R)=D_j. \tag{2.5}$$

In the 0th channel, the Coulomb potential with the charge Z is therefore operative, whereas all other diabatic potential curves are horizontal [see Fig. 1 where diabatic and adiabatic potential curves are shown for the ($N=6$)-state Coulomb model]. The parameter D_α is the diabatic "dissociation limit" for the αth channel. The diabatic potential curves $U_0(R)$ and $U_j(R)$ cross at the points

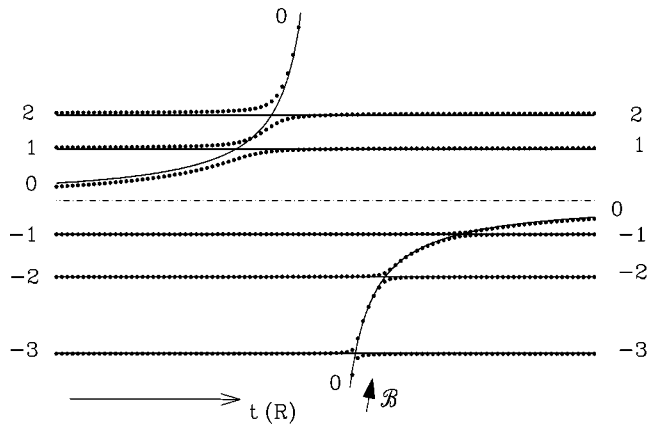

FIG. 1. Diabatic (solid curves) and adiabatic (dots) potential curves for the multistate Coulomb model with $N=6$ as functions of time t. Labeling of diabatic curves is shown. The dash-dotted line indicates asymptote of the Coulomb diabatic curve.

$$R_{cj}=\frac{Z}{D_0-D_j}, \tag{2.6}$$

where $U_0(R_{cj})=U_j(R_{cj})$. In the adiabatic picture considered below, these crossings are replaced by avoided crossings.

III. ADIABATIC BASIS

A. Adiabatic potential curves and dissociation limits

The *adiabatic* potential curves $\mathcal{W}_\alpha(R)$ are R-dependent eigenvalues of the Hamiltonian matrix $\mathbf{H}(R)$ (2.4). These eigenvalues are zeros of the determinant $\Delta(\mathcal{W},R)=\det[\mathcal{W}\mathbf{I}-\mathbf{H}(R)]$, where $\mathbf{I}$ is an $N\times N$ unit matrix:

$$\Delta(\mathcal{W},R)=(\mathcal{W}-D_0+Z/R)\prod_j(\mathcal{W}-D_j)$$
$$-\sum_k|V_k|^2\prod_{j\neq k}(\mathcal{W}-D_j). \tag{3.1}$$

Crossings of diabatic potential curves at the points R_{cj} are replaced by pseudocrossings of adiabatic curves $\mathcal{W}_\alpha(R)$. The long-range behavior of adiabatic potential curves and the related basis states are essential in the subsequent analysis, since they define the form of the wave function's large-$|t|$ asymptotes. First of all, the adiabatic dissociation limits

$$d_\alpha=\lim_{R\to\infty}\mathcal{W}_\alpha(R) \tag{3.2}$$

are different from their diabatic counterparts D_α, being eigenvalues of the separated-atom limit Hamiltonian

$$\mathbf{H}^{(0)}=\lim_{R\to\infty}\mathbf{H}(R). \tag{3.3}$$

They are defined by equations

$$\Delta(d_\alpha)=0 \tag{3.4}$$

with

$$\Delta(E)\equiv\lim_{R\to\infty}\Delta(E,R)=(E-D_0)\prod_j (E-D_j) - \sum_k |V_k|^2\prod_{j\neq k}(E-D_j). \tag{3.5}$$

The determinant $\Delta(E)$ (3.5) is a polynomial factorizable in terms of its roots d_α:

$$\Delta(E)=\prod_\alpha (E-d_\alpha). \tag{3.6}$$

In the limit when $V_j\to 0$ for all j, the adiabatic levels approach diabatic levels: $d_\alpha\to D_\alpha$. For arbitrary couplings V_j, the ordering of adiabatic levels is similar to Eq. (2.3):

$$\cdots<d_{-3}<d_{-2}<d_{-1}<d_0<d_1<d_2<d_3<\cdots. \tag{3.7}$$

B. Large-*R* asymptotes of adiabatic potential curves: Fractional charges

A deviation of the adiabatic potential curve $\mathcal{W}_\alpha(R)$ from its dissociation limit d_α has the Coulomb asymptote

$$\mathcal{W}_\alpha(R)=d_\alpha-\frac{ZA_\alpha}{R}+O(R^{-2}). \tag{3.8}$$

The "effective charge" (ZA_α) in the αth adiabatic channel can be found by expanding expression (3.1) to the order R^{-1}:

$$A_\alpha\frac{d\Delta}{dE}\bigg|_{E=d_\alpha}=\prod_j (d_\alpha-D_j). \tag{3.9}$$

Using representation (3.6), we obtain

$$\frac{d\Delta}{dE}\bigg|_{E=d_\alpha}=\prod_{\gamma\neq\alpha}(d_\alpha-d_\gamma), \tag{3.10}$$

$$A_\alpha=\frac{d_\alpha-D_\alpha}{d_\alpha-D_0}\prod_{\gamma\neq\alpha}\frac{d_\alpha-D_\gamma}{d_\alpha-d_\gamma}, \tag{3.11}$$

where we imply for $\alpha=0$ that the prefactor equals unity: $(d_\alpha-D_\alpha)/(d_\alpha-D_0)\Rightarrow 1$.

The adiabatic basis states $|\alpha)$ can be expanded over the diabatic basis $|\gamma\rangle$ as

$$|\alpha)=\sum_\gamma c_{\alpha\gamma}(R)|\gamma\rangle. \tag{3.12}$$

In the limit $R\to\infty$, we straightforwardly obtain the relation

$$(D_j-d_\alpha)c_{\alpha j}(R\to\infty)=V_j^* c_{\alpha 0}(R\to\infty) \tag{3.13}$$

for expansion coefficients $c_{\alpha\gamma}(R)$. Hence,

$$c_{\alpha j}(R\to\infty)=N_\alpha\frac{V_j^*}{D_j-d_\alpha},\quad c_{\alpha 0}(R\to\infty)=N_\alpha, \tag{3.14}$$

where the normalization factor N_α is determined by

$$N_\alpha^{-2}=1+\sum_j \frac{|V_j|^2}{(D_j-d_\alpha)^2}. \tag{3.15}$$

On considering the term $-Z/R$ in Eq. (2.5) as a perturbation in the basis of $(R\to\infty)$ adiabatic states, we obtain an alternative expression for the adiabatic fractional charge A_α,

$$A_\alpha=|c_{\alpha 0}(R\to\infty)|^2=N_\alpha^2=\left(1+\sum_j\frac{|V_j|^2}{(D_j-d_\alpha)^2}\right)^{-1}. \tag{3.16}$$

It is easy to check that this formula is equivalent to Eqs. (3.11). Representation (3.16) testifies that

$$0<A_\alpha<1. \tag{3.17}$$

In the Appendix, we also prove that

$$\sum_\alpha A_\alpha=1. \tag{3.18}$$

These properties together with formula (3.8) allow us to call A_α the *fractional adiabatic charges*.

Consider now a functional form of the long-range behavior of a time-dependent wave function in the αth adiabatic channel. It is governed by characteristic adiabatic phase factor

$$\exp\left(-i\int^t W_\alpha(vt')dt'\right)\sim\mathcal{F}_\alpha(t), \tag{3.19}$$

which has the same form for $t\to\pm\infty$. Here, the *standard asymptotic solution* is

$$\mathcal{F}_\alpha(t)=|t|^{i\beta_\alpha}\exp(-id_\alpha t) \tag{3.20}$$

with

$$\beta_\alpha=\frac{ZA_\alpha}{v}. \tag{3.21}$$

C. Weak-coupling case

In case of weak coupling, the standard second-order perturbation theory gives the relation

$$d_j-D_j=\frac{|V_j|^2}{D_j-D_0} \tag{3.22}$$

between adiabatic and diabatic dissociation limits. Using these approximations in formula (3.16), we obtain

$$A_j=\frac{|V_j|^2}{(D_j-D_0)^2}+O(V^3), \tag{3.23}$$

$$A_0 = 1 - \sum_j \frac{|V_j|^2}{(D_j - D_0)^2} + O(V^3). \tag{3.24}$$

We see, in the case of weak coupling, that all fractional charges are small ($A_j \sim V_j^2$), except A_0 which is close to unity. For weak coupling, the parameter $2V_j$ signifies the potential curve splitting at the avoided crossing R_{cj}.

IV. SOLUTION OF THE TIME-DEPENDENT PROBLEM IN TERMS OF CONTOUR INTEGRAL

On substituting the Laplace transformation

$$\psi_\alpha(t) = \int_{\mathcal{C}} dE\, \xi_\alpha(E) \exp(-iEt) \tag{4.1}$$

into relations (2.2), the set of coupled equations

$$-i \frac{d}{dE}\left[(D_0 - E)\xi_0 + \sum_j V_j \xi_j \right] - \frac{Z}{v}\xi_0 = 0, \tag{4.2a}$$

$$(D_j - E)\xi_j + V_j^* \xi_0 = 0 \tag{4.2b}$$

for the functions $\xi_\alpha(E)$ can be derived. We find ξ_j from Eq. (4.2b) and substitute this expression into Eq. (4.2a) to get the single first-order differential equation for the function $\xi_0(E)$:

$$i\frac{d}{dE}\left[\left(E - D_0 - \sum_j \frac{|V_j|^2}{E - D_j} \right) \xi_0 \right] - \frac{Z}{v}\xi_0 = 0. \tag{4.3}$$

It is now convenient to introduce the function

$$F(E) = g(E)\xi_0(E), \tag{4.4}$$

where

$$g(E) = E - D_0 - \sum_j \frac{|V_j|^2}{E - D_j}. \tag{4.5}$$

On comparing this latter formula to Eq. (3.5), $g(E)$ is expressed in terms of $\Delta(E)$ as

$$g(E) = \Delta(E) \prod_j (E - D_j)^{-1}. \tag{4.6}$$

The factorization relation (3.6) is utilized to recast Eq. (4.6) as

$$g(E) = (E - d_0) \prod_j \left(\frac{E - d_j}{E - D_j} \right). \tag{4.7}$$

The differential equation for function $F(E)$, Eq. (4.4), is obtained from Eq. (4.3) as

$$i\frac{d}{dE}F(E) = \frac{Z}{v g(E)} F(E). \tag{4.8}$$

In order to carry out integration explicitly, we decompose $1/g(E)$ into the sum of elementary fractions

$$1/g(E) = \frac{1}{E - d_0} \prod_j \left(\frac{E - D_j}{E - d_j} \right) = \sum_\alpha \frac{A_\alpha}{E - d_\alpha}, \tag{4.9}$$

where the coefficients A_α are expressed by formula (3.11). An explicit solution for $F(E)$ is given by

$$F(E) = \exp\left(-i \int^E \frac{Z d\tilde{E}}{v g(\tilde{E})} \right) = \prod_\alpha (E - d_\alpha)^{-i\beta_\alpha}, \tag{4.10}$$

with β_α given by formula (3.21). On taking into account Eqs. (4.7) and (4.4), we finally obtain the contour integral representation of the wave-function components

$$\psi_0(t) = \mathcal{Q} \int_{\mathcal{C}} dE \exp(-iEt) \left[\prod_k (E - D_k) \right] \times \prod_\alpha (E - d_\alpha)^{-i\beta_\alpha - 1}, \tag{4.11a}$$

$$\psi_j(t) = V_j \mathcal{Q} \int_{\mathcal{C}} dE \exp(-iEt) \left[\prod_{k \neq j} (E - D_k) \right] \times \prod_\alpha (E - d_\alpha)^{-i\beta_\alpha - 1}, \tag{4.11b}$$

where $\mathcal{Q}$ is some common normalization factor.

Each solution of the set of N first-order differential equations (2.2) can be considered as a column vector $\boldsymbol{\psi}(t)$ with components $\psi_\alpha(t)$ labeled by subscript α. The set of N first-order differential equations (2.2) has N linear independent solutions, i.e., N different column vectors $\boldsymbol{\psi}^\nu(t)$ labeled by superscript ν, $\nu = 1,2,\ldots,N$. The significance of this superscript is specified as follows. For each ν and for all α, the components $\psi_\alpha^\nu(t)$ are expressed as contour integrals of the same form (4.11), but with different choices of the integration contour $\mathcal{C}^\nu$ in the plane of E, considered as a complex-valued variable.

The simple choice of integration contours refers to the fact that the integrands have exactly N branch points $E_\gamma = d_\gamma$. We choose the integration contour $\mathcal{C}^{\gamma-}$ in the complex-E plane in the following way: it starts at $E = d_\gamma - \varepsilon + i\infty$, where $\exp(-iEt) \to 0$ for $t < 0$ (ε is a small parameter). The contour follows vertically downwards, circumvents the branch point d_γ counterclockwise, and continues vertically upwards back to $E = d_\gamma + \varepsilon + i\infty$ (see Fig. 2). One can say that the contour $\mathcal{C}^{\gamma-}$ hooks on the related branch point d_γ; both its ends go to infinity in direction $E \to +i\infty$ in the complex-E plane. On using these contours in formula (4.11), we obtain exactly N basic linear independent solutions $\boldsymbol{\psi}^{\gamma-}(t)$. For the dynamic problem, behavior of these solutions at $|t| \to \infty$ is essential and is considered in the following section.

V. LARGE-TIME ASYMPTOTES OF SOLUTIONS, $|t| \to \infty$

In order to illustrate the method of calculating the $t \to \infty$ asymptotes for the contour integrals (4.11), we first consider

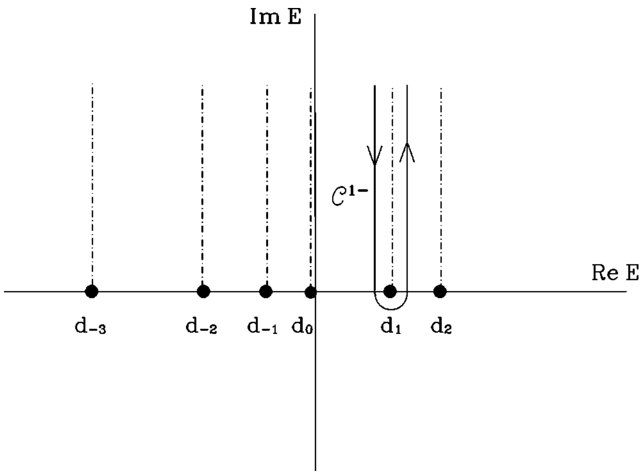

FIG. 2. Complex-E plane with branch points d_γ of the integrand in representation (4.11) for wave function. The cuts (shown by dash-dotted lines) go from branch points upwards, i.e., to $d_\gamma + i\infty$. The branch points are dissociation limits of adiabatic potential curves; the plot corresponds to the six-state Coulomb model of Fig. 1. The integration contour $\mathcal{C}^{1-}$ is also shown, see text.

the $\alpha=0$ component (4.11a) of $\psi_\alpha^{\gamma-}(t)$:

$$\psi_0^{\gamma-}(t)=\mathcal{Q}_{\gamma-}\int_{\mathcal{C}_{\gamma-}} dE\exp(-iEt)\left[\prod_k (E-D_k)\right]\times\prod_\delta (E-d_\delta)^{-i\beta_\delta-1}. \tag{5.1}$$

We rewrite integral (5.1) identically as

$$\psi_0^{\gamma-}(t)=\mathcal{Q}_{\gamma-}\int_{\mathcal{C}_{\gamma-}} dE(E-d_\gamma)^{-i\beta_\gamma-1}\times\exp[-i(E-d_\gamma)t]f_\gamma(E), \tag{5.2}$$

where the factor

$$f_\gamma(E)=\exp(-id_\gamma t)\left[\prod_k (E-D_k)\right]\prod_{\delta\neq\gamma}(E-d_\delta)^{-i\beta_\delta-1} \tag{5.3}$$

is singled out in the integrand. It has no singularity at the point $E=d_\gamma$. For evaluation of integral asymptote it is therefore sufficient to replace $f_\gamma(E)$ by its magnitude at $E=d_\gamma$, i.e., by $f_\gamma(d_\gamma)$. The integration variable is then changed to $y=-i(E-d_\gamma)t$ with the result that the standard integral representation for the Γ function [16]

$$\Gamma(z)=-\frac{1}{2i\sin\pi z}\int_{\tilde{\mathcal{C}}}(-y)^{z-1}e^{-y}dy \tag{5.4}$$

is obtained. Here, the integration contour $\tilde{\mathcal{C}}$ in the complex-y plane starts from $+\infty$, encircles the point $y=0$ counterclockwise, and returns to $+\infty$. Finally, we see that the asymptote is equal to the standard asymptotic solution (3.20) multiplied over some constant (t-independent) factor:

$$\begin{aligned}\psi_0^{\gamma-}(t\to-\infty)&=2\mathcal{F}_\gamma(t)\mathcal{Q}_{\gamma-}\exp(\tfrac{1}{2}\pi\beta_\gamma)\sinh(\pi\beta_\gamma)\Gamma(-i\beta_\gamma)\\&\quad\times\left[\prod_k (d_\gamma-D_k)\right]\prod_{\delta\neq\gamma}(d_\gamma-d_\delta)^{-i\beta_\delta-1}\\&=2\mathcal{F}_\gamma(t)\mathcal{Q}_{\gamma-}\exp(\tfrac{1}{2}\pi\beta_\gamma)\sinh(\pi\beta_\gamma)\Gamma(-i\beta_\gamma)\\&\quad\times A_\gamma\prod_{\delta\neq\gamma}(d_\gamma-d_\delta)^{-i\beta_\delta}\\&=\mathcal{F}_\gamma(t)\mathcal{Q}_{\gamma-}\sqrt{\frac{2\pi v}{Z}}\sqrt{\exp(2\pi\beta_\gamma)-1}N_\gamma\\&\quad\times\exp[-i\arg\Gamma(i\beta_\gamma)]\prod_{\delta\neq\gamma}(d_\gamma-d_\delta)^{-i\beta_\delta},\end{aligned} \tag{5.5a}$$

where we used expression (3.11) for A_γ, relation $\sqrt{A_\gamma}=N_\gamma$ (3.16), and formula

$$|\Gamma(iy)|^2=\frac{\pi}{y\sinh\pi y}. \tag{5.5b}$$

By a similar calculation, we obtain for $\alpha=j$ components of $\psi_\alpha^\gamma(t)$,

$$\psi_j^{\gamma-}(t\to+\infty)=\frac{V_j}{d_\gamma-D_j}\psi_0^{\gamma-}(t\to+\infty). \tag{5.5c}$$

Formulas (5.5c) imply population of a single (γth) adiabatic channel in the limit $t\to-\infty$. Indeed, there is an obvious correspondence between Eqs. (3.13) and (5.5c). We choose the normalization factor $\mathcal{Q}_{\gamma-}$ so that the $t\to-\infty$ asymptote of the solution $\psi_\alpha^{\gamma-}(t)$ corresponds to population of the γth adiabatic channel with unit probability:

$$\psi_0^{\gamma-}(t\to-\infty)=N_\gamma\mathcal{F}_\gamma(t), \tag{5.6a}$$

$$\psi_j^{\gamma-}(t\to-\infty)=N_\gamma\frac{V_j}{d_\gamma-D_j}\mathcal{F}_\gamma(t). \tag{5.6b}$$

Here, N_γ is factor (3.15) introduced earlier. Normalization (5.6) is achieved on taking

$$(\mathcal{Q}_{\gamma-})^{-1}=\sqrt{\frac{2\pi v}{Z}}\sqrt{\exp(2\pi\beta_\gamma)-1}\times\exp[-i\arg\Gamma(i\beta_\gamma)]\prod_{\delta\neq\gamma}(d_\gamma-d_\delta)^{-i\beta_\delta}. \tag{5.7}$$

Another possibility for constructing a set of linear independent solutions is to choose the integration contour in formula (4.11) as $\mathcal{C}^{\gamma+}$, which is obtained from $\mathcal{C}^{\gamma-}$ by rotation counterclockwise over angle π. One can then say that the contour $\mathcal{C}^{\gamma+}$ hooks on the branch point d_γ; both its ends go to infinity in the direction $E\to-i\infty$ in the complex-E plane. We denote such solutions as $\boldsymbol{\psi}^{\gamma+}(t)$. They have asymptotes

$$\psi_0^{\gamma+}(t\to\infty)=N_\gamma\mathcal{F}_\gamma(t), \tag{5.8a}$$

$$\psi_j^{\gamma+}(t\to\infty)=N_\gamma\frac{V_j}{d_\gamma-D_j}\mathcal{F}_\gamma(t), \tag{5.8b}$$

provided the normalization factor is chosen as

$$(\mathcal{Q}_{\gamma+})^{-1}=(\mathcal{Q}_{\gamma-})^{-1}. \tag{5.9}$$

The physical interpretation of $\boldsymbol{\psi}^{\gamma+}(t)$ is now clear: these are such solutions of the nonstationary Schrödinger equation that end up in the *final* $(t\to\infty)$ population of a single (γth) adiabatic state. This can be compared with the meaning of solutions $\psi^{\gamma-}(t)$ that correspond to the *initial* $(t\to-\infty)$ population of a single (γth) adiabatic state.

Most often, model nonstationary problems are considered on the full time axis, $-\infty<t<\infty$. The initial conditions are imposed at $t\to-\infty$. By investigating asymptotes of these solutions at $t\to\infty$ one finds state-to-state transition amplitudes. Mathematically, this implies finding asymptotes of solutions $\psi_j^{\gamma-}(t)$ in the limit $t\to\infty$.

The Coulomb model has an important property: the point $t=0$ corresponds to the essential singularity of solutions $\psi(t)$. In particular, this means that starting from solution $\psi^{\gamma-}(t)$ fixed by initial conditions at $t-\to\infty$, one obtains different results at $t\to\infty$ depending on whether the singular point $t=0$ is circumvented via the upper or lower half plane of complex variable t. The physical interpretation of such solutions requires special analysis [19]. Instead of this, we limit ourselves below to the alternative formulation of the problem on the semiaxis $0<t<\infty$.

VI. THE COULOMB MODEL ON THE SEMIAXIS $0<t<\infty$

A. Imposing initial condition at $t\to+0$

We start with the analyses of a particular solution of form (4.11) with the integration contour different from those discussed in previous sections. Namely, we consider contour $\mathcal{C}^{\mathcal{B}}$ that lies entirely within the large-$|E|$ domain where $|E|\gg|d_\alpha|,|D_\alpha|$. Such a contour starts at $E=A-i\infty$, goes upwards to the $E>0$ half plane, circumvents all the branch points counterclockwise along the semicircle with radius A, and goes downwards to $E=-A-i\infty$; here A is a sufficiently large positive number, $A\gg|d_\alpha|,|D_\alpha|$ for any α [see Fig. 3(a)]. Then, integrals (4.11) are approximately simplified to

$$\psi_0^{\mathcal{B}}(t)=\mathcal{Q}^{\mathcal{B}}\int_{\mathcal{C}^{\mathcal{B}}}dEE^{-i\Sigma_\delta\beta_\delta-1}\exp(-iEt), \tag{6.1a}$$

$$\psi_j^{\mathcal{B}}(t)=V_j\mathcal{Q}^{\mathcal{B}}\int_{\mathcal{C}^{\mathcal{B}}}dEE^{-i\Sigma_\delta\beta_\delta-2}\exp(-iEt). \tag{6.1b}$$

Note that in this approximation, $i\,d\psi_j^{\mathcal{B}}/dt=V_j\psi_0^{\mathcal{B}}$. If we express coefficients β_α via A_α according to formula (3.21) and employ sum rule (3.18), then Eqs. (6.1) are cast as

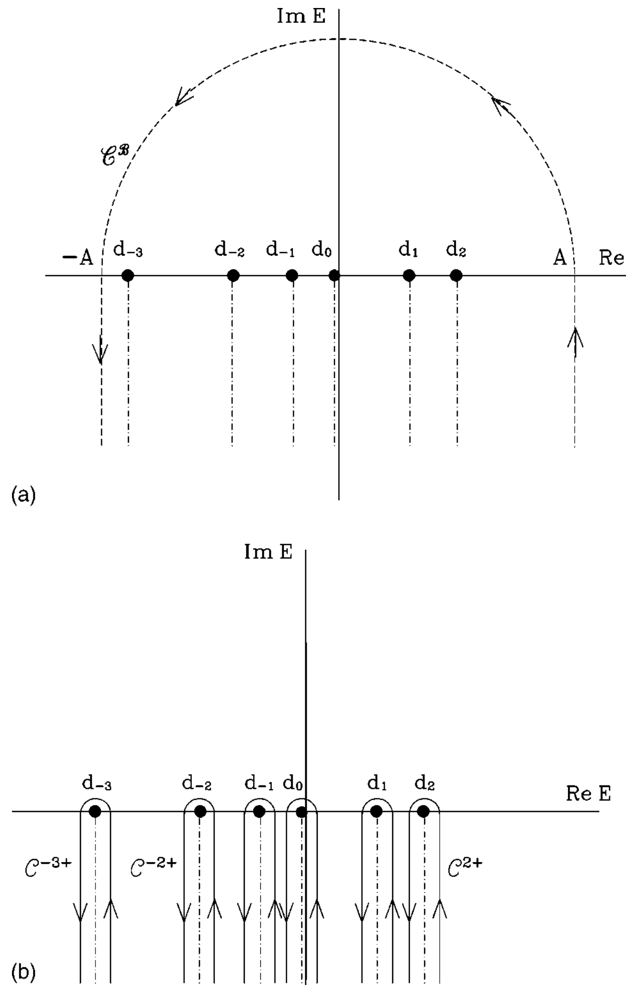

FIG. 3. Same as in Fig. 2, but with different integration contours. The cuts are drawn from the branch points d_γ downwards. Plot (a) shows contour $\mathcal{C}^{\mathcal{B}}$ which corresponds to the initial $(t\to+0)$ population of the emerging potential curve $\mathcal{B}$ shown in Fig. 1; (b) same contour deformed to sequence of contours $\mathcal{C}^{\gamma+}$. The latter representation is convenient to evaluate transition probabilities as $t\to\infty$, see text.

$$\begin{aligned}\psi_0^{\mathcal{B}}(t)&=\mathcal{Q}^{\mathcal{B}}\int_{\mathcal{C}^{\mathcal{B}}}dEE^{-iZ/v-1}\exp(-iEt)\\&=2i\sin(i\pi Z/v)(it)^{iZ/v}\Gamma(-iZ/v)\\&=-\mathcal{Q}^{\mathcal{B}}t^{iZ/v}\sqrt{\frac{2\pi v}{Z}}\sqrt{\exp(2\pi Z/v)-1}\\&\quad\times\exp[-i\arg\Gamma(iZ/v)],\end{aligned} \tag{6.2a}$$

$$\psi_j^{\mathcal{B}}(t)=-\frac{it}{iZ/v-1}V_j\psi_0^{\mathcal{B}}(t). \tag{6.2b}$$

We used here again expressions (5.4) and (5.5b). Formulas (6.2) testify that the solution $\psi^{\mathcal{B}}(t)$ of the nonstationary Schrödinger equation corresponds to the population of the 0th adiabatic state at the instant of time $t\to+0$. (It should be emphasized that at this instant adiabatic and diabatic bases coincide). The related potential curve initially (for $t=+0$)

lies at $E=-\infty$ and *emerges from the abyss* as time increases. Below, we denote this initial state as $\mathcal{B}$. The reader has to keep in mind that this initial adiabatic state generally *does not* correlate smoothly (adiabatically) with the 0th adiabatic state at $t\to\infty$, due to the presence of the pseudocrossings described above. Note that the oscillatory factor in Eq. (6.2a) stems from the characteristic Coulomb phase of the emerging potential curve,

$$\exp\left[-i\int^{t}E(t')dt'\right]\approx\exp\left[-i\int^{t}\left(-\frac{Z}{vt'}\right)dt'\right]\sim t^{iZ/v}. \tag{6.3}$$

The normalization factor $\mathcal{Q}^{\mathcal{B}}$ is to be chosen as

$$(\mathcal{Q}^{\mathcal{B}})^{-1}=\sqrt{\frac{2\pi v}{Z}}\sqrt{\exp(2\pi Z/v)-1}\exp[-i\arg\Gamma(iZ/v)]. \tag{6.4}$$

B. Probability of transitions from the emerging potential curve

The amplitude of transition from the emerging $\mathcal{B}$ state to an arbitrary γ state is obtained by deforming the integration contour as shown in Fig. 3(b) and evaluating the integral over the contour $\mathcal{C}^{\gamma+}$,

$$\begin{aligned}F_{0\to\gamma}&=(\mathcal{Q}^{\mathcal{B}})(\mathcal{Q}_{\gamma+})^{-1}\\&=\sqrt{\frac{\exp(2\pi\beta_\gamma)-1}{\exp(2\pi Z/v)-1}}\exp[i\arg\Gamma(iZ/v)\\&\quad-i\arg\Gamma(i\beta_\gamma)]\prod_{\delta\neq\gamma}(d_\gamma-d_\delta)^{-i\beta_\delta}\\&=\sqrt{\frac{\exp(2\pi\beta_\gamma)-1}{\exp(2\pi Z/v)-1}}\left(\prod_{\delta>\gamma}\exp(\pi\beta_\delta)\right)\exp(i\Phi_\gamma),\end{aligned} \tag{6.5}$$

$$\Phi_\gamma=\arg\Gamma(iZ/v)-\arg\Gamma(i\beta_\gamma)+\arg\left(\prod_{\delta}(d_\gamma-d_\delta)^{-i\beta_\delta}\right). \tag{6.6}$$

In evaluating the product in the formula above, we took into account that $\arg(d_\gamma-d_\delta)=i\pi$ for $\delta>\gamma$. Upon introducing

$$p_\alpha=\exp(-2\pi\beta_\alpha), \tag{6.7}$$

the sum rule (3.18) then becomes

$$\sum_\alpha\beta_\alpha=\frac{Z}{v},\quad\prod_\alpha p_\alpha=\exp\left(-\frac{2\pi Z}{v}\right). \tag{6.8}$$

We use Eqs. (6.7) and (6.8) to finally rewrite the transition amplitude (6.5) as

$$F_{\mathcal{B}\to\gamma}=\sqrt{\frac{1-p_\gamma}{1-\exp(-2\pi Z/v)}}\left(\prod_{\delta<\gamma}p_\delta\right)^{1/2}\exp(i\Phi_\gamma), \tag{6.9}$$

and the related transition probability as

$$P_{\mathcal{B}\to\gamma}=|F_{\mathcal{B}\to\gamma}|^2=\frac{1}{1-\exp(-2\pi Z/v)}(1-p_\gamma)\left(\prod_{\delta<\gamma}p_\delta\right). \tag{6.10}$$

The general relation [13]

$$\sum_\gamma(1-p_\gamma)\left(\prod_{\delta<\gamma}p_\delta\right)=1-\prod_\gamma p_\gamma \tag{6.11}$$

together with formula (6.8) ensures satisfaction of the unitarity relation

$$\sum_\gamma P_{\mathcal{B}\to\gamma}=1. \tag{6.12}$$

C. Interpretation: Crossing and noncrossing mechanism of transitions

If one considers the weak-coupling regime where approximation (3.23) applies, the physical meaning of parameters

$$p_j=\exp\left(-\frac{2\pi ZA_j}{v}\right)\approx\exp\left(-\frac{2\pi Z|V_j|^2}{v(D_j-D_0)^2}\right) \tag{6.13}$$

is revealed. Formula (6.13) is the standard expression for the nonadiabatic transition probability in the two-state Landau-Zener model with coupling V_j and difference of slopes of diabatic potential curves (2.5) at the point of pseudocrossing R_{cj} (2.6):

$$\frac{d}{dR}[U_0(R)-U_j(R)]|_{R=R_{cj}}=\frac{Z}{R_{cj}^2}=\frac{(D_0-D_j)^2}{Z}. \tag{6.14}$$

Formula (6.10) has a clear physical interpretation. The final states $\gamma\leqslant0$ are populated via the passage of series of crossings R_{cj} between the initial-state diabatic potential curve $U_0(R)$ and the final-state curves $U_j(R)$ $(j<0)$, (2.6) [or series of pseudocrossings between the adiabatic potential curves $\mathcal{W}_\gamma(R)$]. Formula (6.10) means diabatic passage of all pseudocrossings $R_{c\delta}$, $\delta<\gamma$, which gives a product of elementary probabilities $(\Pi_{\delta<\gamma}p_\delta)$ and adiabatic passage of the pseudocrossing $R_{c\gamma}$, with probability $1-p_\gamma$. The elementary probabilities p_δ are given by Landau-Zener formula (6.13) in the case of weak coupling. As the couplings increase, the elementary probabilities are appropriately renormalized, being expressed via partial adiabatic charges A_α, as specified above. Besides this, formula (6.10) also contains a kind of normalization factor $[1-\exp(-2\pi Z/v)]^{-1}$ which is close to 1 in the case of weak coupling and low velocity v.

The potential curves $U_j(R)$ with $j>0$ do not experience any crossings in the domain $0<t<\infty$. Therefore, population of the final state $\gamma>0$ cannot be explained in terms of the pseudocrossings passage. Within the simple adiabatic picture these states are not populated at all. According to this the probabilities $P_{0\to j}$ are strongly suppressed due to the factor $p_0 \ll 1$ which enters the product in formula (6.10). Indeed, in the weak-coupling and adiabatic limit one has from Eq. (3.24) $A_0 \approx 1$ and $p_0 \approx \exp(-2\pi Z/v) \ll 1$.

We illustrate these general considerations by application to the six-state model with potential curves shown in Fig. 1. The transition probabilities from the emerging state are as follows:

$$P_{0\to -3} = \frac{1}{1-\exp(-2\pi Z/v)}(1-p_{-3}), \tag{6.15a}$$

$$P_{0\to -2} = \frac{1}{1-\exp(-2\pi Z/v)}p_{-3}(1-p_{-2}), \tag{6.15b}$$

$$P_{0\to -1} = \frac{1}{1-\exp(-2\pi Z/v)}p_{-3}p_{-2}(1-p_{-1}), \tag{6.15c}$$

$$P_{0\to 0} = \frac{1}{1-\exp(-2\pi Z/v)}p_{-3}p_{-2}p_{-1}(1-p_{0}), \tag{6.15d}$$

$$P_{0\to 1} = \frac{1}{1-\exp(-2\pi Z/v)}p_{-3}p_{-2}p_{-1}p_0(1-p_{1}), \tag{6.15e}$$

$$P_{0\to 2} = \frac{1}{1-\exp(-2\pi Z/v)}p_{-3}p_{-2}p_{-1}p_0p_1(1-p_{2}). \tag{6.15f}$$

In the weak-coupling, slow-collision limit one has exponentially small magnitudes $\exp(-2\pi Z/v)$ and p_0, whereas p_{-2}, p_{-1}, p_1, and p_2 are smaller than 1 by some $\sim 1/v$ decrements. Therefore, probabilities of nonadiabatic passage $P_{0\to -2}$ and $P_{0\to -1}$ are of the order of $1/v$, probability of diabatic passage $P_{0\to 0}$ is close to unity (more exactly it is less than 1 by $\sim 1/v$ decrement), and the probabilities of noncrossing transitions $P_{0\to 1}$ and $P_{0\to 2}$ are exponentially small.

It should be emphasized in the model under consideration that there is only one (or none) path that joins initial and final states via passage of a sequence of pseudocrossing. This means that multipath interference effects are not possible. The Demkov-Osherov [1] model has the same property, whereas, in the generalized bow-tie model, multipath interference is operative, although the interference phase cannot be varied continuously [12].

D. Other state-to-state transition probabilities

It is substantially more difficult to find other state-to-state transition probabilities. The transition amplitudes can be written down in terms of solutions $\psi^{\gamma +}(t)$. Indeed, if one considers set of amplitudes $F_{\alpha\to\gamma}$ as a matrix $F_{\alpha\gamma}$, then $(\mathbf{F}^{-1})_{\gamma\alpha} = \psi_j^{\gamma +}(0)$, where

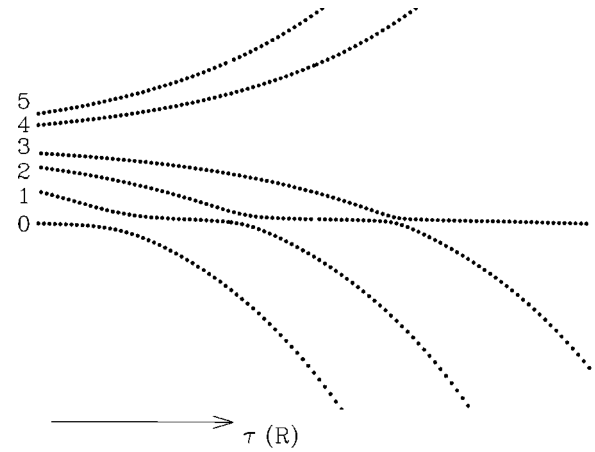

FIG. 4. Adiabatic potential curves for the exactly solvable multistate exponential model of Sec. VII A. The curves $j=1,2,3,4,5$ become degenerate in the limit $t\to -\infty$. For $t\to\infty$ potential curves diverge exponentially.

$$\psi_j^{\gamma +}(0) = V_j \mathcal{Q}_{\gamma +}\int_{\mathcal{C}_{\gamma +}} dE \left[\prod_{k\neq j}(E-D_k)\right]\prod_{\alpha}(E-d_\alpha)^{-i\beta_\alpha -1} \tag{6.16}$$

(note that at $t=0$ the diabatic states actually are simultaneously adiabatic states). However, the analytical evaluation of these contour integrals for the general case seems to be prohibitively difficult.

E. Two-state Coulomb model

Consider now an application of general results to the simplest particular case, the two-state system $(N=2)$. The label j takes only one value that according to our convention could be either 1 or -1.

1. Case when diabatic potential curves cross

The case of crossing diabatic potential curves corresponds to $j=-1$ where

$$d_0 = \tfrac{1}{2}(D_{-1}+D_0+\kappa), \tag{6.17a}$$

$$d_{-1} = \tfrac{1}{2}(D_{-1}+D_0-\kappa), \tag{6.17b}$$

$$A_{-1} = \frac{d_{-1}-D_{-1}}{d_{-1}-d_0} = \frac{1}{2\kappa}(D_{-1}-D_0+\kappa), \tag{6.17c}$$

$$A_0 = 1-A_{-1}, \quad \kappa = \sqrt{(D_{-1}-D_0)^2+4|V_{-1}|^2}, \tag{6.17d}$$

and the probabilities of diabatic and adiabatic passages are, respectively,

$$P_{\mathcal{B}\to 0} = \frac{p_{-1}(1-p_0)}{1-p_{-1}p_0} = \frac{p_{-1}-\exp(-2\pi Z/v)}{1-\exp(-2\pi Z/v)}, \tag{6.18a}$$

$$P_{\mathcal{B}\to -1} = \frac{1-p_{-1}}{1-p_{-1}p_0} = \frac{1-p_{-1}}{1-\exp(-2\pi Z/v)}, \tag{6.18b}$$

$$p_0 = \exp(-2\pi Z A_0/v),$$

$$p_{-1}=\exp(-2\pi ZA_{-1}/v)=\exp(-2\pi Z/v)/p_0, \tag{6.18c}$$

with the unitarity relation

$$P_{\mathcal{B}\to 0}+P_{\mathcal{B}\to -1}=1. \tag{6.18d}$$

Note that in our notations, $P_{\mathcal{B}\to -1}$ is the probability of adiabatic passage.

In the weak-coupling-adiabatic case one has $p_0 \ll 1$, and the transition probabilities are reduced to $P_{\mathcal{B}\to 0}\approx p_{-1}$ and $P_{\mathcal{B}\to -1}\approx(1-p_{-1})$, being straightforwardly interpreted in terms of Landau-Zener-type pseudocrossings.

2. Noncrossing case

Here, $j=1$ and

$$d_0=\tfrac{1}{2}(D_1+D_0-\kappa), \tag{6.19a}$$

$$d_1=\tfrac{1}{2}(D_1+D_0+\kappa), \tag{6.19b}$$

$$A_1=\frac{d_1-D_1}{d_1-d_0}=\frac{1}{2\kappa}(-D_1+D_0+\kappa), \tag{6.19c}$$

$$A_0=1-A_1, \tag{6.19d}$$

and the probabilities of adiabatic and diabatic passages are, respectively,

$$P_{\mathcal{B}\to 0}==\frac{1-p_0}{1-\exp(-2\pi Z/v)}, \tag{6.20a}$$

$$P_{\mathcal{B}\to 1}=\frac{(1-p_1)p_0}{1-\exp(-2\pi Z/v)}, \tag{6.20b}$$

$$p_0=\exp(-2\pi ZA_0/v),$$

$$p_1=\exp(-2\pi ZA_1/v)=\exp(-2\pi Z/v)/p_0. \tag{6.20c}$$

As discussed above, in the weak-coupling-adiabatic case one has $p_0\ll 1$ and the transition probability $P_{\mathcal{B}\to 1}\approx p_0$ is exponentially small. The transition probabilities coincide with those obtained by Tantawi *et al* [15].

VII. RELATED MULTISTATE EXPONENTIAL MODEL

A. Multistate model

Introduce effective time τ instead of t

$$t=\exp(\eta\tau), \tag{7.1}$$

where the constant η is presumed to be positive. For τ passing along real axis from $-\infty$ to ∞, time t varies from 0 to ∞. Therefore, mapping (7.1) is convenient when the nonstationary problem is considered on the semiaxis $0<t<\infty$. In terms of effective time, the nonstationary Schrödinger equation is

$$i\frac{d}{d\tau}|\Psi\rangle=\mathbf{H}_\tau|\Psi\rangle, \tag{7.2a}$$

with the effective Hamiltonian

$$\mathbf{H}_\tau=\eta\exp(\eta\tau)\mathbf{H}=\eta\exp(\eta\tau)\mathbf{H}^{(0)}+\mathbf{C}, \tag{7.2b}$$

where the matrix $\mathbf{H}^{(0)}$ is defined by formula (3.3) and the matrix $\mathbf{C}$ has only one nonzero element: $C_{00}=-\eta Z/v$. Both $\mathbf{H}^{(0)}$ and $\mathbf{C}$ are constant (time-independent) matrices. In particular, $\mathbf{H}^{(0)}$ was introduced in Sec. III as separated-atom limit Hamiltonian; its eigenvalues were denoted as d_α.

Thus, our initial Coulomb model is considered on the semiaxis if t is mapped on the exactly solvable multistate exponential model with Hamiltonian $\mathbf{H}_\tau$. The behavior of potential curves in the exponential model is illustrated by Fig. 4. For $\tau\to-\infty$, there are $(N-1)$ degenerate states $(j=1,2,3,\dots)$ with zero eigenvalues (of course, by the choice of origin of the ordinate axis the eigenvalue could be changed to any constant). The remaining 0th eigenvalue in this limit equals $-\eta Z/v$. As τ increases the degeneracy is lifted, and in the $\tau\to\infty$ asymptotic limit there are N potential curves exponentially diverging as $d_\gamma\eta\exp(\eta\tau)$. Generally, some (pseudo) crossings occur in between. More exactly, the number of pseudocrossings is equal to the number of negative eigenvalues of the operator $\mathbf{H}^{(0)}$ (we presume that $Z>0$).

B. Two-state case: Nikitin model

In the two-state case, $N=2$, the multistate exponential model reduces to the well-known Nikitin model. The Hamiltonian matrix for the latter reads

$$\mathbf{H}_{\text{Nik}}(R)=\begin{pmatrix} Be^{-\alpha R}+\frac{1}{2}\Delta\varepsilon-\frac{1}{2}A\cos\theta e^{-\alpha R} & -\frac{1}{2}A\sin\theta e^{-\alpha R} \\ -\frac{1}{2}A\sin\theta e^{-\alpha R} & Be^{-\alpha R}-\frac{1}{2}\Delta\varepsilon+\frac{1}{2}A\cos\theta e^{-\alpha R}\end{pmatrix}, \tag{7.3}$$

with $R=vt$ and model parameters A, B, θ, $\Delta\varepsilon$, and α (see, for instance, Ref. [20]). Comparing this with expression (7.2b) and identifying $-\alpha R$ with $\eta\tau$, one can see that essentially

$$\eta\mathbf{H}^{(0)}=\begin{pmatrix} B-\frac{1}{2}A\cos\theta & -\frac{1}{2}A\sin\theta \\ -\frac{1}{2}A\sin\theta & B+\frac{1}{2}A\cos\theta\end{pmatrix}, \tag{7.4}$$

and $C_{00}=\Delta\varepsilon$. This allows us to express the parameters of our Coulomb model in terms of Nikitin model parameters as

$$\eta D_1=B-\tfrac{1}{2}A\cos\theta,\quad \eta D_0=B+\tfrac{1}{2}A\cos\theta,$$

$$\eta V_1=-\tfrac{1}{2}A\sin\theta; \tag{7.5a}$$

$$\eta d_1 = B + \tfrac{1}{2}A, \quad \eta d_0 = B - \tfrac{1}{2}A; \tag{7.5b}$$

$$A_1 = \tfrac{1}{2}(1+\cos\theta), \quad A_0 = \tfrac{1}{2}(1-\cos\theta). \tag{7.5c}$$

Our probability (6.20b) of nonadiabatic transition is cast in terms of Nikitin model parameters as

$$P_{0\to1} = \exp\left[-\frac{\pi}{2}\zeta(1-\cos\theta)\right]\frac{\sinh\left[\frac{\pi}{2}\zeta(1+\cos\theta)\right]}{\sinh(\pi\zeta)},$$

$$\zeta = \frac{\Delta\varepsilon}{\alpha v}, \tag{7.6}$$

which reproduces the well-known transition probability of the Nikitin model [20].

VIII. CONCLUSION

Every exactly solvable model improves our understanding of physics and mathematics relevant to nonadiabatic transitions. Of course, more physically realistic models are preferable. Bearing in mind that the Coulomb interaction plays a prominent role in physics, the present Coulomb model appears quite natural and appealing. It has many perspectives of various applications (see, for instance, discussion by Tantawi *et al* [15]). From the same point of view it is physically more natural to consider the model on the semiaxis of time t variable, thus avoiding nonphysical singularity in the origin. Such a statement of the problem corresponds, for instance, to the treatment of half collision when one considers processes that occur as the particles fly apart after close encounter.

The two-state Coulomb model is solvable in terms of the Whittaker functions [18,15] which have an integral representation similar to our formulas (4.11). Whittaker functions satisfy a second-order differential equation that is equivalent to the two coupled first-order equations. From this point of view, the multistate Coulomb model corresponds to a generalization of Whittaker functions. These generalized functions satisfy a set of several coupled first-order differential equations.

The model considered here complements the well-known Demkov-Osherov model and retains its flexibility and richness of parameters. In the present paper, we have provided an analytical treatment and have found closed-form expressions for probabilities of transition from physically interesting state that emerges from the deep energy domain where it corresponds to a very tightly bound and compact system. In the limit of weak coupling, the probabilities were interpreted in terms of pairwise Landau-Zener-type transitions between adiabatic potential curves. The exact solutions also describe deviations from this simple picture, in particular, population without pseudocrossing. We show that our Coulomb model is mapped via introduction of effective time onto the exponential multistate model. For the special two-state case, the related exponential model coincides with the well-known Nikitin model.

APPENDIX

In order to prove the sum rule (3.18) we consider the integral in the complex-E plane

$$I_{\mathcal{C}_1} = \oint_{\mathcal{C}_1} \frac{dE}{g(E)} \tag{A1}$$

along closed contours $\mathcal{C}_1$ that embraces all the poles E_0, E_j of the integrand [see Eq. (4.9)]. It can be expressed via residues of the integrand as

$$I_{\mathcal{C}_1} = 2\pi i \sum_{\alpha} A_{\alpha}. \tag{A2}$$

If we enlarge the contour, the asymptotic approximation for $1/g(E) = 1/E + O(1/E^2)$ (for $|E|\to\infty$) could be employed, as follows from formulas (4.9). By using this asymptote, we obtain

$$I_{\mathcal{C}_1} = 2\pi i. \tag{A3}$$

Comparison of Eqs. (A2) and (A3) completes the proof.

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