Heavy-particle collisions and quantum optics: The parabolic noncrossing model

B. S. Nesbitt, D. S. F. Crothers, and S. F. C. O'Rourke
Theoretical and Computational Physics Research Division, The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland

P. R. Berman
University of Michigan, Ann Arbor, Michigan 48109-1120
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The problem of deriving analytic formulas for transition probabilities in two-level systems is studied. The two-level systems are described by a pair of first-order differential equations coupled by a time-dependent potential. One such model is given by $da_m/dt=-i\beta f(t)a_n e^{(-1)^n i\alpha t}$ $(m,n=1,2;\ m\neq n)$, which describes certain types of ion-atom collisions and some quantum-optics two-level problems. It will be shown that the correct approach in solving the coupled equations is to adopt a Zwaan-Stueckelberg phase-integral analysis of the four-transition-point problem based on the parabolic noncrossing model of Crothers [J. Phys. B **9**, 635 (1976)]. Alternatively, one may obtain an approximation by employing adiabatic perturbation theory, but such an approach can at best provide only weak-coupling solutions and can never guarantee unitarity in the probability amplitudes. The advantage of the phase-integral method is that it produces a strong-coupling approximation by embracing the appropriate asymptotic expansions for cylinder functions of large order and argument [D. S. F. Crothers, J. Phys. A **5**, 1680 (1972)] and it also ensures analyticity, unitarity, and symmetry. [S1050-2947(97)04208-X]

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In many areas of physics one is faced with a complicated many-body quantum-mechanical system. Through a series of approximations one may reduce the problem to a manageable semiclassical form such as a set of first-order differential equations coupled by a time-dependent potential. One such model is the two-state two-parameter parabolic noncrossing model of four closely clustered transition points that can be applied to certain types of ion-atom collisions and some quantum-optics two-level problems. In quantum optics the parabolic model describes the coupling of two levels of an atom by a laser pulse that has a temporal width that is small compared to the natural lifetimes of the levels. Previous work in this field for an arbitrary pulse area $\beta f(t)$ has lead to analytic formulas by Bambini and Berman [1] and perturbation calculations [2,3].

In heavy-particle collisions, the parabolic model describes low-energy inelastic atomic collision processes such as charge transfer through a set of equations describing the quantum-mechanical evolution of the electronic states as the nuclei follow classical trajectories. The charge-transfer mechanism is subject to the noncrossing theory of Rosen and Zener [4] in that the diabatic potential-energy curves do not cross.

In this Brief Report analytic formulas for the transition amplitude are derived from a Zwaan-Stueckelberg phase-integral analysis of the four-transition-point problem developed by Crothers [5]. The advantage of such an approach is that it yields strong-coupling formulas ensuring analyticity, unitarity, and symmetry. The analytic formulas are compared with exact numerical solutions of the coupled equations and perturbation approximations.

The time-dependent noncrossing model is described by the coupled equations

$$\frac{da_1}{dt}=-i\beta f(t)e^{i\alpha t}a_2, \tag{1}$$

$$\frac{da_2}{dt}=-i\beta f(t)e^{-i\alpha t}a_1, \tag{2}$$

where t is the time, α and β are real constants, and $f(t)$ is normalized to unity, in particular $f(t)$ is chosen to be the Lorentzian function

$$f(t)=\frac{1}{\pi(1+t^2)}. \tag{3}$$

Other possible forms of $f(t)$ are

$$f(t)=\frac{1}{\pi(1+t^2)^2} \tag{4}$$

or the hyperbolic secant of the Rosen-Zener model

$$f(t)=\frac{1}{2}\,\mathrm{sech}\left(\frac{\pi t}{2}\right). \tag{5}$$

In quantum optics the parameter α is related to the atom-field detuning and $\beta f(t)$ is defined as the pulse area, whereas in ion-atom collisions α is known as the resonance defect (the energy difference between the two states) and β effectively determines the location of the nonadiabatic transition region.

Asymptotic solutions are sought, particularly in the limit $|\alpha|\gg 1$, subject to the initial conditions $a_1(-\infty)=1$ and $a_2(-\infty)=0$. One can quite easily solve these equations through numerical integration, yet analytical solutions are more useful in understanding the main mechanisms involved. One method of obtaining analytic formulas is to adopt a Zwaan-Stueckelberg phase-integral analysis. The method itself is based on semiclassical JWKB phase integrals and their analytic continuation into the complex plane.

Within the JWKB approximation of Bates and Crothers [6], the two-level system reduces to a set of coupled equations for diabatic amplitudes c_1 and c_2,

$$i\frac{dc_1}{dt}=H_{12}c_2\exp\left(-i\int_0^t(H_{22}-H_{11})dt'\right), \tag{6}$$

$$i\frac{dc_2}{dt}=H_{21}c_1\exp\left(i\int_0^t(H_{22}-H_{11})dt'\right), \tag{7}$$

where the Hamiltonian matrix elements of this particular model are

$$H_{22}-H_{11}=\alpha, \tag{8}$$

$$H_{12}=H_{21}=\beta f(t). \tag{9}$$

According to adiabatic theory [7], applying the usual rotation matrix transformation [8] enables one to obtain the standard straight-line impact parameter adiabatic equations

$$\frac{da_1}{dt}=\frac{dT/dt}{2(1+T^2)}a_2\exp\left(-i\int_0^t\sqrt{4H_{12}^2+(H_{22}-H_{11})^2}dt'\right), \tag{10}$$

$$\frac{da_2}{dt}=\frac{-dT/dt}{2(1+T^2)}a_1\exp\left(i\int_0^t\sqrt{4H_{12}^2+(H_{22}-H_{11})^2}dt'\right), \tag{11}$$

where T is the Stueckelberg variable given by

$$T=\frac{H_{22}-H_{11}}{2H_{12}} \tag{12}$$

and

$$a_m(+\infty)=c_m(+\infty)\exp\left(i\int_0^\infty\sqrt{E_m+E_1-H_{mm}-H_{11}}dt'\right)$$

$$(m=1,2), \tag{13}$$

where a_m are the adiabatic amplitudes and E_m are the adiabatic energies given by

$$2E_m=H_{22}-H_{11}+(-1)^m\sqrt{4H_{12}^2+(H_{22}-H_{11})^2}. \tag{14}$$

The final amplitude $a_2(+\infty)$ is the quantity sought, which is obtained by solving the adiabatic equations subject to the initial conditions $a_1(-\infty)=1$ and $a_2(-\infty)=0$. The strongly coupled adiabatic equations may be specifically written as

$$\frac{da_1}{dt}=\frac{\Omega t}{(1+t^2)^2+\Omega^2}a_2\exp\left(-i\alpha\int_0^t\sqrt{1+\frac{\Omega^2}{(1+t'^2)^2}}dt'\right), \tag{15}$$

$$\frac{da_2}{dt}=\frac{-\Omega t}{(1+t^2)^2+\Omega^2}a_1\exp\left(i\alpha\int_0^t\sqrt{1+\frac{\Omega^2}{(1+t'^2)^2}}dt'\right), \tag{16}$$

where $\Omega=2\beta/\pi\alpha$.

Within the framework of the Zwaan-Stueckelberg phase-integral method and following from the parabolic model analysis [9], one is able to uncouple the equations, reducing the problem to the second-order Weber differential equation. By embracing the appropriate asymptotic expansions for parabolic cylinder functions of large order and magnitude [10], one then obtains the final amplitude

$$a_2(+\infty)=-i\ \sin x\ \mathrm{sech} y, \tag{17}$$

where we have used the method of steepest descent, concentrating on the transition points in the upper half plane. The general Zwaan-Stueckelberg interpretation of the model is

$$x+iy=\int_0^{Z_c}\sqrt{4H_{12}^2+(H_{22}-H_{11})^2}dt' \tag{18}$$

$$=\alpha\int_0^{\sqrt{-1+i\Omega}}dt'\sqrt{1+\frac{\Omega^2}{(1+t'^2)^2}}, \tag{19}$$

which in physical terms is a line integral representing the adiabatic action difference integrated between the classical turning point and the transition point Z_c; the other three complex transition points are Z_c^*, $-Z_c^*$, and $-Z_c$. The complex transition point is given by the zero of the integrand, i.e., $Z_c=\sqrt{-1+i\Omega}$.

A careful analysis of the phase integral yields

$$x+iy=\alpha\sqrt{-1+i\Omega}\sum_{n=0}^{\infty}\frac{(-\frac{1}{2})_n(-\Omega^2)^n}{n!}\times{}_2F_1(\tfrac{1}{2},2n;\tfrac{3}{2};1-i\Omega) \tag{20}$$

$$\approx\frac{\beta}{2}+i\alpha+O(\Omega^2) \tag{21}$$

for small Ω, where $(-\frac{1}{2})_n$ is a Pochhammer symbol. Therefore, the strongly coupled transition probability from a phase-integral abstraction is

$$P_2=|a_2(+\infty)|^2=\sin^2\left(\frac{\beta}{2}\right)\mathrm{sech}^2\alpha. \tag{22}$$

In the limit $|\alpha|\gg1$,

$$P_2\sim4e^{-2\alpha}\sin^2\left(\frac{\beta}{2}\right). \tag{23}$$

Adiabatic perturbation theory offers an alternative approach for obtaining solutions for the coupled equations (10) and (11). For some purposes this approach may be preferable and more convenient than the mathematically intensive Zwaan-Stueckelberg phase-integral analysis, but at best perturbation theory can produce only weak-coupling approximations, which can never guarantee analyticity, unitarity, and symmetry.

Within adiabatic perturbation theory the transition amplitude is given as

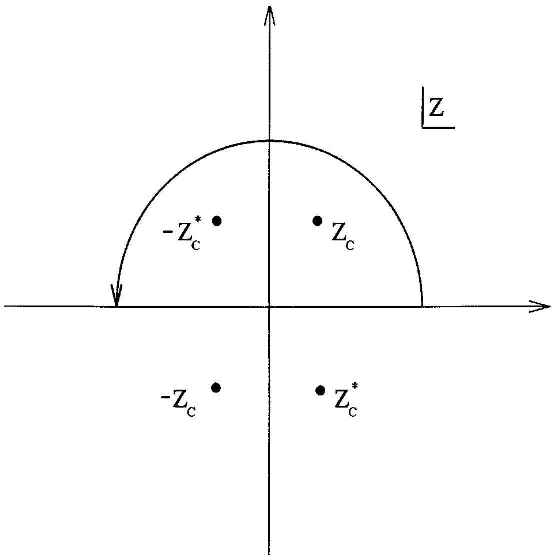

FIG. 1. The four transition points of the parabolic noncrossing model $Z_c = \sqrt{-1+i\Omega}$.

$$a_2(+\infty) = \int_{-\infty}^{+\infty} dt \frac{-dT/dt}{2(1+T^2)} \times \exp\left(i \int_0^t \sqrt{4H_{12}^2 + (H_{22}-H_{11})^2} dt' \right). \tag{24}$$

For the parabolic model this reduces to

$$a_2(+\infty) = -\Omega \int_{-\infty}^{+\infty} dt \frac{t}{\Omega^2 + (1+t^2)^2} \times \exp\left(i\alpha \int_0^t \sqrt{1 + \frac{\Omega^2}{(1+t^2)^2} dt'} \right). \tag{25}$$

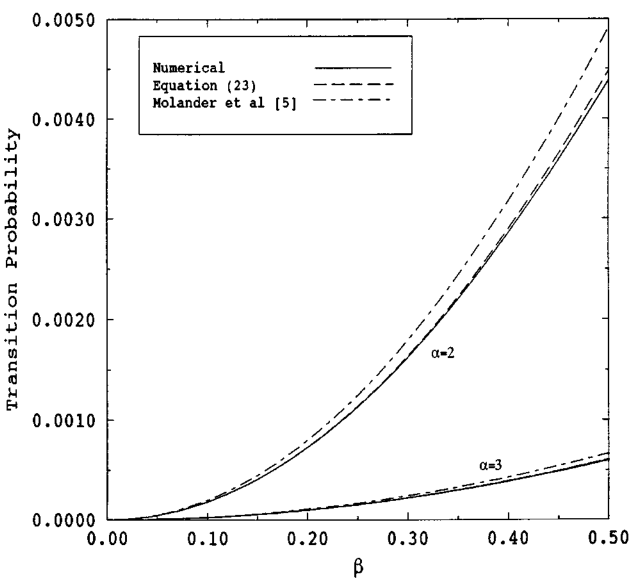

FIG. 2. Transition probability plotted as a function of β, where $0 \leqslant \beta \leqslant 0.5$ and $\alpha = 1,2$. Numerical results and Eq. (23) are shown to be in excellent agreement even when α is not in the limit $\alpha \gg 1$.

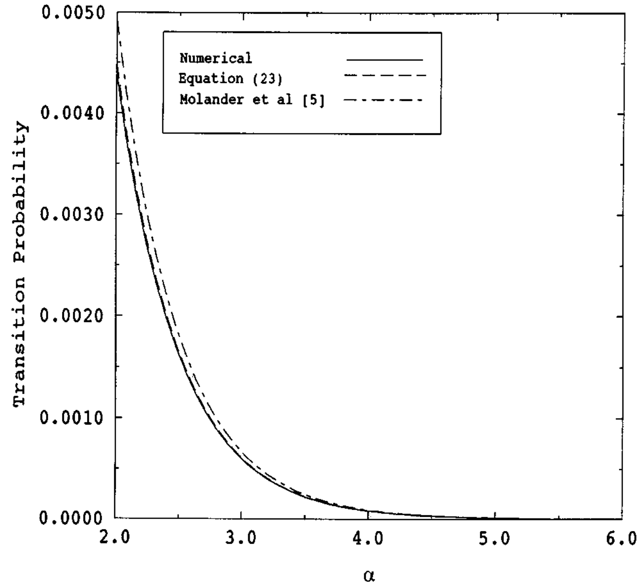

FIG. 3. Transition probability plotted as a function of α, where $2 \leqslant \alpha \leqslant 6$ and $\beta = 0.5$.

Concentrating on the poles in the upper half plane (see Fig. 1) and using Eq. (20) yields

$$P_2 \sim \pi^2 e^{-2\alpha} \sin^2\left(\frac{\beta}{2}\right), \tag{26}$$

which contains an error of $4/\pi^2$ when compared with Eq. (23), showing the inadequacy of perturbation theory when applied to this model.

Another approximation based on perturbation theory [3] yields

$$P_2 \sim \frac{\pi^2}{9} \left| \sum_i (\pm)_i e^{s_i} \right|^2, \tag{27}$$

where

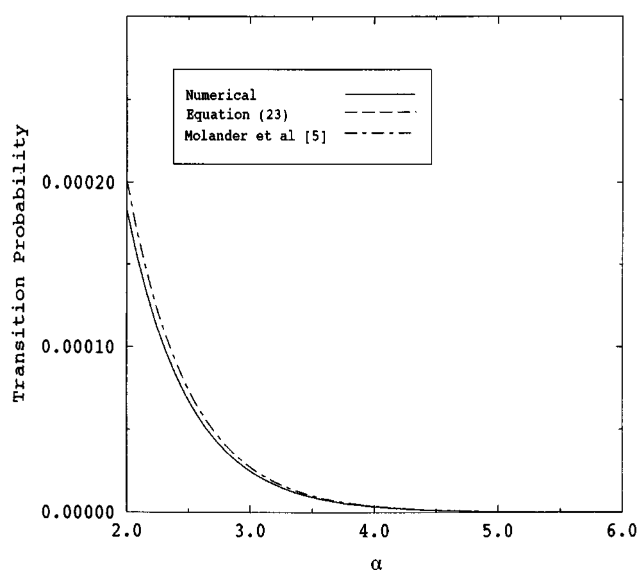

FIG. 4. Transition probability plotted as a function of α, where $2 \leqslant \alpha \leqslant 6$ and $\beta = 0.1$.

$$s_i = i\int_0^{t_i} \sqrt{4H_{12}^2 + (H_{22}-H_{11})^2}\,dt', \tag{28}$$

t_i are the complex transition points in the upper half plane, and the $(\pm)_i$ are chosen according to

$$4H_{12}(t_i) = \pm i(H_{22}-H_{11}).$$

Equation (27) then reduces to

$$P_2 \sim \frac{\pi^2}{9} 4e^{-2\alpha} \sin^2\left(\frac{\beta}{2}\right). \tag{29}$$

In quantum optics P_2 represents the probability that the atom has been excited by the laser pulse and in ion-atom collisions it is the probability of charge exchange occurring.

Equation (23) and the perturbation approximation of Molander *et al.* [3] [Eq. (29)] are compared with the exact numerical solutions of the coupled equations (1) and (2). Figures 2–4 show that Eq. (23) is almost in exact agreement with the numerical solutions, even for comparatively small values of α, for instance, $\alpha=2$. Thus, in practice, the $|\alpha|\gg 1$ limit for Eq. (23) may be interpreted in the usual semiclassical way, namely, as $|\alpha|$ is moderately greater than 1. Of course, for $|\alpha|<1$, which includes $\alpha\approx 0$, Eq. (22) must always be preferred to Eq. (23) or (29). Not surprisingly, for relatively small values of α, the approximation of Molander *et al.* [3] deviates from the numerical solutions, but then they state that their solution is valid only for large α corresponding to a large detuning region. However, large values of α correspond to extremely small transition probabilities, which ultimately have little or no physical significance. Therefore, perturbation theory cannot reveal accurately any of the important physical processes that occur in the region of strong coupling (small α).

The strongly coupled approximations for the transition probability are shown to agree favorably with the exact numerical calculations, within the limit $|\alpha|>1$. It is therefore concluded that the Zwaan-Stueckelberg phase-integral method developed by Crothers [5] produces the correct transition amplitudes when supplemented with the appropriate asymptotic expansions for the parabolic cylinder functions of large order and argument [10]. The main strength of the method is that it incorporates the essential physics into the problem, ensuring analyticity, unitarity, and symmetry. It has also been shown that perturbation theory fails to produce the correct form of the transition amplitude in the case of strong coupling.

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