Occurrence of unit transmissivity in scattering

R. Lefebvre,[1,2] O. Atabek,[1] and V. Leon[3]
[1]Laboratoire de Photophysique Moléculaire du CNRS, Université de Paris-Sud, 91405 Orsay, France
[2]UFR de Physique Fondamentale et Appliquée, Université Pierre et Marie Curie, 75231 Paris, France
[3]Instituto de Física, BUAP, Apartado Postal J-48, Puebla, Puebla 72570, Mexico
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Unit transition probability occurs when a bound state works as a doorway state between two continua. It is shown that in the limit of small coupling this is still true if there is direct coupling between the continua. A cancellation of this coupling occurs in the appropriate element of the transition operator.

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I. INTRODUCTION

It is a textbook example about resonance effects on scattering: if a process is mediated by a resonance, the transition probability reaches the value unity at the resonance energy [1]. This is shown by the form taken by the relevant matrix element of the scattering operator **S**. Let us consider a process involving two continua coupled through a bound state. The entrance continuum wave function with index i is coupled to the exit continuum wave function of index f via an intermediate bound state. The off-diagonal matrix element of the scattering operator **S** can be written as

$$S_{f\leftarrow i}(E)=-2i\pi\frac{v_f v_i^*}{E-E_R+i\pi(|v_i|^2+|v_f|^2)}, \tag{1}$$

where E_R is the resonance position while v_i and v_f are the discrete-continuum couplings between the bound state and the continua i and f. For a symmetric potential with $v_i=v_f$ and $E=E_R$, the square modulus of $S_{f\leftarrow i}$ is 1, even for infinitely small couplings. The transition probability has a Lorentzian shape. An illustration of this situation is resonant tunneling through a double-barrier structure [2], where the resonance is associated with the well between the barriers. Although the usual way to calculate the transmissivity goes through a matching of the wave function and its derivative at each discontinuity of the potential, it is also possible, as shown by Bardeen [3], to evaluate the discrete-continuum couplings of Eq. (1). Other situations with unit transmissivity exist, where interference effects show up, leading to Fano-type profiles [4]. Such profiles are found in the transmissivity of a particle incident on a well and interacting with an oscillating electric field [5], or in the case of an electron incident on an oscillating square potential well [6]. An example implying more than one coordinate is laser assisted reactive scattering [7]. Equation (1) cannot account for this behavior. A so-called background term has to be introduced in the matrix element of the **S** operator [1]. We describe in the next section an example showing this effect. We then develop a simple model to explain that unit transmissivity can persist even when interference reveals the existence of a direct continuum-continuum coupling.

II. INTERFERENCE EFFECTS IN FIELD ASSISTED DOUBLE-BARRIER RESONANT TUNNELING

As an example to show the existence of interference effects in resonant tunneling, let us consider a double barrier enclosing a well. The barriers are narrow and high, so that they behave practically as δ function barriers. The well admits a true bound state of energy E_b, because its bottom is sufficiently below the asymptotic thresholds. The double-barrier structure leads to a set of resonances corresponding to escape processes through the barriers. In the presence of an oscillating field of frequency ω, the dressed state corresponding to the bound state plus a photon acts as an additional doorway state at energy $E_b+\omega$. We have previously analyzed this situation [8] to show that unit transmissivity can be obtained at this energy in the limit of a weak field amplitude. The transmissivity profiles were Lorentzian, showing that the direct continuum-continuum coupling had negligible effects. The present model, as illustrated in Fig. 1, is similar, but the δ function (or close to δ function) barriers ensure enough direct transmission to display the interference effect between direct and resonance-mediated processes. The parameters of the potential are as follows: barrier height $h=25$ a.u., barrier width $\epsilon=0.01$ a.u., well width $2L=2$ a.u., well depth $V_0=1$ a.u., mass of incoming particle $m=1$ a.u.. Such a model provides a simple example to verify the power of a multiple scattering approach. The multiple scattering formula for the field-free transmissivity makes use of the transmission and reflection amplitudes at the two δ function barriers, each written $\Omega\delta(x)$. In the present model Ω can be viewed as $\epsilon\times h$, the width times the height of a barrier. For a particle incident from the left with energy E on the first barrier, with two different thresholds defining a left wave number $k_1=[2mE]^{1/2}$ and a right wave number $k_2=[2m(E+V_0)]^{1/2}$, we derive, along a line similar to that applied to the δ function barrier with equal thresholds [9], the formulas for the amplitudes of transmission t and of reflection r

$$t=\frac{2ik_1}{ik_1+ik_2-2\Omega}, \qquad r=\frac{ik_1-ik_2+2\Omega}{ik_1+ik_2-2\Omega}. \tag{2}$$

For a particle incident on the right barrier the amplitudes are obtained by permuting k_1 and k_2. They are denoted $\tilde{t}$ and $\tilde{r}$. The multiple scattering expression for the transmission

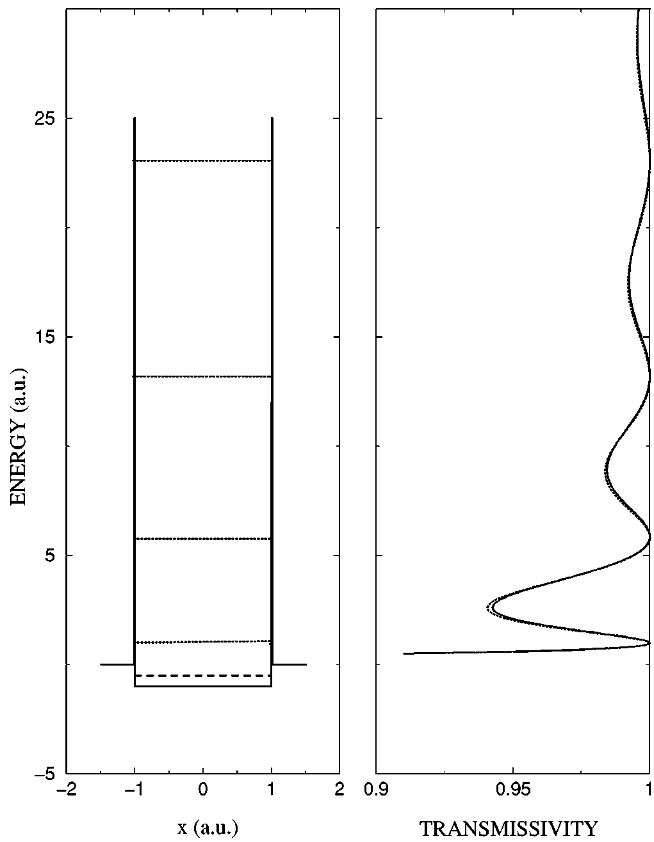

FIG. 1. Transmissivity of a double δ function barrier. The parameters of the potential are as follows: barrier height $h=25$ a.u., barrier width $\epsilon=0.01$ a.u., well width $2L=2$ a.u., well depth $V_0=1$ a.u., mass of incoming particle $m=1$ a.u.. Left panel: the potential, with the bound state energy (dashed horizontal line), and the resonance energies (dotted horizontal lines). Right panel: the field-free transmissivity. Unit transmissivity is reached at each resonance energy associated with the well between the barriers. Solid curve: transfer matrix calculation. Dashed curve: multiple scattering formulation.

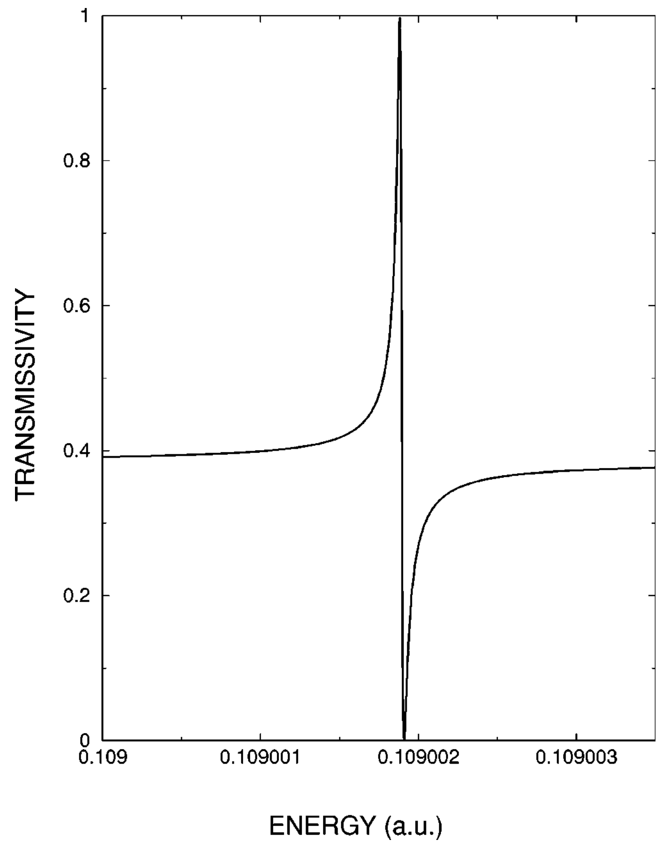

FIG. 2. Transmissivity in the neighborhood of the energy $E_b+\omega$. E_b is the energy of the bound state accommodated by the well below the asymptotic thresholds (true bound state in the absence of the field). The frequency ω is 0.5259 a.u. and the peak field amplitude 0.1×10^{-3} a.u. Solid curve: transfer matrix calculation with the field. Dashed curve: field-free transmissivity.

amplitude is obtained by summation of all wavelets reaching the right asymptotic region after all possible transmissions and reflections of a unit amplitude wave incident from the left. A geometric series is generated:

$$\mathcal{T}=te^{i\beta}\tilde{t}+te^{i\beta}\tilde{r}e^{i\beta}\tilde{r}e^{i\beta}\tilde{t}+te^{i\beta}\tilde{r}e^{i\beta}\tilde{r}e^{i\beta}\tilde{r}e^{i\beta}\tilde{r}e^{i\beta}\tilde{t}+\cdots. \tag{3}$$

β is the phase:

$$\beta=\int_{-L}^{+L}k_2dx. \tag{4}$$

The summation provides for the total transmission amplitude the expression

$$\mathcal{T}=\frac{t\tilde{t}e^{i\beta}}{1-\tilde{r}^2e^{2i\beta}}. \tag{5}$$

We show in Fig. 1 the transmission probability (that is, $|\mathcal{T}|^2$) calculated in two ways: (a) by a transfer matrix technique based on the true parameters of the structure and (b) with the multiple scattering formula. The transmission reaches unity at each resonance energy, as expected. The very good agreement between the two procedures shows that each barrier correctly mimics a δ function barrier. In the following we will need the transmissivity far from a resonance. This transmissivity can be equally well estimated by multiple scattering or the transfer matrix.

We turn now to the effect of an oscillating field interacting with the particle. As explained above (and well documented in the literature [5,6]) a different resonance effect is expected: if ω is the frequency of the field, in the presence of a bound state of energy E_b, there is the possibility of virtual desorption and absorption of a photon. The bound state energy in our case is $E_b\sim-0.51$ a.u. We show in Fig. 2 the transmissivity in the neighborhood of the energy $E_b+\omega$, with $\omega=0.5297$ a.u. and a peak field amplitude $E_0=0.1\times10^{-3}$ a.u. The transmissivity reaches a value very close to unity. We recall [5,8] that this is an indication that, in the escape of a particle initially trapped in the well, only one-photon processes are allowed. However, the profile is not Lorentzian. This is not in accordance with Eq. (1). There is clearly an interference effect giving a Fano-type profile. We also show the field-free transmissivity. The transmissivity is perturbed only in the vicinity of the field-induced resonance.

III. CANCELLATION OF THE DIRECT COUPLING

We develop now an analytic approach to account for the findings of the previous section. The so-called configuration interaction method of Fano [4,10] is adopted. The Hamiltonian is partitioned into $H=H_0+H_1$. The eigenkets of H_0 consist of two energy-normalized continua written $|\alpha_E\rangle$ and $|\beta_E\rangle$ and a bound state of ket $|\phi_i\rangle$ and energy E_i. Residual couplings are due to H_1. All couplings are assumed to be sufficiently smooth to allow them to be taken energy independent. We introduce the notation

$$\langle \alpha_E|H_1|\beta_{E'}\rangle = W,$$
$$\langle \phi_i|H_1|\alpha_E\rangle = \langle \phi_i|H_1|\beta_E\rangle = V. \tag{6}$$

A symmetric pattern of discrete-continuum couplings is assumed. The transition operator $\mathbf{T}$ is written $H_1 + H_1 G H_1$. G is the Green operator $(z-H)^{-1}$. Let us assume first that $W=0$ (no continuum-continuum coupling). We obtain

$$\langle \beta_{\bar{E}}|\mathbf{T}|\alpha_E\rangle = \langle \beta_{\bar{E}}|H_1|\phi_i\rangle\langle \phi_i|G|\phi_i\rangle\langle \phi_i|H_1|\alpha_E\rangle = |V|^2\langle \phi_i|G|\phi_i\rangle. \tag{7}$$

The diagonal matrix element of the Green function is

$$\langle \phi_i|G|\phi_i\rangle = \frac{1}{z-\tilde{E}_i + i\Gamma}. \tag{8}$$

$\tilde{E}_i$ is the shifted bound state energy. The half-width Γ is given by

$$\Gamma = 2\pi|V|^2. \tag{9}$$

The factor 2 accounts for the decay toward the two continua. At the (real) resonance energy $z=\tilde{E}_i$, the matrix element of $\mathbf{T}$ takes the form $-i/2\pi$. From the expression of the scattering operator $\mathbf{S}=\mathbf{1}-2i\pi\mathbf{T}$, we finally obtain

$$|\langle \beta_{\tilde{E}_i}|\mathbf{S}|\alpha_{\tilde{E}_i}\rangle|^2 = 1. \tag{10}$$

This is the explanation, reduced to its essentials, for the unit transition probability observed when a bound state acts as a doorway state between two continua. The result does not depend on the strength of the couplings (provided, of course, they are not zero). However, too small a width of the resonance may forbid the construction of a realistic wave packet that would reveal the phenomenon in a scattering experiment.

We turn now to the case where a direct coupling between the continua is operating. Equation (7) is replaced by

$$\langle \beta_{\bar{E}}|\mathbf{T}|\alpha_E\rangle = \langle \beta_{\bar{E}}|H_1|\alpha_E\rangle + \langle \beta_{\bar{E}}|H_1|\phi_i\rangle\langle \phi_i|G|\phi_i\rangle\langle \phi_i|H_1|\alpha_E\rangle + \int dE'\langle \beta_{\bar{E}}|H_1|\alpha_{E'}\rangle\langle \alpha_{E'}|G|\phi_i\rangle\langle \phi_i|H_1|\alpha_E\rangle + \int dE''\langle \beta_{\bar{E}}|H_1|\phi_i\rangle\langle \phi_i|G|\beta_{E''}\rangle\langle \beta_{E''}|H_1|\alpha_E\rangle + \int\int dE'\,dE''\langle \beta_{\bar{E}}|H_1|\alpha_{E'}\rangle\langle \alpha_{E'}|G|\beta_{E''}\rangle\langle \beta_{E''}|H_1|\alpha_E\rangle. \tag{11}$$

With the assumptions about the couplings [Eq. (6)], this reduces to

$$\langle \beta_{\bar{E}}|\mathbf{T}|\alpha_E\rangle = W^* + |V|^2\langle \phi_i|G|\phi_i\rangle + W^*V\int dE'\langle \alpha_{E'}|G|\phi_i\rangle + W^*V^*\int dE''\langle \phi_i|G|\beta_{E''}\rangle + W^{*2}\int\int dE'\,dE''\langle \alpha_{E'}|G|\beta_{E''}\rangle. \tag{12}$$

The matrix elements of the Green operator are easily found from its definition $G(z-H)=1$. We only provide the results of the integrations present in Eq. (12). We find

$$\int dE'\langle \alpha_{E'}|G|\phi_i\rangle = -i\pi\frac{V^*(1-i\pi W)}{1+\pi^2|W|^2}G_{i,i}, \tag{13}$$

$$\int dE''\langle \phi_i|G|\beta_{E''}\rangle = -i\pi\frac{V(1-i\pi W)}{1+\pi^2|W|^2}G_{i,i}, \tag{14}$$

$$\int\int dE'\,dE''\langle \alpha_{E'}|G|\beta_{E''}\rangle = -\frac{\pi^2 W}{1+\pi^2|W|^2} - \frac{\pi^2|V|^2(1-i\pi W)^2}{(1+\pi^2|W|^2)^2}G_{i,i}. \tag{15}$$

$G_{i,i}$ stands for $\langle \phi_i|G|\phi_i\rangle$ and is given by

$$G_{i,i} = \left(z - E_i + \frac{\pi^2|V|^2(W+W^*)}{1+\pi^2|W|^2} + 2i\pi\frac{|V|^2}{1+\pi^2|W|^2}\right)^{-1}. \tag{16}$$

The resonance energy is shifted even with energy-independent couplings [11]. At the real resonance energy

$$E_R = E_i - \frac{\pi^2 |V|^2 (W + W^*)}{1 + \pi^2 |W|^2}, \tag{17}$$

the matrix element of the transition operator takes the form

$$\langle \beta_{E_R} | \mathbf{T} | \alpha_{E_R} \rangle = W^* - \frac{i}{2\pi}(1 + \pi^2 |W|^2) - \frac{W^*}{2}(1 - i\pi W) - \frac{W^*}{2}(1 - i\pi W) - \pi^2 \frac{W W^{*2}}{1 + \pi^2 |W|^2} + \frac{i\pi W^{*2}}{2} \frac{(1 - i\pi W)^2}{1 + \pi^2 |W|^2}. \tag{18}$$

The last two terms arise from the double integral. We have displayed on purpose the terms corresponding to the two single integrals of Eq. (12) (third and fourth terms), although they give equal contributions. This is to show that terms arising from the $H_1 G H_1$ part of the transition operator *exactly cancel* the term W^* arising from the direct continuum-continuum coupling. Another way to write this matrix element is

$$\langle \beta_{E_R} | \mathbf{T} | \alpha_{E_R} \rangle = -\frac{i}{2\pi} \frac{1 - \pi^2 W^{*2}}{1 + \pi^2 |W|^2}. \tag{19}$$

The dimensionless continuum-continuum coupling contributes only to second order to the transition probability, since for $W \ll 1$ we can write

$$\langle \beta_{E_R} | \mathbf{T} | \alpha_{E_R} \rangle \sim -\frac{i}{2\pi}[1 - \pi^2 (W^{*2} + |W|^2)]. \tag{20}$$

The transition probability is no longer exactly 1 on the resonance. In the absence of discrete-continuum couplings, the transition probability is $4\pi^2 |W|^2$.

IV. LINE SHAPE ANALYSIS

We continue by derivation of the parameters associated with the Fano profile. Let us define

$$\epsilon = \frac{E - E_R}{\tilde{\Gamma}} \tag{21}$$

with E_R given by Eq. (17) and $\tilde{\Gamma}$ being the half-width of the resonance [cf. Eq. (16)]:

$$\tilde{\Gamma} = \frac{2\pi |V|^2}{1 + \pi^2 |W|^2}. \tag{22}$$

We now consider the matrix element of the **T** operator for an off-resonance energy. It is possible to reduce it to the form

$$\langle \beta_E | \mathbf{T} | \alpha_E \rangle = \frac{W^*}{(1 + \pi^2 |W|^2)} \frac{1}{\epsilon + i} \times \left(\epsilon + \frac{1}{2\pi W^*} - \frac{\pi W^*}{2} \right). \tag{23}$$

We have for the transition probability

$$|\langle \beta_E | \mathbf{S} | \alpha_E \rangle|^2 = 4\pi^2 |\langle \beta_E | \mathbf{T} | \alpha_E \rangle|^2 = 4\pi^2 \frac{|W|^2}{(1 + \pi^2 |W|^2)^2} \frac{|\epsilon + q|^2}{\epsilon^2 + 1} \tag{24}$$

with the Fano parameter q:

$$q = \frac{1}{2\pi W^*} - \frac{\pi W^*}{2}. \tag{25}$$

It is easy to check that as the continuum-continuum coupling W goes to zero, one recovers a Lorentzian line shape. For a nonzero and real coupling, there is vanishing of the transition probability at an energy obtained from the condition

$$\epsilon = -\frac{1}{2\pi W} + \frac{\pi W}{2}. \tag{26}$$

Solving this equation in E gives

$$E = E_R - \frac{|V|^2}{W(1 + \pi^2 W^2)} + \frac{\pi^2 |V|^2 W}{(1 + \pi^2 W^2)}. \tag{27}$$

If the dimensionless quantity W is much smaller than unity, the vanishing probability occurs at an energy

$$E = E_R - \frac{|V|^2}{W(1 + \pi^2 W^2)}. \tag{28}$$

The distance between the maximum and the zero increases as W decreases, while the profile is more and more Lorentzian. An estimate of the resonance width and of this distance could lead to an estimate of the direct continuum-continuum coupling.

V. CONCLUSION

From the expression of the transition operator one expects a first order contribution of the direct continuum-continuum coupling. We have shown that on resonance this term is canceled, and the transition amplitude is affected, as compared to that valid in the absence of this coupling, only by second-order terms. The extreme narrowness of the resonance feature in Fig. 2 validates an analysis based on energy-independent couplings.

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