

Tunneling dynamics of a two-atom system

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Abstract. We discuss the quantum tunneling of a diatomic molecule, concentrating on the transmission differences corresponding to different internal states. The evolution picture is constructed basing on introduction of notion of effective potential, the form of which is dependent on interatomic separation. To fully treat the tunneling problem analytically, we slightly modify the effective potential for each internal state. Clear splitting of these resonances enables us to suggest a scheme of molecular interferometer working as a Earth gravity sensor.

1. Introduction

Resonant tunneling is a basic phenomenon in elementary quantum mechanics [1] which appears when a particle tunnels through two (or more) potential barriers, and the incident energy coincides with any quasi-bound energy level inside the double-barrier. This is the matter-wave analog of what happens in an optical Fabry-Perot resonator. It was shown that for tunneling of particles with space-separated centers of mass [2], e.g. two-atom molecules, analogous phenomena is present even in case of bulk, non-split potential barriers. A number of aspects of resonant tunneling of structural particles have been studied theoretically (e.g. [3-6]), using mainly numerical simulations.

In this article we come to analytical expressions for the transmission and reflection amplitudes of symmetric and antisymmetric internal states of a diatomic molecule. On the scale of energies, the resonant transmission proves to be different for these states. As a conclusion, we suggest a scheme of a sensor using this difference to measure the Earth gravitation.

2. Resonant tunneling of symmetric and antisymmetric internal states

Let us consider the quantum tunneling of a molecule composed of two atoms with masses m_1 , m_2 and separated by some distance l . Such 1D molecular structure may be modeled by a potential

$$V_{int} = -\frac{\alpha}{2}(\delta(x+l/2) + \delta(x-l/2)), \quad (1)$$

where parameter α is the characteristic of molecule binding energy and $\delta(x)$ is the Dirac δ -function. In general we take the external (tunneling) potential for both particles in a rectangular form with different widths ($a_{1,2}$) and heights ($U_{1,2}$). Then the Hamiltonian takes the form



$$H = H_{rel} - \frac{\hbar^2}{2M} \frac{d^2}{dy^2} + U_1 \theta \left(\left(a_1 - \frac{m_2 x}{m_1 + m_2} - y \right) \left(a_1 + \frac{m_2 x}{m_1 + m_2} + y \right) \right) + U_2 \theta \left(\left(a_2 + \frac{m_1 x}{m_1 + m_2} - y \right) \left(a_2 - \frac{m_1 x}{m_1 + m_2} + y \right) \right), \quad (2)$$

where x and y denote the relative and the center of mass (c.m.) coordinates,

$$H_{rel} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{int} \quad (3)$$

is the Hamiltonian of relative motion, m and M are reduced and total masses respectively. The eigenvalue and eigenfunction problem $H_{rel} \varphi_{s,a}(x) = -E_{s,a} \varphi_{s,a}(x)$ is a textbook one which has only two bound states, the *symmetric* one:

$$\varphi_s(x) = N_s \left(e^{\chi_s(x+l/2)} \theta(-x-l/2) + \frac{\cosh(\chi_s x)}{\cosh(\chi_s l/2)} \theta((x+l/2)(l/2-x)) + e^{-\chi_s(x-l/2)} \theta(x-l/2) \right), \quad (4)$$

with some energy value E_s determined from the transcendental equation

$$\sqrt{E_s} = \frac{\sqrt{2m}}{4\hbar} \alpha \left(1 - \exp \left(-\frac{\sqrt{2m}}{\hbar} l \sqrt{E_s} \right) \right), \quad (5)$$

and the *antisymmetric* one given by equations

$$\varphi_a(x) = N_a \left(e^{\chi_a(x+l/2)} \theta(-x-l/2) + \frac{\sinh(\chi_a x)}{\sinh(\chi_a l/2)} \theta((x+l/2)(l/2-x)) + e^{-\chi_a(x-l/2)} \theta(x-l/2) \right), \quad (6)$$

$$\sqrt{E_a} = \frac{\sqrt{2m}}{4\hbar} \alpha \left(1 - \exp \left(-\frac{\sqrt{2m}}{\hbar} l \sqrt{E_a} \right) \right), \quad (7)$$

Here $N_{s,a}$ are normalization constants and $\chi_{s,a} = \sqrt{2mE_{s,a}}/\hbar$. Note that the symmetric state exists for any parameters α and l , whereas the antisymmetric state occurs if $\alpha l > 4$.

In the following we will assume that the incident energy of a molecule is smaller than the absolute values of binding energies $E_{s,a}$. Then the continuous spectrum of internal states has no role in the transmission problem and may be omitted from the consideration. As a result,

$$\Psi(x, y) = \psi_s(y) \varphi_s(y) + \psi_a(y) \varphi_a(y), \quad (8)$$

where $\psi_s(y)$ and $\psi_a(y)$ are the wavefunctions of c.m. motion with respect to symmetric and antisymmetric internal states respectively. Starting from the full problem $H \Psi(x, y) = E \Psi(x, y)$, they obey equations

$$\left(-\frac{\hbar^2}{2M} \frac{d^2}{dy^2} + V_s(y) - (E + E_s) \right) \psi_s(y) + V_{sa}(y) \psi_a(y) = 0, \quad (9)$$

$$\left(-\frac{\hbar^2}{2M} \frac{d^2}{dy^2} + V_a(y) - (E + E_a) \right) \psi_a(y) + V_{as}(y) \psi_s(y) = 0, \quad (10)$$

with

$$V_{s,a}(y) = \int_{-\infty}^{\infty} \varphi_{s,a}^2(x) V(x, y) dx, \quad V_{sa}(y) = V_{as}(y) = \int_{-\infty}^{\infty} \varphi_s(x) V(x, y) \varphi_{sa}(x) dx, \quad (11)$$

where $V(x, y)$ is the external potential in the Hamiltonian (2). The integrals in equations (11) are calculated and expressed through the long-length sum of elementary functions.

Homonuclear molecules. In case of same-type atoms $V_{sa}(y) = V_{as}(y) = 0$ and the translational wavefunctions satisfy the following separate equations of Schrödinger form:

$$\left(-\frac{\hbar^2}{2M} \frac{d^2}{dy^2} + V_s(y) \right) \psi_s(y) = (E + E_s) \psi_s(y), \quad (12)$$

$$\left(-\frac{\hbar^2}{2M} \frac{d^2}{dy^2} + V_a(y) \right) \psi_a(y) = (E + E_a) \psi_s(y). \quad (13)$$

Here $V_s(y)$ and $V_a(y)$ become exactly the “effective” potential energies corresponding to two internal states. Unfortunately, Eqs. (12) and (13) with such potential energies don’t have analytic solutions. They will have them if the potential is modeled by a close “replica” form

$$V(y) = \begin{cases} v - v_0 + \frac{v_0}{\exp((-y + l_0)/a_0) + 1} & 0 \leq |y| < y_0 \\ \frac{v}{\exp((y - l_1)/a_1) + 1} & |y| \geq y_0 \end{cases}. \quad (14)$$

Noting that $V_s(y)$ and $V_a(y)$ are symmetric functions of c.m. coordinate y , we proceed with symmetric and antisymmetric basic solutions of Eqs. (12), (13) denoting them as $\psi_{s,sym}(y)$, $\psi_{s,anti}(y)$ and $\psi_{a,sym}(y)$, $\psi_{a,anti}(y)$ respectively. This yields

$$\psi_s(y) = h_{s,sym} \psi_{s,sym}(y) + h_{s,anti} \psi_{s,anti}(y), \quad \psi_a(y) = h_{a,sym} \psi_{a,sym}(y) + h_{a,anti} \psi_{a,anti}(y). \quad (15)$$

So, in case of homonuclear molecules with two internal states, the problem of tunneling of the molecule splits into two separate tunneling problems for each internal state. Simultaneously, the problem of resonances transforms into the question whether the “effective” potentials in Eqs. (11) (or (14)) have internal minima.

Traditional left-side incident-wave geometry can be guaranteed through the well-disposed h -coefficients in Eqs. (15), with respect to asymptotic forms

$$\psi_{s,a}(y \rightarrow -\infty) = e^{ik_{s,a}y} + r_{s,a}e^{ik_{s,a}y}, \quad \psi_{s,a}(y \rightarrow +\infty) = t_{s,a}e^{ik_{s,a}y}, \quad (16)$$

where $r_{s,a}$ and $t_{s,a}$ are the sought reflection and transmission probability amplitudes.

The main question about the form of “effective” potentials is directly linked to the distance l between the atoms, as is exemplified in figure 1. Additionally, the formation of completely isolated barriers takes place at $l \approx 2a$.

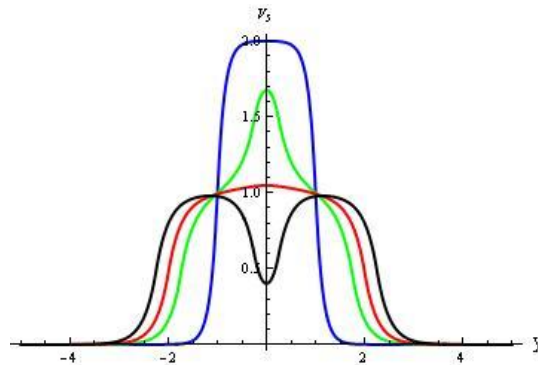


Figure 1. The effective potential $V_s(y)$ for different values of molecular length l for $\alpha/a E_R = 4$. ($E_R = \hbar^2 / 2ma^2$). For blue line $l = 0.1a$, for green $l = 1.5a$, for red $l = 2a$ and for black $l = 2.5a$.

Analytic simulation expresses the transmission and reflection probability amplitudes, $r_{s,a}$ and $t_{s,a}$, through the product of exponential and Gauss hypergeometric functions. They are too cumbersome to be presented in the paper. To go ahead, we choose the length value $l = 3.5a$, when

the difference between effective potentials for the symmetric and antisymmetric internal states is still noticeable (figure 2).

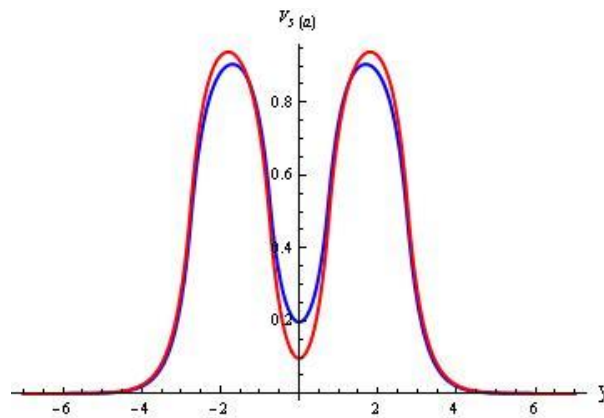


Figure 2. The effective potentials $V_s(y)$ (blue) and $V_a(y)$ (red) at $l = 3.5a$. The parameter of power of interatomic δ -function interaction ($\alpha/aE_R = 2.5$) is somewhat smaller than in figure 1.

It makes perceptible the difference between the corresponding quasi-bound energies and, as a consequence, forms a double-structure in the resonant tunneling picture, as it is depicted in figure 3. In fact, each of resonances works as a separator of symmetric and antisymmetric internal states, guiding them in opposite to barrier directions.

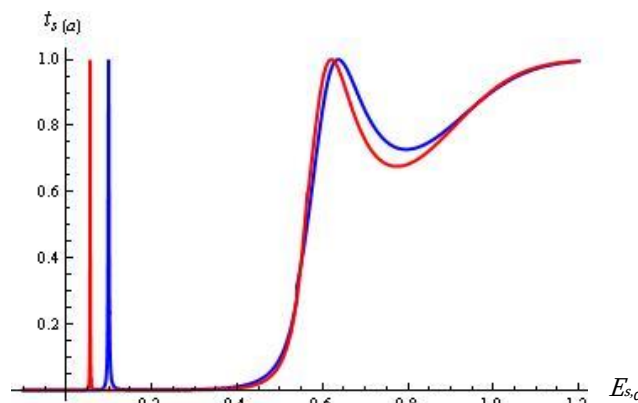


Figure 3. Quantum transparency of a diatomic molecule in its symmetric (blue) and antisymmetric (red) internal states versus the incident energy. Effective potentials are taken from figure 2. The resonances are posed at $E_s = 0.40 E_R$ and $E_a = 0.38 E_R$.

3. Conclusion. A scheme of molecular interferometer

The resonances in the quantum tunneling of a diatomic molecule may be seen as a consequence of constructive interference between the matter waves corresponding to constituent atoms being in different parts of the barrier. The mean interatomic distance must exceed the width of the barrier. This important restriction leaves out of interest the laser induced optical potentials. As a tunneling potential we see perspective in a single-layer atomic structures, such as the famous graphene. Our suggestion assumes a molecular Bose-Einstein condensate, loaded into a potential well over the graphene potential barrier. Switching off the trapping potential, the cold molecular cloud due to gravity falls on the graphene layer having resonant transmission energy for the antisymmetric internal state E_a . The antisymmetric state will tunnel through the layer while the symmetric state will bounce upwards. Immediately after that, the graphene layer will be shifted down to some

appropriate position to match the energy $E_s > E_a$. As a result, the retardation of the symmetric state will be a linear function of the gravitation acceleration down the layer.

Figures 2 and 3, aside the illustration purpose, roughly represent a situation with cold Na_2 molecules [7, 8], where the role of internal states is played by the rotation spectrum. Corresponding resonant transmission energies are about $0.4 \cdot 10^{-4} \text{ eV}$, giving 1.2 m height for the position of the magnetic trap above the graphene layer.

It has to be noted that atomic and molecular interferometers, in parallel to pendulum gravimeters, have repeatedly been used as local gravity sensors (see, for instance, [9-14]). The present scheme of measurement represents a new type on this road: it substitutes material or light-pulse gratings by a single graphene layer. Another principle advantage of the scheme is the irrelevance of complete resonant transmission relative to specific values of parameters of the barrier potential.

Acknowledgement

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