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Coherent tunneling in periodic symmetric multiple well potentials

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Abstract

Based on the numeric solution of a nonstationary Schrödinger equation, features of the coherent wavepacket tunneling dynamics in the *n*-fold ($n = 2, 3, 4, 5$, and 6) periodic potential were analyzed.

Keywords: Coherent tunneling; Internal rotation; Periodic function of potential energy; Time-dependent Schrödinger equation

1. Introduction

Tunneling between potential energy minima is a well-known quantum mechanical phenomenon. Its demonstrations have been observed in molecular spectroscopy [1], semiconductor physics [2], etc. Details of the tunneling process are also of particular interest due to the possibility of observing the parity violation for optical isomers of chiral molecules [3–5].

Dynamics of wavepackets tunneling through potential barriers, interaction of the packets with external fields, the influence exerted by symmetry of the potential function on the formation and structure of molecular spectra have been studied in the last few years in several works (e.g. [6–14]). However, the majority of these works [6, 8, 10–14] are devoted to the problem of tunneling in the non-periodic potential, an excellent example of which is provided by the inversion potential in a molecule of ammonia. Provided minima of the potential energy function are equivalent, a potential turns to be symmetric, and coherent tunneling between these minima is caused by the "interaction" between potential wells [11, 15]. A wavepacket initially localized at one of the minima of this non-periodic potential further will be moving in a certain direction, tunneling to the neighboring minimum, as its propagation in the opposite direction is hindered by an infinitely growing potential wall. In the process the packet form determined by the power function of potential energy is approximately described by Gaussian function.

Specificity of tunneling in the periodic symmetric double-well ($n = 2$) potential that typically shows itself as an internal rotation in non-rigid molecules containing in their structure a hydroxyl group (phenol C_6H_5–OH [16], hydrogen peroxide HO–OH [1, 17]) is associated with identification of the potential function boundary points. According to the principles of quantum mechanics, a particle originally localized in one of the minima of a symmetric periodic potential is tunneling in two directions corresponding to two possible rotation senses of a molecular fragment. Obviously, the probabilities of tunneling through the left and right barriers are identical for equivalent barriers, being distinct for the nonequivalent ones [18]. And the form of a wavepacket determined by the periodic potential function may be greatly different from Gaussian function. Localization of the particle at the second minimum results from tunneling through both barriers but a hypothetical attempt at determining the tunneling direction is similar to trying to find the number of a slit through which a photon or electron is transmitted in a double-slit interference experiment [19], involving elimination of the superposition state and the violated conditions of coherent tunneling.

The principal features of the wavepacket tunneling dynamics in a double-well potential are characteristic for the potential of any multiplicity, whereas just for the multiple well ($n \geq 3$) potential functions, tunneling of a molecular fragment in both senses of rotation is exhibited most markedly. In this case the presence of several minima in the limited angular interval (from 0 to 2π rad) dictates a small width for each of the potential barriers and is liable to result in the initial non-equivalent delocalization of a wavepacket and in its specific dynamics (wave traveling in a particular direction).

This paper presents a study into dynamics of the non-Gaussian form wavepacket tunneling in the *n*-fold ($n \geq 2$) symmetric periodic potential simulating the potential energy function of internal rotation for a non-rigid molecule.

Three-well potentials ($n = 3$) are characteristic for molecular systems whose structure includes an internal top with a 3-fold symmetry axis (methyl group). Most typical representative of such a type non-rigid molecules is ethane CH_3–CH_3 [20]. It seems that four- ($n = 4$) and five-fold ($n = 5$) periodic potentials may be found only in the molecular clusters, for instance formed by a fragment of fullerene or by a molecule including four- (cyclobutane) or five-membered ring (cyclopentane), or else by a water molecule. One of the OH-bonds of a water molecule is oriented to the ring center and the second — to one of the atoms in the ring or to the center of the bond connecting two atoms in the ring. The existence of the like clusters is considered in [21, 22] taking the benzene – water structure as an example. Rotation of a water molecule over the surface of benzene ring in the cluster is accompanied by the origination of a six-fold ($n = 6$) periodic potential. Note that the presence of one or several heteroatoms in the ring structure leads to the origination of an asymmetric periodic potential. As distinct from four- or five-fold periodic functions, the six-fold periodic potential is characteristic not only for weak-bonded molecular clusters but also for some molecular systems, where the top with a 3-fold symmetry axis is involved in hindered internal rotation about the frame with a symmetry plane (nitromethane molecule CH_3–NO_2 [23]).

2. Computation method

It is assumed that a molecular system is in the ground rovibronic state with a single degree of freedom — internal rotation of the molecular top about the frame. Then the associated one-dimensional Hamiltonian (in cm^{-1}) is of the form [1]

$$\hat{H} = \mathbf{B}^{\frac{1}{4}} \hat{J}_\gamma \mathbf{B}^{-\frac{1}{2}} B_{\gamma\gamma} \hat{J}_\gamma \mathbf{B}^{\frac{1}{4}} + V(\gamma)\,, \qquad (1)$$

where γ — internal rotation angle; $\hat{J}_\gamma = -i\dfrac{\partial}{\partial\gamma}$; $B_{\gamma\gamma}$ — (4,4)-element of the matrix inverse to that of the molecular inertia tensor; $\mathbf{B}$ — determinant of the inverse inertia-tensor matrix; $V(\gamma)$ — potential energy function of internal rotation.

Hamiltonian (1) is reduced to the following form:

$$\hat{H} = -B(\gamma)\frac{\partial^2}{\partial\gamma^2} - \frac{\partial B(\gamma)}{\partial\gamma}\frac{\partial}{\partial\gamma} + V_{\mathrm{eff}}(\gamma)\,, \qquad (2)$$

where $B = B_{\gamma\gamma}$ and the effective potential energy function $V_{\mathrm{eff}}(\gamma)$ includes small terms dependent on the inertia parameters $B_{\gamma\gamma}$, $\mathbf{B}$ and their derivatives with respect to the torsional variable. In what follows the subscript «eff» is omitted.

The periodic n-fold potential function of internal rotation $V(\gamma)$ in the symmetric case is represented as a simplest-form Fourier expansion

$$V(\gamma) = \tfrac{1}{2} V_0 (1 + \cos n\gamma)\,,$$

where the value V_0 gives the heights of potential barriers.

A function of the inertia parameter $B(\gamma)$ is assumed to be even and periodic, representing the Fourier expansion

$$B(\gamma) = B_0 + \sum_{k=1} B_k \cos k\gamma\,,$$

Time evolution of a molecular system was found on the basis of a numeric solution for the time-dependent Schrödinger equation with Hamiltonian (2)

$$i\frac{\partial\Psi(\gamma,t)}{\partial t} = \hat{H}\Psi(\gamma,t)\,,$$

The initial wavepacket (at $t = 0$) was formed from the stationary wave functions of the ground state with regard to torsional splitting

$$\Psi(\gamma,0) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \Psi_j(\gamma)\,, \qquad (3)$$

where spatial parts of the stationary wave functions $\Psi_j(\gamma)$ represent linear combinations of the wave functions for the free rotator

$$\Psi_j(\gamma) = \sum_{k=-\infty}^{\infty} C_k^j e^{ik\gamma}\,, \quad C_k^j = C_{-k}^{j*}. \qquad (4)$$

Eigenfunctions (4) and energies of the corresponding stationary states were found by the matrix diagonalization of Hamiltonian (2).

The initial form of a wavepacket is dictated by the potential function multiplicity. For two- and three-fold potentials ($n = 2$ and 3) a practically complete compensation of positive and negative contributions from the parts of wavepacket (3) takes place in different potential wells as the wave functions of distinct states in neighboring wells are actually distinguished by the phase only. This in turn is responsible for localization of the initial packet at one minimum

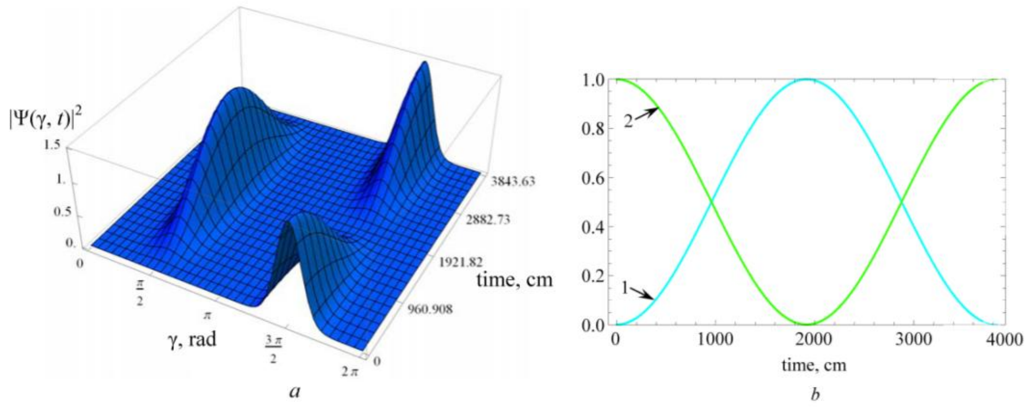


Figure 1. Tunneling of a wavepacket in a symmetric two-well periodic potential: form of the wavepacket (*a*); time dependences of the probabilities P_1 (1) and P_2 (2) (*b*).

of the potential energy. In the case of comparatively narrow potential barriers (at $n > 3$) the eigenfunctions involved in the wavepacket at different minima are distinguished not only by the phase but also, to a great degree, by the form, preventing the formation of the initial packet localized in one of the potential wells.

System's dynamics was studied by the construction of the finite-difference approximation of coupled equations for the real $\varphi(\gamma, t)$ and imaginary $\chi(\gamma, t)$ parts in the stationary-state complex wave function $\Psi(\gamma, t) = \varphi(\gamma, t) + i\chi(\gamma, t)$. The numeric computations were performed with the use of the absolutely stable two-step (three-layer) explicit method [24] enabling one to follow the evolution of a wave packet over considerable time intervals.

3. Results and Discussion

3.1. Double-well potential (n = 2)

In the case of a double-well symmetric potential its tunneling dynamics in greatly determined by the ground-state torsional splitting $\Delta E_{21} = E_2 - E_1$ [18]. For such a potential the probability density function $|\Psi(\gamma, t)|^2$, due to tunneling of the wavepacket, oscillates between minima of the potential function at the frequency Ω_{21} that is equal (in units of $\hbar$) to the quantity ΔE_{21} and has the period $T_{21} = 2\pi/\Omega_{21}$. The quantity $\tau_{21} = \pi/\Omega_{21}$ (time interval between the neighboring probability maxima) in this case may be termed the "tunneling time" because this interval is associated with transition of a wavepacket completely from one minimum of the potential curve to another, whereas the form of this wavepacket becomes recovered. In time τ_{21} the wave packet is "spreading" in opposite directions, being partially reflected from the potential function boundaries and partially penetrating (tunneling) into the adjacent minimum from both sides of the potential barrier to come finally to the center of each minimum of the potential function.

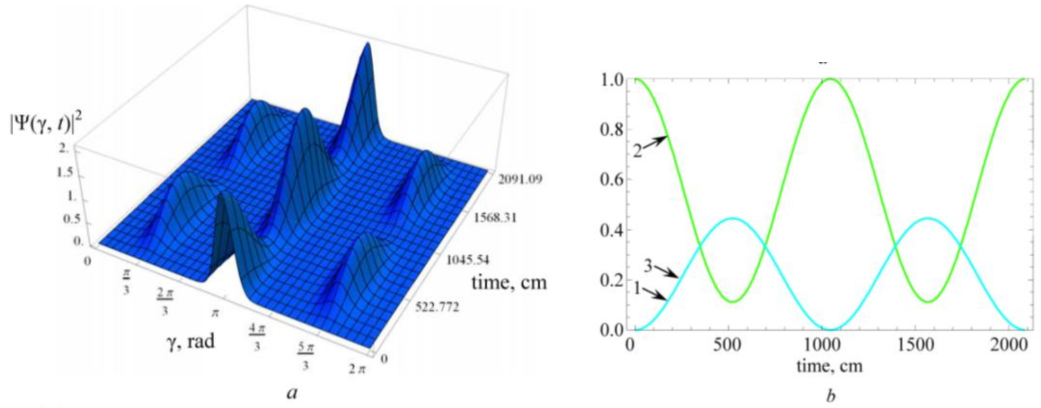
The form of a wavepacket during time $2\tau_{21}$ is shown in Figure 1, *a*. Figure 1, *b* for the same time interval gives the temporal dependences of the probabilities

$$P_1(t) = \int_0^{\pi} |\Psi(\gamma,t)|^2 \, d\gamma \quad \text{and} \quad P_2(t) = \int_{\pi}^{2\pi} |\Psi(\gamma,t)|^2 \, d\gamma$$

associated with localization of the wavepacket at the left and at the right minimum, respectively, of the π-periodic potential for a molecule of phenol. During computations the experimental parameters of a phenol molecule were used [16]: $V_0 = 1215$ cm^{-1}, $B_0 = 22.617$, $B_1 = 0$, $B_2 = 0.005$ cm^{-1}. The computed time characteristics of tunneling dynamics are given in centimeters. To go to time in seconds, one should use the factor $1/c$, where c — speed of light in free space given as cm/s. The above-mentioned parameters B_0 and V_0 for phenol are in line with $\Delta E_{21} = 0.0016$ cm^{-1} and $\tau_{21} = 1921.8$ cm.

3.2. Three-well potential (n = 3)

In the case of three-well symmetric potential with equivalent barriers the situation becomes more complicated because of the internal top has a 3-fold symmetry axis. In consequence, splitting of energy levels results in two rather than three sublevels, one of the levels (upper for the ground torsional state) being doubly degenerate [25]. As energies of two states are coincident ($E_2 = E_3$), similar to the double-well potential case, there is a single non-zero quantity $\Delta E_{31} = \Delta E_{21} = E_2 - E_1 = E_3 - E_1$ associated with the frequency Ω_{31}, period T_{31}, and time interval τ_{31}. But the quantity τ_{31} no longer may be called the "tunneling time",



a *b*

Figure 2. Tunneling of a wavepacket in a symmetric three-well periodic potential: form of the wavepacket (*a*); time dependences of the probabilities P_1 (1), P_2 (2) and P_3 (3) (*b*).

because the computations performed demonstrate that the wavepacket initially localized at one of the minima (e.g., central) subsequently is enable to leave it completely.

The form of a wavepacket in time $4\tau_{31}$ is shown in Figure 2, *a*. Figure 2, *b* for the same time interval gives the time dependences of the probabilities P_1, P_2, and P_3 associated with localization of the wavepacket at the left, central or right minimum, respectively, of the $2\pi/3$-periodic potential for a ethane molecule [20]: $V_0 = 1005$ cm^{-1}, $B(\gamma) = \text{const} = B_0 = 10.68$ cm^{-1}. The indicated values of the parameters B_0 and V_0 for ethane correspond to $\Delta E_{31} = 0.006$ cm^{-1} and $\tau_{31} = 522.8$ cm.

As demonstrated by the computation results, in the case under study the quantity τ_{31} is still associated with a time interval between the neighboring maxima of the probability, whereas recovery of the wavepacket form takes place only after the period of time $T_{31} = 2\tau_{31}$ and exactly in the same potential well, where the initial wavepacket was localized. During time $2\tau_{31}$ the wavepacket is symmetrically spreading to the side potential wells to "come together" finally in the central one. In the process the probability of its detection at the central minimum in these time intervals never goes to zero. A minimal value of the probability of detecting a wavepacket at the central minimum is independent of the parameters V_0 and B_0, being equal to 0.1111.

3.3. Four-well potential (n = 4)

In the case of a four-well symmetric potential with equivalent barriers energy levels are splitting into three sublevels, one of them (second) being doubly degenerate. As the energies of two states are coincident ($E_2 = E_3$), two splitting values (two frequencies) are the case: $\Delta E_{31} = \Delta E_{21} = E_2 - E_1 = E_3 - E_1 = \Omega_{31}$ and $\Delta E_{43} = \Delta E_{42} = E_4 - E_3 = E_4 - E_2 = \Omega_{43}$ corresponding to the time intervals τ_{31}, τ_{43} and to the periods $T_{31} = 2\tau_{31}$, $T_{43} = 2\tau_{43}$. The overall splitting of the ground state $\Delta E_{41} = E_4 - E_1$ associated with the frequency Ω_4 leads to the third, "reduced", time interval $\tau_{41} = \tau_{31}\tau_{43}/(\tau_{31} + \tau_{43})$ and to the "reduced" period $T_{41} = 2\tau_{41}$. As compared to the three-fold potential, barriers become narrower causing a greater torsional splitting of energy levels and hence reduced (by several orders) times τ.

The form of a wavepacket and time dependences for the probabilities P_1, P_2, P_3 и P_4 of its localization in one of four potential wells are presented in Figure 3. The computations were performed using the simulation parameters: $V_0 = 1000$ cm^{-1}, $B(\gamma) = \text{const} = B_0 = 22.60$ cm^{-1}. The indicated potential barrier height is rather typical for non-rigid molecules. A value of the inertia parameter corresponds to the moment of inertia for hydroxyl group OH. These values of the parameters V_0 and B_0 are associated with the frequencies $\Omega_{31} = 2.677$ cm^{-1}, $\Omega_{43} = 2.775$ cm^{-1}, $\Omega_{41} = 5.452$ cm^{-1} and with the time intervals $\tau_{31} = 1.174$ cm, $\tau_{43} = 1.132$ cm, $\tau_{41} = 0.576$ cm.

As distinct from double- and three-well potentials, for the probability density function in the case under consideration there occurs some kind of a traveling wave whose propagation direction is determined by the initial phases of eigenfunctions (4) forming the initial wavepacket. Each of the Fourier spectra for all the four probabilities P_1, P_2, P_3, and P_4 involves three frequencies: Ω_{31}, Ω_{43}, and Ω_{41}. According to data in Figure 3, *a*, one half of the "reduced" period $\tau_{41} = T_{41}/2$ corresponds to a time interval between neighboring maxima of the probability density. Since τ_{31} and τ_{43} are not integers, the initial form of a wavepacket may be completely recovered only after several thousands of such time intervals. Nevertheless, as seen from data in Figure 3, *b*, in the period $T = 64.265$ cm the probability distribution of the wavepacket localization in a certain potential well takes the form close to the initial one. This period is

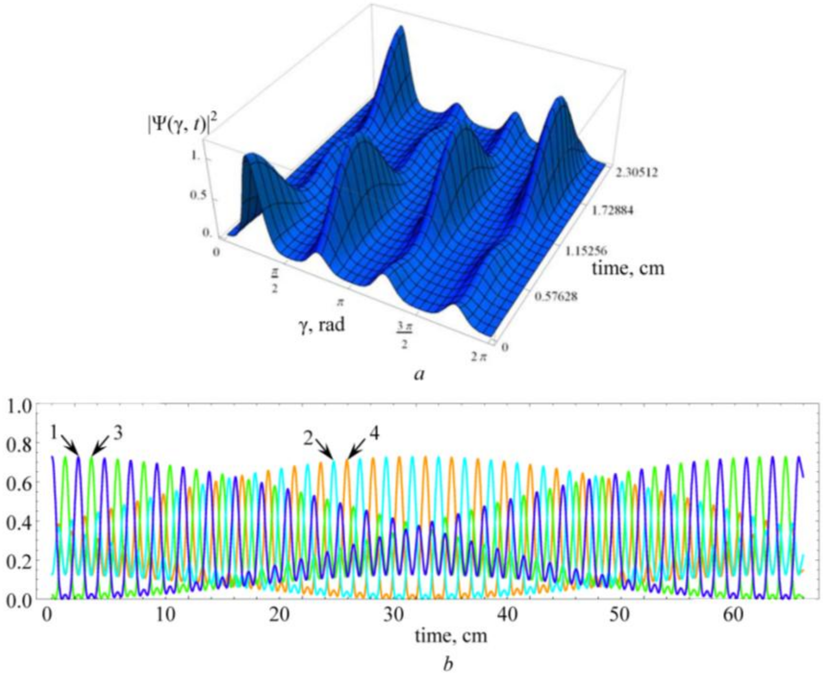


Figure 3. Tunneling of a wavepacket in a symmetric four-well periodic potential: form of the wavepacket in the time interval $4\tau_{41}$ (*a*); time dependences of the probabilities P_1 (1), P_2 (2), P_3 (3) and P_4 (4) in the time interval $T = 64.265$ cm (*b*).

associated with the difference frequency $\Delta\Omega = \Omega_{43} - \Omega_{31} = 0.098$ cm^{-1} that is exhibited as an envelope of the probability curve in each of the potential wells.

3.4. Five-well potential (n = 5)

Splitting of energy levels for the five-well symmetric potential with equivalent barriers also gives three sub-levels two of which (second and third) are doubly degenerate. Despite the presence of three periods only (τ_{31}, τ_{53}, and "reduced" τ_{51}), however, dynamics of tunneling is more complex in its character. The computations were performed with the same values of the parameters V_0 and B_0 as for a four-well potential. In this case we have: $\Omega_{31} = 7.032$ cm^{-1}, $\Omega_{53} = 12.519$ cm^{-1}, $\Omega_{51} = 19.551$ cm^{-1}, $\tau_{31} = 0.447$ cm, $\tau_{53} = 0.251$ cm, $\tau_{51} = 0.161$ cm.

Also, Fourier spectra for the probabilities P_1, P_2, P_4, and P_5 have three frequencies (Ω_{31}, Ω_{53}, Ω_{51}) each. A Fourier spectrum for the probability P_3 has a single frequency (Ω_{31}) because the probability density of the wavepacket localization is changed, with a well defined period ($T_{31} = 2\tau_{31}$), only in the central (third) well, see Figure 4, *a*. And the probability of the wavepacket localization in the third well comes to 0.4 (Figure 4, *b*).

In the first and fifth potential wells the probability density functions are in opposite phases — a maximum of the function $|\Psi(\gamma, t)|^2$ in the first well is corresponding to a minimum in the fifth well. A similar situation is observed for the second and fourth potential maxima too. Maximal values of the probabilities for the wavepacket localization in the first and fifth wells are above 0.8, while in the second and fourth wells they are hardly approaching 0.3. For other values of the parameters V_0 and B_0 the above-mentioned probabilities are comparable. As a rule, the overall probability maxima for localization of a wavepacket in the first and fifth (second and fourth) wells fall at minima (maxima) of the third (Figure 4, *b*).

Unlike a four-well potential, in the case considered the difference frequency $\Delta\Omega = \Omega_{53} - \Omega_{31} = 5.487$ cm^{-1} and the period $T = 2\pi/\Delta\Omega = 1.154$ cm are of the same order of magnitude, with the frequencies Ω_{53}, Ω_{31} and periods T_{53}, T_{31} respectively. Because of this, the envelope of these probabilities, being no pronounced in character, is still traced in Figure 4, *b*.

3.5. Six-well potential (n = 6)

For a six-well symmetric potential with equivalent barriers energy levels are splitting into four sub-levels two of which (second and third) are doubly degenerate. In this case there are three non-zero values of ΔE (ΔE_{31}, ΔE_{53}, ΔE_{65}) associated with three time intervals τ (τ_{31}, τ_{53}, τ_{65}), whereas the overall splittings ΔE_{51}, ΔE_{63}, ΔE_{61} are associated with the "reduced" periods τ_{51}, τ_{63}, τ_{61}. The described computations have been performed with the same values of the parameters V_0 and B_0 as in the case of the four-

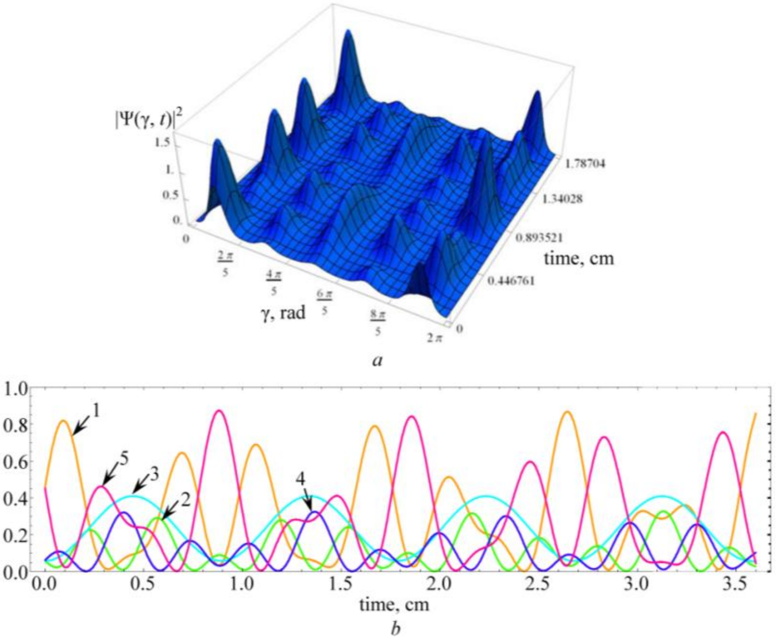


Figure 4. Tunneling of a wavepacket in a symmetric five-well periodic potential: form of the wavepacket in the time interval $4\tau_{31}$ (*a*); time dependences of the probabilities P_1 (1), P_2 (2), P_3 (3), P_4 (4) and P_5 (5) in the time interval $8\tau_{31}$ (*b*).

fold potential. Then we have: $\Omega_{31} = 11.725$ cm^{-1}, $\Omega_{53} = 27.098$ cm^{-1}, $\Omega_{65} = 16.117$ cm^{-1}, $\Omega_{51} = 38.823$ cm^{-1}, $\Omega_{63} = 43.215$ cm^{-1}, $\Omega_{61} = 54.940$ cm^{-1}, $\tau_{31} = 0.268$ cm, $\tau_{53} = 0.116$ cm, $\tau_{65} = 0.195$ cm, $\tau_{51} = 0.081$ cm, $\tau_{63} = 0.073$ cm, $\tau_{61} = 0.057$ cm. The computation results are given in Figure 5.

Fourier spectra for the probabilities P_1, P_3, P_4, and P_6 involve all the six frequencies mentioned above. Fourier spectra for the probabilities P_2 and P_5 have only three frequencies (Ω_{31}, Ω_{63}, Ω_{61}) each. A great number of the fundamental and sum Ω as well as difference $\Delta\Omega$ frequencies in the case of a six-well potential results in a more and more complex tunneling dynamics compared to the five-well case (Figure 5, *a*). Note that most characteristics for a six-well potential is the greatest delocalization degree of a wavepacket.

Figure 5, *b* demonstrates the probabilities P_1 and P_3 for the wavepacket localization in the first and third wells in the time interval $T = 8.582$ cm during which the form of a wavepacket in these wells is recovered with a sufficient degree of accuracy. Recovery of the wavepacket form for the fourth and sixth potential wells (Figure 5, *d*) occurs during the same time interval T for which the approximate

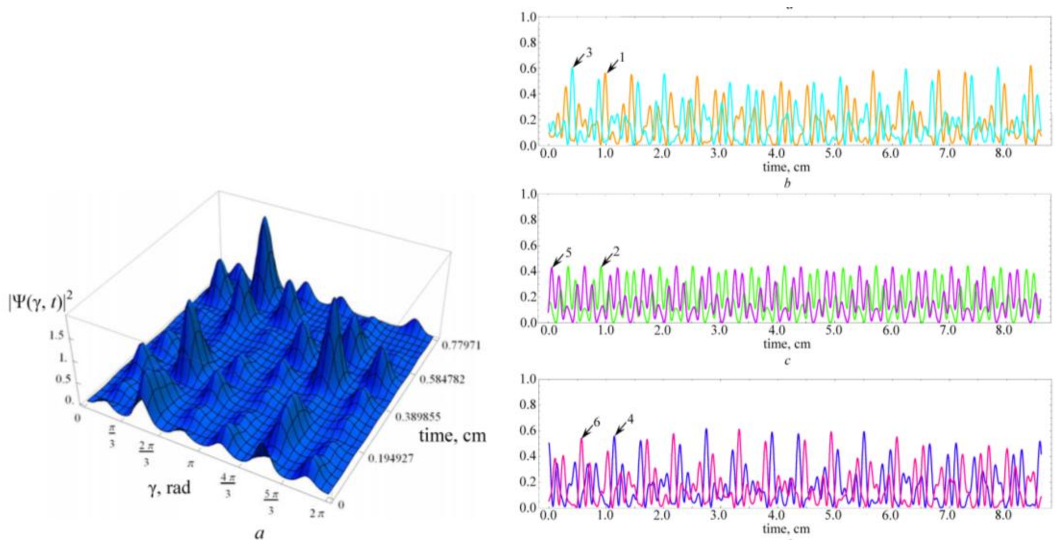


Figure 5. Tunneling of a wavepacket in a symmetric six-well periodic potential: form of the wavepacket in the time interval $4\tau_{65}$ (*a*); time dependences of the probabilities P_1 (1) and P_3 (3) (*b*), P_2 (2) and P_5 (5) (*c*), P_4 (4) and P_6 (6) (*d*) in the time interval 8.582 cm.

equalities $T \approx 21T_1 \approx 15T_2 \approx 6T_3$ are true, and the periods $T_1 = 2\pi/\Delta\Omega_1$, $T_2 = 2\pi/\Delta\Omega_2$, $T_3 = 2\pi/\Delta\Omega_3$ are determined by the difference frequencies $\Delta\Omega_1 = \Omega_{53} - \Omega_{31}$, $\Delta\Omega_2 = \Omega_{53} - \Omega_{65}$, $\Delta\Omega_3 = \Omega_{65} - \Omega_{31}$. In the second and fifth potential wells (Figure 5, *c*) the form of a wavepacket is recovered much faster during the time period T' that is equal to 1.597 cm, for which the approximate equalities $T' \approx 8T_4 \approx 11T_{63} \approx 14T_{61}$ are also true, where $T_4 = 2\pi/\Delta\Omega_4 = 2\pi/(\Omega_{63} - \Omega_{31})$. In this way several difference frequencies influence greatly the tunneling dynamics of a wavepacket in multiple well periodic potentials.

The probabilities for the wavepacket localization in the first and third wells are in opposite phases. A similar situation is observed for the second and fifth as well as for the fourth and sixth wells. Maximal values of the probabilities in the first, third, fifth, and sixth well are over 0.61, whereas in the second and fourth wells they only approximate 0.42. For other values of the parameters V_0 and B_0 the indicated probabilities are comparable.

4. Conclusions

Tunneling of a wavepacket in two directions associated with two possible rotation senses of a quantum system fragment is the principal feature of the coherent tunneling dynamics in a periodic potential. Multiplicity of a potential in the tunneling process is responsible for its character. In a two-fold potential the wavepacket initially localized in one of the minima of the potential function goes completely to the neighboring minimum. In the case of a three-fold potential the wavepacket initially localized at a central maximum is symmetrically tunneling to side minima and then returns back, making the probability of its localization at a central minimum always other than zero. In the case of a four-fold potential the time dependence of the probability density function appears as a traveling wave. And the form of this distribution is determined by values of the "reduced" period (overall state splitting) and of the period associated with the difference frequency. Dynamics of tunneling for the potentials of great multiplicity is less systematic in character due to numerous fundamental, sum, and difference frequencies.

A dynamic description of the torsional tunneling process makes it possible to follow the evolution of the fragments in a non-rigid molecular system in detail and to establish the conditions for realization of the tunneling transitions between its equilibrium configurations, directly influencing the formation of a fine torsion-rotation structure in molecular spectra.

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