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BIFURCATION AND CHAOS IN TWO-DIMENSIONAL SYSTEMS OF QUANTUM DOTS AND QUANTUM MOLECULESA.K. Aringazin^{1,2}, V.D. Krevchik^{2,3}, M.B. Semenov^{2,3}¹Institute for Basic Research, Eurasian National University, Astana, Kazakhstan, aringazin@emu.kz²Institute for Basic Research, FL, USA, ³Penza state University, Penza, Russia, physics@pnzgu.ru

Methods developed in the approach to quantum tunneling with dissipation are applied to a dissipative tunneling in the systems of coupled quantum molecules. We study two-dimensional (2D) effects of cleavage and thermally controlled extrema in tunnel probability function on asymmetry parameter; thermally dependent blockage effect; effect of edge temperature in the case when radii of quantum dots (QD) in quantum molecules (QM) are bigger than radii of final state QD; bifurcations in the temperature dependence and in coupling constant in interacting QM systems. 2D tunnel transitions are chaotic in the case of antiparallel 2D transfers and this chaotization occurs as a phase transition of second order, whereas in the case of parallel 2D transfers the bifurcations occur as a phase transition of first order.

Keywords: quantum tunneling, dissipation, bifurcations, chaotization, phase transition.

Dynamics of transfer processes in two-dimensional (2D) nonlinear systems exhibits bifurcation and chaos at some range of their parameters. Such phenomena were studied theoretically in two-dimensional systems of interacting Josephson contacts, in low-temperature two-dimensional adiabatic chemical kinetics of molecules like 7-azaindole [10, 11, 17]. Experimental observation of such bifurcations in two dimensions is difficult. For the system of Josephson contacts the experimental identification was obscured by essential background fluctuations. In the case of porphyrin molecules, bifurcations have been experimentally found but they appear to be of unstable character.

However, the situation becomes different with the appearance of artificial nanostructures properties of which are under some control. These include quantum dots (QD) and quantum molecules (QM) as well as pairs of QD and QM bound by a quantum tunnel effect. We studied 2D dissipative tunneling in the systems of interacting QM, in a quasiclassical (instant on) approximation. We showed particularly that one observes the effect of blockage of two-particle wave function in the system of interacting QM accounting for the effect of bifurcation of tunnel trajectories when QD in QM have the same radii. When the interaction of the system with thermostat is switched off the blockage effect is replaced by the effect of cleavage in the plot of tunnel probability as a function of the QM asymmetry parameter.

There is growing interest in electron transport in tunnel bound nanostructures [1-17]. Some studies concern control parameters of nanostructures and mesoscopic systems (MS) when one accounts for their nonlinear properties [10, 12]. When studying MS one should note that physics and chemistry related to electron transport at nanoscales share a number of common features. MS are like macromolecules and, as usual, they interact with matrix or thermostat [9-11]. From this point of view, the term quantum molecule is suitable when one deals with quantum dots bound by tunnel effects. This allows considering physics of MS in combination with dissipative multidimensional tunneling, which happens not only in MS but also in many chemical reactions.

Quasiclassical study of quantum particle dynamics interacting with thermostat is one of the exciting problems from theoretical viewpoint [1-12]. Revival interest to quantum tunneling in the presence of thermostat is due to studies on tunnel bound MS [4-7, 13-16] which could be treated as reacting molecular complexes. It is of particular interest that in the artificial nanostructures with QD and QM nonlinear effects, such as bifurcation and cleavage, may occur, which, in contrast to the usual chemical reaction case, exhibit rather stable character [10-11]. This quasiclassical approach is

of much interest since it allows obtaining most results in an analytical form while other known approaches fail when one tries to account for the thermostat.

Applicability of the instanton approach [1-3, 8-11] in calculating temperature dependence of tunnel probability Γ for QD based on InSb can be estimated by comparing characteristic size of the system with de Broglie wavelength of the tunneling particle, or in terms of rare gas of instanton-antiinstanton pairs [9-11]:

$$\left\{ \begin{array}{l} R \gg \frac{\hbar}{(2-\sqrt{3})\sqrt{2m^*U_0}} \\ R \gg \frac{\hbar}{\sqrt{8m^*k_B T}} \end{array} \right. \quad (1)$$

$$\left\{ \begin{array}{l} R \gg \frac{\hbar}{\sqrt{8m^*k_B T}} \end{array} \right. \quad (2)$$

Here, U_0 is height of the potential barrier, m^* is the effective mass of tunneling electron. Due to Eq. (1) the radius R of QD should be much bigger than de Broglie wavelength of the tunneling particle. Eq. (2) is the condition of applicability of the gas of instanton-antiinstanton pairs [9-11]. One can check that Eqs. (1) and (2) both fulfill at $T \geq 50 K$ and $U_0 \approx 0.2\epsilon_B$ that may correspond to QD based on InSb.

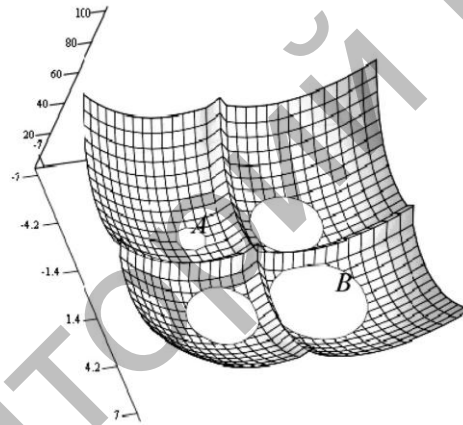


Fig. 1 Potential energy surface (3) in the case of parallel transfer of two tunneling particles: $a=2, b=2.5, \alpha^*=0.0001$. A and B denote initial and final two-point states respectively

The minimum at B of this 2D potential is lower than local minimum at A. The other two (intermediate) local minima are between the levels of A and B.

In this paper, we study dissipative tunneling in the system of interacting QM. Experimental aspects of this problem are discussed in [16]. In accord to [10], 2D model potential for this system (Fig. 1) can be represented as:

$$U_1(R_1, R_2) = \frac{\omega^2(R_1+a)^2}{2}\theta(-R_1) + \left[-\Delta I + \frac{\omega^2(R_1-b)^2}{2} \right] \theta(R_1) + \frac{\omega^2(R_2+a)^2}{2}\theta(-R_2) + \left[-\Delta I + \frac{\omega^2(R_2-b)^2}{2} \right] \theta(R_2) - \frac{\alpha(R_1-R_2)^2}{2} \quad (3)$$

The corresponding instanton action is found in the form [10]:

$$S\{R_1, R_2\} = \int_{-\beta/2}^{\beta/2} d\tau \left\{ \frac{\dot{R}_1^2}{2} + \frac{\dot{R}_2^2}{2} + V(R_1, R_2) + \right. \quad (4)$$

$$+ \frac{1}{2} \int_{-\beta/2}^{\beta/2} d\tau' D(\tau - \tau') [R_1(\tau) + R_2(\tau)] [R_1(\tau') + R_2(\tau')] \Big\}$$

2D quasiclassical trajectory (instant on), which minimizes the action S can be determined from the set of equations of motion

$$\frac{\delta S}{\delta R_1} = 0, \quad \frac{\delta S}{\delta R_2} = 0. \quad (5)$$

The instants τ_1 and τ_2 («centers» of instantons), at which two particles pass top points of the barriers along the coordinates of tunneling are determined by the conditions:

$$R_1(\tau_1) = 0, \quad R_2(\tau_2) = 0 \quad (6)$$

The resulting action S as a function of τ_1 and τ_2 is:

$$S = 2a(b+a)(\tau_1 + \tau_2)\omega^2 - \frac{\omega^2(a+b)^2(\tau_1 + \tau_2)^2}{\beta} - \frac{\omega^4(a+b)^2(\tau_1 - \tau_2)^2}{(\omega^2 - 2\alpha)\beta} - \frac{2\omega^4(a+b)^2}{\beta} \sum_{n=1}^{\infty} \left\{ \frac{(\sin v_n \tau_1 + \sin v_n \tau_2)^2}{v_n^2(v_n^2 + \omega^2 + \xi_n)} + \frac{(\sin v_n \tau_1 - \sin v_n \tau_2)^2}{v_n^2(v_n^2 + \omega^2 - 2\alpha)} \right\} \quad (7)$$

In the case of essential character of interaction with some local mode ω_L of the thermostat (C is the interaction constant of tunneling particle for the local mode ω_L), the action (7) as a function of the parameters ε^* and τ^* , ($\varepsilon = \varepsilon^* \omega = (\tau_1 - \tau_2) \omega$; $\tau = 2\tau^* \omega = (\tau_1 + \tau_2) \omega$; $\beta^* = \beta \omega / 2$; $\alpha^* = 2\alpha / \omega^2$; $b^* = b/a$, $b \geq a$) can be rewritten as:

$$S = (b+a)(3a-b)\omega^2\tau^* - \frac{\omega^4(a+b)^2\varepsilon^*}{2(\omega^2 - 2\alpha)} - \frac{4\omega^2(a+b)^2(\tau^*)^2}{\beta} - \frac{\omega^4(a+b)^2(\varepsilon^*)^2}{(\omega^2 - 2\alpha)\beta} - \frac{\omega^2(a+b)^2}{2\tilde{\gamma}} \left\{ \frac{(\omega^2 - \tilde{x}_2)}{\sqrt{\tilde{x}_1}} \left(\operatorname{cth} \left(\frac{\beta}{2} \sqrt{\tilde{x}_1} \right) - \frac{1}{\operatorname{sh} \left(\frac{\beta}{2} \sqrt{\tilde{x}_1} \right)} \left(\operatorname{ch} \left[\left(\frac{\beta}{2} - 2\tau^* \right) \sqrt{\tilde{x}_1} \right] - \operatorname{ch} \left[\left(\frac{\beta}{2} - \varepsilon^* \right) \sqrt{\tilde{x}_1} \right] + \frac{1}{2} \operatorname{ch} \left[\left(\frac{\beta}{2} - \varepsilon^* - 2\tau^* \right) \sqrt{\tilde{x}_1} \right] + \frac{1}{2} \operatorname{ch} \left[\left(\frac{\beta}{2} - 2\tau^* + \varepsilon^* \right) \sqrt{\tilde{x}_1} \right] \right) \right\} - \frac{(\omega^2 - \tilde{x}_1)}{\sqrt{\tilde{x}_2}} \left(\operatorname{cth} \left(\frac{\beta}{2} \sqrt{\tilde{x}_2} \right) - \frac{1}{\operatorname{sh} \left(\frac{\beta}{2} \sqrt{\tilde{x}_2} \right)} \left(\operatorname{ch} \left[\left(\frac{\beta}{2} - 2\tau^* \right) \sqrt{\tilde{x}_2} \right] - \operatorname{ch} \left[\left(\frac{\beta}{2} - \varepsilon^* \right) \sqrt{\tilde{x}_2} \right] + \frac{1}{2} \operatorname{ch} \left[\left(\frac{\beta}{2} - \varepsilon^* - 2\tau^* \right) \sqrt{\tilde{x}_2} \right] + \frac{1}{2} \operatorname{ch} \left[\left(\frac{\beta}{2} - 2\tau^* + \varepsilon^* \right) \sqrt{\tilde{x}_2} \right] \right) \right\} \Big\}$$

$$-\frac{\omega^4(a+b)^2}{2(\omega^2-2\alpha)^{3/2}} \left\{ -\operatorname{cth}\left(\frac{\beta}{2}\sqrt{\omega^2-2\alpha}\right) + \frac{1}{\operatorname{sh}\left(\frac{\beta}{2}\sqrt{\omega^2-2\alpha}\right)} \left(\operatorname{ch}\left[\left(\frac{\beta}{2}-\varepsilon^*\right)\sqrt{\omega^2-2\alpha}\right] - \right. \right. \\ \left. \left. -\operatorname{ch}\left[\left(\frac{\beta}{2}-2\tau^*\right)\sqrt{\omega^2-2\alpha}\right] + \frac{1}{2}\operatorname{ch}\left[\left(\frac{\beta}{2}-\varepsilon^*-2\tau^*\right)\sqrt{\omega^2-2\alpha}\right] + \right. \right. \\ \left. \left. + \frac{1}{2}\operatorname{ch}\left[\left(\frac{\beta}{2}-2\tau^*+\varepsilon^*\right)\sqrt{\omega^2-2\alpha}\right] \right) \right\}, \quad (8)$$

where

$$\tilde{x}_{1,2} = \frac{1}{2} \left(\omega^2 + \omega_L^2 + \frac{C^2}{\omega_L^2} \right) \mp \frac{1}{2} \sqrt{\left(\omega^2 + \omega_L^2 + \frac{C^2}{\omega_L^2} \right)^2 - 4\omega^2\omega_L^2}, \\ \tilde{\gamma} = \sqrt{\left(\omega^2 + \omega_L^2 + \frac{C^2}{\omega_L^2} \right)^2 - 4\omega^2\omega_L^2}.$$

Accounting for the system of transcendent equations (6) this formula allows revealing a number of dissipative tunnel effects for the system of interacting quantum molecules. Inverse temperature dependence of the action (8) (tunnel probability Γ) with bifurcation effect is shown in Fig. 2.

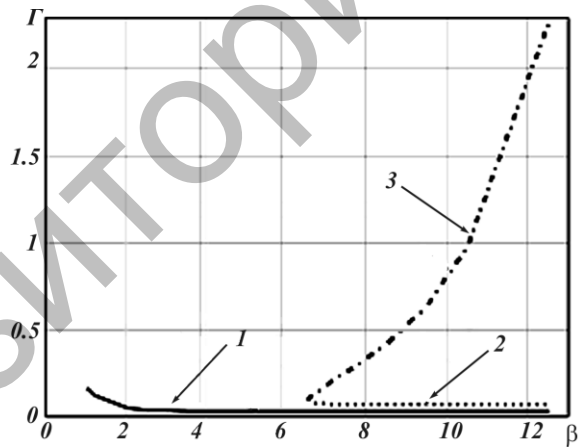


Fig. 2 Tunnel probability Γ as a function of inverse temperature β^* : 1 – $\varepsilon = 0, \alpha^* = 0.1, b = 1.1$; 2 and 3 – $\varepsilon \neq 0, \alpha^* = 0.1, b = 1.1$

Similar to the case of tunneling in one dimension, in the structures like quantum molecules it appears possible to find effect of blockage of two-particle wave function in the limit when radii of quantum dot pairs, which form interacting quantum molecules, coincide. Also, this effect essentially depends on thermostat presence. Observing dependence of the action on the asymmetry parameter (sharp extremum at $b^* = b/a = 1$, minimum of Γ) responsible for the blockage effect, one can observe bifurcation, i.e. appearance of additional asynchronous tunnel regimes of transfer. In the case when thermostat effect is negligible, one can see the cleavage effect instead of characteristic blockage effect (minimum of $\Gamma(b^*)$), either in the action or in $\Gamma(b^*)$ as a function of asymmetry parameter b^* (for example, it can be controlled by an external electric field).

The bifurcation is not disappearing. One can observe strong nonlinear dependence of the action (5) and of Γ on the coupling parameter α^* . One can also demonstrate that the blockage is controlled: with increasing temperature the distance $\Delta\Gamma$ between extrema of $\Gamma(b^*)$ decreases while with increase of the potential barrier U_0^* it increases.

In conclusion, we show applicability of well-known methods of quantum tunneling with dissipation to a dissipative tunneling in the systems of coupled quantum molecules. We theoretically predict 2D effects of cleavage and thermally controlled extrema in tunnel probability function on asymmetry parameter; thermally dependent blockage effect; effect of edge temperature in the case when radii of QD in QM are bigger than radii of final state QD; bifurcations in the temperature dependence and in coupling constant in interacting QM systems.

Chaotization on two-dimensional tunnel transitions is observed in the case of antiparallel 2D transfers and occurs as a phase transition of second order, whereas in the case of parallel 2D transfers the bifurcations occur as a phase transition of first order.

Studied effect of controlled blockage in the case of electrically interacting QD could be used to construct structures like qubit. We hope that these theoretical results will be checked in experiments with STM/AFM.

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