ISOELECTRONIUM CORRELATIONS AS A NONLINEAR TWO-DIMENSIONAL TWO-PARTICLE TUNNEL EFFECT

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Abstract

In this paper, we study a nonlinear two-dimensional two-particle quantum tunnel effect with dissipation in diatomic H-H system. We use an instanton technique based on path integral approach, and present analytical solutions, in a linearized reaction coordinates and harmonic potential approximation. It appears that the tunnel effect leads to a specific correlation between two electrons interacting with each other by Coulomb potential. This effect can be viewed as a mechanism supporting the isoelectronium recently proposed by Santilli and Shillady within the framework of isochemical model of the hydrogen molecule. We show that, under a condition of effective two-dimensional motion, contribution of the quantum tunnel correlated configurations is essential in the electron dynamics. Temperature dependence of the probability of the two-electron tunnel transitions per unit time has been studied.

1 Introduction

In a recent paper, Santilli and Shillady [1] suggested a new isochemical model of the hydrogen molecule characterized by a bond at short distances of the two valence electrons into a singlet quasi-particle state called isoelectronium has been introduced. Namely, the isochemical model suggests introducing of attractive short-range Hulten potential interaction between the electrons, in addition to the usual Coulomb repulsive potential. An origin of the short-range attractive potential has been assumed due to a deep overlapping of wavepackets of the electrons giving rise to nonlinear and other effects.

Both the unstable and stable isoelectronium cases corresponding to the general four-body and the restricted three-body problems, respectively, have been analyzed, in Born-Oppenheimer approximation. Standard Boys-Reeves numerical three-body and four-body calculations [1], exact analytic three-body solution based study [2], and analytic four-body Ritz variational study [3] of the model have been carried out. The Hulten potential V_h, which contains two parameters, appeared to lead to rather complicated calculations so that the other potentials, the Gaussian-screened-Coulomb potential V_g and the exponential-screened-Coulomb potential V_e, have been used in the above papers, to mimic the Hulten potential at long and short distance asymptotics. A comparison of the obtained results with experimental data on H_2 molecule showed that the approximation of stable pointlike isoelectronium (three-body problem) does not fit the data while for the unstable isoelectronium case (the general four-body problem) exact representation of the experimental binding energy and bond length of H_2 molecule can be achieved by fitting the correlation length parameter of the potential. The ground state energy based estimation [3] showed that the contribution of the attractive interelectron potential V_e (i.e., contribution of the isoelectronium related potential) should be about 1%...6% of that of the usual repulsive interelectron Coulomb potential, to meet the experimental data. In ref. [3] some relation between the two parameters of the Hulten potential was used, thus only one parameter has been used for the fitting. This relation arose from consideration of the two-electron system governed by the Hulten potential, with the assumption that the electrons could form one-level bound state.

The effect of electron correlations made by the introduced attractive short-range interelectron potentials (i.e., the unstable isoelectronium), with the correlation length parameter value of about 0.01 bohr appeared to be helpful in achieving exact representation of the experimental data on H_2 molecule. Also, within the Boys-Reeves framework the isoelectronium based approach appeared to provide an essentially (at least 1000 times) faster computer calculations [1], in comparison to a standard C.I. calculation. This approach has been extended to the case of other diatomic molecules [1] and water molecule [4].

In the present paper, we study two-electron correlations arising from the *two-dimensional* tunnel effect with dissipation which can take place in diatomic molecules subjected to strong external electromagnetic field. More specifically, we take H_2 molecule as a simple example and assume that the three-dimensional potential can be effectively reduced to a two-dimensional one under the action of

the external field. Also, we assume that the H_2 molecule is a part of molecular association. Due to obtained results, the two-particle tunnel effect leads to a contribution which resembles that of the above isoelectronium correlations in two-dimensions. However, we should to emphasize that we do not introduce any attractive interelectron potential. Namely, the characteristic two-electron correlation arises naturally as a consequence of the two-dimensional two-particle tunnel effect with dissipation.

Present consideration is strongly motivated by recent studies of a light gas called MagneGas^{TM}, consisting, due to a standard chemical analysis, mainly of carbon monoxide CO (41%) and hydrogen H_2 (48%) gases, produced by the Santilli's PlasmaArcFlow^{TM} chemical reactor [5, 6]. Gas-chromatography mass-spectrometry and infrared spectroscopy data obtained at room temperatures clearly indicate presence of high molecular mass species (up to 1000 a.m.u.) in MagneGas, in a macroscopic percentage. They have no strong infrared signature of conventional chemical bonds, except for that of carbon monoxide CO and, also, carbon dioxide CO_2, which is present in MagneGas^{TM} in some small percentage. The GC-MS/IR search results using a library of about 138,000 chemical species did not indicate any matches with these high molecular mass species. The main hypothesis on the origin of these species called *magnecules* is that they are formed from the usual molecules (CO, H_2, etc.) bonded to each other in some way, under the initial action of strong external electromagnetic field produced by underwater arc in the Santilli's PlasmaArcFlow^{TM} reactor [5]. We refer the interested reader to refs. [5, 6] for more detailed information on MagneGas^{TM} and Santilli's PlasmaArcFlow^{TM} reactor, and their applications.

We conjecture that the two-dimensional tunnel effects play an essential role at the stage of forming of the high molecular mass species (magnecules) inside the reactor, where the influence of the strong external electromagnetic field takes place. Main details of a rather complicated physico-chemical process inside the reactor can be studied elsewhere. In general, an importance of studying of the tunnel effects is grounded on the fact that a tunnel effect is known to be as a mechanism in forming of formaldehyde ($CH_2{=}O$) polymer structure.

In the present paper, we concentrate on the study of consequences implied by the eventual 'magnetic freezing' (lowering of the effective temperature due to the effect of external electromagnetic field) of the hydrogen molecule in molecular association. The magnetic freezing is characterized by an effective reducing of the three-dimensional potentials to some two-dimensional ones ('polarizing of orbits'). We should to emphasize that the system under study is not a separate H_2 molecule as such because of the effective two-dimensional treatment of it and presence of the neighbor molecules in association; herebelow, the system under study is referred to as H-H system.

We use oscillator potentials as an approximation to superposition of Coulomb potentials in the H-H system in molecular association. Such an approximation is naturally used in low-temperature chemical kinetics, with parameters of the oscillator potential being adjusted to reproduce a ground state energy level. The interelectron potential is taken as a Coulomb one. We note that the ground state energy of the "magnetically frozen" H_2 molecule (the H-H system) is lower than

that of the ordinary H_2 molecule. As the result the binding energy of the H-H system is bigger than that of H_2 molecule. Detailed study of the effect of external electromagnetic field will be made in a subsequent paper.

Set up of the model is the following. We consider two-dimensional (planar) motion of two electrons around fixed nuclei of two H atoms. The electrons thus move in a nonlinear potential $U(q_1, q_2)$, where the reaction coordinates q_1 and q_2 of the electrons in the H-H system can be linearized in the first order approximation as shown in Fig. 1. The linearization assumes introducing of *four* centers, instead of the original two centers (protons).
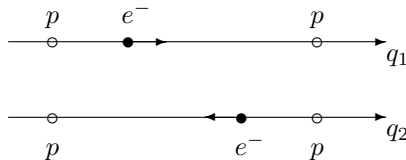

Figure 1: The linearized reaction coordinates q_1 and q_2.

The resulting approximate nonlinear potential $U(q_1, q_2)$ represents two-dimensional potential surface modelling the two-dimensional potential of the original system (two protons and two electrons moving in plane). This surface has the highest points at a half proton-proton distance, and four lowest points at the protons.

Dynamics of two interacting electrons in this two-dimensional potential is due to the ordinary quantum mechanics to which the energy barrier lying between the protons makes specific contribution: two-dimensional quantum tunnel effect of two-electron transitions. The tunnel component of the probability of two-electron transitions becomes essential in the case when the ordinary over-barrier two-electron transitions are suppressed.

Clearly, the tunnel transitions can greatly affect both the character and strength of the chemical bond in diatomic molecule. As a consequence, they can give an essential contribution to electron dynamics in the magnecules consisting of such molecules.

We remark that usually a tunnel effect is considered for the case of one particle in one dimension, which is a simplest case studied to much extent. In this paper, we consider tunnel effect with *dissipation* for the case of *two interacting* particles in *two-dimensional* potential.

The tunnel correlation of electrons is considered on the background of a formed two-dimensional potential of the H-H system which is assumed to be a part of molecular association (magnecule). So, we study temperature effects by introducing interaction of the H-H system with a heat bath.

2 The two-dimensional tunnel model

Details on using of the theory of quantum tunnelling with dissipation [7]-[14] in chemical kinetics can be found in the literature [15]-[17]. Below, we turn to determining of the two-dimensional nonlinear potential for two interacting electrons.

For the case of non-interacting electrons the potential energies of first and second electrons, as functions of the reaction coordinates, q_1 and q_2, are taken in the following form:

$$U(q_1) = \frac{1}{2}\omega^2(q_1 + a)^2\theta(-q_1) + \frac{1}{2}\omega^2(q_1 - a)^2\theta(q_1),$$
$$U(q_2) = \frac{1}{2}\omega^2(q_2 - a)^2\theta(q_2) + \frac{1}{2}\omega^2(q_1 + a)^2\theta(-q_2), \tag{1}$$

where $2a$ is distance between two nuclei in the H-H system ($2a \simeq 1.40$ bohr, for H_2 molecule in vacuum), mass of electron is $m = 1$, and ω is a frequency. In Fig. 2, the potentials $U(q_1)$ and $U(q_2)$ are shown.
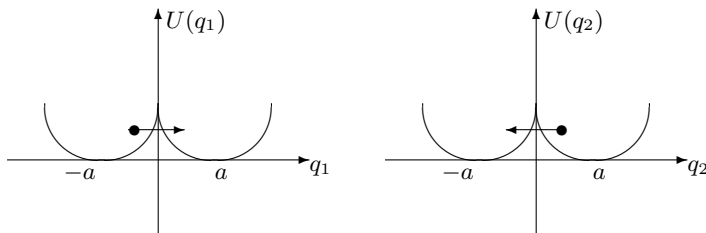

Figure 2: The potentials $U(q_1)$ and $U(q_2)$ as functions of linearized coordinates.

The interaction between the two electrons is taken in the following form:

$$V_{int}(q_1, q_2) = -\frac{1}{2}\alpha(q_1 - q_2)^2, \tag{2}$$

where α is a positive constant, and $(q_1 - q_2)$ is distance between the electrons. Note that V_{int} has the form of *attractive* harmonic potential. Indeed, in the xy-plane the x-component of the mutual distance of two interacting electrons in two dimensions are much bigger than the y-component, $q_0 \gg a$, as shown in Fig. 3

So, the interaction potential can be expanded in small parameter $(q_{1y} - q_{2y})^2/q_0^2$, where q_{1y} and q_{2y} are coordinates of tunneling. The Coulomb repulsion potential between the electrons with electric charges $-e$ is then

$$V_C = \frac{e^2}{\varepsilon_0|q|} = \frac{e^2}{\varepsilon_0\sqrt{q_0^2 + (q_{1y} - q_{2y})^2}}$$
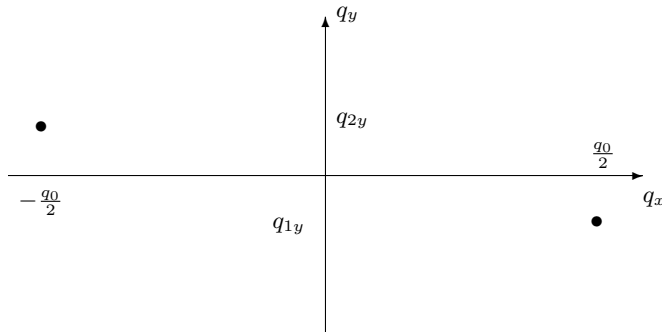
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Figure 3: Transition of two interacting electrons.

$$\simeq \frac{e^2}{\varepsilon_0 q_0} - \frac{e^2}{2\varepsilon_0 q_0} \frac{(q_{1y} - q_{2y})^2}{q_0^2}, \tag{3}$$

where ε_0 is dielectric constant. The negative (second) term in the series expansion (3) is the effective attractive potential (2) so that the constant α is found as

$$\alpha = \frac{e^2}{2\varepsilon_0 q_0}. \tag{4}$$

The first term, $e^2/(\varepsilon_0 q_0)$, is responsible for repulsion between the electrons, and is constant along the reaction coordinates so that it can be absorbed by redefining $U(q_1)$ and $U(q_2)$. Obviously, in general the interaction potential V_C is always repulsive but one can see that only its effective *attractive* part given by Eq. (2), as a function of the reaction coordinates, appears to contribute to the reaction dynamics.

In general, the *attractive* character of the interelectron potential $V_{int}(q_1, q_2)$ resembles the attractive interelectron Hulten potential $V_h(r)$ of the isochemical model [1]. The difference is that V_{int} is formulated in terms of reaction coordinates, has a harmonic form, and naturally arises as an effective long-range potential in the two-dimensional approach. So, V_{int} can be viewed as a potential essentially supporting the isoelectronium in two dimensions.

Thus, the general form of the total potential is a sum of $U(q_1)$, $U(q_1)$, and $V_{int}(q_1, q_2)$,

$$\tilde{U}(q_1, q_2) = U(q_1) + U(q_2) + V_{int}(q_1, q_2),$$

which we redefine as

$$U(q_1, q_2) = \frac{2\tilde{U}(q_1, q_2)}{\omega^2} = (q_1+a)^2\theta(-q_1)\theta(q_1)+(q_2-a)^2\theta(q_2)\theta(-q_2)-\frac{\alpha^*}{2}(q_1-q_2)^2. \tag{5}$$

Here, we have denoted

$$\alpha^* = \frac{2\alpha}{\omega^2},$$

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which is a dimensionless parameter, $\alpha^* < 1$. In Fig. 4 section of the potential (5), at some energy level, is schematically depicted. In Figs. 5 and 6, three-dimensional plots of the potential, at different values of the renormalized inter-electron coupling parameter, $\alpha^* = 0.1$ (weak coupling) and $\alpha^* = 0.5$ (strong coupling), are shown. Here, the ovals corresponding to sections of the potential by a horizontal plane at some energy level are depicted for the reader convenience. We recall that q_1 and q_2 are the reaction coordinates (not coordinates of real configuration space of the system).
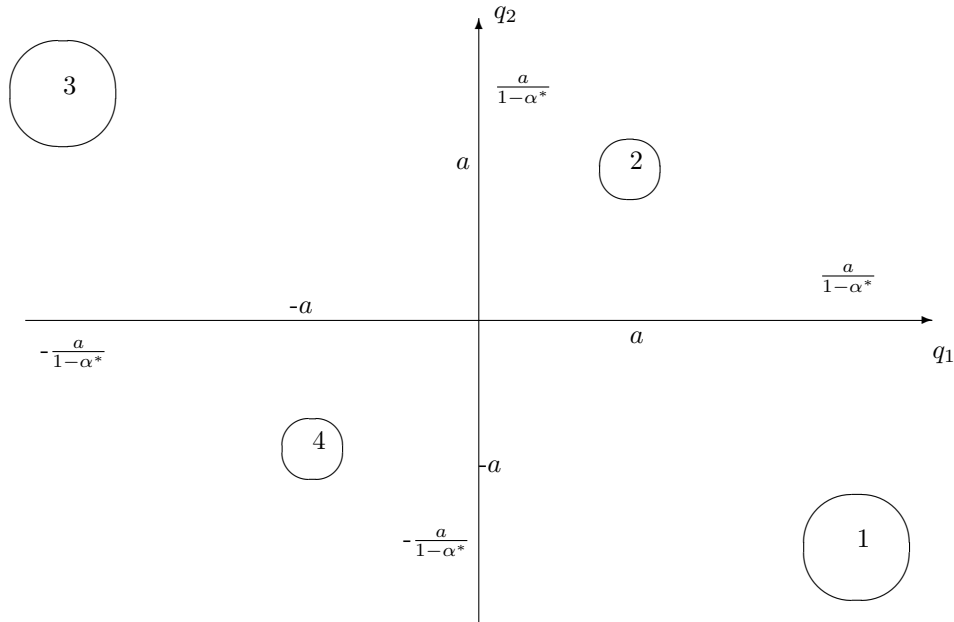

Figure 4: Level lines (1,2,3,4) of the potential $U(q_1, q_2)$; α^* is the renormalized coupling parameter.

3 Probability of the two-electron transition

Since the hydrogen molecule is assumed to be a part of an association of molecules (magnecule), we introduce interaction of the H-H system with external oscillators, a heat bath. Dynamics of the heat bath is defined by the oscillator Hamiltonian

$$H_{hb} = \frac{1}{2}\sum_i (p_i + \omega_i^2 Q_i^2). \tag{6}$$
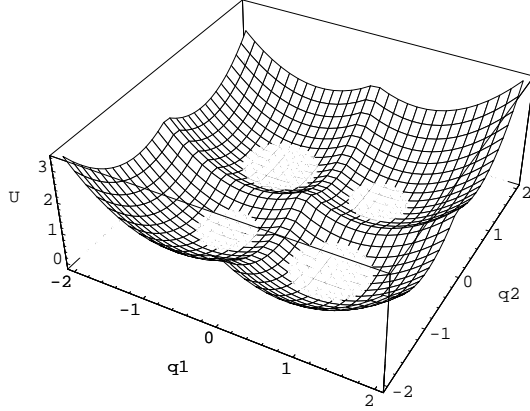
Figure 5: A three-dimensional plot of the potential $U(q_1, q_2)$; $\alpha^* = 0.1$, $a = 0.7$.

We assume that each of the electrons linearly interacts with the oscillators, namely, the interaction potentials are

$$V_{e-hb}^{(1)}(q_i, Q_i) = q_1 \sum_i C_i Q_i, \qquad V_{e-hb}^{(2)}(q_i, Q_i) = q_2 \sum_i C_i Q_i, \qquad (7)$$

The probability of the two-electron transition per unit time is given by

$$\Gamma = 2T \frac{\text{Im}Z}{\text{Re}Z}, \qquad (8)$$

where, as usual, the most important part is the exponential part of Γ. At zero temperature, for the case of metastable levels we have

$$\Gamma = -2\text{Im}E, \qquad E = E_0 - \frac{i}{2}\Gamma, \qquad (9)$$

from which Eq. (8) follows as the generalization to the case of finite temperature T. Indeed,

$$\Gamma = \frac{2\sum_i \exp(-E_{0i}/T)\text{Im}E_i}{\sum_i \exp(-E_{0i}/T)} = \frac{2T\text{Im}\sum_i \exp(-E_i/T)}{\text{Re}\sum_i \exp(-E_i/T)} = 2T\frac{\text{Im}Z}{\text{Re}Z}. \qquad (10)$$

Here, i runs over energy levels of the metastable states, and Z is statistical sum of the total system. The imaginary part of Z corresponds to a decay of the energy levels.

To calculate Γ it is convenient to represent Z as a path integral [7]-[14]

$$Z = \prod_i \int Dq_1 Dq_2 DQ_i \exp[-S(q_1, q_2, Q_i)], \qquad (11)$$
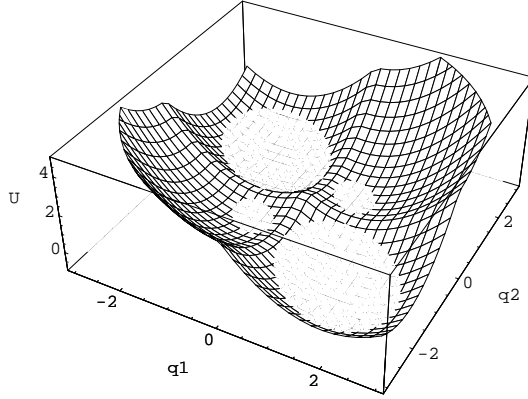
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Figure 6: A three-dimensional plot of the potential $U(q_1, q_2)$; $\alpha^* = 0.5$, $a = 0.7$.

where S is the action of the total system. An imaginary part of Z corresponds to decay of the initial energy levels. One can perform functional integral over Q_i exactly, and obtain

$$Z = \prod_i \int Dq_1 Dq_2 \exp[-S(q_1, q_2)],$$

where

$$S(q_1, q_2) = \int\limits_{-\beta/2}^{\beta/2} d\tau \left\{ \frac{1}{2}\dot{q}_1^2 + \frac{1}{2}\dot{q}_2^2 + V(q_1, q_2)) + \right. \tag{12}$$

$$\left. \frac{1}{2} \int\limits_{-\beta/2}^{\beta/2} d\tau' D(\tau - \tau')(q_1(\tau) + q_2(\tau))(q_1(\tau') + q_2(\tau')) \right\},$$

where

$$D(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} D(\nu_n) e^{i\nu_n \tau} \tag{13}$$

is Green function for the oscillators, with

$$D(\nu_n) = -\sum_i \frac{C_i^2}{\omega_i^2 + \nu_n^2}, \tag{14}$$

$\beta = \hbar/k_B T$ is the inverse temperature parameter, and ν_n is Matsubara's frequency.

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The quasiclassical trajectory minimizing the action S in two-dimensional space is defined by the equations of motion,

$$-\ddot{q}_1+\Omega_0^2 q_1+\alpha_1 q_2+\int_{-\beta/2}^{\beta/2} d\tau' K(\tau-\tau')(q_1(\tau')+q_2(\tau'))+\omega^2 a\theta(-q_1)-\omega^2 a\theta(q_1)=0$$

(15)

and

$$-\ddot{q}_2+\Omega_0^2 q_2+\alpha_1 q_1+\int_{-\beta/2}^{\beta/2} d\tau' K(\tau-\tau')(q_1(\tau')+q_2(\tau'))-\omega^2 a\theta(q_2)+\omega^2 a\theta(-q_2)=0.$$

(16)

Here, the kernel K is defined by

$$K(\tau)=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}\xi_n e^{i\nu_n\tau},$$

(17)

where ξ_n is determined from the redefined Eq. (14), namely,

$$D(\nu_n)=-\sum_i\frac{C_i^2}{\omega_i^2}+\xi_n.$$

(18)

This redefinition has been made in order to extract a zero mode term.

We seek for solutions of the set of Eqs. (15) and (16) in the form of Fourier series expansions in frequencies ν_n,

$$q_1=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}q_n^{(1)}e^{i\nu_n\tau},\qquad q_2=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}q_n^{(2)}e^{i\nu_n\tau}.$$

(19)

The renormalized frequency, Ω_0 and renormalized coupling constant α_1 are defined by

$$\Omega_0^2=\omega^2-\sum_i\frac{C_i^2}{\omega_i^2}-\alpha,\qquad \alpha_1=\alpha-\sum_i\frac{C_i^2}{\omega_i^2}.$$

(20)

Inserting Eqs. (19) into the set of equations (15) and (16), we get the following equations:

$$q_0^{(1)}+q_0^{(2)}=\frac{4\omega^2 a\varepsilon}{\Omega_0^2+\alpha_1},$$

$$q_0^{(1)}-q_0^{(2)}=-\frac{2\omega^2 a\beta}{\Omega_0^2-\alpha_1}+\frac{8\omega^2\tau_0}{\Omega_0^2-\alpha_1},$$

(21)

for the case $n=0$, and

$$q_n^{(1)}+q_n^{(2)}=\frac{4\omega^2 a(\sin\nu_n\tau_1-\sin\nu_n\tau_2)}{\nu_n(\nu_n^2+\Omega_0^2+\alpha_1+2\xi_n)},$$

$$q_n^{(1)}-q_n^{(2)}=\frac{4\omega^2 a(\sin\nu_n\tau_1+\sin\nu_n\tau_2)}{\nu_n(\nu_n^2+\Omega_0^2-\alpha_1)},$$

(22)

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for the case $n \neq 0$. Here, we have denoted

$$\varepsilon = \tau_1 - \tau_2, \qquad \tau_0 = \frac{1}{2}(\tau_1 + \tau_2), \tag{23}$$

and τ_1 and τ_2 are the values of time τ at which first and second electron, respectively, passes through the maximum of the potential barrier. Namely, τ_1 and τ_2 are determined from the following equations:

$$q_1(\tau_1) = 0, \qquad q_2(\tau_2) = 0. \tag{24}$$

These two equations can be used to change arguments of the above θ-functions. As the result, the θ-functions become depending on the time values τ_1 and τ_2, instead of the coordinates q_1 and q_2, and the Eqs. (15) and (16) take a *linear* form. Note that, quasiclassically, the time values $\pm\tau_1$ and $\pm\tau_2$ correspond to the times when first and second electron, respectively, are at the top of the potential barrier.

Inserting the trajectories defined by Eqs. (19), (21), and (22) into Eqs. (12), we obtain the quasiclassical (instanton) action in the form

$$S = \frac{8\omega^4 a^3 \tau_0}{\Omega_0^2 - \alpha_1} - \frac{4\omega^4 a^2 \varepsilon^2}{\beta(\Omega_0^2 + \alpha_1)} - \frac{16\omega^4 a^2 \tau_0^2}{\beta(\Omega_0^2 - \alpha_1)}$$

$$- \frac{32\omega^4 a^2}{\beta} \sum_{n=1}^{\infty} \left[\frac{\sin^2 \nu_n \tau_0 + \cos^2 \nu_n \varepsilon/2}{\nu_n^2(\nu_n^2 + \Omega_0^2 - \alpha_1)} + \frac{\sin^2 \nu_n \varepsilon/2 + \cos^2 \nu_n \tau_0}{\nu_n^2(\nu_n^2 + \Omega_0^2 + \alpha_1 + 2\xi_n)} \right]. \tag{25}$$

The quasiclassical action S describes probability of a two-particle tunnel transition per unit time, with an exponential accuracy. For the case of *antiparallel* motion of the electrons, the above instanton action S, at $\xi_n = 0$ (no heat bath), takes the form

$$S = -2\omega a^2 \left\{ |\varepsilon|(1 - \frac{1}{1 - \alpha^*}) + \frac{\sinh(|\varepsilon|\sqrt{1 - \alpha^*})}{(1 - \alpha^*)^{3/2}} - \sinh|\varepsilon| \right.$$

$$+ \frac{\cosh(|\varepsilon|\sqrt{1 - \alpha^*}) + 1}{(1 - \alpha^*)^{3/2}} \cdot \frac{\cosh((\beta^* - \tau)\sqrt{1 - \alpha^*}) - \cosh(\beta^*\sqrt{1 - \alpha^*})}{\sinh(\beta^*\sqrt{1 - \alpha^*})} \tag{26}$$

$$\left. + \frac{(\cosh\varepsilon - 1)(\cosh(\beta^* - \tau) + \cosh\beta^*)}{\sinh\beta^*} \right\}.$$

Here, we have denoted

$$\alpha^* = \frac{2\alpha}{\omega^2}, \quad \beta^* = \frac{\beta\omega}{2}, \quad \varepsilon = (\tau_1 - \tau_2)\omega, \quad \tau = (\tau_1 + \tau_2)\omega,$$

and the parameters ε and τ obey the following set of equations:

$$-\sinh\varepsilon[\coth\beta^* + \cosh\tau \coth\beta^* - \sinh\tau] + \frac{1}{1 - \alpha^*}\sinh(\varepsilon\sqrt{1 - \alpha^*})[\coth(\beta^*\sqrt{1 - \alpha^*})$$

$$- \cosh(\tau\sqrt{1 - \alpha^*})\coth(\beta^*\sqrt{1 - \alpha^*}) + \sinh(\tau\sqrt{1 - \alpha^*})] = 0,$$

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$$-1 - \frac{1}{1-\alpha^*} + (\cosh\varepsilon - 1)(\sinh\tau\coth\beta^* - \cosh\tau) + \cosh\varepsilon \qquad (27)$$

$$+\frac{1}{1-\alpha^*}\left\{[\cosh(\varepsilon\sqrt{1-\alpha^*}) + 1][\sinh(\tau\sqrt{1-\alpha^*})\coth(\beta^*\sqrt{1-\alpha^*})\right.$$

$$\left. - \cosh(\varepsilon\sqrt{1-\alpha^*})] - \cosh(\varepsilon\sqrt{1-\alpha^*})\right\}.$$

Solution of the Eq. (27) is

$$\varepsilon = (\tau_1 - \tau_2)\omega = 0, \quad \alpha < \frac{1}{2}\omega^2, \quad \forall\beta, \qquad (28)$$

$$\tau_1 = \tau_2 = \frac{\tau}{2\omega} = \frac{\beta}{4}.$$

At low temperatures, $\omega\beta \gg 1$, we then have

$$e^{-\tau\sqrt{1-\alpha^*}} \simeq \alpha^*(1-\alpha^*)^\gamma\left\{1 - (1-\alpha^*)^\gamma(\frac{\alpha^*}{1-\sqrt{1-\alpha^*}} - 1)\right\}^{-1}, \qquad (29)$$

$$e^\varepsilon \simeq \frac{1}{1-\alpha^*}\frac{(\alpha^* - e^{-\tau\sqrt{1-\alpha^*}})}{e^{-\tau\sqrt{1-\alpha^*}}},$$

where

$$\gamma = \frac{\sqrt{1-\alpha^*}}{1-\sqrt{1-\alpha^*}}.$$

The approximate solution (29) is valid at

$$\frac{1}{4} < \frac{2\alpha}{\omega^2} < 1$$

and $\beta > \beta_c$, where the critical temperature is

$$\beta_c = -\frac{1}{\omega\sqrt{1-\alpha^*}}\ln\left\{\frac{\alpha^*(1-\alpha^*)^\gamma}{1 - (1-\alpha^*)^\gamma(\frac{\alpha^*}{1-\sqrt{1-\alpha^*}} - 1)}\right\}. \qquad (30)$$

As one can see, a characteristic critical temperature, $\beta_c = \hbar/(k_B T_c)$, of the system arises and it depends mainly on the value of the interelectron coupling parameter α^*.

At $\varepsilon = 0$, for the case of symmetric two-dimensional potential the solution (28) yields

$$S = \frac{4\omega a^2}{(1-\alpha^*)^{3/2}}\tanh\frac{\omega\sqrt{1-\alpha^*}}{4}\beta \qquad (31)$$

At $\varepsilon \neq 0$, the resulting expression for the action S is cumbersome so that we do not represent it here. However, it can be shown that, at $\beta > \beta_c$,

$$S_{(\varepsilon=0)} < S_{(\varepsilon\neq 0)} \qquad (32)$$

so that the value $\varepsilon = 0$ minimizes the action. As the result, the values $\varepsilon \neq 0$ correspond to splitted trajectories which appear to be unstable; see Fig. 7.
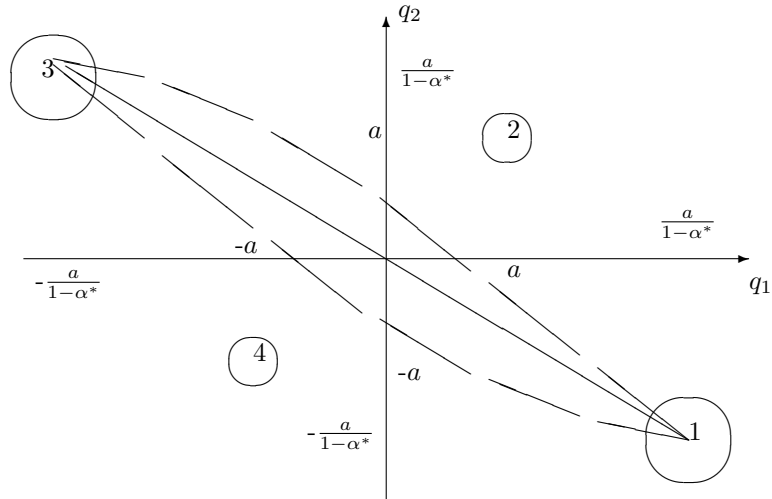
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Figure 7: A schematic picture of the tunnel trajectories at $\varepsilon = 0$ (solid line) and at $\varepsilon \neq 0$ (dash lines).

The instanton solution with $\varepsilon = 0$ corresponds to a strongly correlated antiparallel motion of the two tunnelling electrons. Namely, the two electrons *simultaneously* pass the tops of the potentials. This correlation of the two electrons depends on value of the electron-electron (attraction) coupling constant α^* naturally arising within the framework of the model.

Such a correlation resembles the isoelectronium correlation introduced in ref. [1] where the correlation is governed by the short-range attractive electron-electron (Hulten) potential.

4   Conclusions

At $\beta > \beta_c$, the basic single trajectory is splitted to two degenerated trajectories as shown in Fig. 7 (dash lines). In contrast to the case of parallel transition, this splitting (bifurcation) takes place at any values of the parameters of the potential $U(q_1, q_2)$. Also, at $\beta > \beta_c$, we have $S_{(\varepsilon \neq 0)} > S_{(\varepsilon = 0)}$ so that the trajectory with $\varepsilon = 0$ make a leading contribution. At $\beta < \beta_c$, the two degenerated trajectories become a single basic trajectory characterized by $q_1 = -q_2$.

We see that in contrast to the case of one tunnelling particle at which only one trajectory (instanton) is realized, in the case of two tunnelling particles in the two-dimensional potential the situation is more complicated. As we have shown in general there are two types of trajectories, a single basic trajectory and splitted degenerated trajectory, both making contribution to the tunnel effect. The splitted trajectory is characterized by nonsimultaneous ($\tau_1 \neq \tau_2$) transition of the two particles through the top points of the barriers, so that the time

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correlation between the particles' motion is lost. It is highly remarkable that in the case of symmetric two-dimensional potential such splitted trajectories in both the cases of parallel and antiparallel motion of the two particles are unstable. At small α^* and $\beta < \beta_c$, the splitted degenerated trajectory is not realized so that there is only the basic single trajectory $(q_1 = -q_2)$. This trajectory is characterized by simultaneous $(\tau_1 = \tau_2)$ transition of the two particles through the top points of the barriers, so that there is a strong correlation between the particles' motion.

The chosen form of the interelectron interaction does not affect the motion of the center of mass $(q_1 = q_2)$. So, for the parallel transition along the basic trajectory $(q_1 = q_2)$ the quasiclassical (instanton) action does not depend on the coupling parameter. In this case,

$$S = 4\omega a^2 \tanh \frac{\omega\beta}{4}. \tag{33}$$

Since the motion with maximal value of the relative coordinate, i.e. $q_1 = -q_2$, is energetically preferable it becomes clear why for the parallel transition along the degenerate trajectory the action decreases with increase of the coupling parameter while for the antiparallel transition along the degenerate trajectory the action increases with increase of the coupling parameter.

Thus, in the case of antiparallel tunnel transition of two interacting electrons the preferable trajectory is a single basic one which is characterized by strong (isoelectronium-like) correlation between the electrons $(\tau_1 = \tau_2)$. Here, the uncorrelated motion ("decay" of the isoelectronium-like state) is suppressed because it makes bigger contribution to the instanton action.

As to a heat bath, it appears to be possible to study analytically the effect of, for example, one local mode ω_L to the two-electron transition probability. The result is that the heat bath does not change the qualitative conclusions made above. Temperature dependence of the action S for the antiparallel motion case $(\varepsilon = 0)$ at two different values of the renormalized coupling parameter, $\alpha^* = 0.1$ and $\alpha^* = 0.5$, is shown in Fig. 8
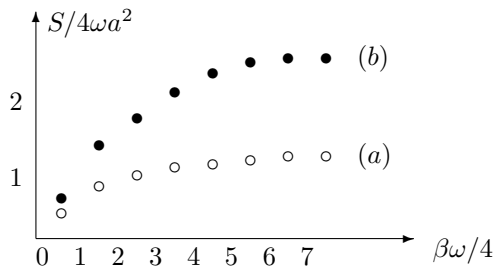

Figure 8: The action $(\varepsilon = 0$, antiparallel motion) as a function of inverse temperature $\beta = \hbar/k_B T$; (a) $\alpha^* = 0.1$, (b) $\alpha^* = 0.5$.

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In this paper, we used the assumption that dynamics of the two interacting electrons can be taken approximately as a two-dimensional. This is due to the viewpoint [1] that strong external electromagnetic field confines, to some degree, the usual three-dimensional motion of the electrons so that consideration of *two-dimensional* effects in molecules, as well as in associations of molecules, becomes highly important. The main two-dimensional effect, namely, the two-electron tunnel effect with dissipation, for the antiparallel transition, has been studied in this paper.

Within the one-instanton linearized reaction coordinates approximation and using an ideal gas of instanton-antiinstanton pairs ($\beta\omega \ll 16U_{barrier}/\omega$), we have shown that the *correlated isoelectronium-like motion* of the two tunnelling electrons in two-dimensional H-H system with dissipation takes place and appears to be the *most stable* configuration. Thus, the tunnel correlations can be viewed as a mechanism supporting the isoelectronium configurations introduced by Santilli and Shillady.

Detailed study of the effect of strong external electromagnetic field, as well as the implications of the results of this paper, will be made in a subsequent paper.

Application of the formalism presented in this paper to carbon monoxide molecule CO is of much interest as well. Study of the transition rates, $\Gamma = e^{-S}$, for the case of association of molecules (intramolecular tunnelling) could be important in investigating electron charge distribution and bonds in magnecules.

Acknowledgment

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