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Research Article

Quantum Tunneling in a Time-Periodic Double-Well Potential as a Driver of LENR

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Abstract

At sufficiently low temperatures, the reaction rates in solids are controlled *by quantum* rather than by thermal fluctuations. We solve the Schrödinger equation for a Gaussian wave packet in a *nonstationary* harmonic oscillator and derive simple analytical expressions for the increase of its mean energy and dispersion with time induced by *time-periodic* modulation. Applying these expressions to the modified Kramers theory, we demonstrate a strong increase of the rate of escape out of a time-periodic potential well at a *constant height* of the potential barrier, when the driving frequency of the well *position* equals its eigenfrequency, or when the driving frequency of the well *width* exceeds its eigenfrequency by a factor of ~ 2. Physical realization of the time-periodic driving modes can be induced by *localized anharmonic vibrations* (LAVs), a.k.a. *discrete breathers*, in which the amplitude of atomic oscillations greatly exceeds the amplitude of *zero-point oscillations*. At low temperatures LAVs can be excited by external triggering (such as irradiation by fast particles or by a laser), which can result in strong catalytic effects due to amplification of the Kramers rate. Numerical solution of Schrodinger equation for time-periodic double well potential is obtained, which agrees qualitatively with modified Kramers rate theory. Application of the present theory to low-energy nuclear reactions is discussed.

Keywords: Localized anharmonic vibrations in solids; zero-point oscillations; Kramers escape rate; chemical and nuclear catalysis

1. Introduction

Theory of escape rates over a potential barrier, first proposed by Kramers in 1940 [1] is an archetype model for chemical reactions, and it has many applications in chemistry kinetics, diffusion in solids, nucleation and other phenomena [2]. The model considers a Brownian particle moving in a symmetric double-well potential *U(x)* (Fig. 1a). The position of the particle represents the (free) energy of a system including the 'reaction site'. The particle is subject to fluctuational

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forces that cause transitions between the neighboring potential wells at a rate given by the celebrated Kramers rate:

$$R_K = \frac{\omega_0}{2\pi} \exp\left[-E_0/D\left(T, E_{ZPO}\right)\right], \omega_0^2 = U''\left(x_m\right)/m \tag{1}$$

where T is the temperature, E_{ZPO} is the energy of *zero-point oscillations,* $\omega_0/2\pi$ is the natural attempt frequency, ω_0 being the angular frequency of the harmonic oscillator, E_0 is the height of the potential barrier separating the two stable states, corresponding to the reactants and products, and $D(T, E_{ZPO})$ is the strength of the Gaussian white noise induced by thermal and quantum fluctuations. In a general case, $D(T, E_{ZPO})$ is given by [3]

$$D\left(T, E_{ZPO}\right) = E_{ZPO} \coth\left(E_{ZPO}/k_B T\right) \approx \begin{cases} E_{ZPO},\ T << E_{ZPO}/k_B \\ k_B T,\ T >> E_{ZPO}/k_B \end{cases},\ E_{ZPO} = \frac{\hbar\omega_0}{2}, \tag{2}$$

where, $\hbar$ is the Plank constant, k_b is the Boltzmann constant. It is quite natural to use the noise strength (2) in the calculation of the Kramers escape rate of the potential well, which results in a non-vanishing escape rate even if $T \to 0$ [3]. At sufficiently high temperatures, the noise strength becomes equal to $k_B T$, and the Kramers rate (1) provides a theoretical basis for the Arrhenius law, whereas at low temperatures, significant deviations from this low are predicted due to quantum effects.

The original Kramers model assumes a stationary potential landscape for a Brownian particle, which can be questioned in the situations where the reaction site is in the vicinity of *localized anharmonic vibrations* (LAVs) of atoms known also as 'discrete breathers' [4]–[8] or 'intrinsic localized modes' [9], [10], a sub-class of LAVs arising in regular crystals. In contrast to phonons, LAVs are large amplitude and *periodic in time*, and therefore they can induce a time-periodic modulation (driving) of the reaction potential landscape. It can involve the time-periodic oscillation of the potential barrier *height* and *shape*. The former case was analyzed by Dubinko et al. [4], [5] who showed that if the driving frequency Ω is about or lower than the natural frequency, $\Omega \leq \omega_0$, one can use an 'adiabatic' approximation (Fig. 1a). In this case, the reaction rate $\langle R_K \rangle$, averaged over times exceeding the driving period, has been shown to increase with respect to the ground value R_K according to the following expression:

$$\langle R_K \rangle \approx R_K \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} \exp\left(\frac{V\cos\left(\Omega t\right)}{k_b T}\right) dt = R_K I_0\left(\frac{V}{k_b T}\right), \tag{3}$$

where the amplification factor can be approximated by the zero order, modified Bessel function of the first kind $I_0\left(x\right)$ with the argument determined by the ratio of the driving amplitude V to the temperature, and it weakly depends on the driving frequency or the barrier height [5].

Figure 1b shows that the LAV-induced periodic driving of the barrier height can amplify the average reaction rate very strongly if the ratio $V/k_B T$ is high enough. That is expected to be the case in the reaction site interacting with a nearby LAV, since molecular dynamics simulations using realistic interatomic potentials of various materials show that a typical deviation of the potential energy of atoms within a LAV is of the order of several fractions of electron-volts [7]–[10].

In a general case with account of quantum effects, the escape rate (3) can be written as follows:

$$\langle R_K \rangle \approx R_K \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} \exp\left(\frac{V\cos\left(\Omega t\right)}{D\left(T, E_{ZPO}\right)}\right) dt = R_K I_0\left(\frac{V}{D\left(T, E_{ZPO}\right)}\right), \tag{3a}$$

It should be noted that numerous authors have worked a lot on problems of escape of particles out of potential wells with a barrier *height* driven by noise and periodic modulations. The list of relevant publications includes Refs. [8], [13], [15], [25], [37], [38], [39], [48], [53] available at https://www.physik.uni-bielefeld.de/∼ reimann/Publ.html.

In contrast to these papers, the present paper considers effects due to the periodic driving of the potential landscape *shape*, which are not taken into account by the amplification factor (3a) that is sensitive only to the modulation of

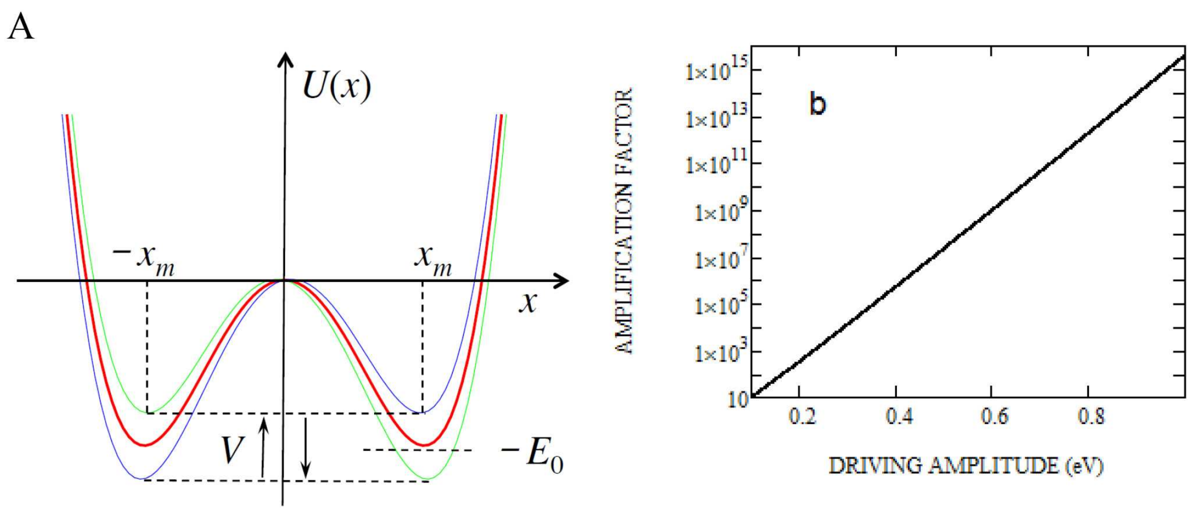

Figure 1. (a) Sketch of the double-well potential $U(x) = (1/4)bx^4 - (1/2)ax^2$ (red curve) The minima are located at $\pm x_m$, where $x_m = (a/b)^{1/2}$. These are stable states before and after the reaction, separated by a potential 'barrier' with the height $E_0 = a^2/4b$ changing periodically within the V band. The green and blue curves represent the two maximally tilted energy landscapes. (b) Amplification factor for the escape rate of a thermalized Brownian particle at $T = 300$ K from a periodically driven potential well vs. the driving amplitude, according to eq. (3) [5].

the barrier *height*. Driving of the potential landscape shape (without changing the barrier height), can result in the time-periodic modulation (i) of the curvature and (ii) of the positions of the potential minima. In sections 2 and 3, we will consider the corresponding effects separately, since the quantum dynamics of the oscillating wave functions in these limiting cases are qualitatively different. In section 4, the modified Kramers escape rate will be derived taking into account time-periodic driving of the potential shape in these two limiting cases. In section 5, a numerical solution of the Schrödinger equation for a particle in a time-periodic double-well potential is presented, which describes the quantum tunneling through potential barrier at super low temperature when thermal effects are negligible. In section 6, the present results are compared with a theory of resonance tunneling, a.k.a. *Euclidean resonance*, and in section 7, the results are summarized, and outstanding problems are discussed.

2. Solution of the Schrödinger Equation for a Harmonic Oscillator With Time-Periodic Eigenfrequency

The initial state of the system (reactants) can be described by a wave function of the Gaussian form placed near the first energy minimum that can be approximated by a parabolic potential [11]:

$$\psi\left(x_0, t_0 = 0\right) = \frac{1}{\sqrt[4]{\pi\xi^2}} \exp\left(-\frac{x_0^2}{2\xi^2}\right), \xi = \sqrt{\hbar/m\omega_0}, \tag{4}$$

Time-periodic modulation of the potential curvature will result in time-periodic modulation of the harmonic oscillator eigenfrequency. A harmonic oscillator with time-dependent frequency for a particle with the mass *m* obeys the nonstationary Schrödinger equation of the form:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{m\omega^2\left(t\right)}{2}x^2\psi. \tag{5}$$

The solution of the equation (5) can be expressed using the Green's function (or the propagator) and the following initial condition [12]:

$$\psi(x,t)=\int_{-\infty}^{+\infty}dx_0 G(x,t;x_0,t_0)\,\psi(x_0,t_0)\,,\ \lim_{t\to\tau+0}G(x,t;x_0,t_0)=\delta(x-x_0) \tag{6}$$

The expression for the propagator has the form [12]:

$$G(x,t;x_0,t_0)=\sqrt{\frac{m}{2\pi i\hbar Z}}\exp(\theta_G)\,,\theta_G=\frac{im}{2\hbar Z}\left[\frac{dZ}{dt}x^2-2xx_0+Yx_0^2\right], \tag{7}$$

where the functions $Y=Y(t)$, $Z=Z(t)$ are defined by the following equations and initial conditions that can be derived from the condition (7):

$$\frac{d^2Y}{dt^2}+\omega^2(t)\,Y=0,\frac{dY(t_0)}{dt}=0,Y(t_0)=1, \tag{8}$$

$$\frac{d^2Z}{dt^2}+\omega^2(t)\,Z=0,\frac{dZ(t_0)}{dt}=1,Z(t_0)=0, \tag{9}$$

$$Y(t)\frac{dZ(t)}{dt}-Z(t)\frac{dY(t)}{dt}=1. \tag{10}$$

Then the expression for the wave function for the arbitrary moment of time $\forall t>t_0=0$ can be obtained in the following form:

$$\psi(x,t)=\frac{1}{\sqrt[4]{\pi\xi^2}}\frac{\exp(\theta_\psi)}{\sqrt{Y+i\omega_0 Z}},\theta_\psi=-\frac{x^2}{2\xi^2}\frac{1}{i\omega_0 Z}\left[\frac{dZ}{dt}-\frac{1}{Y+i\omega_0 Z}\right] \tag{11}$$

The probability density of finding the particle at *(x, t)* is given by the square of the wave function:

$$|\psi(x,t)|^2=\frac{B(t)}{\xi\sqrt{\pi}}\exp\left\{-\frac{x^2}{\xi^2}B^2(t)\right\},B(t)=\frac{1}{\sqrt{Y^2(t)+\omega_0^2Z^2(t)}}, \tag{12}$$

while dispersions of coordinate and momentum are given by:

$$\sigma_x(t)=\left\langle(x-\langle x\rangle)^2\right\rangle=\frac{\hbar}{2m\omega_0}\left[Y^2+\omega_0^2Z^2\right], \tag{13}$$

$$\sigma_p(t)=\left\langle(p-\langle p\rangle)^2\right\rangle=\frac{\hbar m\omega_0}{2}\left[\left(\frac{1}{\omega_0}\frac{dY}{dt}\right)^2+\left(\frac{dZ}{dt}\right)^2\right], \tag{14}$$

At *constant eigenfrequency:* $\omega(t)=\omega_0=const$, the x and p dispersions are constant as well as the mean oscillator energy $\langle E\rangle=\frac{1}{2m}\sigma_p+\frac{m\omega^2}{2}\sigma_x$, i.e. the zero point oscillator energy E_{ZPO} and the maximum mean square displacement from the equilibrium position, i.e. the ZPO amplitude A_{ZPO}:

$$\sigma_x=\frac{\hbar}{2m\omega_0},\quad \sigma_p=\frac{\hbar m\omega_0}{2},\langle E\rangle=E_{ZPO}=\frac{\hbar\omega_0}{2},A_{ZPO}=\sqrt{\frac{\hbar}{2m\omega_0}}. \tag{15}$$

In a special case of *parametric time-periodic modulation* of the eigenfrequency with the driving frequency $\Omega=2\omega_0$, the equations (8), (9) are the Mathieu equations [12]:

$$\ddot{x}+\omega_0^2\left[1-g\cos(2\omega_0 t)\right]x=0 \tag{16}$$

which solution can be written explicitly in the first approximation to the small modulation amplitude $g << 1$, when one obtains the first approximations for dispersion of the coordinate and momentum, which describe fully the evolution of the Gaussian wave packet in time:

$$\sigma_x(t) = \frac{\hbar}{2m\omega_0}\cosh\left(\frac{g\omega_0 t}{2}\right)\left[1+\tanh\left(\frac{g\omega_0 t}{2}\right)\sin(2\omega_0 t)\right], \tag{17}$$

$$\sigma_p(t) = \frac{\hbar m\omega_0}{2}\cosh\left(\frac{g\omega_0 t}{2}\right)\left[1-\tanh\left(\frac{g\omega_0 t}{2}\right)\sin(2\omega_0 t)\right], \tag{18}$$

In particular, the ZPO mean energy and amplitude increase with time as:

$$E_{ZPO}(t) = \frac{\hbar\omega_0}{2}\cosh\frac{g\omega_0 t}{2}, A_{ZPO}(t) = \sqrt{\frac{\hbar}{2m\omega_0}\cosh\frac{g\omega_0 t}{2}}. \tag{19}$$

Fig. 2a shows that the parametric modulation of a parabolic potential well increases the dispersion of the wave packet with increasing number of oscillation periods, $N = \omega_0 t/2\pi$, which results in rapidly increasing probability to find the oscillating particle far beyond the characteristic length of the stationary well $\xi = A_{ZPO}(0)\sqrt{2}$. Another significant effect of the modulation is the *continuous* increase of the ZPO energy (Fig. 2b), which is different from the *quantum* energy increase to the higher oscillation levels: $E_n = \hbar\omega_0(1/2+n)$, when the probability density becomes concentrated at the classical "turning points". In contrast to that, we clearly deal with the ground (zero-point) state, in which the probability density is concentrated at the origin, which means that the particle spends most of its time at the bottom of the potential well, whereas the dispersion of its position and momentum increases along with its zero-point energy due to the parametric modulation.

Although an analytical solution of the problem for an arbitrary modulation frequency cannot be obtained, numerical analysis shows that the maximum effect is produced by a parametric modulation at $\Omega = 2\omega_0$. In the following section, we will consider another type of the harmonic well modulation that conserves its eigenfrequency but changes the position of the well minimum.

3. Solution of the Schrödinger Equation for a Harmonic Oscillator With Time-Periodic Position of the Potential Minimum

In this case, the Schrödinger equation takes the following form:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + \frac{m\omega_0^2}{2}[x - X(t)]^2\psi(x,t). \tag{20}$$

Its solution is given by eq. (6) with the Green function of the form [13]

$$G(x,t;x_0,t_0=0) = \sqrt{\frac{m\omega_0}{2\pi i\hbar\sin(\omega_0 t)}}\exp\{\theta(x,t;x_0,0)\}, \tag{21}$$

$$\begin{aligned}\theta(x,t;x_0,0) = &-\frac{im\omega_0^2}{2\hbar}\int_0^t d\tau X^2(\tau) + \frac{i\hbar}{2m}\int_0^t d\tau a^2(\tau) + a(t)x \\ &+ \frac{m\omega_0}{\hbar}\frac{[x+s(t)\exp(i\omega_0 t)]^2}{1-\exp(i2\omega_0 t)} - \frac{m\omega_0}{2\hbar}\left(x^2 - x_0^2\right),\end{aligned} \tag{22}$$

$$a(t) = \frac{im\omega_0^2}{\hbar}\int_0^t d\tau X(\tau)\exp[i\omega_0(\tau - t)], s(t) = -x_0 + \frac{i\hbar}{m}\int_0^t d\tau a(\tau)\exp(-i\omega_0\tau), \tag{23}$$

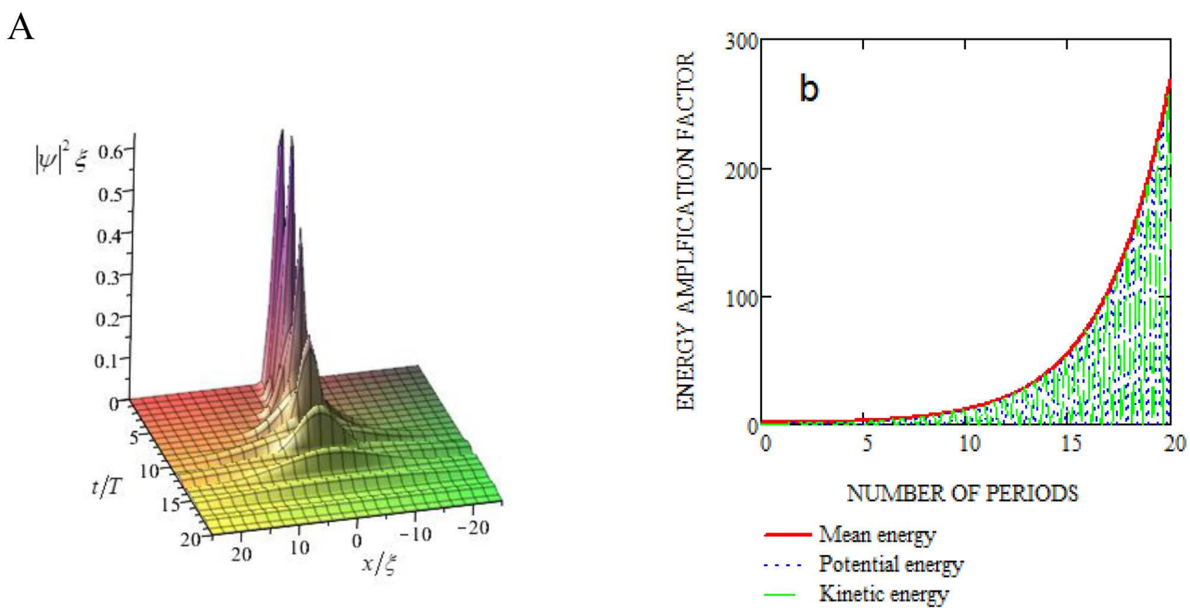

Figure 2. (a) Localization probability distribution vs. the number of oscillation periods $N = \omega_0 t/2\pi = t/T$ in the parametric regime $\Omega = 2\omega_0$ at $g = 0.1$ according to eq. (12). (b) Ratio of the zero-point energy to its stationary value in the parametric regime at $g = 0.1$ according to eq. (19).

Then for the initial wave packet given by eq. (4), an expression for the wave function for the arbitrary moment of time $\forall t > t_0 = 0$ can be obtained in the following form:

$$\psi(x,t) = i\sqrt[4]{\frac{m\omega_0}{\pi\hbar}}\exp\left\{-\frac{m\omega_0}{2\hbar}\left[x^2 + 2x\omega_0\int_0^t d\tau X(\tau)\sin\omega_0(\tau - t) - F(t)\right] - iJ(x,t)\right\}, \tag{24}$$

$$F(t) = 2\omega_0^3\int_0^t d\tau\left(\int_0^\tau d\tau' X(\tau')\sin\omega_0(\tau' - \tau)\right)\cdot\left(\int_0^\tau d\tau'' X(\tau'')\cos\omega_0(\tau'' - \tau)\right), \tag{25}$$

$$J(x,t) = \frac{m\omega_0^2}{2\hbar}\left\{\int_0^t d\tau U^2(\tau) + \frac{\hbar t}{m\omega_0} - \omega_0^2 I_1(t) - 2xI_2(t)\right\}, \tag{26}$$

$$I_1(t) = \int_0^t d\tau\left[\left(\int_0^\tau d\tau' U(\tau')\sin\omega_0(\tau' - \tau)\right)^2 - \left(\int_0^\tau d\tau' U(\tau')\cos\omega_0(\tau' - \tau)\right)^2\right], \tag{27}$$

$$I_2(t) = \int_0^t d\tau U(\tau)\cos\omega_0(\tau - t), \tag{28}$$

Accordingly, the probability density distribution is given by:

$$|\psi(x,t)|^2 = \sqrt{\frac{m\omega_0}{\pi\hbar}}\exp\left\{-\frac{m\omega_0}{\hbar}\left[x^2 + 2x\omega_0\int_0^t d\tau X(\tau)\sin\omega_0(\tau - t) - F(t)\right]\right\}, \tag{29}$$

Time-periodic modulation has a maximum effect on the oscillator when the modulation frequency equals the eigenfrequency, when one has a wave packet concentrated around a ‘centre of mass’ with a coordinate $\lambda(t)$ that oscillates

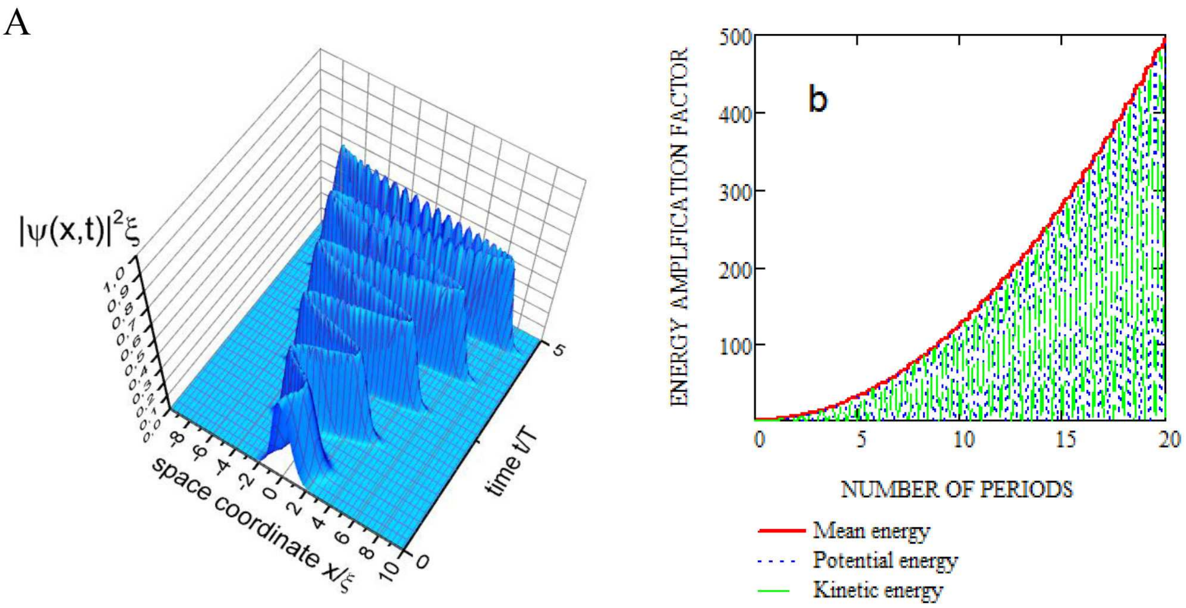

Figure 3. (a) Localization probability distribution by eq. (31) and (b) ratio of the mean energy to its stationary value by eq. (32) vs. the number of oscillation periods $N = \omega_0 t/2\pi = t/T$ at $\Omega = \omega_0, g_A = 0.5$.

with amplitude linearly increasing in time (Fig. 3a) and the mean energy that increases as t^2(Fig. 3b):

$$X\left(t\right) = g_A A_{ZPO} \sin\left(\omega_0 t\right), \psi\left(x,t\right) = i\sqrt[4]{\frac{m\omega_0}{\pi\hbar}} \exp\left\{-\frac{m\omega_0}{2\hbar}\left[x+\lambda\left(t\right)\right]^2 - iJ(x,t)\right\}, \tag{30}$$

$$\lambda\left(t\right) = \frac{g_A A_{ZPO}}{2}\omega_0 t\left(\cos\omega_0 t - \frac{\sin\omega_0 t}{\omega_0 t}\right), \quad g_A\text{- the modulation factor,} \tag{31}$$

$$\langle E\rangle = \frac{\hbar\omega_0}{2} + \frac{\left(g_A A_{ZPO}\right)^2 m\omega_0^2}{8}\left[\omega_0^2 t^2 + \omega_0 t\sin 2\omega_0 t + \sin^2\omega_0 t\right], A_{ZPO} = \sqrt{\frac{\hbar}{2m\omega_0}}, \tag{32}$$

The driving of the well position does not affect the wave packet dispersions in the p and x space that remain constant:

$$\sigma_x = \frac{\hbar}{2m\omega_0}, \quad \sigma_p = \frac{\hbar m\omega_0}{2}, A_{ZPO} = \sqrt{\frac{\hbar}{2m\omega_0}}, \tag{33}$$

which means that the wave packet deviates from the well bottom as a whole and the uncertainty of the particle position does not increase with time, in a marked contrast to the well eigenfrequency modulation considered in the previous section (Fig. 2).

In the following section, we will discuss the applications of the above analysis of quantum dynamics of non-stationary harmonic oscillators to the modified Kramers rate of escape out of a potential well taking into account the time-periodic driving.

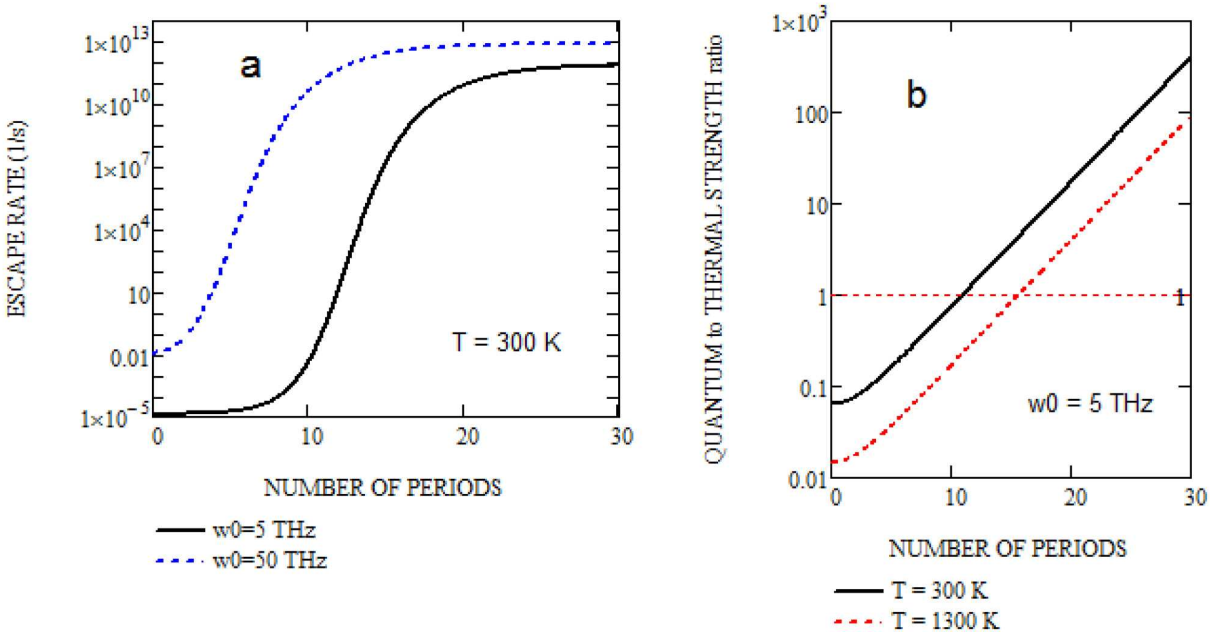

Figure 4. (a) Escape rate from a well of a depth $E_0 = 1$ eV, eigenfrequency 5 THz (solid curve) and 50 THz (dashed curve) at 300 K vs. the number of oscillation periods in the parametric regime $\Omega = 2\omega_0$ at $g = 0.1$. (b) Increase of the quantum to thermal noise strength, E_{ZPO}/k_bT, with increasing number of oscillation periods at different temperatures 300 K and 1300 K.

4. Modified Kramers Rate

It is known that the tunnel effect is inherently related to the operation of the uncertainty principle similar to the ZPO energy, the difference being that for the tunnel effect the coordinate is one in which the potential energy passes through a maximum, whereas for ZPO energy it passes through a minimum [14]. This thesis is well illustrated by the Kramers model of escape out of a potential well modified with account of ZPO energy [3], according to which the strength of the Gaussian white noise is determined by a synergetic action of *thermal* and *quantum* fluctuations, as described by eq. (2).

In Section 2, we demonstrated that the parametric modulation of the well eigenfrequency increases the *strength of quantum fluctuations* manifested by the wave packet broadening and by the increase of its ZPO energy given by eq. (19). Substituting eq. (19) into eqs. (1), (2) one can evaluate the rate of escape from a well with given parameters, which will increase with increasing number of oscillation periods, as illustrated in Fig. 4a for a potential well with a depth of 1 eV, and with eigenfrequency ranging from 5 to 50 THz.

Such a well depth is typical for many chemical reactions, and the lower frequency limit of ~5 THz is typical for the oscillation frequencies of metal (heavy) atoms while 50 THz is closer to the frequencies of light atoms such as hydrogen etc. embedded in a crystal lattice of heavier atoms. A characteristic example is hydrogen or deuterium atoms in metal hydrides/deuterides, such as NiH or PdD, in the vicinity of *gap breathers*- a subclass of LAV arising in a regular lattice [15]. The large mass difference between H or D and the metal atoms provides a gap in phonon spectrum, in which gap breathers can be excited either by thermal fluctuations at elevated temperatures or by external driving such as irradiation at low temperatures [16]. As has been argued in [15], the interplay between harmonic and anharmonic forces operating in the gap breather can result in a parametric driving of the potential wells of neighboring light atoms with a double frequency in relation to their eigenfrequencies. Accordingly, various reactions involving hydrogen atoms can be greatly accelerated by external energy input producing LAVs, in agreement with experimental results [17].

Another important consequence of the parametric driving of the well eigenfrequency is the increase of the quantum noise strength as compared to the thermal noise strength represented by the ratio E_{ZPO}/k_bT that increases with increasing number of oscillation periods (Fig. 4b). This means that one can expect quantum effects to dominate over the thermal ones even at elevated temperatures, which may be manifested by a strong deviation from the Arrhenius law.

The parametric driving $\Omega = 2\omega_0$ considered above requires rather special conditions similar to those in gap breathers in diatomic crystals [15], while in many other systems [7], e.g., in metals [8]–[10], oscillations of atoms in a discrete breather have different amplitudes but the same frequency. This case is closer to the driving of the potential well positions with $\Omega \approx \omega_0$, which also results in increasing mean energy of the quantum oscillator (eq. (32)), but it does not increase the quantum noise strength since the wave packet dispersion remains constant (eq. (33)). Accordingly, one could expect an acceleration of the escape from a well to occur due to the effective decrease of the well depth given by

$$R_K = \frac{\omega_0}{2\pi}\exp\left[-\left(E_0 - \langle E\rangle\right)/D\left(T\right)\right], D\left(T\right) = \frac{\hbar\omega_0}{2}\coth\left(\hbar\omega_0/2k_BT\right), \tag{34}$$

where $\langle E\rangle$ is the mean oscillator energy increasing with time according to eq. (32). The corresponding rate of escape from a well with a given parameter in this driving regime is presented in Fig. 5 for a potential well with a depth of 1 eV. It can be seen that the oscillator energy gradually increases up to the activation energy value resulting in a significant increase of the reaction rate, especially at low temperatures.

Note that in a real situation, anharmonicity of the potential well could limit the energy gained by the driving, which should be considered in order to make quantitative evaluations of the reaction acceleration by the present mechanism.

5. Tunneling in a Time-Periodic Double Well Potential at Zero Temperature

Consider Schrödinger equation for a wave function $\psi\left(x,t\right)$ of a particle with a mass *m* in the non-stationary double-well potential $V\left(x,t\right)$:

$$i\hbar\frac{\partial}{\partial t}\psi\left(x,t\right) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi\left(x,t\right) + V\left(x,t\right)\psi\left(x,t\right), \tag{35}$$

$$V\left(x,t\right) = \frac{m\omega_0^2}{2}\left[\frac{a\left(t\right)}{x_0^2}x^4 - b\left(t\right)x^2\right], x_0 = \sqrt{\frac{\hbar}{m\omega_0}}, \tag{36}$$

where $a(t)$ and $b\left(t\right)$ are the dimensionless parameters that determine the form and the driving mode of the potential shown in Fig. 6.

$$a\left(t\right) = \frac{1}{2\sqrt{\alpha}}\left[\alpha - \beta\cos\left(\Omega t\right)\right], b\left(t\right) = \frac{1}{2\sqrt{\alpha}}\sqrt{\alpha - \beta\cos\left(\Omega t\right)}, \tag{37}$$

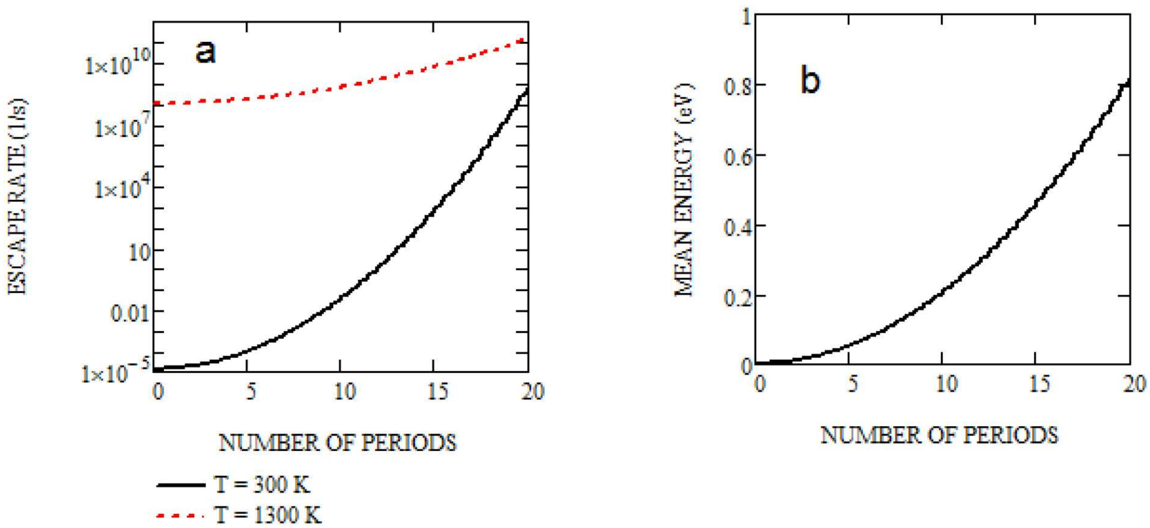

Figure 5. Escape rate from a well of a depth E_0 = 1 eV, eigenfrequency 5 THz at different temperatures (a) and the oscillator mean energy (b) vs. the number of oscillation periods at $\Omega = \omega_0, g_A = 0.5$.

Ω is the driving frequency of the eigenfrequencies ω_{eigen} and positions $x_{\min}$ of the potential wells in the vicinity of the minima given by:

$$\frac{\omega_{eigen}}{\omega_0} = \sqrt{2b} = \sqrt[4]{1 - \frac{\beta}{\alpha}\cos(2\omega_0 t)} \approx \left[1 - \frac{\beta}{4\alpha}\cos(2\omega_0 t)\right], \quad g_\omega = \frac{\beta}{2\alpha} << 1, \tag{38}$$

$$\frac{x_{\min}}{x_0} = \pm\sqrt{\frac{b}{2a}} = \pm\frac{1}{\sqrt{2}}\frac{1}{\sqrt[4]{\alpha - \beta\cos(2\omega_0 t)}} = \frac{1}{\sqrt{2}}\frac{1}{\alpha^{1/4}\sqrt[4]{1 - \frac{\beta}{\alpha}\cos(2\omega_0 t)}}$$

$$\approx \frac{x_{\min}(0)}{x_0}\left(1 + \frac{\beta}{4\alpha}\cos(2\omega_0 t)\right), \quad g_x \equiv \frac{\beta}{4\alpha} << 1, \tag{39}$$

From eqs (9), (10) it follows that the driving under consideration results in a *simultaneous* time-periodic modulation of the potential well *positions* and *eigenfrequencies* with amplitudes g_x and g_ω, respectively. Therefore, we are dealing here with a synergetic effect of the two mechanisms considered separately for a harmonic oscillator in sections 2 and 3.

Initial state of the system is described by a wave function of the Gaussian form placed near the first energy minimum (Fig. 7a):

$$\psi(x, t_0 = 0) = \frac{1}{\sqrt[4]{\pi x_0^2}}\exp\left(-\frac{(x - x_{\min})_0^2}{2x_0^2}\right), \tag{40}$$

The probability distribution of finding the particle at the point x is given by $\rho(x, t_0 = 0) = |\psi(x, t_0 = 0)|^2$, which is shown in Fig. 7b. It can be seen that the probability density is concentrated at $x_{\min} \approx 4.73$, which means the particle spends most of its time at the bottom of the potential well.

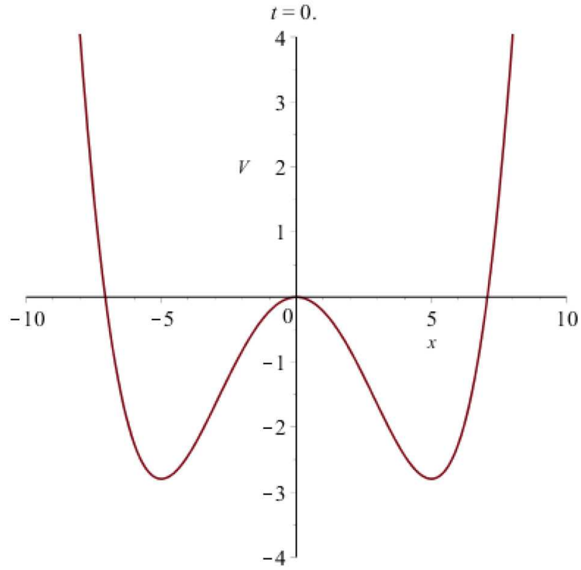

Figure 6. Double-well potential given by eq. (7) at α= 0.0005, β = 0.0001, which corresponds to the ratio of the potential depth to ZPV energy given by $1/8\sqrt{\alpha} \approx 5.6$.

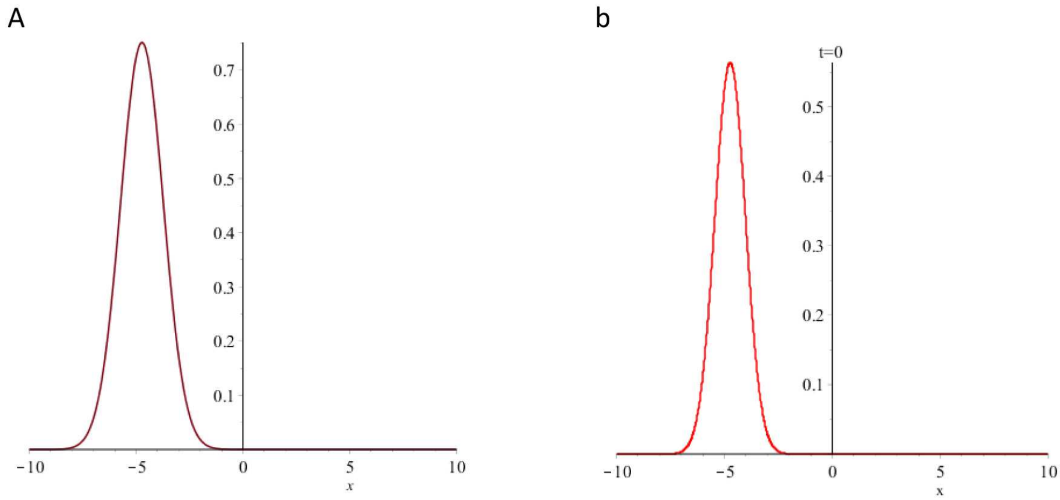

Figure 7. (a) Initial wave function $\psi\left(x, t_0 = 0\right)$ and (b) the probability distribution to find the particle at the point x:$\rho\left(x, t_0 = 0\right) = \left|\psi\left(x, t_0 = 0\right)\right|^2$ in the left potential well shown in Fig. 7.

At the selected parameters, the potential depth to ZPV energy ratio is given by $1/8\sqrt{\alpha} \approx 5.6$, which is a typical ratio for solid state chemical reactions. It means that the particle energy is 5.6 times lower than the energy required to

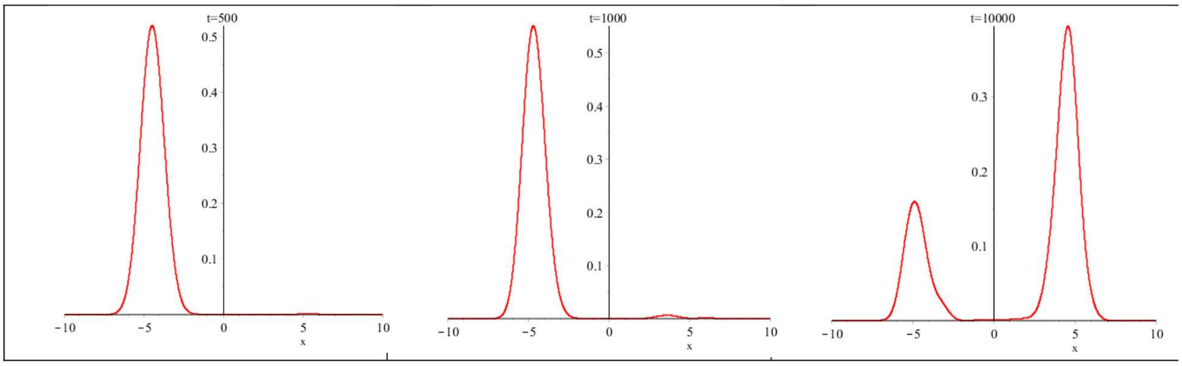

Figure 8. The probability distribution of the particle at different moments of time $t = 2\pi/\omega_{eigen}$ in *stationary potential wells*: α= 0.0005; β = 0.

'jump' over the barrier into another well. The mean time of tunneling through the barrier from a stationary potential well is very large as can be seen from Fig. 8 showing the probability distribution of the particle at different moments of time $t = 2\pi/\omega_{eigen}$, measured in the oscillator periods. For example, t = 1000 corresponds to 1000 'attempts' to escape from the left well. However, one can see that the probability to find the particle in the right well is still negligibly small. Only at t = 10000, it becomes higher than the probability to find the particle in the left well.

The situation becomes dramatically different in the case of time-periodically driven wells as demonstrated in Fig. 9 for the two driving frequencies $\Omega = \omega_{eigen}$; $\Omega = 2\omega_{eigen}$. In both cases, already at $t = 100$, the probability of finding the particle in the right well becomes comparable with the probability to find the particle in the left well. This means that the mean escape (tunneling) time has decreased by $\sim$2 orders of magnitude due to the driving with a comparatively small driving amplitude $g_\omega = 2g_x = 0.1$.

The driving frequency effect is different from that obtained for a harmonic oscillator in sections 2 and 3, where two sharp peaks were observed at resonant frequencies $\Omega = \omega_{eigen}$ and $\Omega = 2\ \omega_{eigen}$. Due to a simultaneous time-periodic modulation of the potential well positions and eigenfrequencies, the accelerating effect of driving depends non-monotonously on the driving frequency with a several maximums lying between $= \omega_{eigen}$ and 2 ω_{eigen}.

Finally, dependence of the tunneling time on the driving amplitude is shown in Fig. 10. It appears that increasing the amplitude by a factor of 2 results in decreasing the mean tunneling time by an order of magnitude. This example demonstrates the importance of the time-periodic driving of the potential wells in the vicinity of LAVs in the reactions involving quantum tunneling.

6. Discussion

The described effect is novel, and it differs qualitatively from a well-studied effect of resonance tunneling, a.k.a. *Euclidean resonance* [22] (an easy penetration through a classical nonstationary barrier due to under-barrier interference). In the latter case, the tunneling rate has a sharp peak as a function of the particle energy when it is close to a certain *resonant value* defined by the nonstationary field. Therefore, it requires an extremely specific parametrization of the tunneling conditions. In contrast to that, the time-periodic driving of the potential wells considered above, results, first, in a sharp and continuous (not quantum) increase of the ZPO amplitude and energy [6], [13], which in its turn increases the tunneling rate.

The present theory can be applied to the problem of penetration through the Coulomb barrier required for the explanation of low-energy nuclear reactions (LENR) as was demonstrated by Dubinko and Laptev in [15]–[20].

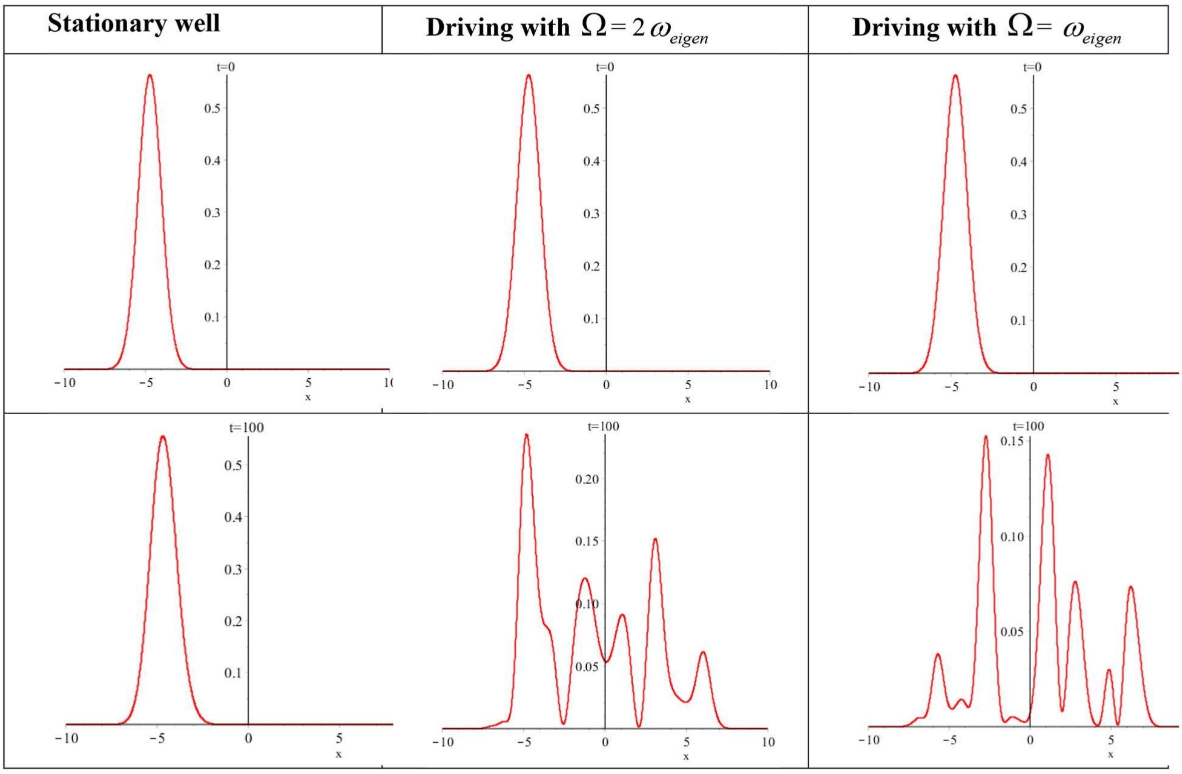

Figure 9. The probability distribution of the particle at different moments of time $t = 2\pi/\omega_{eigen}$ in stationary potential wells ($\alpha = 0.0005$; $\beta = 0$) and under the potential driving ($\alpha = 0.0005$; $\beta = 0.0001$) corresponding to $g_\omega = \beta/2\alpha = 0.1$; $g_x == \beta/4\alpha = 0.05$. The driving frequency Ω is indicated in the figure.

7. Summary and Outlook

Analytical solution of the Schrödinger equation for a periodically driven harmonic oscillator is derived, which shows that the oscillator wave packet dispersion and zero-point energy increases in response to parametric modulation of the oscillator eigenfrequency at $\Omega = 2\omega_0$. Based on that, a large increase of the escape rate with increasing number of modulation periods is demonstrated in the framework of the modified Kramers theory, which considers the quantum noise strength that increases due to the time-periodic driving. On the other hand, time-periodic driving of the potential well positions at $\Omega = \omega_0$ results in increasing mean energy of the quantum oscillator at a constant dispersion of the wave packet. This results in lowering of the effective activation barrier, which may amplify the escape rate significantly, especially at low temperatures.

A numerical solution of Schrodinger equation for time-periodic double well potential is obtained, which agrees qualitatively with Kramers rate theory.

It should be noted that the results were obtained for time-periodic driving of the potential *well shape* and *position* in contrast to numerous works on the escape of particles out of potential wells with a *barrier height* driven by noise and periodic modulations.

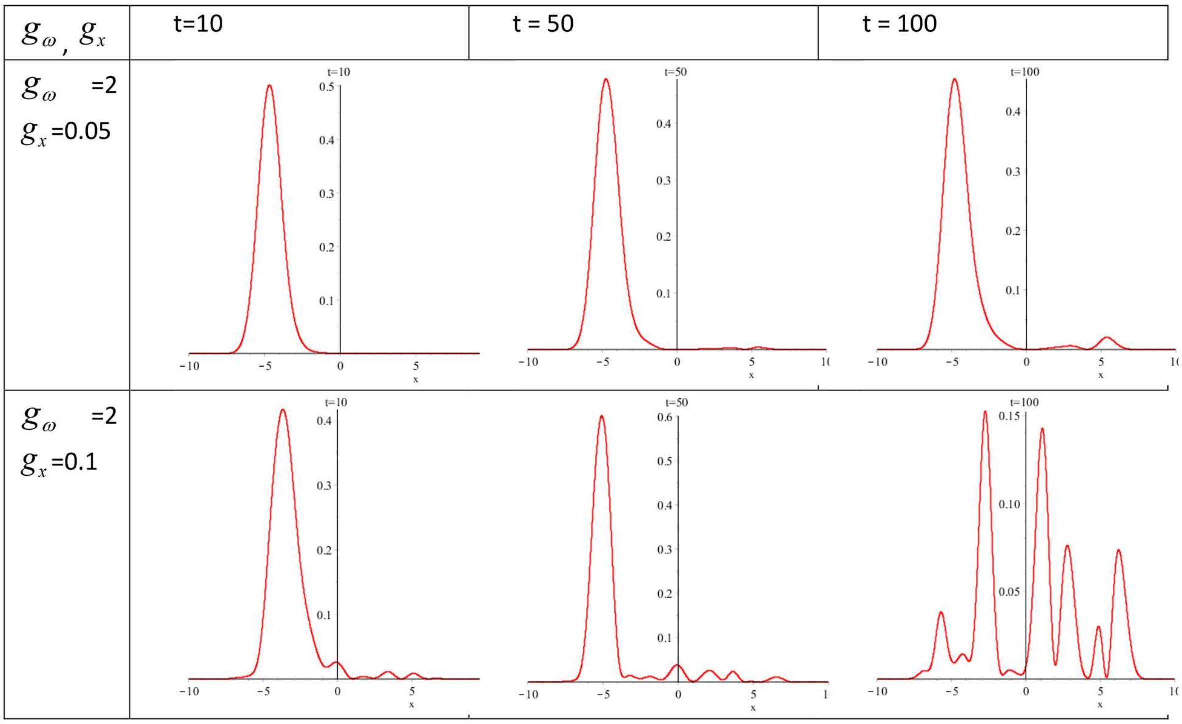

Figure 10. The probability distribution of the particle at different moments of time under the potential driving at $\Omega = \omega_{eigen}$, $\alpha = 0.0005$; $\beta = 0.00005 \div 0.0002$, corresponding to different driving amplitudes g_ω, g_x as indicated in the figure.

Physical realization of the time-periodic driving modes can be induced by *localized anharmonic vibrations*, a.k.a. *discrete breathers* that can be excited in a crystal bulk or at crystal defects either thermally or by external triggering such as irradiation [16], which can result in strong catalytic effects, such as nuclear catalysis resulting in LENR. It should be noted that, in reality, discrete breathers are *time-quasiperiodic* including a noise component [23]. Further investigations of the noise effect on the escape rate from *time-quasiperiodic* potential well are worthwhile and will be considered elsewhere.

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