# ON TRAPPING AND SLOWDOWN OF MOLECULES IN COLLIMATED BEAMS BY ELECTROMAGNETIC POTENTIAL WELLS DEEPENING OVER TIME

**S.T. HUSEYNOVA, A.Ch. IZMAILOV***
*Institute of Physics, Azerbaijan National Academy of Sciences,*
*Javid av. 131, Baku, Az-1143, AZERBAIJAN*
**e-mail: azizm57@rambler.ru*

We have shown possible increase of the spectroscopy resolution of molecules in a collimated beam due to their capture and deceleration at their passage of controlled potential electromagnetic well, which deepens to some limit during a certain period of time. The calculations were carried out in the model of such a one-dimensional rectangular well, which can be created in an area of local quasi-homogeneous electric (or magnetic) field in the path of a beam of molecules exhibiting an electric (or magnetic) dipole moment in their ground quantum state. It is shown that fractions of molecules in the beam captured and slowed down in this way significantly depend not only on the limiting depth of the electromagnetic well, but also on the rate of its deepening.

**Keywords:** electromagnetic well, molecular beam, one-dimensional rectangular well, high-resolution spectroscopy
**PACS:** 45.50.-j, 41.20.-q, 42.62.Fi

## 1. INTRODUCTION

Atomic and molecular beams have played central roles in many experiments in physics and chemistry, from seminal tests of fundamental aspects of quantum mechanics to molecular reaction dynamics, and have found a wide range of applications [1]. The motion of neutral molecules in a beam can be manipulated and controlled with inhomogeneous electric and magnetic fields [2].

Electromagnetic "cooling" and localization of microparticles (in particular, atoms and molecules) under conditions of the high vacuum are very important for a number of directions of physics and technologies, including ultra-high resolution spectroscopy of such particles [3]. In papers [4, 5], new methods for the slowdown and trapping of various microparticles (including atoms and molecules in the ground quantum state) were proposed by means of external electromagnetic fields which induce (for such particles) potential wells having fixed spatial distributions but deepening over time up to some limit. It is assumed that considered particles are under conditions of the high vacuum and forces acting on these particles are not dissipative, that is they move without friction. Depending on whether the particles have electric (magnetic) moment, it is possible to use the controllable electric (magnetic) field or far-off-resonance laser radiation for inducing of corresponding potential wells for given particles. Paper [6] presents the brief review on these methods.

Now we will analyze features of particle dynamics in the case of a one-dimensional rectangular electromagnetic potential well deepening over time. Such a well can be created in the area of local quasi-homogeneous electric (or magnetic) field in the path of a collimated beam of molecules exhibiting an electric (or magnetic) dipole moment. During a certain time, interval in which the strength of the given field is increasing, such a potential well (with the fixed spatial distribution) can trap or slowdown molecules in the beam. This, in particular, would allow controlling collimated beams of atoms or molecules in their ground quantum state for spectroscopic applications.

## 2. BASIC EQUATIONS

Assume that a point particle of mass $m$ freely moving with velocity $v_0 > 0$ along the $x$ axis (fig.1) from area $x < 0$ and reaches the boundary $x = 0$ of the following one-dimensional rectangular potential well at time $t$:

$$U(x,t) = -J_0\eta(L-x)\eta(x)\varphi(t), \qquad (1)$$

where $J_0 > 0$ is a constant quantity with the dimension of energy, $1 \geq \varphi(t) \geq 0$ is a nondecreasing function of time $t \geq 0$, and $\eta(y)$ is the step function ($\eta(y) = 1$ for $y \geq 0$ and $\eta(y) = 0$ if $y < 0$). The well (1) has the fixed spatial distribution but deepens over time up to some limit. The particle velocity increases jump like from the initial value $v_0$ to $v \geq v_0$ at the time moment $t$ when the particle reaches the boundary point $x = 0$ (fig.1) of the potential well (1). The relation between quantities $v$ and $v_0$ can be found from the total energy $E$ of a particle at the moment $t$

$$E(x = 0\,, t) = 0.5mv_0^2 = 0.5mv^2 - J_0\varphi(t). \qquad (2)$$

This particle will continue moving inside the rectangular potential well (fig.1) with constant velocity $v$ until it reaches the opposite potential-well boundary with coordinate $x = L$ at the moment $(t + L / v)$.

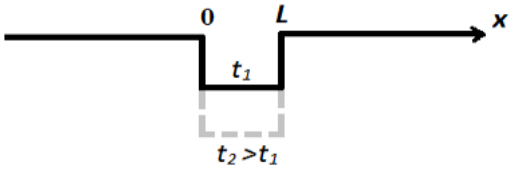


*Fig.1.* The scheme of the rectangular potential well deepening over time $t$.

131, H.Javid ave, AZ-1143, Baku
ANAS, Institute of Physics
E-mail: jophphysics@gmail.com

First, let us analyze the situation in which the particle is unable to overcome the potential well (1). This happens when the total energy $E$ of the particle becomes negative as function $\varphi(t)$ (1) increases with time $t$, i.e., under the condition

$$0.5mv^2 - J_0\varphi\left(t + {}^{L}/_{v}\right) < 0. \qquad (3)$$

When condition (3) holds, the particle reflects back from the well boundary at $x = L$ (fig.1) and starts moving backward at velocity $(-v)$ until it arrives to the opposite well boundary at $x = 0$ at time $(t + 2L/v)$. Due to the relation $\varphi\ (t + 2L/v) \geq \varphi\ (t + L/v)$, such motion of the particle with velocity $v$ from the potential-well boundary located at $x = 0$ to the opposite boundary at $x = L$ (fig. 1) repeats itself again and again. Hence, according to (3), maximum possible velocity $v_{\max}(t)$ of particles trapped into potential well (1) at time $t$ is determined by the equation

$$0.5mv_{\max}^2 = J_0\varphi\left(t + {}^{L}/_{v_{\max}}\right). \qquad (4)$$

Having found velocity $v_{\max}(t)$ from (4), we then obtain from (2) the maximum possible initial velocity $\tilde{v}_0(t)$ of free particles that remain localized in potential well (1) after reaching it at the time $t$:

$$\tilde{v}_0(t) = \sqrt{v_{\max}^2(t) - \frac{2J_0\varphi(t)}{m}}. \qquad (5)$$

Minimum velocity of particles $v_{\min}(t)$ captured into the discussed trap at time $t$ can be found from expression (2) by setting $v_0 = 0$:

$$v_{\min}(t) = \sqrt{\frac{2J_0\,\varphi(t)}{m}}. \qquad (6)$$

Let us now consider the case of relatively fast particles that have velocity $v_0$ exceeding $\tilde{v}_0(t)$ (4), (5) at the moment $t$ when they enter the potential well (fig.1). Similar to relations (2) and (3), the following expression governing the total energy of the particle reaching the well boundary $x = L$ at time $(t + L/v)$ can be obtained:

$$E\left(L, t + {}^{L}/_{v}\right) = 0.5mv_f^2 = 0.5mv^2 - J_0\varphi\left(t + {}^{L}/_{v}\right) > 0, \qquad (7)$$

where $v$ and $v_f$ are velocities of the particle inside the well and after leaving it, respectively. According to (7), the final velocity $v_f \leq v_0$ is given by

$$v_f = \sqrt{v^2 - \frac{2J_0}{m}\,\varphi\left(t + {}^{L}/_{v}\right)}, \qquad (8)$$

while velocity $v$ can be found straightforwardly from relation (2):

$$v = \sqrt{v_0^2 + \frac{2J_0\varphi(t)}{m}}. \qquad (9)$$

Next, we will analyze the dynamics of the passage through the potential well (1) of a group of collimated beam molecules that do not interact with each other, according to the visual scheme in fig. 2.

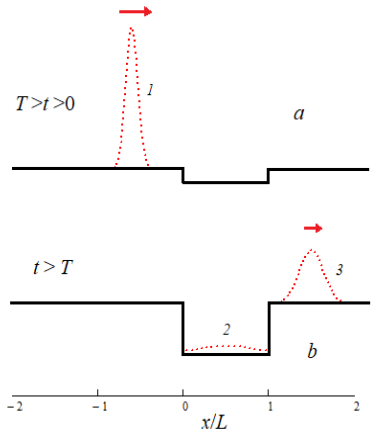


*Fig.2.* Scheme of propagation of a group of molecules through a rectangular potential well, deepening in the time interval $T \geq t \geq 0$. Here *1* is the given group of molecules before falling into this well, *2* and *3* are the fractions of this group of molecules captured into this well and passing through it, respectively.

It is assumed that at the moment $t = 0$ there is a distribution of the given group of molecules along the coordinate $x < 0$ and velocity $v_0 \geq 0$. During time $t > 0$, these molecules move towards the potential well (fig. 2a).

Until this well is reached, they are not acted upon by external forces and the distribution of the considered molecules is described by the function $f(x - v_0t, v_0)$. Thus, directly on the border $x = 0$ of the well (fig. 1) the distribution of the corresponding molecules by velocity $v_0$ is determined by the function $f(-v_0t, v_0)$. As they fall into this well, which deepens over time $T \geq t \geq 0$, some of these molecules will be localized in it, and the other part will overcome it (fig. 2b). Consider, for example, the distribution $f(x, v_0)$ of the considered molecules, which takes place at the moment $t = 0$ in a limited range of coordinates $x_2 > x > x_1$ with normalization to unity of the total number of these molecules, i.e.

$$\int_{x_1}^{x_2}\left(\int_0^{\infty} f(x, v_0)dv_0\right)dx = 1. \qquad (10)$$

Then, according to the relations (1)-(5), the relative fraction $p(t) \leq 1$ of these molecules, localized in the potential well by the time $t > 0$, is determined by the following formula:

$$p(t) = \int_0^t\left(\int_0^{\tilde{v}_0(t_1)} f(-v_0t_1, v_0)v_0dv_0\right)dt_1, \qquad (11)$$

where $\tilde{v}_0(t)$ (4), (5) is the maximum possible initial velocity of free particles that remain localized in the potential well (1) after reaching it at the time $t$.

Another part of the molecules of the initial group will overcome this well (fig. 2b). However, according to relations (7)-(9), their speeds will decrease from the initial value $v_0$ to $v_f < v_0$ in the process of deepening

this well. We will characterize such a "cooling" of these molecules by the following dimensionless parameter $r(t) < 1$:

$$r(t) = \Delta K(t)/K_0, \qquad (12)$$

where

$$\Delta K(t) = 0.5m \int_0^t \left[\int_{\tilde{v}_0(t_1)}^{\infty} (v_0^2 - {v_f}^2(t_1)) f(-v_0 t_1, v_0) v_0 dv_0\right] dt_1,$$

$$K_0 = 0.5m \int_0^T \left[\int_{\tilde{v}_0(t_1)}^{\infty} f(-v_0 t_1, v_0) v_0^3 dv_0\right] dt_1,$$

here $\Delta K(t)$ is the decrease of the kinetic energy of these molecules at the time $t$, $K_0$ is their total initial kinetic energy before passing through the potential well, which deepens in the time interval $T \geq t \geq 0$, speeds $\tilde{v}_0(t)$ and $v_f(t)$ are described by formulas (5) and (8), respectively.

## 3. DISCUSSION OF RESULTS

We will consider the following function $\varphi(t)$ of the potential well (1):

$$\varphi(t) = \left(\frac{t}{T}\right)^n \eta(T-t) + \eta(t-T), (n > 0,\ t \geq 0). \qquad (13)$$

According to (13), the depth of the well (1) increases from 0 to $J_0$ during the time interval $0 \leq t \leq T$ and retains maximum value $J_0$ at $t > T$. It is convenient to introduce the following characteristic quantities $w$ and $K$ for potential well (1), (13) which have the dimensions of velocity and energy, respectively:

$$w = {}^{L}/_{T}\,, \quad K = 0.5mw^2. \qquad (14)$$

Fig.3 presents time dependences of the function $\varphi(t)$ (13) and corresponding particles velocity $\tilde{v}_0(t)$ (4), (5) for various parameters $n$, which determine the deepening rate of the potential well (1), (13). It can be seen that the capture of molecules stops starting from the time $t = T$, since the potential well becomes stationary and $\tilde{v}_0(t) = 0$.

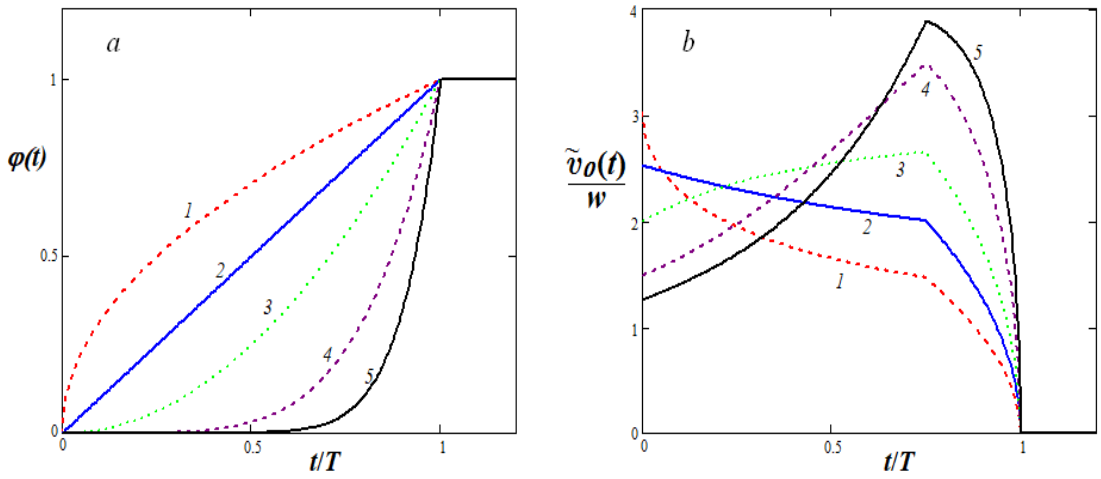


*Fig.3.* Dependences of the function φ(t) (*a*) and velocity $\tilde{v}_0(t)$ (*b*) on time $t$ for different values of the parameter $n = 0.5$ (curve 1), 1 (2), 2 (3), 5(4) and 10 (5), when $J_0 = 16\ K$.

Next, we will calculate the characteristics of trapped and slowed down molecules using formulas (11) and (12) for the following initial distribution $f(x, v_0)$ of these molecules at time $t = 0$ as an example:

$$f(x, v_0) = 1.274 \frac{{v_0}^2}{dw^3} exp\left(-\frac{{v_0}^2}{w^2}\right) exp\left[-\frac{(x-x_0)^2}{d^2}\right] \qquad (15)$$

where the value of $w$ is defined in (14), and $d$ is the characteristic extent of this distribution near its central position $x_0$. Note that the distribution (15) satisfies the normalization condition (10).

Fig. 4 shows the dependences of the characteristics $p(t)$ (11) and $r(t)$ (12) on time $t$ for various parameters $n$. The fraction $p(t)$ (11) of trapped molecules increases during the entire time interval $T \geq t \geq 0$ of the deepening of the potential well and reaches a constant value $p_{\max}$ when $t \geq T$ (fig. 4a). The value of $r(t)$ (12) also first increase with time $t$ (fig. 4b). However, unlike the dependencies $p(t)$ in fig.4a, the output of the functions $r(t)$ to constant values $r_{\max}$ can occur before the moment

$t = T$. Indeed, over time $t > 0$, more and more slow molecules from their initial distribution (15) will fall into the potential well. In accordance with the dependences for the velocity $\tilde{v}_0(t)$ (fig. 3b), all such relatively slow molecules with the initial velocity $v_0 < \tilde{v}_0(t)$ will be localized in this well at $t < T$. Therefore, they will not contribute to the characteristic $r(t)$, which describes the deceleration of molecules as a result of their passage through the considered potential well. According to fig. 4, the increase in $p(t)$ and $r(t)$ with time $t$ also significantly depends on the parameter $n$, which determines the deepening rate of the potential well (1), (13).

Fig. 5. shows the dependences on this parameter $n$ for the maxima $p_{\max}$ and $r_{\max}$ of the values $p(t)$ (11) and $r(t)$ (12), which they reach by the moment $t = T$ (Fig. 4). The fraction $p_{\max}$ of the molecules trapped in the potential well obviously increases with the growth of the maximum depth $J_0$ (1) of this well (Fig. 4a). According to Fig. 4b, the most effective deceleration of molecules, that have passed through the considered well, takes place in the range of values $2 \geq n \geq 1$ of the parameter $n$ of the function (13).

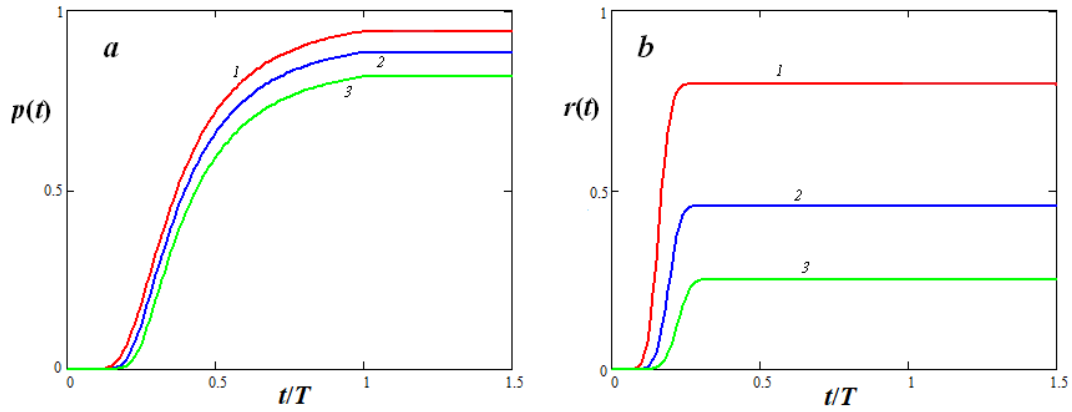


*Fig.4.* Dependences of $p(t)$ (*a*) and $r(t)$ (*b*) on time *t* for different values of the parameter $n = 1$ (curve 1), 5 (2), and 10 (3), when $J_0 = 16\,K$, $x_0 = -0.4L$ and $d = 0.1L$.

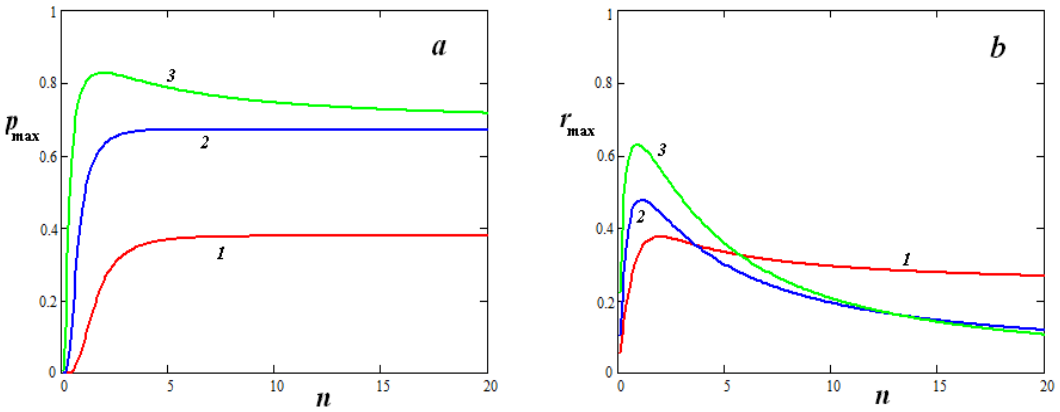


*Fig.5.* Dependences of $p_{\max}$ (*a*) and $r_{\max}$ (*b*) on the parameter *n* for different values of $J_0 = K$ (curve 1), $2K$ (2) and $5K$ (3), when $x_0 = -0.4L$ and $d = 0.1L$.

Fig. 6 shows the dependence of the values $p_{\max}$ and $r_{\max}$ on the position $x_0$ of the center of the initial distribution of molecules $f(x, v_0)$ (15). The form of these dependences $p_{\max}(x_0)$ and $r_{\max}(x_0)$ is also largely determined by the parameter $n$, which characterizes the deepening rate of the potential well (1), (13). Indeed, the coordinate $x_0$ of the initial distribution (15) determines the characteristic times $t$ for the molecules to reach the boundary $x = 0$ (Figs. 1, 2) of the considered rectangular potential well (1). In this regard, the dependence $\tilde{v}_0(t)$ (5) will play a critical role, which can change radically with a change of the parameter $n$ (Fig. 3b). Depending on the value of the initial velocity $v_0 < \tilde{v}_0(t)$ or $v_0 > \tilde{v}_0(t)$, the molecule will either be localized in the given well or leave it with a final velocity $v_f \leq v_0$. Naturally, as the distance $x_0$ of the initial distribution of molecules $f(x, v_0)$ (15) decreases from the boundary $x = 0$ of the potential well, the fraction $p_{\max}$ of molecules trapped in this well will increase (Fig. 6a).

Fig. 4-6 present our numerical calculations of the characteristics $p$ (11) and $r$ (12) on the particular example of the initial distribution of molecules $f(x, v_0)$ (15) at the time $t = 0$. However, the qualitative results obtained in this work can certainly be used in the analysis of the features of capture and

deceleration of molecules from a collimated beam by electromagnetic potential wells deepening with time also for other initial molecular distributions $f(x, v_0)$. Thus, it is possible to determine the optimal conditions for ultrahigh resolution spectroscopy of such molecules.

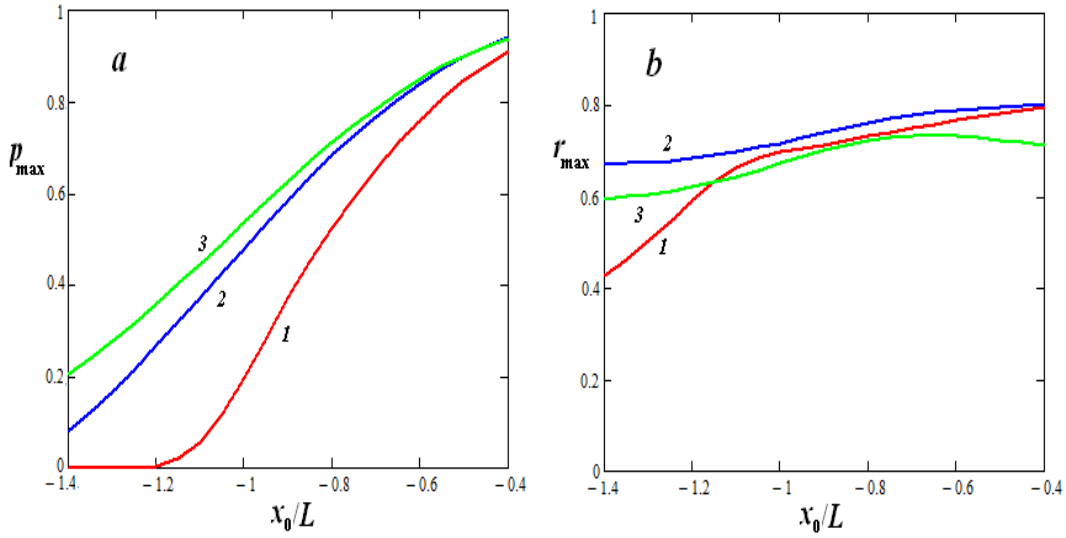


*Fig.6.* Dependences of $p_{\max}$ (*a*) and $r_{\max}$ (*b*) on the coordinate $x_0$ for different values of the parameter $n = 0.5$ (curve 1), 1 (2), и 2 (3), when $J_0 = 16\ K$ and $d = 0.1L$.


[1] *G. Scoles*, Ed. Atomic and Molecular Beam Methods; Oxford University Press: New York, 1988 and 1992; Vols. 1 and 2.

[2] *S.Y.T van de Meerakker, H.L. Bethlem, N. Vanhaecke,* and *G. Meijer*. Manipulation and control of molecular beams. Chemical Reviews, 2012, V. 112, N 9, pp. 4828–4878.

[3] *W. Demtroder.,* Laser Spectroscopy: Basic Concepts and Instrumentation. (Springer, 2003).

[4] *A.Ch. Izmailov*. Trapping of classical particles by an electromagnetic potential well deepening over time. Optics and Spectroscop., 2015, V. 119, N5, p. 883-886.

[5] *A.Ch. Izmailov*. On motion control of microparticles by an electromagnetic field amplifying over time for spectroscopy problems. Optics and Spectroscopy, 2017, V. 122, N2, pp. 315-321.

[6] *A.Ch. Izmailov*. New electromagnetic methods of slowdown and trapping of particles. AJP FIZIKA, 2018, V. XXIV, N 3, Section En, pp. 15-18.