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Development and Application of a Simple Model for Calculating the Quantum Diffusion Parameters of Rubidium, Hydrogen, and Deuterium Atoms

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Abstract

Relevance. The tunnelling effect is used in various modern devices, such as quantum interference devices and superconducting qubits of quantum computers, therefore, the theoretical calculation and experimental observation of the parameters of the quantum diffusion of atoms during tunnelling are of particular relevance.

Purpose. Theoretical evaluation of the parameters of the quantum diffusion of rubidium, hydrogen, and deuterium based on a simple quantum-mechanical model of atomic tunnelling.

Methods. The study uses quantum mechanical calculations and diffusion equations of solid-state physics.

Results. It is shown that the probabilities of detecting a particle in different regions of space change with time, and an equation is proposed for calculating the time after which the probability of the particle remaining outside the potential barrier would exceed the probability of its localisation inside the potential well. It is established that the time of Bose-condensed rubidium atoms in a potential well when tunnelling through a barrier of 1.3 microns in size is a macro-value of 0.43 s. The model parameters for the quantum diffusion of hydrogen and deuterium on the ice surface are calculated.

Conclusions. For Bose-condensed rubidium atoms, the estimated time of their stay in the potential well and the experimental time of overcoming the optical barrier with a width of 1.3 microns have similar values. It is found that the estimated time of the hydrogen atom in the potential well is 1.61010^{-8} s., and for deuterium – $0.57 \cdot 10^{-6}$ s., and the estimated coefficient of quantum diffusion of hydrogen is almost two orders of magnitude greater than that for deuterium, which corresponds to the experimental results. It is shown that thermally activated diffusion does not affect the diffusion of hydrogen, but makes a certain contribution to the total diffusion of deuterium on the ice surface at a temperature of 10°K

Keywords: tunnelling, atom, detection probability, potential well, crystal lattice, diffusion coefficient

Introduction

Tunnelling is one of the most unusual phenomena in quantum physics, where particles are able to overcome barriers that are classically impossible to overcome. The tunnelling effect manifests itself, for example, in quantum diffusion [1], in the process of photosynthesis and is used in various modern devices, from superconducting quantum interference devices (SQUID) to superconducting qubits for quantum computers. Therefore, the theoretical calculation and experimental observation of tunnelling parameters, such as the time spent by the particle in the potential well and potential barrier, are extremely relevant.

It is known that the group delay [2] is the time of arrival of the peak of the transmitted wave packet on the far side of the barrier, which can be less than the barrier thickness divided by the speed of light, without violating the causal relationship. This has been confirmed by many experiments [3-10], and in [11] it is stated that the tunnelling of particles occurs almost instantly. On the contrary, in 1980, M. Buttiker and R. Landauer calculated the time spent by the particle in the potential barrier through which it tunnels [12], which is close to the classical time of its movement. In [13-19], models were proposed that specify the time when a particle is located in a potential well and passes through a potential barrier. In [20-23],

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Bose-condensed ^{87}Rb atoms tunnelling through the optical barrier were directly studied and its time was measured.

At the same time, the estimation of particle lifetime in a potential well is usually considered to be related to the estimation of the tunnelling time [24-27]. On the other hand, in the formulation of the problem with two potential barriers, this time is calculated as the inverse of the attenuation coefficient (decay constant) with a coefficient of 2 [26-27]. However, as direct calculations for real physical systems show, these theoretical estimates can be much less than the classical time of passage of a potential well by a particle, which is also a contradiction. Therefore, the question of the probability and residence time of particles in a potential well during tunnelling remains open. This study considers another theoretical estimate of these parameters.

In solid-state physics, the corresponding quantum mechanical models are widely used in calculating the parameters of the interaction of particles with a crystal lattice [28-31]. These models contain interaction parameters in the form of potential pits of different heights and widths. On their basis, the main regularities of the interaction of neutral atoms with the crystal lattice of a solid body are explained. At the same time, in models with several potential wells or barriers, it should be taken into account that tunnelling leads to a shift in the energy levels of the particle by a certain amount [24; 30-31]. At the same time, in [24], small additives were discarded, which lead to a shift in the energy levels of the particle during tunnelling, which affected the accuracy of the model and made it difficult to calculate the parameters of quantum diffusion. It is of great interest to modify a simple tunnelling model so that the resulting relations can then be used to perform specific calculations on quantum diffusion.

The purpose of this study is to theoretically evaluate the parameters of the quantum diffusion of rubidium, hydrogen, and deuterium based on a simple quantum mechanical model of atomic tunnelling.

Materials and Methods

To describe the tunnelling of an impurity atom through a potential barrier, the study uses a quantum mechanical model of a particle with mass m_0 located in a rectangular potential well with width a, bounded on one side by an infinitely high wall ($x=0$), and on the other ($x=l$) by a potential barrier with height U_0 and width $a=l_1-l$. If at some time $t<0$ the width of the potential barrier a$\to\infty$, then the particle is localised inside the "space" (0, l) and its wave function inside the potential well has a discrete spectrum $E = E_0$ (Fig. 1).

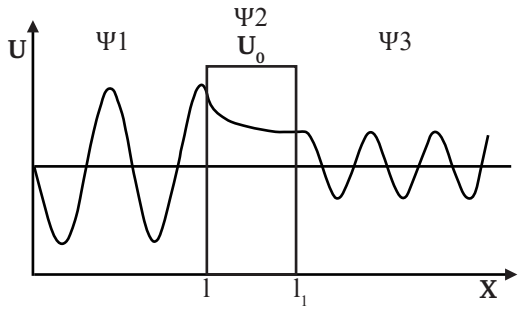

Figure 1. Model of quantum diffusion of an atom through a potential barrier

Source: [24]

The wave function of a particle at an arbitrary time $t\geq 0$ for three regions: 1 ($0<x<l$), 2 ($l<x<l_1$), and 3 ($l_1<x$) will have the form [24]:

$$\Psi_1 = A_1 \sin kx \quad (1.1)$$

$$\Psi_2 = A_2 e^{-\eta(x-l)} + B_2 e^{\eta(x-l)} \quad (1.2)$$

$$\Psi_3 = A_3 e^{ik(x-l1)} \quad (1.3)$$

where $k^2 = \frac{2m_0}{\hbar^2} E$ $\hbar$ – Planck constant,

$\eta^2 = \frac{2m_0}{\hbar^2}(U_0 - E) > 0$

The solution Ψ_1 for the first region is chosen in such a way that at $x=0$ it turns to zero, and in the solution in the third region, only the wave leaving the barrier is left. This leads to the appearance of a quasi-discrete spectrum consisting of quasi-levels in the system [24-27]. From the condition of continuity of the wave function of the particle at the boundaries of the barrier, the docking conditions are found:

When $x=l$:

$$A_1 \sin kl = A_2 + B_2 \quad (2.1)$$

$$A_1 \cos kl = (B_2 - A_2)\, k/\eta \quad (2.2)$$

When $x=l_1$:

$$A_2 e^{-\eta a} + B_2 e^{\eta a} = A_3 \quad (3.1)$$

$$A_2 e^{-\eta a} - B_2 e^{\eta a} = -ikA_3/\eta \quad (3.2)$$

where $a=l_1-l$.

From the last two equations, the relations follow:

$$A_2 = \frac{1 - ik/\eta}{2} e^{\eta a} A_3 \quad (4.1)$$

$$B_2 = \frac{1 + ik/\eta}{2} e^{-\eta a} A_3 \quad (4.2)$$

Substituting the relations (4.1-4.2) into the equations (2.1-2.2) leads to the equation for determining the energy:

$$\frac{1 + ik/\eta}{1 - ik/\eta} e^{-2\eta a} = \frac{tgkl + k/\eta}{tgkl - k/\eta} \quad (5)$$

At the initial moments of time ($t\geq 0$), the amplitude of the outgoing wave A_3 will be much less than the amplitude of the standing wave in the well A_1, i.e., the probability

of detecting a particle in region 3 is much less than in region 1:

$$|A_3| \sim A_1 e^{-\eta a} \quad (6)$$

For a→∞, the solution in region 3 turns to zero ($A_3=0$), following by equation (5) to determine the discrete energy levels in the potential well in region 1:

$$tg\ k_0 l = -k_0/\eta_0 \quad (7)$$

where the index 0 denotes the values k and η for a →∞.

Taking into account exponentially small terms of the order $A_1 e^{-2pa}$ under the condition $\eta a >> 1$ and $\eta l >> 1$, the solution of equation (7), as is known [24-27], describes quasi-levels. To calculate them, a small imaginary part of k' in the value k is selected, and in the real part, in contrast to [24], the resulting additives are taken into account:

$$k = k_0 - ik' \quad (8)$$

where k_0 is related to the discrete energy spectrum E_0 of the particle in region 1 by the usual relation:

$$k_0^2 = \frac{2m_0}{\hbar^2} E_0 \quad (9)$$

Then, substituting the value k in the form (8) in equation (5), taking into account (7) and the condition $nl >> 1$, in the first order of magnitude $e^{-2\eta a}$, the value k' is found:

$$k'l = \frac{4(k_0/\eta_0)^2}{[1+(k_0/\eta_0)^2]^2} e^{-2\eta a} \quad (10)$$

In this case, for the energy E of the particle, is found, taking into account (8):

$$E = \frac{\hbar^2 k^2}{m_0} = \frac{\hbar^2}{m_0}\left[k_0^2 - k'^2 - 2ik'k_0\right] = E' - i\hbar\lambda, \quad (11)$$

– quasi-discrete spectrum of the particle energy,

$$E' = E_0 - \Delta E = \frac{\hbar^2}{m_0}\left[k_0^2 - k'^2\right] \quad (12)$$

$$\lambda = 2v_0 k' = D_0 \frac{v_0}{2l} exp\left[-2a\sqrt{\frac{2m_0}{\hbar^2}(U_0 - E_0)}\right] \quad (13)$$

$$v_0 = \frac{\hbar k_0}{m_0} \quad (14)$$

– the velocity of the particle corresponding to the discrete energy spectrum in the region 1:

$$D_0 \cong \frac{16(k_0/\eta_0)^2}{[1+(k_0/\eta_0)^2]^2} \quad (15)$$

Results and Discussion

The presence of the addition of ΔE in the expression for the particle energy (12) means that in the quasi-discrete spectrum, the particle energy decreases by the value of ΔE compared to the discrete spectrum. This state of the system corresponds to the velocity of the particle in region 3:

$$v' = \frac{\hbar}{m_0}\sqrt{k^2 - k'^2} \quad (16)$$

Therefore, when passing the energy barrier, the atom loses speed and, therefore, radiates, reducing its energy by ΔE. The presence of the imaginary part in the expression for the energy (11) indicates that the wave function of the particle in the potential well will decrease exponentially over time. In this case, for the square of the modulus of the wave function:

$$|\psi|^2 = Ae^{-\lambda t} \quad (17)$$

where λ – the so-called decay constant – characterises the decreasing probability of finding a particle inside a potential well. However, beyond the potential barrier in region 3, the solution should increase with distance from the barrier due to a small addition to the wave number k':

$$|\psi_3|^2 = Ae^{2k'x} \quad (18)$$

And therefore, the normalisation integral for the function Ψ_3 should be modified for large values of x. However, the growth of the function outside the barrier at $x \to \infty$ is compensated by its exponential decrease at $t \to \infty$ according to equality (17), which ensures the fulfilment of the continuity equation [24]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0 \quad (19)$$

where p – probability density, j – current density.

Next, the study considers the implementation of the continuity equation for three domains. In the first area, the equation has the form:

$$\frac{\partial j}{\partial x} = v_0 \frac{\partial \rho}{\partial x} = 2v_0 k' \rho \quad (20.1)$$

$$\frac{\partial \rho}{\partial t} = -\lambda \rho \quad (20.2)$$

$$-\lambda\rho + 2v_0 k'\rho = 0 \quad (20.3)$$

In the second area, the change in the energy of the system by the value of ΔE (and hence the velocity of the particle) is taken into account. Then the continuity equation can be represented as:

$$\frac{\partial j}{\partial x} = v\frac{\partial \rho}{\partial x} + \rho\frac{\partial v}{\partial x} = 2vk'\rho + \rho v_x \quad (21.1)$$

$$\frac{\partial \rho}{\partial t} = -\lambda\rho = -2v_0 k'\rho \quad (21.2)$$

$$-\lambda\rho + 2vk'\rho + \rho v_x = 0 \quad (21.3)$$

From (21.3) it follows:

$$v_x = 2(v_0 - v)k' = 2\Delta v \cdot k' \quad (22)$$

When $x=l$ $v_x=0$, when $x=l_1$ $v_x=2\Delta vk'$.
In the third domain, then, it should be assumed:

$$\frac{\partial j}{\partial x} = v'\frac{\partial \rho}{\partial x} = 2v'k'\rho \quad (23.1)$$

$$\frac{\partial \rho}{\partial t} = -\lambda'\rho \quad (23.2)$$

$$-\lambda'\rho + 2v'k'\rho = 0 \quad (23.3)$$

Thus, the attenuation coefficients in regions 1 and 2 (inside the crystal lattice) and 3 (outside the crystal lattice) differ by a small amount, equal to $v_x=2\Delta vk'$. This

means that the probability of detecting a particle in region 1 changes with time, as $|\psi_1|^2=A_1^2e^{-\lambda t}$, and the probability of detecting a particle in region 3, as $|\Psi_3|^2=A_3^2e^{-\lambda'\tau}$, where $\lambda'=2v'k'$ – decay constant for region 3.

Using the expression (6), the following equality is obtained:

$$|\psi_1(\tau)|^2 = |\psi_3(\tau)|^2 \Rightarrow A_1^2 e^{-\lambda\tau} = A_1^2 e^{-2\eta a} e^{-\lambda'\tau} \quad (24)$$

After finding the time τ, the amplitudes of the wave functions in regions 1 and 3 will have the same value:

$$\tau = 2\eta a/v_x \quad (25)$$

Therefore, after the time τ, determined by equation (25), the probability of the particle staying in region 3 outside the potential barrier will be equal to the probability of its localisation inside the potential well. Therefore, the time τ can also be called the period when the atom is in the potential well.

Returning to the discussion about the passage of a potential barrier by a particle, the "classical" time of its tunnelling can be introduced in a simple model. Indeed, if in region 1, before passing the barrier, the velocity of the particle is v, and after passing it – v', then the "classical" time of the particle passing through the potential barrier of width a is:

$$\tau_c = \frac{2a}{(v+v')} \quad (26)$$

In contrast to data from [3-11], this time has a significant value. The above simple model is largely applicable to the description of the quantum diffusion of atoms of elements (hydrogen, nitrogen, carbon) at a sufficiently low temperature. Next, the study considers this issue with some concrete examples.

Parameters of quantum diffusion of Bose-condensed rubidium atoms. The developed model was applied to calculate the parameters of a physical system consisting of Bose-condensed ^{87}Rb atoms tunnelling through an optical barrier with a thickness of 1.3 microns, given in [23]. Next, the study considers the case $E/U_0=0.5$, the velocity of the rubidium ion $v=3.7\ mm/s$.

From these data, the energy value of the Bose-condensed rubidium ion is found:

$$\boldsymbol{E} = \frac{m_0 v^2}{2} = \frac{87\times 1.66\cdot 10^{-27}\times (3.7\cdot 10^{-3})^2}{2} \approx 1\cdot 10^{-30} J$$

and the parameter k_0 corresponding to this energy value:

$$k_0 = \frac{m_0 v}{h} = \frac{87\times 1.66\cdot 10^{-27}\times 3.7\cdot 10^{-3}}{6.63\cdot 10^{-34}} = 8.06\cdot 10^5 m^{-1}$$

From the conditions (1.1-1.3) it is also found that in this case $\eta=k_0$.

Assuming further that the width of the potential pit is equal to the width of the potential barrier, from the equation (10) the value of the parameter k' is found:

$$k' = \frac{e^{-2\eta a}}{a} = 9.4\cdot 10^4 m^{-1}$$

The velocity of the particle after passing the potential barrier is found from equation (16):

$$v' = v_0\sqrt{1-\frac{k'^2}{k^2}} = 3.674\cdot 10^{-3} m/s$$

Using this velocity value, it is possible to find the probable time of finding rubidium atoms in a potential well. Substituting the expression v_x from (22) into (25), obtain:

$$\tau = \frac{\eta a}{\Delta v\cdot k'} = 0.43 s \quad (27)$$

Thus, it is established that the time spent by Bose-condensed rubidium atoms in a potential well when tunnelling through a barrier with a size of 1.3 μm is a macro-value of 0.43 s. For a Bose particle system, this parameter also shows the likely time that 50% of the particles will be outside the potential barrier during tunnelling. This result may well pass a practical test.

The "classical" time of the particle passing through the potential barrier in a simple model was also calculated:

$$\tau_c = \frac{2a}{(v+v')} = 0.353\ ms \quad (28)$$

This time, within the error of calculations and experiment, corresponds to the experimental result given in [23].

Parameters of the quantum diffusion of hydrogen and deuterium on the ice surface at a temperature of 10°K. Next, the study calculates the quantum diffusion parameters for hydrogen atoms located on the ice surface at a temperature of 10°K [32]. For the estimation, a simple one-dimensional model is used and it is assumed that the dimensions of the potential pit l and the potential barrier a are equal to half the period of the ice crystal lattice (0.23 nm).

The energy of hydrogen atoms at a temperature of 10°K is equal to:

$$E = \frac{3kT}{2} = \frac{3\times 1.38\cdot 10^{-23}\times 10}{2} \approx 2.07\cdot 10^{-22} J$$

This energy value corresponds to the value of the velocity of the hydrogen atom and the parameter k_0:

$$v = \sqrt{2E/m} = 500\ m/s$$

$$k_0 = \frac{m_0 v}{h} = \frac{1.66\cdot 10^{-27}\times 500}{6.63\cdot 10^{-34}} = 1.25\cdot 10^9 m^{-1}$$

For a simple model, the condition $nl>1$ must be satisfied, from where $\eta>4.4\cdot 10^9$. Assuming that $n=4k_0=5\cdot 10^9\ m^{-1}$ and the width of the potential well l is equal to the width of the potential barrier, from the equation (10) the value of the parameter k' is found:

$$k' = \frac{4(k_0/\eta)^2}{[1+(k_0/\eta)^2]^2 l} e^{-2\eta a} = 0.97\cdot 10^8 m^{-1}$$

The velocity of the particle after passing the potential barrier is found from equation (16):

$$v' = v_0\sqrt{1-\frac{k'^2}{k^2}} = 499.25\ m/s$$

Using this value of the atomic velocity difference, it is possible to find the estimated time of equal probability density of finding hydrogen atoms inside the potential well and outside the barrier. The following is obtained:

$$\tau_H = \frac{\eta a}{\Delta v \cdot k'} = 1.6 \cdot 10^{-8} s$$

For hydrogen atoms located on the ice surface, this period characterises the probable time of the particle's stay in the potential well. Formally, the diffusion coefficient of hydrogen on the surface of a two-dimensional ice lattice can be calculated using the classical equation (4 in the numerator occurs when diffusion occurs on the surface) [33]:

$$D = d^2/4\tau \quad (29)$$

Substituting in (29) the numerical values of the d – period of the ice crystal lattice and the time of the hydrogen atom in the potential well τ_H, an estimate of the quantum diffusion coefficient of hydrogen on the ice surface is obtained:

$D_H = 3.2 \cdot 10^{-12}\ m^2/s = 3.2 \cdot 10^{-8}\ cm^2/s$

For comparison, the study calculates the quantum diffusion parameters for deuterium atoms located on the ice surface at a temperature of 10°K. The energy of hydrogen atoms at a temperature of 10°K is equal to:

$$E = \frac{3kT}{2} \approx 2.07 \cdot 10^{-22} J$$

This energy value corresponds to the value of the velocity of the hydrogen atom and the parameter k_0:

$$v = \sqrt{2E/m} = 353\ m/s$$

$$k_0 = \frac{m_0 V}{h} = \frac{2 \cdot 1.66 \cdot 10^{-27} \times 353}{6.63 \cdot 10^{-34}} = 1.77 \cdot 10^9 m^{-1}$$

Assuming that in this case $\eta = 4k_0$ and the width of the potential well is equal to the width of the potential barrier, from the equation (10) the value of the parameter k' is found:

$$k' = \frac{4(k_0/\eta)^2}{[1 + (k_0/\eta)^2]^2 l} e^{-2\eta a} = 0.37 \cdot 10^8 m^{-1}$$

The velocity of the particle after passing the potential barrier is found from equation (16):

$$v' = v_0 \sqrt{1 - \frac{k'^2}{k^2}} = 352.923\ m/s$$

Using this velocity value, it is possible to find the estimated time of equal probability density of finding deuterium atoms inside the potential well and outside the barrier. The following is obtained:

$$\tau_D = \frac{\eta a}{\Delta v \cdot k'} = 0.57 \cdot 10^{-6} s$$

It is found that the period of the deuterium atoms in the potential well is 570 ms. Substituting in (29) the numerical values of the period of the ice crystal lattice and the time of the hydrogen atom in the potential well τ_H, an estimate of the quantum diffusion coefficient of hydrogen on the ice surface is obtained:

$D_D = 0.9 \cdot 10^{-13}\ m^2/c = 0.9 \cdot 10^{-9}\ cm^2/s$

The value of the quantum diffusion coefficient of deuterium is almost two orders of magnitude less than the quantum diffusion coefficient of hydrogen, if the energy barrier of these elements is the same. This has been experimentally confirmed in [32].

Comparison of the parameters of quantum and thermally activated diffusion of hydrogen and deuterium atoms. A comparison of the parameters of quantum diffusion and thermally activated diffusion is of interest. In [34], an expression for the zero-diffusion coefficient is obtained:

$$D_0 = 1.14 \cdot d \cdot \frac{N_e^2}{\rho} \cdot T^2\ cm^2/s \quad (30)$$

where, for the hydrogen atoms on the water surface, the atomic weight is $N_e = 1$, the ice crystal lattice period is $d = 0{,}454\ nm$, and the ice density is $p = 0.9\ g \cdot m^{-3}$. At a temperature of 10°K, the calculated value of D_0 for hydrogen is:

$D_{0H} = 0.58 \cdot 10^{-7}\ cm^2/s$

If the activation energy of hydrogen is assumed to be equal to the value of the energy barrier per 1 mole of hydrogen, then:

$U_0 = 4E = 6kT_0,\ E_a = 6RT_0$

$$D_H^T = 0.58 \cdot 10^{-7} \cdot e^{-\frac{E_a}{RT}} = 1.44 \cdot 10^{-10} cm^2/s$$

This value is two orders of magnitude less than the quantum diffusion coefficient, and thermally activated diffusion makes almost no contribution to the diffusion of hydrogen at 10°K.

Similar calculations are performed for deuterium. The calculated value of D_0 for deuterium is 4 times greater than that of hydrogen:

$D_{0H} = 2.32 \cdot 10^{-7}\ cm^2/s$

If the activation energy of hydrogen is assumed to be equal to the value of the energy barrier per 1 mole of hydrogen, then:

$$D_D^T = 2.32 \cdot 10^{-7} \cdot e^{-\frac{E_a}{RT}} = 0.58 \cdot 10^{-9} cm^2/s$$

This value is close to the value of the quantum diffusion coefficient of deuterium, and, therefore, thermally activated diffusion makes a certain contribution to the diffusion of deuterium on the ice surface at a temperature of 10°K.

Conclusions

1. A simple quantum-mechanical model of tunnelling an atom through a potential barrier is developed. It is shown that the decay constants in the region inside the potential well and outside the potential barrier differ by an amount equal to $v_x = 2\Delta v k'$ and, consequently, the probabilities of detecting an impurity particle in these regions change with time.

2. An equation is proposed for calculating the time τ, after which the probability of a particle remaining outside the potential barrier would exceed the probability of its localisation inside the potential well. It is shown that

for Bose-condensed rubidium atoms, this time of their stay in the potential well when tunnelling through a potential barrier of 1.3 μm is 0.43.

3.The model parameters for the quantum diffusion of hydrogen and deuterium on the ice surface are calculated. It is found that the estimated time of the hydrogen atom in the potential well is $1{,}61010^{-8}$ s, and for deuterium $-0.57 \cdot 10^{-6}$ s, and the estimated coefficient of quantum diffusion of hydrogen is almost two orders of magnitude greater than that for deuterium.

4. It is shown that thermally activated diffusion does not affect the diffusion of hydrogen, but makes a certain contribution to the total diffusion of deuterium on the ice surface at a temperature of 10°K.

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Розробка і застосування простої моделі для розрахунку параметрів квантової дифузії атомів рубідію, водню і дейтерію

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Анотація

Актуальність. Ефект тунелювання використовується у різних сучасних пристроях, таких як квантові інтерференційні пристрої і надпровідні кубіти квантових комп'ютерів, тому теоретичний розрахунок і експериментальне визначення параметрів квантової дифузії атомів є надзвичайно актуальними.

Мета. Теоретична оцінка параметрів квантової дифузії рубідію, водню і дейтерію на основі простої квантово-механічної моделі тунелювання атомів.

Методи. У роботі використані квантово-механічні розрахунки й дифузійні рівняння фізики твердого тіла.

Результати. Показано, що ймовірність виявлення частки у різних областях простору змінюються з часом і запропонована формула для розрахунку часу, після закінчення якого ймовірність перебування частки за межами потенційного бар'єру буде перевищувати ймовірність її локалізації всередині потенційної ями. Встановлено, що час знаходження бозе-конденсованих атомів рубідію у потенційній ямі за тунелювання через бар'єр розміром 1,3 мкм становить макровеличину 0,43 с. Розраховані параметри моделі для квантової дифузії водню і дейтерію на поверхні льоду.

Висновки. Для бозе-конденсованих атомів рубідію розрахунковий час їх перебування у потенційній ямі та експериментальний час подолання оптичного бар'єру шириною 1,3 мкм мають близькі значення. Встановлено, що розрахунковий час перебування атома водню у потенційній ямі становить $1{,}6 \cdot 10^{-8}$ с., а дейтерію – $0{,}57 \cdot 10^{-6}$ с. Оцінний коефіцієнт квантової дифузії водню майже на два порядки більше такого для дейтерію, що відповідає експериментальним результатам. Показано, що термічно активована дифузія не впливає на дифузію водню, але вносить певний вклад у загальну дифузію дейтерію на поверхні льоду за температури 10 °К

Ключові слова: тунелювання, атом, ймовірність виявлення, потенційна яма, кристалічна решітка, коефіцієнт дифузії