Research Article

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Low-temperature separation of helium-helion mixture

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Abstract: The research is devoted to the problem of designing materials with an adjustable property of permeability. The obtained tool for property regulation allows achieving hyper-selectivity in relation to separation of helium isotope mixtures, as well as some other gas mixtures. The research is theoretical in nature; however, it suggests a clear direction of activity for experimenters. The result obtained is valid for ultrathin barriers of any form. As a result, a new exact solution of the Schrödinger equation of wave dynamics, which is valid for the case of two-barrier systems, is found. This solution allows for comprehensive consideration of the process of wave passage through a barrier and identification of the causes leading to super-permeability of individual components.

Keywords: membrane permeability, Schrödinger equations, selectivity of gas mixtures

1 Introduction

Porous graphenes and porous boron nitride are best suited as elements of a composite membrane. Such materials can be obtained by epitaxy [1, 2] or by vapour deposition onto a substrate containing a defect-free graphene or porous boron nitride [3, 4]. However, there is another entire group of stable sheets with a thickness of one atom which can be converted into a porous 2D material at the stage of synthesis or after mechanical peeling. Thus, GeH sheets

which are thermally stable at the temperature of up to 75°C are investigated in [5]. Another known material is silicon which is an equivalent to graphenes [6, 7]; it has great prospects for new applications. In [8] the authors consider black phosphorus as a layered material from which it is possible to obtain a phosphorene — a monoatomic layer whose physical properties differ significantly from its bulk counterpart. The work [9] reports on successful manufacturing of a two-dimensional stanene based on Sc by the method of molecular beam epitaxy. In [10] it is suggested that functionalization of hexagonal boron nitride by amine molecules causes exfoliation of the layered structure which leads to the formation of boron nitride sheets. The authors of [11] state that the development of new layered materials has evolved from graphenes to metallic oxides and metallic chalcogenide nanosheets. Additionally, in [12] the authors mention metal dichalcogenides as the latest 2D materials and give an example of a material based on MoS₂. In [13] the electronic properties of the following metal dichalcogenides with a two-dimensional structure are observed: MoS₂, WS₂, WTe₂, TiSe₂, NbS₂, VSe₂, NbSe₂, TaS₂. All the materials can be adapted for separation of gases with an application of an appropriate method for their synthesis or subsequent processing leading to the formation of pores. In [14] a layered two-dimensional network structure, which contains uniformly distributed holes and is based on C₂N stoichiometry is reported.

Thus, a significant number of two-dimensional materials have already been synthesized, and they can be used in works on quantum sifting of isotopes. The *r*-C₃N₄ membrane is of great interest in terms of quantum screening of ³He/⁴He mixtures. Using this membrane makes it possible to achieve a degree of separation equal to 18 units [15]. In [16] it is suggested that tunnelling problems improve understanding of chemical phenomena. In [17] the authors consider a numerical solution to the problem of quantum-mechanical transitions through barriers. The proposed method was tested on some discontinuous potential distributions. Theoretical studies were carried out and demonstrated that efficient separation of ³He/⁴He can be achieved using a porous graphene-like material from carbon nitride with application of the quantum sieving ef-

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fect [18]. Mixtures of H_2/T_2 , $^3\text{He}/^4\text{He}$, CH_4/CD_4 , H_2/HD are studied in [19]. The work presents a simple theory for calculating selectivity at zero pressure due to quantum sieving in nanopores. In [20] the authors use molecular dynamics modelling, as well as the Monte Carlo method and experimental neutron scattering data, to study adsorption and diffusion of hydrogen and deuterium in zeolite in the temperature range of 30–150 K. In [21] molecular sieving of hydrogen and deuterium through a zeolite membrane at low temperatures is observed. There occurs an inverse kinetic scattering effect which consists in the fact that the heavier isotope, deuterium, diffuses faster than hydrogen. At 65 K scattering selectivity reaches 46 units. A number of works suggest that a porous graphene of a certain structure can be used for quantum screening of a helium–helium mixture [22]. Naturally, porous boron nitride, as well as any nanoporous membrane with a thickness of one atom of a given substance, is also suitable for these purposes. Several pore structures for separation of hydrogen from methane or helium from other noble gases are presented in [23–26]. The authors in [27–32] mainly analyse single-layer materials. There are works on controlled separation [33]. These studies assume that temperature plays the role of the control parameter. In addition, the case of a tunable potential barrier is analysed in [34]. In [35, 36] diffusion membranes are considered. In [37, 38] authors investigate membranes for industrial applications. Bimaterial is considered in [39]. Helium enrichment by resonant tunnelling through bilayers is presented in [40]. Works [41–52] consider application of classical mechanics in molecular sieving problems. However, at temperatures of the order of 50–60 K, the Schrödinger wave dynamics should be used for the problems under consideration.

2 The Schrödinger differential equation

Passage of matter waves and their reflection from a potential barrier $U(x)$ are described by the stationary Schrödinger differential equation:

$$\frac{d^2\psi}{dx^2} + [k^2 - 2mU(x)]\psi = 0. \quad (1)$$

It is assumed that the barrier $U(x)$ and the desired function $\psi(x)$ are defined on the entire real axis x , and the wave which is incident on the left side of the barrier has the form:

$$\psi_0 = e^{ikx} \quad (2)$$

If the values m and E represent the dimensionless mass and the energy of the material particle, the wave parameter k is equal to:

$$k = \sqrt{2mE}. \quad (3)$$

Numerous literature sources devoted to solving the Schrödinger equation (1) [53, 54] describe various methods of solution. Exact solutions are known for a potential barrier $U(x)$ of a rectangular shape, as well as for a barrier having the form:

$$U(x) = \frac{1}{\text{ch}^2(ax)}. \quad (4)$$

For barriers of other shapes approximate numerical methods of calculation are usually used. They are based on the assumption that, firstly, it is necessary to calculate two linearly independent solutions $\Phi_1(x)$ and $\Phi_2(x)$ of differential equation (1) within a certain interval $0 < x < L$ adjacent to the $U(x)$ barrier region. Such solutions can be found by various numerical methods, using, for example, the Runge – Kutta method, or other modifications of finite-difference schemes. Figure 1 shows one of the results of such calculations for a barrier of a numerically specified shape.

Figure 1: Fundamental solutions of stationary Schrödinger equation for barriers of given shape

It should be noted that the process of finding the functions $\Phi_1(x)$ and $\Phi_2(x)$ from equation (1) written in the difference form can be significantly facilitated by using the null(**M**) subroutine which is available in the MatLab system. Factually, the difference form of equation (1) is as follows:

$$\mathbf{M} \cdot \boldsymbol{\psi} = 0, \quad \mathbf{M} = \mathbf{D2} + \text{diag} [k^2 + 2mU(x)], \quad (5)$$

$\boldsymbol{\psi}$ – the vector of grid values of the desired function,

$\mathbf{D2}$ – the matrix analogue of the second derivative with respect to x .

If we remove the first and the last rows of the matrix **M** obtained in such a way and apply the null(**M**) opera-

tion, we will, as a result, obtain two desired column vectors $\Phi_1(x)$ and $\Phi_2(x)$. Moreover, they are immediately issued by the null(M) program in an orthonormal form.

The graphs of linearly independent functions $\Phi_1(x)$ and $\Phi_2(x)$ satisfying the Schrödinger equation (1), shown in Figure 1, were calculated by this method. This method completely replaces the “sweep method” known in computational mathematics and even surpasses it in terms of the solution accuracy.

On determining the functions $\Phi_1(x)$ and $\Phi_2(x)$ we continue the solution with reference to the entire real axis x by cross-linking with the solutions outside the barrier interval. It is assumed that the solutions in different areas have the following form:

$$\begin{aligned}\psi(x) &= e^{ikx} - D \cdot e^{-ikx} & x < 0, \\ \psi(x) &= A \cdot \Phi_1(x) + B \cdot \Phi_2(x) & 0 < x < L, \\ \psi(x) &= C \cdot e^{ik(x-L)} & x > L.\end{aligned}\quad (6)$$

The latter expressions imply that within the region in front of the barrier there are both an incident and a reflected wave, and behind the barrier there is only one passing wave. The problem of cross-linking the solutions consists in determining the four coefficients A, B, C, D from the condition that the ψ function values are equal to its derivative at the contact points of the adjacent solutions. This leads to a system of four linear algebraic equations:

$$\begin{pmatrix} \Phi_1(0) & \Phi_2(0) & 0 & -1 \\ \Phi_1'(0) & \Phi_2'(0) & 0 & -ik \\ \Phi_1(L) & \Phi_2(L) & -1 & 0 \\ \Phi_1'(L) & \Phi_2'(L) & -ik & 0 \end{pmatrix} \cdot \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \begin{pmatrix} 1 \\ ik \\ 0 \\ 0 \end{pmatrix} \quad (7)$$

Since the coefficients A, B, C, D obtained from system (7) are complex quantities, the function $\psi(x)$ expressed by formulas (6) is also a complex quantity.

In quantum mechanics the function $\psi(x)$ expressed by formulas (6) and (7) is less significant than the square of its module $\rho = |\psi|^2$ because it is equal to the density of probability that the particle is at a point with the coordinate x . If the graph of the function $\rho(x)$ is displayed, it usually fluctuates strongly with a doubled spatial frequency equal to $2k$ due to the interference of the incident and the reflected waves. Therefore, such a graph is rarely presented on the screen. Instead, more informative parameters appear to be the current transmission coefficient $a = |C|^2$ and the reflection coefficient $b = |D|^2$.

The system of equations given in (7) is particular as the following equation is always observed:

$$|C|^2 + |D|^2 = 1 \quad (8)$$

That is, the sum of the transmission and the reflection coefficients is equal to unity, and this equality can be used

as a control tool for calculations. The current values of $C(x)$ and $D(x)$ can be determined from the same system of equations (7) in which the letter L is replaced by the letter x .

Figure 2 shows how the graphs of the functions $\rho(x) = |\psi|^2$ and $a(x)$ look against the background of the composite potential barrier $U(x)$ given in the numerical form.

Figure 2: Result of numerical solution of Schrödinger differential equation

The calculation was carried out according to formulas (6) and (7) observing that the mass m and the energy E of the particle had the following dimensionless values: $E = 0.5$; $m = 4$.

Thus, the described method of cross-linking applied for linearly independent solutions gives acceptable results in some cases. However, since it is only numerical, it does not allow for complete evaluation of the shape of the barrier influencing the transmission coefficient of particles.

3 The Schrödinger integral equation

In addition to the cross-linking method of solutions, there is also an approach based on the fact that the Schrödinger differential equation (1) can be reduced to the corresponding integral equation, which has the form:

$$\psi(x) - \frac{2m}{2ik} \int_{-\infty}^{\infty} e^{ik|x-\zeta|} U(\zeta) \psi(\zeta) d\zeta = e^{ikx}. \quad (9)$$

Such an integral equation is given in the well-known book by Morse and Feshbach [53].

This large book pays much attention to the description of various approximate methods for solving equation (9), such as the iterative-perturbation Born approximations, the Fredholm series, long-wave approximations, short-wave approximations, and WKBJ-approximations. The abbreviation WKBJ stands for the first letters of the names G.

Wentzel, H.A. Kramers, L. Brillouin, and H. Jeffreys. These researchers more or less independently discovered this method in connection with solving various problems.

However, such approximate methods are no longer of great necessity as in reality it is possible to formally obtain the exact solution for integral equation (9) because it is similar to an integral equation with a degenerate kernel in its form. To show this we use the following identity which, in essence, is the expansion of the $f(x-h)$ function at the point x :

$$f(x-h) \equiv e^{-h \frac{d}{dx}} f(x). \quad (10)$$

Applying identity (10) to equation (9) we can write it in the form:

$$\psi(x) - \lambda \left(\int_{-\infty}^{\infty} U(\zeta) \psi(\zeta) e^{-\zeta \frac{d}{dx}} d\zeta \right) e^{ik|x|} = e^{ikx}, \quad (11)$$

$$\text{where } \lambda = \frac{m}{ik} = \frac{1}{2i} \sqrt{\frac{2m}{E}}.$$

The integral expression in parentheses in the last formula represents some analytic function of the parameter $p = d/dx$. Let us introduce the following notation for it:

$$\int_{-\infty}^{\infty} U(\zeta) \psi(\zeta) e^{-\zeta \frac{d}{dx}} d\zeta = \int_{-\infty}^{\infty} U(\zeta) \psi(\zeta) e^{-\zeta p} d\zeta = G(p), \quad (12)$$

$$p = \frac{d}{dx}.$$

Then equation (11) can be rewritten in the following form:

$$\psi(x) - \lambda \cdot G(p) \cdot e^{-ik|x|} = e^{ikx}. \quad (13)$$

Here the form of the differential operator $G(p)$ acting on the function to the right is not known because the function ψ in formula (12) is not known, either. However, it can be found from expression (13). Multiplying (13) by $U(x) \exp(-xp)$ and performing integration in infinite limits, we get:

$$\begin{aligned} & \left(\int_{-\infty}^{\infty} U(x) \psi(x) e^{-xp} dx \right) \\ & - \lambda G(p) \cdot \left(\int_{-\infty}^{\infty} e^{ik|x|} U(x) e^{-xp} dx \right) \\ & = \left(\int_{-\infty}^{\infty} e^{ikx} U(x) e^{-xp} dx \right). \end{aligned} \quad (14)$$

Or:

$$\begin{aligned} G(p) \cdot \left[1 - \lambda \int_{-\infty}^{\infty} e^{ik|x|} U(x) \cdot e^{-xp} dx \right] \\ = \int_{-\infty}^{\infty} e^{ix(k+ip)} U(x) dx. \end{aligned} \quad (15)$$

Hence, the expression for the differential operator $G(p)$ has the form:

$$\lambda G(p) = \frac{\lambda \int_{-\infty}^{\infty} e^{ix(k+ip)} U(x) dx}{1 - \lambda \int_{-\infty}^{\infty} e^{ik|x|} U(x) e^{-xp} dx} \quad (16)$$

In addition, if we assume (without loss of generality) that the function $U(x)$ is identically different from zero only for $x > 0$, the integrals in the numerator and the denominator of formula (16) will coincide.

Thus, introducing (16) into (13) we obtain the solution of the Schrödinger integral equation (9) in the following differential operator form:

$$\begin{aligned} \psi(x) = e^{ikx} + \left[\frac{\lambda \int_{-\infty}^{\infty} e^{ix(k+ip)} U(x) dx}{1 - \lambda \int_{-\infty}^{\infty} e^{ix(k+ip)} U(x) dx} \right] \cdot e^{ik|x|}, \quad (17) \\ p = \frac{d}{dx} \end{aligned}$$

It is known that if some differential operator $Q(p)$ acts on an exponential function, the result will be the following expression:

$$Q\left(\frac{d}{dx}\right) \cdot e^{\mu x} = Q(\mu) \cdot e^{\mu x} \quad (18)$$

However, in formula (17) the differential operator acts on the exponential of the module of the argument, therefore, formula (18) is incorrect in this case. At the same time the exponent of the module of the argument can be reduced to an exponential form if to use the Fourier identity which is valid for any function $f(x)$:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega x} d\omega \int_{-\infty}^{\infty} e^{i\omega \alpha} f(\alpha) d\alpha \quad (19)$$

Introducing (19) in (17) we obtain:

$$\begin{aligned}\psi(x) &= e^{ikx} + \left[\frac{\lambda \int_{-\infty}^{\infty} e^{ix(k+ip)} U(x) dx}{1 - \lambda \int_{-\infty}^{\infty} e^{ix(k+ip)} U(x) dx} \right] \\ &\cdot \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega x} d\omega \int_{-\infty}^{\infty} e^{i\omega \alpha} e^{ik|\alpha|} d\alpha \\ &= e^{ikx} + \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega x} \left[\frac{\lambda \int_{-\infty}^{\infty} e^{ix(k+\omega)} U(x) dx}{1 - \lambda \int_{-\infty}^{\infty} e^{ix(k+\omega)} U(x) dx} \right] d\omega \\ &\cdot \int_{-\infty}^{\infty} e^{ik|\alpha|} \cdot e^{i\omega \alpha} d\alpha.\end{aligned}\quad (20)$$

For further transformations of formula (20) it is convenient to introduce the concept of the spectrum of the potential barrier $B(\omega)$ and calculate the integral over the variable α in the explicit form:

$$\begin{aligned}B(\omega) &= \int_{-\infty}^{\infty} U(x) e^{i\omega x} dx, \\ \int_{-\infty}^{\infty} e^{ik|\alpha|} \cdot e^{i\omega \alpha} d\alpha &= \frac{2ik}{k^2 - \omega^2}\end{aligned}\quad (21)$$

Then formula (20) takes the form:

$$\begin{aligned}\psi(x) &= e^{ikx} \\ &+ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega x} \left[\frac{\lambda \cdot B(\omega + k)}{1 - \lambda \cdot B(\omega + k)} \right] \frac{2ik}{k^2 - \omega^2} d\omega\end{aligned}\quad (22)$$

This is the solution of the Schrödinger integral equation (9) written as an integral along the real axis ω in the spectral region. The factor enclosed in square brackets is responsible for the influence of the shape of the barrier on the de Broglie wave passing through it. Since the integrand has two poles $\omega = \pm k$ and possibly other poles of the denominator of the fraction in square brackets, the integrand is considered to be meromorphic. If we knew all its poles, integral (22) could be found as the sum of the residues. In numerical integration, integral (22) should be taken along a line parallel to the real axis and lying slightly below it.

4 Further transformations of the solution

A solution of form (22) can be transformed in such a way that it is expressed as an integral along the real axis x . To

do this we need to introduce a new function $K(x)$ related to the spectrum of the potential barrier $U(x)$ by the relations known from the theory of integral Fourier transforms:

$$\frac{\lambda B(\omega + k)}{1 - \lambda B(\omega + k)} = \int_{-\infty}^{\infty} K(x) \cdot e^{i\omega x} dx, \quad (23)$$

$$K(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[\frac{\lambda B(\omega + k)}{1 - \lambda B(\omega + k)} \right] \cdot e^{-i\omega x} d\omega$$

Then formula (22) can be written as a sequence of three integrals:

$$\begin{aligned}\psi(x) &= e^{ikx} \\ &+ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega x} d\omega \int_{-\infty}^{\infty} K(\beta) \cdot e^{i\omega \beta} d\beta \int_{-\infty}^{\infty} e^{ik|\alpha|} e^{i\omega \alpha} d\alpha \\ &= e^{ikx} \\ &+ \int_{-\infty}^{\infty} K(\beta) d\beta \int_{-\infty}^{\infty} e^{ik|\alpha|} d\alpha \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(-x+\beta+\alpha)} d\omega \right).\end{aligned}\quad (24)$$

The last integral in this formula, with respect to the variable ω , is the Dirac delta function, therefore, we obtain:

$$\begin{aligned}\psi(x) &= e^{ikx} + \int_{-\infty}^{\infty} K(\beta) d\beta \int_{-\infty}^{\infty} e^{ik|\alpha|} \delta(\alpha - (x - \beta)) d\alpha \\ &= e^{ikx} + \int_{-\infty}^{\infty} K(\beta) \cdot e^{ik|x-\beta|} d\beta.\end{aligned}\quad (25)$$

Thus, instead of formula (22), to find the wave function $\psi(x)$ we can use a more compact expression:

$$\psi(x) = e^{ikx} + \int_{-\infty}^{\infty} K(\zeta) \cdot e^{ik|x-\zeta|} d\zeta \quad (26)$$

For its calculation it is necessary to find numerically the function $K(x)$ associated with the barrier spectrum by formulas (23).

5 The reflection and transmission coefficients

Solving the Schrödinger equation using the integral equation method does not provide observation of the cross-linking condition. Therefore, it is necessary to make sure that the boundary conditions are satisfied at $x = \pm \infty$. For

this purpose, we will rewrite equation (27) in more detail:

$$\psi(x) = e^{ikx} \left[1 + \int_{-\infty}^x K(\zeta) e^{-ik\zeta} d\zeta \right] + e^{-ikx} \int_x^{\infty} K(\zeta) e^{ik\zeta} d\zeta \quad (27)$$

From here we see that at a great distance $|x| \rightarrow \infty$ the function $\psi(x)$ behaves as follows:

$$\begin{aligned} \psi(x) &\approx e^{ikx} \left[1 + \int_{-\infty}^{\infty} K(\zeta) e^{-ik\zeta} d\zeta \right], \quad x \rightarrow \infty, \\ \psi(x) &\approx e^{ikx} + e^{-ikx} \int_{-\infty}^{\infty} K(\zeta) e^{ik\zeta} d\zeta, \quad x \rightarrow -\infty. \end{aligned} \quad (28)$$

That is, behind the barrier only the incident wave is preserved, and in front of the barrier there are both the incident and the reflected wave of the matter. Therefore, the boundary conditions of the problem at infinity are satisfied.

We can now immediately get the expression for the reflection coefficient:

$$b = \left| \int_{-\infty}^{\infty} K(\zeta) e^{ik\zeta} d\zeta \right|^2 \quad (29)$$

Further, we note that the reflection coefficient (29) can also be written explicitly through the spectrum of the potential barrier $B(\omega)$. Applying formula (23) we find:

$$b = \left| \frac{\lambda B(2k)}{1 - \lambda B(2k)} \right|^2 \quad (30)$$

After the reflection coefficient is found, the passage coefficient can be determined by the formula:

$$a = 1 - b. \quad (31)$$

6 Examples

There are cases when the spectral function of the potential barrier is found analytically.

For example, for a barrier in the form of the Gaussian pulse we get:

$$U(x) = e^{-\beta^2 x^2}, \quad B(\omega) = \frac{\sqrt{\pi}}{\beta} \cdot e^{-\frac{\omega^2}{4\beta^2}} \quad (32)$$

In this case, formula (30) for the reflection coefficient takes the form:

$$\begin{aligned} b(m, E) &= \left| \frac{\lambda \beta^{-1} \sqrt{\pi} e^{-\frac{k^2}{\beta^2}}}{1 - \lambda \beta^{-1} \sqrt{\pi} e^{-\frac{k^2}{\beta^2}}} \right|^2, \quad \text{where } k = 2mE, \\ \lambda &= \frac{2m}{2ik} \end{aligned} \quad (33)$$

Figure 3 shows the shape of the potential barrier and the graphs of the reflection coefficient $b(m, E)$ calculated by formula (33).

Figure 3: Single barrier (left) and reflection coefficient depending on particle energy (right)

These graphs demonstrate that particles with a larger mass at the same energy E are reflected more strongly for this type of barrier, while smaller particles with a very small mass pass through it being weakly reflected at sufficiently high energies.

Let us now consider the question of how the compound potential barrier which, for example, consists of two identical barriers spaced apart by a distance of d affects the reflection coefficient. The shape of such a barrier is as follows:

$$U(x) = e^{-\beta^2 x^2} + e^{-\beta^2 (x-d)^2} \quad (34)$$

Calculating its spectrum, we obtain:

$$\begin{aligned} B(\omega) &= \int_{-\infty}^{\infty} e^{-\beta^2 x^2} e^{i\omega x} dx + \int_{-\infty}^{\infty} e^{-\beta^2 (x-d)^2} e^{i\omega x} dx \\ &= \int_{-\infty}^{\infty} e^{-\beta^2 x^2} e^{i\omega x} dx + e^{i\omega d} \int_{-\infty}^{\infty} e^{-\beta^2 (x-d)^2} e^{i\omega (x-d)} dx \\ &= \int_{-\infty}^{\infty} e^{-\beta^2 x^2} e^{i\omega x} dx \cdot [1 + e^{i\omega d}] \\ &= \frac{\sqrt{\pi}}{\beta} e^{-\frac{\omega^2}{4\beta^2}} \cdot [1 + e^{i\omega d}]. \end{aligned} \quad (35)$$

Thus, the addition of a new barrier introduces only an additional factor in its spectrum.

Formula (33) for the reflection coefficient, therefore, takes the form:

$$b(m, E, d) = \left| \frac{\lambda \beta^{-1} \sqrt{\pi} e^{-\frac{k^2}{\beta^2}} \cdot (1 + e^{2ikd})}{1 - \lambda \beta^{-1} \sqrt{\pi} e^{-\frac{k^2}{\beta^2}} \cdot (1 + e^{2ikd})} \right|^2 \quad (36)$$

Due to the presence of an additional factor in formula (36), it is always possible to find such values of the distances d between two barriers at which the reflection coefficient $b(m, E_0, d)$ automatically vanishes at energy values $E = E_0$. Equating the factor (in parentheses) to zero we get:

$$e^{2ikd} = -1 = e^{i\pi(2n+1)}, \quad d = \frac{\pi(n + \frac{1}{2})}{k} = \frac{\pi(n + \frac{1}{2})}{\sqrt{2mE_0}}, \quad (37)$$

$$n = 0, 1, 2, 3 \dots$$

Choosing the distance d in formula (36) in this way we achieve the selectivity effect, i.e. a particle with the mass m and energy E_0 freely passes, without any reflection, through a potential barrier consisting of two pulses.

Figure 4 shows the position of the composite potential barrier $U(x)$ and the result of calculating the reflection coefficient by formula (36).

Figure 4: Composite barrier (left) and reflection coefficient (right, dotted line - reflection coefficient of single barrier)

The dashed line on the right side shows, for comparison, a graph of the reflection coefficient for a single barrier. It can be seen from this calculation that the double barrier significantly reduces the reflection coefficient, compared with the single barrier, and turns it to zero for a discrete series of energy values E , as predicted by formula (36).

When the Schrödinger equation (1) was solved by the numerical method of cross-linking for composite barriers, significant fluctuations in the reflection coefficient b and the transmission coefficient a with a change in energy E were also quite often observed. The method of cross-linking is purely numerical in nature, and it is difficult to understand the reason why a particle passes through a double barrier more easily than through a single barrier. As

a result, there has been a tendency to attribute this effect to counting errors.

As for formulas (36) and (37), they are a consequence of the exact solution of the Schrödinger integral equation (9) and, therefore, are not in doubt. Compound potential barriers are accompanied by potential wells the bound states of which resonate with the incident wave.

Let the composite barrier have the form of two Gaussian pulses: $U(x) = \exp(-\beta^2 x^2)$, $U(x) = \exp(-\beta^2 (x - d)^2)$. We will consider the nature of passage of isotopes with a change in the distance d between the vertices of the pulses. Figure 5 shows the permeability distributions of helion a_3 and helium a_4 , as well as the degree of separation for the mixture $\chi = a_3/a_4$.

Figure 5: Change in permeability and selectivity with increasing distance between barriers

The change in permeability takes place in the form of vibrations. Moreover, these fluctuations nearly occur in antiphase. Because of this, there arise bursts of selectivity. Figures 6, 7 show the distributions of the same characteristics, but for the cases $E = 0.49$ and $E = 0.475$. We can observe a quantum character of the change in selectivity with the distance between the barriers, as well as a sharp increase in the degree of separation of the mixture in narrow bands.

Figure 6: Change in permeability and selectivity

Figure 7: Change in permeability and selectivity with increasing distance between barriers

Figures 8, 9 show that at low temperatures there are areas that correspond to super-permeability of the composite membrane with respect to helion. Moreover, the system as a whole is characterized by hyper-selectivity. In addition, with a decrease in temperature, an expansion of the super-permeability bands is observed.

Figure 8: Selectivity at particle energy value $E = 0.375$

7 Conclusion

The solution of the Schrödinger integral equation in the differential operator form was obtained. The expressions for the reflection and transmission coefficients immediately follow from this form. Due to the presence of the second barrier, the reflection coefficient vanishes in a sequence of values along the distances between the barriers. This means that at these values the transmission coefficient of helium is equal to unity. At the same time, the helium isotope, helion, has a different mass; therefore, it has a non-

Figure 9: Selectivity at particle energy $E = 0.3$

zero reflection coefficient at the found values of the distance between the barriers. Thus, one of the components passes through the system of barriers, while the other does not pass at all. As a result, we get an effective system for sifting isotopes. This system can be configured for screening by changing the distance between the barriers. Moreover, the conclusions turn out to be true for ultrathin barriers made of any materials.

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