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PENETRATION OF PARTICLES THROUGH MULTI-BARRIER SYSTEMS

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Abstract. The paper gives a theoretical justification for the effect of increasing permeability of ultra-thin membranes by altering their internal material structure, namely through the process of creating one or two energy voids within the permeable layer. An effective computing technology for solving the stationary Schrödinger equation is also described.

1 Introduction

Molecular dynamics is widely used in studies of physical processes in nanoporous structures [1-15], as well as in studying mechanical behaviour of nanoporous crystals [18-22]. However, for problems associated with passage of molecules through a barrier, wave dynamics appears to be more effective [23, 24]. In multi-barrier systems, in comparison with the case of a monolayer, particles are accumulated in a potential well, and thereby particle concentration in front of the barrier and behind it is increased. Since all this occurs in the wave mode of mass concentration and in the centre of the well there is the maximum amplitude of oscillations, the system with energy wells show generation of more intense transmitted waves, which drives a great mass over the barrier. Material particles: electrons, protons and atoms are associated with the de Broglie wave. If the wave frequency coincides with the frequency of one of the energy wells enclosed between two barriers, the system shows resonance phenomena which lead to an increase in particle concentration in the whole near-barrier area, in particular, behind the barrier, which means that there is an increase in the particle transmission coefficient. Since the authors were only interested in the final result concerning the integral permeability of the membrane instead of wave dynamics as such, all the conclusions reached in the work are based on the results of solving the stationary Schrödinger equation. The results of such studies may be interesting from the standpoint of technologies for creating effective functional layers with atomic selective permeability, as well as gas separation membranes for separation of helium from natural gas and others.

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2 The method for solving the stationary Schrödinger equation

In problems of particle penetration through an energy barrier the following equation is used [25, 26]:

$$\frac{d^2\psi}{dx^2}+m\left[\lambda^2-U(x)\right]\psi=0. \tag{1}$$

This equation is commonly called the one-dimensional stationary Schrödinger equation and it describes the quantum-mechanical motion of a particle in one dimension. Here, the function $U(x)$ is the potential, λ^2 is the energy of the particle, and m is its mass. The desired function ψ is such that the square of its module determines the density of the probability of particle localization at the point x. Equation (1) is written here in the dimensionless normalized form, when the potential $U(x)$ and the energy of the particle λ^2 are attributed to the dimensional value of the potential barrier U_0, so that the maximum value of the potential $U(x)$ is assumed to be equal to 1. The mass of the particle m in equation (1) is also a dimensionless quantity referring to a certain standard value in accordance with the scales of the phenomenon under study. Clearly, equation (1) possesses not only a quantum sense. It is applicable to many other problems of theoretical physics which may consist in determining the resonant frequencies of acoustic or electromagnetic waves within an inhomogeneous cavity [27]. Equation (1) plays an important role in solutions of nonlinear partial differential equations where the method of inverse scattering is used [28]. In these problems it is necessary to restore the potential $U(x)$ when the function $\psi(x)$ is known.

The general solution of equation (1) can be obtained as a linear combination of two linearly independent solutions $w_1(x)$ and $w_2(x)$ which can be found using the traditional Runge-Kutta method by comparing the obtained result with the known exact solutions. The accuracy of calculations is controlled by the value of the Wronskian determinant $W=w_1(x)w_2'(x)-w_2(x)w_1'(x)$, as well as by the accuracy of following the equality $|B|^2+|A|^2=1$. The first item on the left side of this equation is the reflection coefficient and the second - the transmission coefficient. To meet these criteria in the numerical method of the Runge-Kutta type, one has to use a step of calculation which is too small and this greatly increases the computational time. In this connection, in this paper we propose to use a non-standard operation matrix analysis which is available in modern mathematical packages such as MatLab [29] or SciLab. This operation allows finding an orthonormal basis (null-space) for rectangular matrices.

For example, let the matrix **M** consist of 8 rows and 10 columns. Then, by carrying out the command **B**=null(**M**) we get the rectangular matrix **B** which has 10 rows and two columns each of which is orthogonal to all the rows of the matrix **M**. Additionally, the result is obtained with almost a maximum machining precision. In this method, equation (1) must be written in the finite difference form:

$$\psi_{n-1}+\left[-2+h^2m\left(\lambda^2-U_n\right)\right]\psi_n+\psi_{n+1}=0. \tag{2}$$

Next for equation (2) we construct a corresponding three-diagonal matrix, eliminate its last two lines and get the matrix **H** as a result. Calculating the null-space of the matrix **H**: **w**=null(**H**) gives a numerical representation of the fundamental solutions $w_1(x)$ and $w_2(x)$ of equation (1) in the form of two vector columns. The accuracy of the solution by this method is independent of the parameter λ and does not require a small step, which permits reliable calculation of both the function $\psi(x)$ and the transmission coefficient $D(m,\lambda)=|A|^2$ for particles passing through potential barriers of complex shapes.

2 Examples of calculations

The typical view of the graph $|\psi|^2(x)$ obtained by the numerical method is shown in fig.1, where the shape of the barrier is marked by a dotted line.

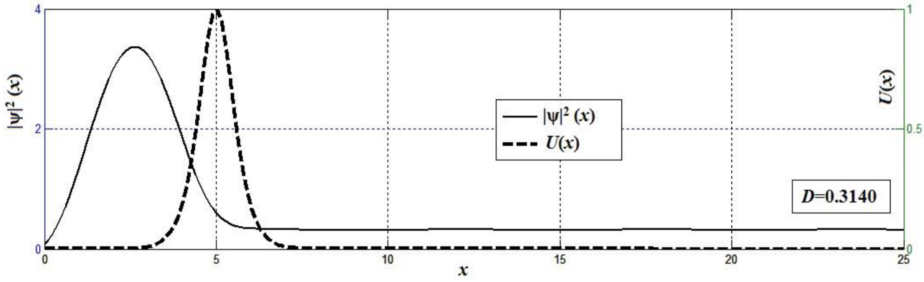

Fig. 1. Particle of parameters: m=1, λ=0.5 passing single barrier.

The transmission coefficient D in this case is of a little value equal to 0.3140. It would seem that addition of new barriers should reduce the general transmission coefficient. But, as is clear from fig.2, an increase in the number of barriers, by contrast, leads to an increase in the transmission coefficient. This is due to the fact that the density of probabilities $|\psi|^2$ in wells reaches its maximum values, which facilitates penetration of particles through the barriers.

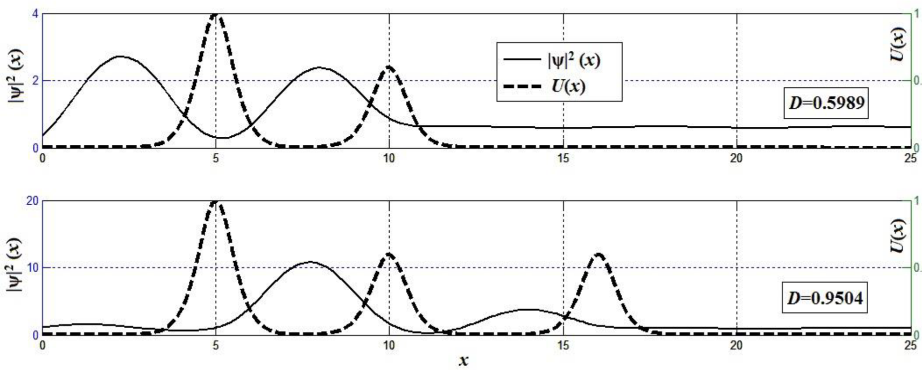

Fig. 2. Effect of adding new barriers on distribution of density of probabilities $|\psi|^2$ and particle transmission coefficient $D(m, \lambda)$.

Here we deal with a resonance effect of interaction between bound particles in potential wells and an oncoming particle. This phenomenon is observed only for certain values of the parameter λ and it is clearly seen on graphs of the function $D(\lambda)$ for a given shape of the potential barrier.

Calculations revealed that the effect of increasing permeability of a composite membrane refers only to certain particle energy. Changing the energy of particles falling onto the membrane, we inevitably get reduction of permeability for the same barrier system. Therefore, in practical problems of gas separation it is necessary to consider the Maxwell distribution of particle according to energies.

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