# An Analytical Solution to the Problem of Hydrogen Isotope Passage through Composite Membranes Made from 2D Materials 

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#### Abstract

An analytical solution to the problem of wave transport of matter through composite hyperfine barriers is constructed. It is shown that, for a composite membrane consisting of two identical ultra-thin layers, there are always distances between the layers at which the resonant passage of one of the components is realized. Resonance makes it possible to separate de Broiler waves of particles with the same properties, which differ only in masses. Broad bands of hyper-selective separation of a hydrogen isotope mixture are found at the temperature of 40 K .


Keywords: wave dynamics; compound barriers; resonant transmission; the Schrödinger equation; analytical solutions

## 1. Introduction

It becomes necessary to solve the Schrödinger equation, which is one of the most important equations of mathematical physics in modeling the processes of low-temperature separation of gas components. A fairly large number of modern works are devoted to solving the nonlinear Schrödinger equation (NLSE). In particular, a method for constructing a class of exact analytical solutions of the NLSE model with varying dispersion, nonlinearity, as well as gain or absorption, is developed in [1]. Using the Lie symmetry method, new solutions for nonlinear Schrödinger systems are constructed in [2]. Two cases of exact solutions of the NLSE and an analytical solution of the three-dimensional timeindependent equation for a charged particle in the field of an exact electric dipole are found in $[3,4]$. A functional integral, representing the solution of the wave equation, is obtained in [5]. Various properties of solutions of the extended nonlinear Schrödinger equation, the fractional nonlinear diffusion equation, and the fractional nonlinear Schrödinger equation are studied in [6,7]. A number of works are devoted to the study of solitons [8] and their stability [9], as well as to the question of soliton perturbations [10]. In [11], the authors suggest an exact analytical resolution method for stationary Schrödinger equations with polynomial potentials.

On the basis of various types of potential used in the equation, it is possible to single out works on solving the NLSE for an inseparable complex potential [12], the potential function of the Morse oscillator for a periodic external field [13], an arbitrary potential that determines bound states [14], a non-central generalized inverse quadratic potential of Yukawa within the Nikiforov-Uvarov framework [15]. Analytical solutions of the Schrödinger equation for some diatomic molecular potentials with any angular
momentum are obtained in [16]. Using the Nikiforov-Uvarov method, an exact solution of the N -dimensional radial Schrödinger equation with a generalized Cornell potential is obtained in [17], and one- and two-dimensional NLSE solutions with a double-well potential and a Stark-type perturbing term are presented in [18]. The work presented in [19] proposes a solution to the one-dimensional Schrödinger equation for a potential of a special form. The solution is presented in terms of non-integer order Hermite functions. Finally, in [20] the authors find and analyze the analytical Schrödinger equations with a singular potential of fractional degree called the potential of the second Exton.

The Linear Schrödinger Equation (LSE) is considered learned. However, the problem of wave transport through composite barriers is of great interest for membrane technologies of low-temperature gas separation.

## 2. Materials and Methods

### 2.1. The Schrödinger Differential Equation

The differential equation of wave dynamics is:

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \Delta \Psi+U \Psi+\frac{\hbar}{i} \frac{\partial \Psi}{\partial t}=0 \tag{1}
\end{equation*}
$$

where $\Psi$ is the wave function; $\hbar$ is the Planck's constant; $U$ is the energy of interaction between the particle and the environment; $m$ is the mass of the particle, $\Delta$ is the Laplace operator; $i$ is the imaginary unit.

In the special case in which the potential energy $U$ is clearly independent of time, the solution to Equation (1) is found in the form:

$$
\begin{equation*}
\Psi=\psi e^{-i E t / \hbar} \tag{2}
\end{equation*}
$$

where $E$ is the particle energy and $\psi$ is the wave function of coordinates.
Then, the following stationary Schrödinger equation can be used to find the amplitude of the wave $\psi$ :

$$
\begin{equation*}
\Delta \psi+\frac{2 m}{\hbar^{2}}(E-U) \psi=0 \tag{3}
\end{equation*}
$$

Below, we will present some analytical constructions which prove to be very effective in analysing problems of isotope transmission through composite membranes. With problems concerning the low-temperature membrane separation of gas mixtures, the direction of transfer, perpendicular to the membrane surface, is of decisive importance. Therefore, only a one-dimensional Schrödinger equation is enough to consider.

It is also convenient to have a dimensionless form of the equation of wave transfer of matter.
If the particle mass is referred to as $m_{0}$, which is the mass of a hydrogen atom, the energy scale is $U_{0}$, which is the depth of the potential well in the distribution of the energy of a pair of interactions between the membrane substance and mobile particles, and the length of the scale is taken as:

$$
\begin{equation*}
L=\hbar / \sqrt{m_{0} U_{0}} \tag{4}
\end{equation*}
$$

then the dimensionless equation of wave dynamics does not contain the Planck's constant $\hbar$ :

$$
\begin{equation*}
\frac{d^{2} \psi}{d x^{2}}+2 m(E-U(x)) \psi=0 \tag{5}
\end{equation*}
$$

In record (5), all quantities are dimensionless, including the coordinate $x$.
Thus, we reduced the number of problem constants by one. This is essential for further analytical calculations.

### 2.2. The Integral Schrödinger Equation and Its Transformations

The implementation of numerical methods for solving the Schrödinger differential equation is focused on the finite region of variations of the independent variable, as well as on matching the obtained numerical data with asymptotic distributions of the calculated value. Normally, the conditions of matching are understood as the equality of the wave function itself and its derivative. However, there is no justification for using this form of conditions. The size of the finite region of integration also requires substantiation. In this
connection, aiming to carry out integration along the entire real axis is important. This can be done analytical methods. The Schrödinger integral equation is quite suitable for analytical analysis:

$$
\begin{equation*}
\psi(x)-\frac{2 m}{2 i k} \int_{-\infty}^{\infty} e^{i k|x-\zeta|} U(\zeta) \psi(\zeta) d \zeta=e^{i k x} \tag{6}
\end{equation*}
$$

where $k=\sqrt{2 m E}$. In their book, Morse and Feshbach note the equivalence of the differential and integral description of propagation of matter waves [21].

Equation (6) is similar in form to an integral equation with a degenerate kernel. However, in fact, it is not the same. In order to separate the variables in the integral term of Equation (6), it is necessary to use the operational calculus. A function of one variable and a differential operator $d / d x$ can be distinguished in the kernel of the equation. To do this, one is only required to use the definition of the shift operator:

$$
\begin{equation*}
e^{-h \frac{d}{d x}} f(x)=f(x-h) \tag{7}
\end{equation*}
$$

It is easy to verify that (7) is true if the operator exponent on the left is expanded in a Taylor series in a neighborhood of zero, and the function $f(x-h)$ is expanded in a neighborhood of the point $x$. Applying equality (7) to (6), we can rewrite the original equation in the following form:

$$
\begin{equation*}
\psi(x)-\lambda\left(\int_{-\infty}^{\infty} U(\zeta) \psi(\zeta) e^{-\zeta \frac{d}{d x}} d \zeta\right) e^{i k|x|}=e^{i k x}, \lambda=\frac{m}{i k}=\frac{1}{2 i} \sqrt{\frac{2 m}{E}} \tag{8}
\end{equation*}
$$

Let us pay attention to the expression in parentheses. This expression is a differential operator and, at the same time, is an analytical function of some parameter $p$ :

$$
\begin{equation*}
\int_{-\infty}^{\infty} U(\zeta) \psi(\zeta) e^{-\zeta \frac{d}{d x}} d \zeta=\int_{-\infty}^{\infty} U(\zeta) \psi(\zeta) e^{-\zeta p} d \zeta=L(p), p=\frac{d}{d x} \tag{9}
\end{equation*}
$$

Taking into account the introduced notation, we can write Equation (8) in the following form:

$$
\begin{equation*}
\psi(x)-\lambda L(p) e^{i k|x|}=e^{i k x} \tag{10}
\end{equation*}
$$

The form of a differential operator acting on the exponential function on the right of it is still unknown. However, it can be found. Multiplying (10) by $U(x) \exp (-x p)$ and performing integration in infinite limits, we obtain:

$$
\begin{equation*}
\left(\int_{-\infty}^{\infty} U(x) \psi(x) e^{-x p} d x\right)-\lambda L(p)\left(\int_{-\infty}^{\infty} e^{i k|x|} U(x) e^{-x p} d x\right)=\left(\int_{-\infty}^{\infty} e^{i k x} U(x) e^{-x p} d x\right) \tag{11}
\end{equation*}
$$

Two differential operators appear here, for which we introduce the following notation:

$$
\begin{equation*}
B(p)=\int_{-\infty}^{\infty} e^{i k x} U(x) e^{-x p} d x, Q(p)=\int_{-\infty}^{\infty} e^{i k|x|} U(x) e^{-x p} d x \tag{12}
\end{equation*}
$$

Taking into account these notations, operator equality (11) takes the form:

$$
\begin{equation*}
L(p)[1-\lambda Q(p)]=B(p) \tag{13}
\end{equation*}
$$

Hence, we get:

$$
\begin{equation*}
L(p)=\frac{B(p)}{1-\lambda Q(p)} \tag{14}
\end{equation*}
$$

Sometimes integrals (12) can be calculated analytically. In a general sense, the result of numerical integration obtained on the basis of the simplest quadrature formulas of the trapezoid method is suitable. In any case, these integrals depend only on the shape of the potential barrier.

Using (14), Equation (10) can be rewritten as:

$$
\begin{equation*}
\psi(x)=e^{i k x}+\frac{\lambda B(p)}{1-\lambda Q(p)} e^{i k|x|} \tag{15}
\end{equation*}
$$

The operators $B(p)$ and $Q(p)$, which are included in the last equation, as can be seen from (12), can be determined based on the given shape of the barrier $U(x)$. In principle, relation (15) already determines the desired distribution of $\psi(x)$. However, it still has an operator form, so let us return to relation (10).

If the differential operator $L(p)$ acted on an exponential function of the usual form, the result would be as follows:

$$
\begin{equation*}
L\left(\frac{d}{d x}\right) e^{\mu x}=L(\mu) e^{\mu x} \tag{16}
\end{equation*}
$$

However, in formula (10) this operator acts on the exponent of the modulus of the argument. Therefore, direct application of (16) is impossible. Nevertheless, the exponent from the modulus of the argument can be reduced to the usual exponent if we use the Fourier identity:

$$
\begin{equation*}
e^{i k|x|}=\frac{1}{2 \pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i \omega x} e^{i \omega \alpha} e^{i k|\alpha|} d \alpha d \omega \tag{17}
\end{equation*}
$$

Applying rules (16) and (17) to formula (10) we obtain:

$$
\begin{equation*}
\psi(x)=e^{i k x}+\frac{1}{2 \pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} L(-i \omega) e^{-i \omega x} e^{i k|\alpha|} e^{i \omega \alpha} d \alpha d \omega \tag{18}
\end{equation*}
$$

Expression (18) is exactly the solution of the Schrödinger integral equation written as a double integral along the spectral axis. As can be seen, in contrast to (6), its right-hand side contains all known quantities since the functions $B(-i \omega)$ and $Q(-i \omega)$ which make up $L(-i \omega)$ and are called the spectra of the barrier are determined only by its shape, i.e., are known functions of the problem statement. In addition to the shape of the barrier, we know the character of the asymptotic behavior of the solution with respect to the physical variable $x$.

By this stage of integration, we have already got rid of the differential operator $L(p)$ having replaced it by the function $L(-i \omega)$ using rule (16). Let us denote the function $L(-i \omega)$ by $G(\omega)$. Then, taking into account (14), we get:

$$
\begin{equation*}
G(\omega)=\frac{\lambda B(-i \omega)}{1-\lambda Q(-i \omega)}=\frac{\lambda \int_{-\infty}^{\infty} U(x) e^{i x(\omega+k)} d x}{1-\lambda \int_{-\infty}^{\infty} U(x) e^{i k|x|} e^{i \omega x} d x} \tag{19}
\end{equation*}
$$

As a result, we have:

$$
\begin{equation*}
\psi(x)=e^{i k x}+\frac{1}{2 \pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i \omega x} G(\omega) e^{i k|\alpha|} e^{i \omega \alpha} d \alpha d \omega \tag{20}
\end{equation*}
$$

Let us also suppose that function $G(\omega)$ is the spectrum of some function $K(x)$. This means that the following conditions are observed:

$$
\begin{equation*}
G(\omega)=\int_{-\infty}^{\infty} K(x) e^{i \omega x} d x, K(x)=\frac{1}{2 \pi} \int_{-\infty}^{\infty} G(\boldsymbol{\omega}) e^{-i \omega x} d \omega \tag{21}
\end{equation*}
$$

Introducing (21) in (20), we find:

$$
\begin{align*}
& \psi(x)=e^{i k x}+\frac{1}{2 \pi} \int_{-\infty}^{\infty} e^{-i \omega x} \int_{-\infty}^{\infty} K(\beta) e^{i \omega \beta} \int_{-\infty}^{\infty} e^{i k|\alpha|} e^{i \omega \alpha} d \alpha d \beta d \omega= \\
& =e^{i k x}+\int_{-\infty}^{\infty} K(\beta) \int_{-\infty}^{\infty} e^{i k|\alpha|}\left(\frac{1}{2 \pi} \int_{-\infty}^{\infty} e^{i \omega(-x+\beta+\alpha)} d \omega\right) d \alpha d \beta \tag{22}
\end{align*}
$$

The integral in parentheses of the last expression is the Dirac delta function. Therefore, we can further write:

$$
\begin{equation*}
\psi(x)=e^{i k x}+\int_{-\infty}^{\infty} K(\beta) d \beta \int_{-\infty}^{\infty} e^{i k|\alpha|} \delta(\alpha-(x-\beta)) d \alpha=e^{i k x}+\int_{-\infty}^{\infty} K(\beta) e^{i k|x-\beta|} d \beta \tag{23}
\end{equation*}
$$

Thus, the most compact form of the solution, in which the integral is taken in the direction of variation of the physical variable, is as follows:

$$
\begin{equation*}
\psi(x)=e^{i k x}+\int_{-\infty}^{\infty} K(\zeta) e^{i k|x-\zeta|} d \zeta \tag{24}
\end{equation*}
$$

When solving the Schrödinger equation by the method of the integral equation, the fulfilment of the matching conditions is not provided. In this case, it is only necessary to check how the solution behaves at $x= \pm \infty$. For this purpose, we will rewrite solution (24) in terms of integrals with a variable upper or lower limit:

$$
\begin{equation*}
\psi(x)=e^{i k x}\left[1+\int_{-\infty}^{x} K(\zeta) e^{-i k \zeta} d \zeta\right]+e^{-i k x}\left[\int_{x}^{\infty} K(\zeta) e^{i k \zeta} d \zeta\right] \tag{25}
\end{equation*}
$$

Based on this form of writing the distribution $\psi(x)$, we can draw a conclusion about the asymptotic behavior of the wave function:

$$
\begin{align*}
& \psi(x) \approx e^{i k x}\left[1+\int_{-\infty}^{\infty} K(\zeta) e^{-i k \zeta} d \zeta\right], x \rightarrow \infty  \tag{26}\\
& \psi(x) \approx e^{i k x}+e^{-i k x} \int_{-\infty}^{\infty} K(\zeta) e^{i k \zeta} d \zeta, x \rightarrow-\infty
\end{align*}
$$

As can be seen from these relations, after the barrier, there is a passing wave, and before the barrier there are both the incident and the reflected waves. Thus, solution (24) correctly reflects the asymptotic behavior of the desired function.

### 2.3. The Reflection Coefficient

It was found in [22] that the Fourier spectrum for the wave function $\psi$ has the form:

$$
\begin{equation*}
G(\omega, k)=\int_{-\infty}^{\infty} \psi(x) e^{i \omega x} d x=\frac{\lambda B(\omega, k)}{1-\lambda B(\omega, k)} \tag{27}
\end{equation*}
$$

Here, parameters $k$ and $\lambda$ are determined by the particle mass $m$ and the energy $E$ :

$$
\begin{equation*}
k=\sqrt{2 m E}, \lambda=\frac{m}{i k} \tag{28}
\end{equation*}
$$

As for expression $B(\omega, k)$, this depends on the shape of the potential barrier $U(x)$ and is represented by the following integral:

$$
\begin{equation*}
B(\omega, k)=\int_{-\infty}^{\infty} U(x) e^{i x(\omega+k)} d x \tag{29}
\end{equation*}
$$

The reflection coefficient $R$ of the particle flux has the following formula:

$$
\begin{equation*}
R(k, \lambda)=\left|\frac{\lambda B(\omega, k)}{1-\lambda B(\omega, k)}\right|_{\omega=k}^{2} \tag{30}
\end{equation*}
$$

In particular cases of forms of the potential barrier $U(x)$ integral, (29) can be calculated explicitly; then, the corresponding final formulas can be obtained for the reflection coefficient $R$.

## 3. Results

### 3.1. Determining the $B(\omega, k)$ Integral

It is convenient to distinguish between even and odd forms of the potential barrier $U(x)$, since formulas (29) are then written in the form of one-sided integrals. For example, in the case of an even function $U(x)$ integral, (29) is written in the form:

$$
\begin{equation*}
B(\omega, k)=2 \int_{0}^{\infty} U(x) \cos (\omega+k) x d x \tag{31}
\end{equation*}
$$

Formula (31) means that it is enough to know only one function, $B_{0}(\omega)$, which is the cosine Fourier transform for the potential barrier. Using it, we can calculate function $B(\omega, k)$ :

$$
\begin{equation*}
B_{0}(\omega)=\int_{0}^{\infty} U(x) \cos \omega x d x, B(\omega, k)=2 B_{0}(\omega+k) \tag{32}
\end{equation*}
$$

In this case, the reflection coefficient (30) is equal to:

$$
\begin{equation*}
R(k, \lambda)=\left|\frac{\lambda B_{0}(2 k)}{1-\lambda B_{0}(2 k)}\right|^{2}, B_{0}(\omega)=2 \int_{0}^{\infty} U(x) \cos \omega x d x \tag{33}
\end{equation*}
$$

If we carry out similar transformations of integral (29) for an odd function $U(x)$, we get the following result:

$$
\begin{equation*}
B_{0}(\omega)=\int_{0}^{\infty} U(x) \sin \omega x d x, B(\omega, k)=i B_{0}(\omega+k), R(k, \lambda)=\left|\frac{\lambda i B_{0}(2 k)}{1-\lambda i B_{0}(2 k)}\right|^{2} \tag{34}
\end{equation*}
$$

Thus, the difference between an odd barrier and an even one is that the cosine Fourier transform of the barrier is replaced by its sinus transformation and the imaginary factor $i$ appears at parameter $\lambda$.

There is a significant difference in writing analytical formulas between the cosine and sine Fourier transform of the same function. For example:

$$
\begin{aligned}
& \int_{0}^{\infty} e^{-\beta x^{2}} \cos \omega x d x=\frac{1}{2} \sqrt{\frac{\pi}{\beta}} e^{-\omega^{2} / 4 \beta} \\
& \int_{0}^{\infty} e^{-\beta x^{2}} \sin \omega x d x=\frac{\omega}{2 \beta} \sum_{s=1}^{\infty} \frac{1}{(2 s-1)!!}\left(-\frac{\omega^{2}}{4 \beta}\right)^{s-1} .
\end{aligned}
$$

### 3.2. The Double Potential Barrier

By a double potential barrier, we mean such a function $U(x)$ which for an even barrier has the form:

$$
\begin{equation*}
U(x)=U_{0}(x+d)+U_{0}(x-d) \tag{35}
\end{equation*}
$$

That is, the double potential barrier consists of the sum of two separate symmetric barriers $U_{0}(x)$ which are shifted relative to each other by a distance of $\pm d$, as shown in Figure 1.


Figure 1. Shape of double potential barrier.
It is clear that, in this case, the value $B(\omega, k, d)$ depends, apart from the parameters $\omega$ and $k$, on the distance $d$ between the barriers.

In order to find the dependence of the integral $B(\omega, k, d)$ on the distance $d$, we use the formula for the shift of the argument which has the form:

$$
\begin{equation*}
\int_{-\infty}^{\infty} U_{0}(x+d) e^{i x(\boldsymbol{\omega}+k)} d x=\int_{-\infty}^{\infty} U_{0}(\mu) e^{i(\boldsymbol{\omega}+k)(\mu-d)} d \mu=e^{-i(\boldsymbol{\omega}+k) d} \int_{-\infty}^{\infty} U_{0}(x) e^{i(\boldsymbol{\omega}+k) x} d x \tag{36}
\end{equation*}
$$

This means that the spectra of the shifted and the non-shifted barrier momentum differ only by the factor $\exp [-i(\omega+k) d]$.

For a barrier of form (35), therefore, we obtain:

$$
\begin{align*}
& B(k+\omega, d)=\int_{-\infty}^{\infty}\left[U_{0}(x+d)+U_{0}(x-d)\right] e^{i(\omega+k) x} d x= \\
& =\int_{-\infty}^{\infty} U_{0}(x) e^{i(\omega+k) x} d x\left[e^{-i(\omega+k) d}+e^{i(\omega+k) d}\right]=2 \cos (\omega+k) d \int_{-\Delta}^{\infty} U_{0}(x) e^{i(\omega+k) x} d x . \tag{37}
\end{align*}
$$

Let us introduce the so-called basic spectral function $B_{0}(\omega, d)$ for the barrier $U_{0}(x)$ as follows:

$$
\begin{equation*}
B_{0}(\omega, d)=2 \cos \omega d \int_{-\infty}^{\infty} U_{0}(x) e^{i \omega x} d x \tag{38}
\end{equation*}
$$

Then, the spectrum of the double barrier and the reflection coefficient are equal to:

$$
\begin{equation*}
B(\omega+k, d)=B_{0}(\omega+k, d), R=\left|\frac{\lambda B_{0}(2 k, d)}{1-\lambda B_{0}(2 k, d)}\right|^{2} \tag{39}
\end{equation*}
$$

As can be seen, for a double barrier, the basic function $B_{0}(\omega, d)$ is a periodic function of the distance $d$ between local barriers. Therefore, the reflection coefficient is repeated by increasing the distance $d$ with a period equal to $\pi / k$.

Noticing that $\lambda=-i m / k$ we can write the reflection coefficient $R$ in the following form:

$$
\begin{equation*}
R=\left|\frac{-i \frac{m}{k} B_{0}(2 k, d)}{1+i \frac{m}{k} B_{0}(2 k, d)}\right|^{2}=\frac{(m / k)^{2} B_{0}^{2}(2 k, d)}{1+(m / k)^{2} B_{0}^{2}(2 k, d)} \tag{40}
\end{equation*}
$$

From formula (40) it can be seen that the reflection coefficient $R$ is always included in the interval $0 \leq R \leq 1$.

### 3.3. An Example of Calculations

For model calculations, it is convenient to use a potential barrier:

$$
\begin{equation*}
U_{0}(x)=e^{-\beta x^{2}} \tag{41}
\end{equation*}
$$

The basic functions $B_{0}(\omega, d)$ for this is equal to:

$$
\begin{equation*}
B_{0}(\omega, d)=2 \cos \omega d \sqrt{\frac{\pi}{\beta}} e^{-\omega^{2} / 4 \beta} \tag{42}
\end{equation*}
$$

Using formula (40), it is possible to construct graphs of the reflection coefficient $R(d)$ or the transmission coefficient of particles $C=1-R$, depending on the distance $d$ between local barriers.

Figure 2 shows an example of calculating the transmission coefficients of a double barrier for particles with masses $m_{1}=2$ and $m_{2}=5$. Such masses correspond to $\mathrm{H}_{2}$ and DT molecules. The particle energy $E$ and the barrier width parameter $\beta$ in the calculations were taken to be equal to the following: $E=0.8, \beta=4$.


Figure 2. Two graphs of dependence of particle transmission coefficient on distance $d$ between barriers.
The solid line corresponds to the graph for a particle with a mass $m=2$; the dotted line-to $m=5, E=0.8, \beta=4$.

Since the oscillation periods of these graphs (depending on the distance $d$ ) do not coincide, there is a possibility of such a choice of the distance $d$ between the barriers that gives an advantage for one of the substances under consideration to pass through the double barrier.

It is possible that other graphic information is more suitable for a comparative analysis of the permeability of two substances with different masses equal to $m_{1}$ and $m_{2}$, for example, when graphs of relative values are displayed on the screen:

$$
\begin{equation*}
S_{1}(d)=\frac{C_{1}(d)-C_{2}(d)}{C_{1}(d)} \text { and } S_{2}(d)=\frac{C_{2}(d)-C_{1}(d)}{C_{2}(d)} . \tag{43}
\end{equation*}
$$

Under the condition, $S_{1}(d)>0$, the graph of the function $S_{1}(d)$ shows how better the first substance passes through the double barrier than the second at the same distance $d$ between the barriers.

The same can be said for the graph of the function $S_{2}(d)$.
Figure 3 shows graphs of relative deviations for the same calculations, as shown in Figure 2.


Figure 3. Graphs of relative deviations of transmission coefficients for particles with masses $m=2$ and $m=5$.

It is clearly seen in Figure 3 that it is possible to adjust the distance $d$ between the barriers in such a way that only particles with the required mass will pass through the barrier well.

Therefore, it can be stated that there is an effect of separation for particles that differ only in mass. By adjusting the distance $d$ between the barriers, it is possible to provide passage of one of the particles, while passage of the other will be completely blocked.

## 4. Discussion

In its form, the Schrödinger integral equation is analogous to an integral equation with a degenerate kernel. In the kernel of this equation the variables are not separated due to the presence of the modulus of the difference between the two available variables. Along with this, in relation to the required function, it is a recursion. Thus, in the course of constructing a solution, it is necessary to solve two subproblems: to remove the modulus of the variable difference and to eliminate recursion. The key to implementing these steps is the use of the shift operator. With the use of this operator, the exponential function of the modulus of the variable difference, which is available in the record of the Schrödinger integral equation, is divided into two parts. In case of such a separation one of the variables falls into the operator part, with the other falling into the usual functional dependence. At the operator level it is possible to get rid of recursion with respect to $\psi$ in the original equation.

For this purpose, the original wave equation in integral form is multiplied by $U(x) \exp (-x p)$ and integrated in infinite limits. As a result, an operator relation is obtained which allows finding $L(p)$ as an operator function determined only by the value of the barrier energy. Using the Fourier identity and the properties of a differential operator acting on the exponential function the transition from operator relations to ordinary functional dependences is carried out and the integral representation for the wave function is written in terms of the shape of the barrier. As a result, an integral relation for ordinary functions, in the integral term of which there is no recursion in $\psi$, is obtained. The last relation determines the solution of the Schrödinger integral equation. The solution is valid on the entire real axis and does not require boundary conditions. Therefore, it only remains necessary to check its asymptotic behaviour. The check allows for finding a compact formula for the total reflection coefficient $R$. A very important advantage of the exact solution, in comparison with solutions obtained using numerical matching methods, is that this solution allows for calculating the total reflection coefficient $R$ for the potential barrier $U(x)$ of a given shape.

In the case of composite barriers consisting of monolayers of the same shape, according to the formula obtained for $R$, the zeros of the reflection coefficient are found. It appears that the reflection coefficient vanishes not for one, but for many values of the distance $d$ between single barriers.

The result is an efficient isotope screening system. This system can be configured to separate components by varying the distance between the barriers.

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