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Multichannel Scattering Amplitudes of Microparticles in a Quantum Well with Two-Dimensional δ-Potential

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Abstract—The quasi-one-dimensional scattering of a quantum particle on the two-dimensional δ-potential is considered. Analytical expressions for multi-channel transmission t_n and reflection r_n amplitudes are given. The problem is solved for the case of finite number of channels that is equal to N when the particle is incident on the potential while moving in l channel. The case of three-channel scattering was examined in details. As was shown within the frameworks of this problem, the "overpopulation" of particles in the second and third channels occurs when $k_2 \to 0$ and $k_3 \to 0$. The location points of δ-potential that provide the complete "overpopulation" of channels were also obtained.

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1. INTRODUCTION

For one-dimensional systems the problem of description of microparticle motion in inhomogeneous or discrete media is well developed [1–7]. Particularly, some exact methods for finding the wave functions, the energy spectrum, the density of states, the localization radius etc. were proposed. As for practically important 2D and 3D systems, the finding of analytical solutions for this class of problems faces the insurmountable mathematical difficulties. For this reason the consideration of quasi-one-dimensional models [8–12], in which the scattering of particles on the given (non-one-dimensional) potential occurs in one direction, whereas the motion of particle in the perpendicular direction is constrained by permeability barriers, appears to be a breakthrough in this field. The limitation is the transverse motion result in discrete energy spectrum; the total energy is a sum of energies of transverse and longitudinal motion. The main difference from the case of one-dimensional motion is that, due to the elastic scattering in the longitudinal direction the particle may make transition to another quantized level in the transverse motion, and, hence, there arises a new scattering channel with different value of the wave vector. Thus, the scattering in the quasi-one-dimensional system always is multichannel one.

The aim of the present work is to investigate the multichannel scattering based on an example of exactly solvable model that is a rectangular quantum well with a built-in two-dimensional δ-potential. The relevant mathematical problem includes the consideration of a system of coupled differential equations.

2. SCHRÖDINGER EQUATION FOR THE PROBLEM OF MULTICHANNEL SCATTERING

Let us consider the motion of a particle in xy plane. The particle motion in the y direction is limited by impenetrable walls $(0 < y < a)$. The motion in the direction of x axis is restricted. Inside the well the particle is in the potential field $U(x,y)$. The stationary states of particle under these conditions are described by the two-dimensional Schrödinger equation

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Psi(x,y)+\left(\chi^2-V(x,y)\right)\Psi(x,y)=0\,, \tag{1}$$

where $(2M/\hbar^2)E=\chi^2$ and $(2M/\hbar^2)U(x,y)=V(x,y)$. The solution of equation (1) subject to the boundary conditions $V(x,0)=V(x,a)=\infty$ may be represented in the form of expansion [8–10]

$$\Psi(x,y)=\sum_{n=1}^{\infty}\Psi_n(x)\Phi_n(y)\,. \tag{2}$$

Here $\Phi_n(y)$ are basis functions that together with conditions $\Phi_n(0)=\Phi_n(a)=0$ are solutions of equations

$$\frac{d^2\Phi_n(y)}{dy^2}+\chi_n^2\Phi_n(y)=0, \qquad n=1,2,...,\infty \tag{3}$$

and have the form

$$\Phi_n(y)=\sqrt{\frac{2}{a}}\sin\frac{\pi n}{a}y, \qquad \chi_n=\frac{\pi n}{a}. \tag{4}$$

The functions $\Psi_n(x)$, that are the coefficients in expansion (2), are solutions of the system of coupled equations

$$\frac{d^2\Psi_n(x)}{dx^2}+k_n^2\Psi_n(x)-\sum_{m=1}^{\infty}V_{nm}(x)\Psi_m(x)=0, \tag{5}$$

where

$$k_n^2=\chi^2-\chi_n^2, \tag{6}$$

$$V_{n,m}(x)=\int_0^a\Phi_n^*(y)V(x,y)\Phi_m(y)dy\,. \tag{7}$$

The value k_n^2 plays the role of kinetic energy of the longitudinal motion of particle in the n-th channel. The functions $V_{nm}(x)$ form a symmetrical matrix, the diagonal elements $V_{nn}(x)$ of which determine the potential energy in x point of the n-th channel. The nondiagonal elements $V_{nm}(x)$ describe the couplings between different channels n and m. The indices n and m take an infinite number of values. It is assumed in what follows that n is a countable number and varies from 1 to N.

3. AMPLITUDES OF MULTICHANNEL SCATTERING

Now find the scattering amplitudes for a particular form potential that is a two-dimensional δ-function, placed in $(0,y_0)$ point:

$$V(x,y)=V_0\delta(x)\delta(y-y_0)\,. \tag{8}$$

After substitution of (8) in (7) we have

$$V_{nm}(x)=a_{nm}\delta(x), \tag{9}$$

where

$$a_{nm} = \frac{2V_0}{a}\sin(\chi_n, y_0)\sin(\chi_m, y_0)\,. \tag{10}$$

At the substitution of (10) in (5) we obtain

$$\frac{d^2\Psi_n(x)}{dx^2} + k_n^2\Psi_n(x) - \delta(x)\sum_{m=1}^{N} a_{nm}\Psi_m(x) = 0, \qquad n = 1,2,...,N\,. \tag{11}$$

Now assume that the particle with energy k_l^2 $(l < N)$ moves along x axis and passes through the potential barrier. The asymptotical solutions of system (11) are the wave functions of free motion:

$$\Psi_l(x) = \begin{cases} \exp(ik_l x) + r_l \exp(-ik_l x)\,, & x < 0, \\ t_l \exp(ik_l x)\,, & x > 0, \end{cases} \tag{12}$$

$$\Psi_{n\neq l}(x) = \begin{cases} r_n \exp(-ik_n x)\,, & x < 0, \\ t_n \exp(ik_n x)\,, & x > 0, \end{cases} \tag{13}$$

where t_n, r_n are the transmission and reflection amplitudes. The standard conditions for "matching" of wave functions (12), (13) and of their derivatives at the passage through the singular point $x = 0$ have the form

$$\Psi_n(+0) = \Psi_n(-0)\,, \tag{14}$$

$$\Psi'_n(+0) - \Psi'_n(-0) = \sum_{m=1}^{N} a_{nm}\Psi_m(0)\,. \tag{15}$$

After substitution of formulas (12) and (13) in (14) and (15) we get

$$\begin{cases} t_l = 1 + r_l, \\ t_m = r_m, \quad m \neq l, \\ \sum_{m=1}^{N}{}' a_{lm} t_m + a_{ll} t_l = 2ik_l t_l - 2ik_l, \\ \sum_{m=1}^{N}{}' a_{nm} t_m + a_{nl} t_l = 2ik_n t_n, \quad n \neq l, \end{cases} \tag{16}$$

where the prime by the summation symbol means that at summation over m the terms with $m = l$ are omitted. The system of linear equations (16) contains $2N$ unknowns t_n and r_n. Eliminating r_n and replacing t_l and $t_{n\neq l}$ by new unknowns $z_l = 1/t_l$ and $z_{n\neq l} = t_n/t_l$ we obtain

$$\begin{cases} \sum_{m=1}^{N}{}' a_{lm} z_m + 2ik_l z_l = -b_{ll}, \\ \sum_{m=1}^{N}{}' a_{nm} z_m - 2ik_n z_n = -a_{nl}, \quad n \neq l, \end{cases} \tag{17}$$

where $b_{ll} = a_{ll} - 2ik_l$. Now in (17) let us separate z_l out of all N unknowns. It is determined by means of the Cramer's formula

$$z_l = D/D_l\,, \tag{18}$$

where

$$D_l = \begin{vmatrix} b_{11} & a_{12} & \dots & a_{1,l-1} & 0 & a_{1,l+1} & \dots & a_{1N} \\ a_{21} & b_{22} & \dots & a_{2,l-1} & 0 & a_{2,l+1} & \dots & a_{2N} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{l1} & a_{l2} & \dots & a_{l,l-1} & 2ik_l & a_{l,l+1} & \dots & a_{lN} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{N1} & a_{N2} & \dots & a_{N,l-1} & 0 & a_{N,l+1} & \dots & b_{NN} \end{vmatrix}. \tag{19}$$

The determinant D is obtained from D_l by replacing the l-th column with the one of constant terms of system (17). D_l can be exactly calculated. Now we make use of the fact that a_{nm} coefficients can be represented as $a_{nm} = p_n q_m$, where $p_n = \left(2V_0/a\right)\sin(\chi_n y_0)$ and $q_m = \sin(\chi_m y_0)$, and take into account that $a_{nm} = a_{mn}$ and $a_{nm}a_{km} = a_{nk}a_{mm}$. Using the factorization method of linear factors in determinant (19) we obtain the formula

$$D_l = 2ik_l(1 + i\sum_{n=1}^{N}{}' \frac{p_n q_n}{b_{nn} - p_n q_n})\prod_{m=1}^{N}{}'(b_{mm} - p_m q_m), \tag{20}$$

(as before, the prime sign in both symbols of sum and product means that the terms with $n, m = l$ shall be omitted). Returning to previous notations $p_n q_n = a_{nn}$ and $b_{nn} - a_{nn} = -2ik_n$, we obtain

$$D_l = -(1 + i\sum_{n=1}^{N}{}' \frac{a_{nn}}{2k_n})\prod_{m=1}^{N}(-2ik_m). \tag{21}$$

The expression for determinant D is obtained in a similar way:

$$D = -(1 + i\sum_{n=1}^{N} \frac{a_{nn}}{2k_n})\prod_{m=1}^{N}(-2ik_m). \tag{22}$$

From formulas (18), (21), (22) it follows that

$$z_l = \frac{1 + i\sum_{n=1}^{N} \frac{a_{nn}}{2k_n}}{1 + i\sum_{n=1}^{N}{}' \frac{a_{nn}}{2k_n}} = 1 + \frac{i\frac{a_{ll}}{2k_l}}{1 + i\sum_{n=1}^{N}{}' \frac{a_{nn}}{2k_n}}. \tag{23}$$

Obtaining exact formulas for $z_{n\neq l}$ unknowns on the basis of the Cramer's formulas would entail some mathematical difficulties. However, one can avoid these difficulties by using formula (23). Let us represent the first of equations (17) in the following form:

$$z_l = 1 + i\frac{a_{ll}}{2k_l} + i\sum_{n=1}^{N}{}' \frac{a_{ln}}{2k_l} z_n . \tag{24}$$

The equality of the right-hand sides of formulas (23) and (24) and the property $a_{ln}^2 = a_{ll}a_{nn}$ result in:

$$\sum_{n=1}^{N}{}' a_{ln}\left(z_n + \frac{i\frac{a_{ln}}{2k_n}}{1 + i\sum_{m=1}^{N}{}' \frac{a_{mm}}{2k_m}} \right) = 0 . \tag{25}$$

As a_{ln} coefficients differ from zero and the values of $z_{n\neq l}$ are linearly independent, then to satisfy the equation (25) it is necessary and sufficient that the expression in the brackets be equal to zero, that is

$$z_{n\neq l} = -\frac{i\dfrac{a_{ln}}{2k_n}}{1+i\sum\limits_{m=1}^{N}{}'\dfrac{a_{mm}}{2k_m}}. \tag{26}$$

With formula (26) the set task to obtain exact formulas for scattering amplitude of particle undergoing a multi-channel scattering of any order in a quantum well with the built-in two-dimensional δ-potential, proves completed.

4. THREE-CHANNEL SCATTERING

To investigate the density of particles scattered in different channels, we consider the three-channel scattering problem when the particles are incident on the potential while being in the second channel. If the energy of particle is not sufficient for excitation of the fourth channel, then the scattering would proceed via the first three channels. This means that the particles may pass to the third and the first channels and be scattered in these. Since the elastic scattering, the energy of longitudinal motion of particle decreases in the first case, and increases in the second one, i.e., $k_3 < k_2 < k_1$.

One can find the ratios of the densities of scattered particles n_1/n and n_3/n, where n_1 and n_3 are the densities of particles scattered in the first and the third channels, respectively, and n is the total number of particles, that is $n = n_1 + n_2 + n_3$. It is easy to see that the relative density of particles scattered in the second channel is

$$\frac{n_2}{n} = 1 - \frac{n_1}{n} - \frac{n_3}{n}. \tag{27}$$

Based on the above formulas (23) and (24) we can write

$$\frac{|t_1|^2}{|t_2|^2} = \frac{\dfrac{a_{12}^2}{4k_1^2}}{1+\left(\dfrac{a_{11}}{2k_1}+\dfrac{a_{33}}{2k_3}\right)^2}, \qquad \frac{|t_3|^2}{|t_2|^2} = \frac{\dfrac{a_{23}^2}{4k_3^2}}{1+\left(\dfrac{a_{11}}{2k_1}+\dfrac{a_{33}}{2k_3}\right)^2},$$

$$\frac{1}{|t_2|^2} = \frac{1+\left(\dfrac{a_{11}}{2k_1}+\dfrac{a_{22}}{2k_2}+\dfrac{a_{33}}{2k_3}\right)^2}{1+\left(\dfrac{a_{11}}{2k_1}+\dfrac{a_{33}}{2k_3}\right)^2}. \tag{28}$$

In addition, the law of particle flux conservation is the case, i.e.,

$$|t_2|^2 + |r_2|^2 = 1 - 2\frac{k_1}{k_2}|t_1|^2 - 2\frac{k_3}{k_2}|t_3|^2. \tag{29}$$

We have for the total density of particles

$$n \sim 2\left(|t_1|^2 + |t_3|^2\right) + |t_2|^2 + |r_2|^2,$$

or taking into account (29),

$$n \sim 2\left(1-\frac{k_1}{k_3}\right)|t_1|^2 + 2\left(1-\frac{k_3}{k_2}\right)|t_3|^2 + 1. \tag{30}$$

The densities of particles in the first and third channels are respectively proportional to

$$n_1 \sim 2|t_1|^2 \quad \text{and} \quad n_3 \sim 2|t_3|^2 . \tag{31}$$

In view of (30) and (31) it is easy to determine the relative densities of particles in the first and third channels that are respectively

$$\frac{n_1}{n} = \frac{2\left|\frac{t_1}{t_2}\right|^2}{D}, \qquad \frac{n_3}{n} = \frac{2\left|\frac{t_3}{t_2}\right|^2}{D}, \tag{32}$$

where

$$D = \frac{1}{|t_2|^2} + 2\left(1-\frac{k_1}{k_2}\right)\frac{|t_1|^2}{|t_2|^2} + 2\left(1-\frac{k_3}{k_2}\right)\frac{|t_3|^2}{|t_2|^2}. \tag{33}$$

Taking into consideration formulas (28) we finally obtain

$$\frac{n_1}{n} = \frac{1}{\left(1+\left(\frac{a_{11}}{2k_1}+\frac{a_{22}}{2k_2}+\frac{a_{33}}{2k_3}\right)^2\right)\frac{2k_1^2}{a_{12}^2}+\left(1-\frac{k_1}{k_2}\right)+\left(1-\frac{k_3}{k_2}\right)\frac{a_{23}^2}{a_{12}^2}\frac{k_1^2}{k_3^2}}, \tag{34.1}$$

$$\frac{n_3}{n} = \frac{1}{\left(1+\left(\frac{a_{11}}{2k_1}+\frac{a_{22}}{2k_2}+\frac{a_{33}}{2k_3}\right)^2\right)\frac{2k_3^2}{a_{23}^2}+\left(1-\frac{k_1}{k_2}\right)\frac{a_{12}^2}{a_{23}^2}\frac{k_3^2}{k_1^2}+\left(1-\frac{k_3}{k_2}\right)}. \tag{34.2}$$

Analysis of obtained formulas (34) with due regard for $k_3 < k_2 < k_1$ shows, that in case of small k_3 the “overpopulation” of particles in the third channel may occur. It is of interest because the energy is maximum in the third channel and in case of $k_3 \to 0$ the initial energy of particle as a whole passes into the energy of transverse motion, i.e., the particle does not almost move in the scattering direction and is in the quantum state with maximum transverse energy. As we will show in what follows, under this condition ($k_3 \to 0$) the number of particles in the first and second channels is strongly reduced. The value of ratio n_3/n depends on the position of δ-potential and is maximal when the potential is in $y_0 = a/3$ and $y_0 = 2a/3$ points. Actually, it is easy to find from formulas (34) that

$$\lim_{k_3 \to 0} \frac{n_3}{n} = \frac{1}{1+B}, \tag{35}$$

where

$$B = \frac{a_{33}^2}{2a_{23}^2} = \frac{a_{33}^2}{2a_{22}a_{33}} = \frac{a_{33}}{2a_{22}}. \tag{36}$$

As for the values of n_1/n and n_2/n, in case of $k_3 \to 0$ we have

$$\frac{n_1}{n} = \frac{a_{12}^2}{a_{32}^2}\frac{k_3^2}{k_1^2} \to 0, \qquad \frac{n_2}{n} = \frac{B}{1+B}. \tag{37}$$

Thus, when $k_3 \to 0$ the scattering in the first channel does not take place, that is the particles are scattered in the incidence (the second) channel and in the third channel.

Now consider the case when the scattering occurs only in the third channel. According to (35)–(37), in this case it is required that $B=0$ or $a_{23}=0$. This condition leads to equation $\sin(3\pi y_0/a)=0$, whence it is easy to find two solutions $y_0=a/3$ and $y_0=2a/3$ of this equation. And so, if the δ-potential is in these points, then the particles completely transfer from the second channel to the third one and the total "overpopulation" of particles occurs at much higher energy level of transverse motion.

Consider also the case, when the flux of particles in the first channel is incident on the potential. After interaction with the potential the particles are scattered into three channels. Analogous simple calculations of the relative densities of particles scattering into different channels give the following formulas:

$$\frac{n_2}{n}=\frac{1}{\left(1+\left(\frac{a_{11}}{2k_1}+\frac{a_{22}}{2k_2}+\frac{a_{33}}{2k_3}\right)^2\right)\frac{2k_2{}^2}{a_{12}^2}+\left(1-\frac{k_2}{k_1}\right)+2\left(1-\frac{k_3}{k_1}\right)\frac{a_{13}^2}{a_{12}^2}\frac{k_2^2}{k_3^2}}, \tag{38.1}$$

$$\frac{n_3}{n}=\frac{1}{\left(1+\left(\frac{a_{11}}{2k_1}+\frac{a_{22}}{2k_2}+\frac{a_{33}}{2k_3}\right)^2\right)\frac{2k_3{}^2}{a_{23}^2}+\left(1-\frac{k_1}{k_2}\right)\frac{a_{12}^2}{a_{23}^2}\frac{k_3^2}{k_1^2}+\left(1-\frac{k_3}{k_2}\right)}, \tag{38.2}$$

$$\frac{n_1}{n}=1-\frac{n_2}{n}-\frac{n_3}{n}. \tag{38.3}$$

Since the relative densities of particles scattering into different channels depend on the longitudinal momenta of particles k_2 and k_3, it is of interest to investigate the scattering process for extremely small values of these momenta, i.e., for $k_2\to 0$ and $k_3\to 0$.

If the first condition is satisfied $(k_2\to 0)$, then it is easy to see that the initial longitudinal momentum of the particle is not sufficient for excitation of the third channel. And we obtain from equation (38.1)

$$\lim_{k_2\to 0}\frac{n_2}{n}=\frac{1}{1+B_2}, \qquad B_2=\frac{a_{22}}{2a_{11}}. \tag{39}$$

As was shown in [13], the maximal value of $n_2/n=1$ is obtained when the δ-potential is near the centre of potential well. Indeed, in this case $B_2\sim\cos(\pi y_0/a)$ and when $y_0\to a/2$, $B_2\to 0$ and $n_2/n\to 1$.

When the second condition $(k_3\to 0)$ is fulfilled, then the excitation of the second, as well as the third channels are energetically possible. However, as it is seen from formula (38), here only the third channel is excited. Actually, according to formula (38.1), for $k_3\to 0$ the ratio n_2/n is proportional to k_3^2 and tends to zero together with k_2. The particles are mainly excited in the third channel, and the ratio n_3/n in case of $k_3\to 0$ is expressed by formula

$$\lim_{k_3\to 0}\frac{n_3}{n}=\frac{1}{1+B_3}, \qquad B_3=\frac{a_{33}}{2a_{11}}. \tag{40}$$

In this case also the maximal value of $n_3/n=1$ is realized if the condition $B_3=0$ is satisfied. According to formula (10), B_3 is

$$B_3=\sin^2\left(\frac{3\pi y_0}{a}\right)\Big/\sin^2\left(\frac{\pi y_0}{a}\right),$$

and, hence, the condition $B_3=0$ is satisfied at $y_0=a/3$ and $y_0=2a/3$. So, there are two positions of δ-potential when the complete "overpopulation" of electrons in the third channel is realized. Analogous results were obtained for the case, when the particles were initially moving in the second channel.

5. CONCLUSIONS

The quasi-one-dimensional scattering of a quantum particle on the two-dimensional δ-potential was considered. Analytical expressions for amplitudes of multi-channel transmission t_n and reflection r_n were obtained. The problem was solved for the case when number of channel is finite and equal to N, and the particle is incident on the potential at its motion along the l-th channel.

The obtained expressions may be used for determination of particle densities in different scattering channels. The distribution of particles in the scattering channels would depend on the parameters of incident and scattered beams, as well as on the parameters of scattering potential. One can realize any preassigned particle distribution by means of proper choice of these parameters. So, the "overpopulation" of particles in the second and third channels occurs when conditions $k_2 \to 0$ and $k_3 \to 0$ are met. Also, there are location points of δ-potential such that the complete "overpopulation", i.e., the equality of n_2/n and n_3/n ratios to unity, is provided.

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