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ALGEBRAIC DESCRIPTION OF MULTILAYER SYSTEMS WITH RESONANCES

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A multiple reflection method is applied to multilayer systems to demonstrate the appearance of resonances, their splitting, and tunneling through magnetic layers in neutron optics.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

Алгебраическое описание многослойных систем с резонансами

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С помощью метода многократного отражения волн рассчитывается отражение от многослойной системы, демонстрируется возникновение и расщепление резонансов и исследуется туннелирование через магнитные пленки в нейтронной оптике.

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1. INTRODUCTION

To find reflection and transmission amplitudes for a neutron incident on a multilayer system (MS) one (as shown in many text books) usually solves a one-dimensional quantum mechanical problem with rectangular potentials (Fig. 1). Wave functions inside ith potential (i=a,b,c...) of height u_i can be represented in the form:

$$\psi_i = A_i \exp(ik_i x) + B_i \exp(-ik_i x),$$

where $k_i = \sqrt{k_0^2 - u_i}$, k_0 are the neutron wave-numbers in the potential and in vacuum, respectively. All the wave functions and their derivatives should be matched at all the interfaces, which gives two equations at every interface for determination of A_i and B_i. Thus,

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if there are n interfaces in the potential, one obtains $2n$ linear algebraic equations. The solution of these equations is a very tedious problem, and the result is usually very difficult to interpret. We show here how to avoid this tedious process and to obtain a transparent analytical result without multiple matching. Only one (almost trivial) matching at a single interface is sufficient.

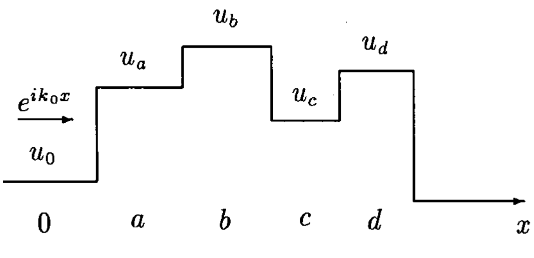

Fig. 1. Multilayer system potential

Many papers devoted to simplification of MS have been published in mathematical and popular journals. Among them are some very famous ones [1–3], however we use the different approach elaborated in [4–8], and hope that it will give additional insight into the physics of interaction of radiation with MS.

We shall consider first spinless neutrons, and after that take into account their magnetic interaction characteristics. We shall show how resonances appear in a middle layer of a three-layer system, and demonstrate how these resonances split, if two-side layers are replaced by more complicated MS. Following that, we shall consider magnetic MS, and describe resonances and tunneling in them.

Sometimes formulas represented here, especially in magnetic case, seem to be complicated, however, and we want to stress it, the algorithm of their derivation is elementary. Thus one can easily construct them, and after that can straightforwardly calculate all the necessary magnitudes. In magnetic case it requires only the knowledge how to calculate product and inverse of 2x2 matrices.

2. A POTENTIAL STEP

First we suppose that the particle, we shall investigate in this section, is a spinless scalar one, like a neutron in the absence of a magnetic field. Let us consider propagation of such a particle in the potential shown in Fig. 2 and given by:

$$V(x) = u_a\theta(x > 0),$$

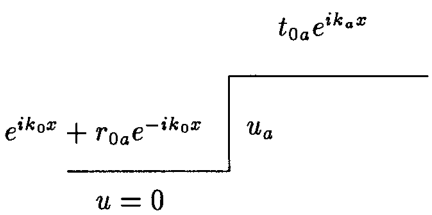

Fig. 2. Reflection and transmission at a potential step

which represents a step of height u_a. This finite step potential models, e.g., nuclear scattering of neutrons. Here Heaviside θ-function is equal to 1 or 0 depending on whether the inequality in its argument is satisfied or not, respectively. The one-dimensional Schrödinger equation describing neutron propagation in this system is:

$$[d^2/dx^2 + k_0^2 - V(x)]\Psi(x) = 0. \tag{1}$$

If we seek for a solution containing the incident neutron described by the plane wave, $\exp(ik_0x)$, propagating from the left to the right, we find it in the form:

$$\Psi(x) = \theta(x < 0)[\exp(ik_0x) + r_{0a}\exp(-ik_0x)] + \theta(x > 0)t_{0a}\exp(ik_ax), \tag{2}$$

where $k_a = \sqrt{k_0^2 - u_a}$, r_{0a} and t_{0a} are reflection and transmission amplitudes, respectively. Matching of the function and its first derivative at the point $x = 0$ gives equations for r_{0a} and t_{0a}:

$$1 + r_{0a} = t_{0a}, \quad k_0[1 - r_{0a}] = k_a t_{0a},$$

which have the solution:

$$r_{0a} = \frac{k_0 - k_a}{k_0 + k_a}, \quad t_{0a} = \frac{2k_0}{k_0 + k_a}. \tag{3}$$

For this solution it does not matter whether the potential step u_a is positive, i.e., a barrier, as shown in Fig. 2, or negative, i.e., a well, and it does not matter, whether it is real or complex.

From (3) we can immediately find reflection r_{a0} and transmission t_{a0} amplitudes from inside to outside of the potential. In that case we seek for a solution of (1) with the incident particle propagating toward the step at $x = 0$ from the right, i.e., with the incident plane wave $\exp(-ik_a x)$. From (3), purely from symmetry considerations, it follows that r_{a0} and t_{a0} are:

$$r_{a0} = \frac{k_a - k_0}{k_0 + k_a} = -r_{0a}, \quad t_{a0} = \frac{2k_a}{k_0 + k_a} = \frac{k_a}{k_0} t_{0a}. \tag{4}$$

These formulas can be generalized for the interface between two potentials u_a and u_b:

$$r_{ab} = -r_{ba} = \frac{k_a - k_b}{k_a + k_b}, \quad t_{ab} = \frac{k_a}{k_b} t_{ba} = \frac{2k_a}{k_a + k_b}, \tag{5}$$

where $k_{a,b} = \sqrt{k_0^2 - u_{a,b}}$, and k_0 denotes the neutron's vacuum wave number.

As the reader may have noticed, the left indices in r_{ab}, t_{ab} denote the space containing the incident wave, so the amplitudes t_{ba} and r_{ba} can be immediately obtained from r_{ab}, t_{ab} by simply interchanging a and b.

In the case where $u_{a,b}$ are real, and $k_0^2 > u_{a,b}$, the wave-numbers k_a, k_b and the coefficients r_{ab} and t_{ab} are also real. However because of losses $u_{a,b}$ usually contain small imaginary parts, thus the k's also contain small imaginary parts, however for simplicity, in the following we shall neglect imaginary parts of $u_{a,b}$, which means that we shall neglect the losses.

If $k_0^2 < u_b$ the number k_b becomes imaginary: $k_b = i\kappa_b$, where $\kappa_b = \sqrt{u_b - k_0^2}$. If at the same time $k_0^2 > u_a$, the amplitudes r_{ab}, t_{ab} also become complex:

$$r_{ab} = \frac{k_a - i\kappa_b}{k_a + i\kappa_b} = e^{2i\phi_{ab}}, \quad \phi_{ab} = -\arctan\left(\frac{\kappa_b}{k_a}\right), \tag{6}$$

$$t_{ab} = 2\cos(\phi_{ab})e^{i\phi_{ab}}, \quad t_{ba} = -2i\sin(\phi_{ab})e^{i\phi_{ab}} \tag{7}$$

with the phase ϕ_{ab} being real. This phase increases with energy, from $-\pi/2$ up to 0, when k_0^2 grows from u_a up to u_b. It is important to note that it is the general property of the phase for reflection from a potential barrier of any form.

2.1. Magnetic Systems. In the presence of a magnetic field, the spin of the neutron and the spinor nature of the neutron wave function must be taken into account. With a magnetic field $\boldsymbol{B}_i$ inside the ith region (i=a,b) the total potential becomes $\hat{V}(x) = \hat{u}_a^+\theta(x<0)+\hat{u}_b^+\theta(x>0)$, where $\hat{u}_i^+ \equiv u_i(\boldsymbol{\sigma\omega}_i) = u_i + \boldsymbol{\sigma\omega}_i$ includes both nuclear (u_i) and magnetic ($\boldsymbol{\sigma\omega}_i$) parts. The magnetic term contains the Pauli matrices $\boldsymbol{\sigma}$, and vector $\boldsymbol{\omega} = -(2m/\hbar^2)\mu\boldsymbol{B}$, in which μ is the neutron magnetic moment equal to -1.91 of the nuclear magneton.

The neutron wave number in the ith region now becomes an operator $\hat{k}_i^+ \equiv \hat{k}_i(\boldsymbol{\sigma\omega}_i) = \sqrt{k_0^2 - \hat{u}_i^+}$. Thus incident neutrons propagating from the left to the interface are described by the plane wave $\exp(i\hat{k}_a^+x)\xi_0$, and those propagating from the right are described by the plane wave $\exp(-i\hat{k}_b^+x)\xi_0$, where ξ_0 is spinor part of the incident wave. The solution of (1) in the first case becomes

$$\Psi(x) = \{\theta(x<0)[\exp(i\hat{k}_a^+x) + \hat{r}_{ab}^+\exp(-i\hat{k}_l^+x)] + \theta(x>0)\hat{t}_{ab}^+\exp(i\hat{k}_b^+x)\}\xi_0. \tag{8}$$

Matching this function at the interface $x=0$ gives the equations:

$$1+\hat{r}_{ab}^+ = \hat{t}_{ab}^+, \qquad \hat{k}_a^+(1-\hat{r}_{ab}^+) = \hat{k}_b^+\hat{t}_{ab}^+,$$

which have the solution

$$\hat{r}_{ab}^+ = (\hat{k}_a^+ + \hat{k}_b^+)^{-1}(\hat{k}_a^+ - \hat{k}_b^+), \qquad \hat{t}_{ab}^+ = (\hat{k}_a^+ + \hat{k}_b^+)^{-1}2\hat{k}_a^+. \tag{9}$$

If all the fields in different regions are collinear, the magnetic case is identical to the non-magnetic one because the neutrons polarized along or opposite the fields can be treated independently as scalar particles. Of more interest is the case of noncollinear fields, which became important following recent reports of theoretical [4] and experimental [9,10] advances.

All the magnitudes in (9) are 2x2 matrices of the type $f(\boldsymbol{\sigma\omega})$, which can be represented as

$$\hat{f}(\boldsymbol{\omega\sigma}) = F_+ + \frac{\boldsymbol{\sigma\omega}}{\omega}F_-, \quad F_\pm = [f(\omega)\pm f(-\omega)]/2. \tag{10}$$

Such a representation can be used for all the $\hat{k}_i(\boldsymbol{\sigma\omega}_i)$ in (9) and for $\hat{r}_{ab}^+$, $\hat{t}_{ab}^+$, and we need only to find the form of the function $f(\boldsymbol{\sigma\omega})$.

For instance, $\hat{k}_i^+ \equiv k_i(\boldsymbol{\sigma\omega}_a)$ has the representation (10) with $K_{\pm,i} = (k_i^+ \pm k_i^-)/2$, and $k_i^\pm \equiv k_i(\pm\omega_i) = \sqrt{k_0^2 - u_i \mp \omega_i}$. The factor $(\hat{k}_a^+ + \hat{k}_b^+)^{-1} \equiv 1/(\hat{k}_a^+ + \hat{k}_b^+)$ in $\hat{r}_{ab}^+$, $\hat{t}_{ab}^+$ can be reduced to the form (10) after multiplication of nominator and denominator by $\hat{k}_a^- + \hat{k}_b^-$, where $\hat{k}_i^- \equiv \hat{k}_i(-\boldsymbol{\sigma\omega}_i) = \sqrt{k_0^2 - \hat{u}_i^-}$ and $\hat{u}_i^- \equiv \hat{u}_i(-\boldsymbol{\sigma\omega}_i) = u_i - \boldsymbol{\omega}_i\boldsymbol{\sigma}$ $(i=a,b)$.

This operation gives:

$$(\hat{k}_a^+ + \hat{k}_b^+)^{-1} = (\hat{k}_a^- + \hat{k}_b^-)/N, \tag{11}$$

where

$$N = (\hat{k}_a^+ + \hat{k}_b^+)(\hat{k}_a^- + \hat{k}_b^-) = k_a^+k_a^- + k_b^+k_b^- + \hat{k}_b^+\hat{k}_a^- + \hat{k}_a^+\hat{k}_b^- =$$

$$(k_a^+ + k_b^+)(k_a^- + k_b^-) + 4K_{-,a}K_{-,b}\sin^2(\vartheta_{ab}/2), \tag{12}$$

and ϑ_{ab} is the angle between $\boldsymbol{\omega}_a$ and $\boldsymbol{\omega}_b$ in adjacent spaces: $\cos\vartheta_{ab} = (\boldsymbol{\omega_a}\boldsymbol{\omega}_b)/\omega_a\omega_b$. To get the expression (12) we used the easily checkable relations:

$$f(\boldsymbol{\sigma\omega})f(-\boldsymbol{\sigma\omega}) = f(\omega)f(-\omega), \quad (\boldsymbol{\sigma\omega}_1)(\boldsymbol{\sigma\omega}_2) = (\boldsymbol{\omega_1\omega_2}) + i(\boldsymbol{\sigma}[\boldsymbol{\omega_1\omega}_2]),$$

where $(\boldsymbol{AB})$ and $[\boldsymbol{AB}]$ denote scalar and vector product of vectors $\boldsymbol{A}$ and $\boldsymbol{B}$, respectively.

After the transformation (11) we obtain

$$\hat{r}^+_{ab} = \frac{1}{N}(k^+_a k^-_a - k^+_b k^-_b + \hat{k}^-_b \hat{k}^+_a - \hat{k}^-_a \hat{k}^+_b) =$$

$$\frac{1}{N}\left(k^+_a k^-_a - k^+_b k^-_b + 2K_{+,b}K_{-,a}\frac{\boldsymbol{\sigma\omega}_a}{\omega_a} - 2K_{+,a}K_{-,b}\frac{\boldsymbol{\sigma\omega}_b}{\omega_b} + 2iK_{-,a}K_{-,b}\frac{\boldsymbol{\sigma}[\boldsymbol{\omega_a\omega}_b]}{\omega_a\omega_b}\right), \tag{13}$$

$$\hat{t}^+_{ab} = \frac{2}{N}(k^+_a k^-_a + \hat{k}^-_b \hat{k}^+_a) =$$

$$\frac{2}{N}\left(k^+_a k^-_a + K_{+,b}K_{+,a} + K_{+,b}K_{-,a}\frac{\boldsymbol{\sigma\omega}_a}{\omega_a} - K_{+,a}K_{-,b}\frac{\boldsymbol{\sigma\omega}_b}{\omega_b} + 2iK_{-,a}K_{-,b}\frac{\boldsymbol{\sigma}[\boldsymbol{\omega_a\omega}_b]}{\omega_a\omega_b}\right), \tag{14}$$

It is clear that, if the magnetic field is zero in both regions, then $k^+_i = k^-_i = k_i$, and for any ϑ we recover the amplitudes for scalar case:

$$\hat{r}^+_{ab} = \frac{k_a^2 - k_b^2}{(k_a + k_b)^2} = \frac{k_a - k_b}{k_a + k_b} \equiv r_{ab}, \qquad \hat{t}^+_{ab} = \frac{2k_a(k_a + k_b)}{(k_a + k_b)^2} = \frac{2k_a}{k_a + k_b} \equiv t_{ab}.$$

2.2. Reflection and Transmission of a Rectangular Potential Barrier. Now we shall consider a rectangular potential barrier (Fig. 3), and show how to find expressions for the reflection R_a and the transmission T_a amplitudes without matching the wave-function on two interfaces.

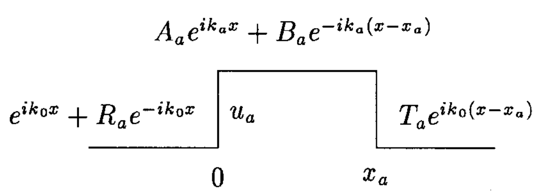

Fig. 3. Reflection and transmission of a rectangular potential barrier

The reflection amplitude is composed of two parts. The first one describes a single reflection from the interface at $x = 0$, and the second one contains multiple reflections and propagations inside the potential between the two interfaces at $x = 0$ and $x = x_a$:

$$R = r + t'er'e[1 + r'er'e + (r'er'e)^2 + \cdots]t =$$

$$r + (tt'r'e^2)/(1 - e^2r'^2), \tag{15}$$

where for simplicity we omit indices and use the notation $r = r_{0a}$, $r' = r_{a0}$, $t = t_{0a}$, $t' = t_{a0}$ and $e = \exp(ik_a a)$.

The transmission amplitude is obtained in a similar fashion:

$$T = t'[1 + r'er'e + (r'er'e)^2 + \cdots]et = t'et/(1 - e^2r'^2). \quad (16)$$

Using the trivial relationship $tt' = 1 - r^2$, we obtain the final expressions:

$$R_a = r_{0a}\frac{1 - \exp(2ik_ax_a)}{1 - r_{a0}^2\exp(2ik_ax_a)}, \quad T_a = \exp(ik_ax_a)\frac{1 - r_{0a}^2}{1 - r_{a0}^2\exp(2ik_ax_a)}. \quad (17)$$

For arbitrary k_a we can directly show that:

$$|R_a|^2 + |T_a|^2 = 1, \quad (18)$$

which is a consequence of unitarity.

For real k_a the amplitude R_a exhibits decaying oscillations, and T_a exhibits growing oscillations with energy. When $2k_ax_a = 2\pi n$ with integer n we have $R_a = 0$, $T_a = (-1)^n$. For the first maxima of T_a, when $r_{0a} \approx 1$, it is useful to represent (17) in the form

$$R_a = r_{0a}\frac{\exp(-2ik_ax_a) - 1}{\exp(-2ik_ax_a) - r_{a0}^2}, \quad T_a = \exp(-ik_ax_a)\frac{1 - r_{0a}^2}{\exp(-2ik_ax_a) - r_{a0}^2}, \quad (19)$$

and to expand denominator over $E_0 - E_m$ near maxima of transmissions, where $E_0(\equiv k_0^2) = E_m = (\pi m/x_a)^2 + u_a$, and m are integers:

$$R_a = r_{0a}\frac{E_0 - E_m}{E_0 - E_m + i\Gamma/2} = r_{0a}\left(1 - \frac{i\Gamma_1}{E_0 - E_m + i\Gamma/2}\right), \quad (20)$$

$$T_a = (-1)^m\frac{i\Gamma_2}{E_0 - E_m + i\Gamma/2},$$

where $\Gamma = \Gamma_1 + \Gamma_2 = (1 - r_{0a}^2)2\pi m/x_a^2$, $\Gamma_1 = \Gamma_2 = \Gamma/2$.

Besides R_a and T_a, the wave-function inside the barrier

$$\Psi(x) = \theta(0 \le x \le a)[A_a\exp(ik_ax) + B_a\exp(-ik_a\{x - x_a\})] \quad (21)$$

can also be found without matching. Indeed, the amplitudes A_a, B_a of the waves propagating to the right and to the left, respectively are related to reflection and transmission amplitudes as follows:

$$A_a = t + r'eB_a, \qquad B_a = r'eA_a, \quad (22)$$

from which it is easy to find

$$A_a = \frac{t_{0a}}{1 - r_{a0}^2\exp(2ik_ax_a)}, \quad B_a = \frac{r_{a0}\exp(ik_ax_a)t_{0a}}{1 - r_{a0}^2\exp(2ik_ax_a)}. \quad (23)$$

3. RELATIONS BETWEEN R AND T FOR ARBITRARY POTENTIALS

For the rectangular potential of Fig. 3 the phases ϕ_R and ϕ_T of the complex amplitudes $R_a = |R_a| \exp(2i\phi_{Ra})$ and $T_a = |T_a| \exp(2i\phi_{Ta})$ are related to each other in a simple way: $2\phi_{Ra} = 2\phi_{Ta} \pm \pi/2$. To prove this we need only put down (17) in the form

$$R_a = \left[e^{-ik_a x_a} - e^{ik_a x_a}\right] \frac{r_{0a} \exp(ik_a x_a)}{1 - r_{a0}^2 \exp(2ik_a x_a)}, \quad T_a = \left[\frac{1}{r_{0a}} - r_{0a}\right] \frac{r_{0a} \exp(ik_a x_a)}{1 - r_{a0}^2 \exp(2ik_a x_a)}, \tag{24}$$

and to observe that for real k_a the first factor in R_a is imaginary, and it is equal to $-2i \sin(k_a x_a)$, while the first factor in T_a is real. In the case, when $k_a = i\kappa_a$ is an imaginary value, the first factor in R_a is a real magnitude $2\mathrm{sh}(\kappa_a x_a)$, while the first factor in T_a is imaginary: $-2i \sin(2\phi_{0a})$, where ϕ_{0a} is defined by (6).

From these considerations and from unitarity (18) it follows that

$$R_a^2 - T_a^2 = \exp(4i\phi_{Ra}). \tag{25}$$

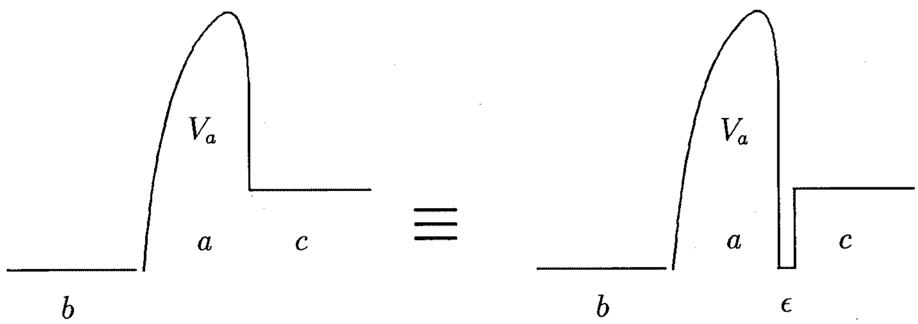

Fig. 4. An arbitrary potential with two different energy levels on both sides

These relations were obtained for a potential like that one shown in Fig. 3, however it is valid for any symmetric potential, because the reflection and transmission amplitudes from both sides are the same for such a potential.

For a general, nonsymmetrical potential V_a, like the one shown in Fig. 4, it is not difficult to prove that the reflection amplitudes R_{cb} from the right and R_{bc} from the left, and the analogous transmission amplitudes T_{bc} and T_{cb} satisfy the relations:

$$R_{bc,cb} = \exp(2i\zeta_{bc,cb})|R_{cb}|, \quad T_{bc} = \frac{k_b}{k_c} T_{cb}, \quad R_{bc}R_{cb} - T_{bc}T_{cb} = \exp(4i\phi_{Ra}), \tag{26}$$

where $\phi_{Ra} = (\zeta_{bc} + \zeta_{cb})/2$. From (26) it follows that reflections from both sides differ only by a phase, and the ratio of the transmission amplitudes is reciprocal to the ratio of the neutron velocities $k_{b,c} = \sqrt{k_0^2 - u_{b,c}}$ on both sides of the potential V_a.

If the potential level on both sides of the potential is the same, then the transmission amplitudes from the left and from the right become identical for arbitrary potential V_a.

To prove (26) we use something like mathematical induction method. We find the reflection and transmission amplitudes for the potential shown in Fig. 4 splitting it by an infinitesimal gap of the width ϵ with the same potential level inside it as at b to the left of V_a. We show that, if the relations (26) are valid for the asymmetric potential V_a, they are also valid for the full potential of Fig. 4.

The reflection and transmission amplitudes for potential with the gap may be written in a straight-forward fashion using our multiple reflection formalism inside the gap:

$$R_{bc} = \frac{R_a - r_{\epsilon c}(R_a^2 - T_a^2)}{1 - R'_a r_{\epsilon c}}, \quad R_{cb} = \frac{r_{c\epsilon} - (r_{\epsilon c} r_{c\epsilon} - t_{\epsilon c} t_{c\epsilon}) R'_a}{1 - R'_a r_{\epsilon c}}, \tag{27}$$

$$T_{bc} = \frac{T_a t_{\epsilon c}}{1 - R'_a r_{\epsilon c}}, \quad T_{cb} = \frac{T_a t_{c\epsilon}}{1 - R'_a r_{\epsilon c}},$$

where $r_{\epsilon c} \equiv r_{bc}$, $r_{c\epsilon} \equiv r_{cb}$, $t_{\epsilon c} \equiv t_{bc}$, $t_{c\epsilon} \equiv t_{cb}$ are the amplitudes of the interaction with a potential step defined by (3), (4), and satisfying the relation $r_{\epsilon c} r_{c\epsilon} - t_{\epsilon c} t_{c\epsilon} = -1$.

If for the same potential level on both sides of the potential V_a the reflection amplitudes R_a, R'_a from the left and right, respectively satisfy the relations (26), i.e., differ by a phase, and transmission amplitudes T_a, T'_a of the potential V_a from both sides are identical, then it is easy to see that the full reflection and transmission amplitudes in (3) satisfy relations (26) for different potential levels on both sides.

It is easy to check that if we chose the potential level in the gap different from the side b, and supposed R and T amplitudes of the left part of the potential satisfiy (26), we would obtain again that for the reflection and transmission amplitudes of the total potential in Fig. 4 the relations (26) are also valid.

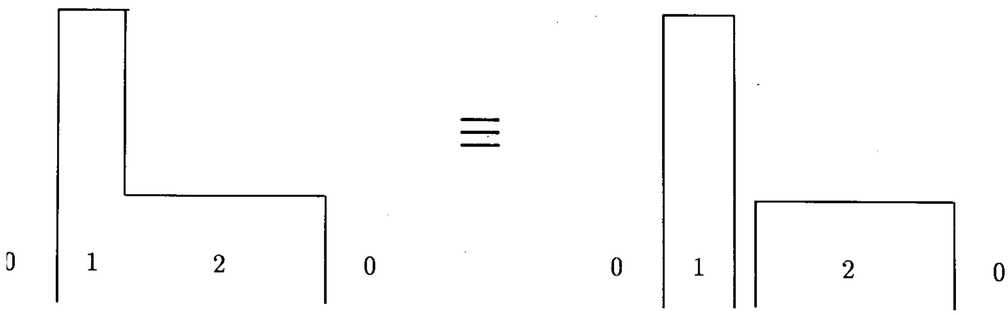

Fig. 5. Any potential can be split by an infinitesimal gap into two ones

To illustrate (26) on a simple model let us consider the asymmetrical potential of Fig. 5, consisting of two rectangular potentials. The reflection and transmission amplitudes may be found using the same relations as (15,16) but with $e \equiv 1$, because propagation phase in the infinitesimal gap is itself infinitesimal and can be put equal to 0. Thus:

$$R_{12} = \frac{R_1 - R_2(R_1^2 - T_1^2)}{1 - R_1 R_2}, \quad R_{21} = \frac{R_2 - R_1(R_2^2 - T_2^2)}{1 - R_1 R_2}, \quad T_{12} = \frac{T_1 T_2}{1 - R_1 R_2} \equiv T_{21}. \tag{28}$$

Applying relation (25), it is easy to see that:

$$R_{12} = \exp(4i[\phi_{R1} - \phi_{R2}])\frac{R_1^* - R_2}{R_2^* - R_1}R_{21} = \exp(2i\chi_{12})R_{21}, \tag{29}$$

which means that the reflection amplitudes from two opposite sides differ by a phase-factor.

4. THE BREIGHT–WIGNER RESONANCE IN MS

Now we shall consider an arbitrary potential with a well inside it (Fig. 6), and show how to get the Breight–Wigner (BW) resonant form for the transmission and the reflection amplitudes and to calculate the wave function inside the well. We shall study only the case of the incident wave propagating from the left, where the potential is zero.

4.1. A Single Resonance. Transmission $T_{0\to c}$ and reflection $R_{0\to c}$ amplitudes for the whole potential (Fig. 6) can be obtained in the same way as was shown in (15) and (16). Indeed, let us suppose that the reflection and transmission amplitudes for the left barrier are ρ_{0a}, ρ_{a0}, τ_{0a}, τ_{a0} and those for the right barrier are ρ_{ca}, ρ_{ac}, τ_{ca}, τ_{ac}.

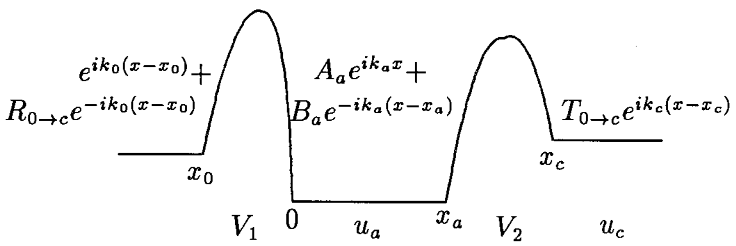

Fig. 6. A potential with a well inside it

The reflection $R_{0\to c}$ and transmission $T_{0\to c}$ amplitudes from the left for the whole potential are

$$R_{0\to c} = \rho_{0a} + \frac{\tau_{a0}\exp(2ik_a x_a)\tau_{0a}\rho_{ac}}{1 - \exp(2ik_a x_a)\rho_{a0}\rho_{ac}}, \quad T_{0\to c} = \frac{\tau_{ac}\exp(ik_a x_a)\tau_{0a}}{1 - \exp(2ik_a x_a)\rho_{ac}\rho_{a0}}, \tag{30}$$

and the amplitudes A_a and B_a of the wave-function inside the well obtained as in (22) are

$$A_a = \frac{\tau_{0a}}{1 - \exp(2ik_a x_a)\rho_{a0}\rho_{ac}}, \quad B_a = \frac{\rho_{ac}\exp(ik_a x_a)\tau_{0a}}{1 - \exp(2ik_a x_a)\rho_{ac}\rho_{a0}}. \tag{31}$$

All the magnitudes in (30,31) behave resonantly at those energies k_0^2 for which the phase $\xi(k_0)$ of the second term in denominator is $2\pi n$ with integer n, i.e.:

$$\xi_a(k_0) \equiv 2k_a x_a + 2\zeta_{a0} + 2\zeta_{ac} = 2\pi n, \tag{32}$$

where $2\zeta_{a0}$, $2\zeta_{ac}$ are the phases of two complex amplitudes ρ_{a0} and ρ_{ac}, respectively.

To get the BW form of R and T we use the same technique that was successful in obtaining (19, 2.2), i.e., we divide the numerator and the denominator of expressions (30) by

$\exp(i\xi_a(k_0))$ and expand $\exp(-i\xi_a(k_0))$ near $k_0 = k_n$, where k_n is defined as a solution of $\xi_a(k_n) = 2\pi n$. This yields:

$$R_{0\to c} = \rho_{0a}\left[1 - \frac{i\gamma_1}{E_0 - E_n + i\Gamma_a/2}\right], \quad T_{0\to r} = (-1)^n \frac{\exp(i\zeta_{0a} + i\zeta_{ca})\gamma_2}{E_0 - E_n + i\Gamma_a/2}, \tag{33}$$

where $E_{0,n} = k_{0,n}^2$, and $2\zeta_{(0,c)a}$ are the phases of the appropriate reflection amplitudes: $\rho_{0a,ca} = |\rho_{0a,ca}|\exp(2i\zeta_{0a,ca})$ at the point $k_0 = k_n$. The magnitudes γ and Γ_a are defined as follows

$$\gamma_1 = 2k_n \frac{|\rho_{ac}/\rho_{0a}| - |\rho_{ac}\rho_{0a}|}{d\xi_a(k_n)/dk_n}, \quad \gamma_2 = 2k_n \frac{|\tau_{0a}\tau_{ac}|}{d\xi_a(k_n)/dk_n}, \quad \Gamma_a = 2k_n \frac{2(1 - |\rho_{a0}\rho_{ac}|)}{d\xi_a(k_n)/dk_n}. \tag{34}$$

We should take into account that the resonant representation has distinct BW resonant behavior only if the widths are narrow enough, which means that both $\rho_{a0,ac}$'s are very close to unity and $|\tau| \ll 1$. In this case

$$\rho_{a0,ac} = \sqrt{1 - |\tau_{a0,ac}|^2 k_{0,c}/k_a} \approx |\tau_{a0,ac}|^2 k_{0,c}/2k_a, \quad k_{c,a} = \sqrt{k_0^2 - u_{c,a}}, \quad \text{and} \quad k_0 = k_n.$$

The derivative $d\xi_a/dk_n$ can be calculated as follows:

$$\frac{d\xi_a(k_n)}{dk_n} = \frac{d\xi_a(k_a)}{dk_a}\frac{dk_a}{dk_n} = 2x'_a \frac{k_n}{k_a}, \quad x'_a = x_a + \Delta x_a, \quad \Delta x_a = \frac{d\zeta_{ac}(k_a)}{dk_a} + \frac{d\zeta_{a0}(k_a)}{dk_a}.$$

Now all the γ magnitudes can be approximated as follows:

$$\gamma_1 = \frac{k_a}{x'_a}|\tau_{0a}\tau_{a0}|, \quad \gamma_2 = \frac{k_a}{x'_a}|\tau_{0a}\tau_{ac}|, \quad \Gamma_a = \frac{k_a}{x'_a}(|\tau_{a0}|^2 k_0/k_a + |\tau_{ac}|^2 k_c/k_a). \tag{35}$$

$$\gamma_1 = \frac{k_a}{x'_a}|\tau_{0a}\tau_{a0}|, \quad \gamma_2 = \frac{k_a}{x'_a}|\tau_{0a}\tau_{ac}|, \quad \Gamma_a = \frac{k_a}{x'_a}(|\tau_{a0}|^2 k_0/k_a + |\tau_{ac}|^2 k_c/k_a). \tag{36}$$

The reflection and the transmission coefficients can be represented in the BW form now:

$$|R_{0\to c}|^2 = |\rho_{0a}|^2\left[1 - \frac{\sqrt{\Gamma_0\Gamma_1}\Gamma_a}{(E_0 - E_n)^2 + (\Gamma_a/2)^2} + \frac{\Gamma_0\Gamma_1}{(E_0 - E_n)^2 + (\Gamma_a/2)^2}\right], \tag{37}$$

$$|T_{0\to c}|\frac{k_c}{k_0} = \frac{\Gamma_0\Gamma_2}{(E_0 - E_n)^2 + \Gamma_a^2/4}. \tag{38}$$

The first term in (37) represents a potential scattering (reflection from the first barrier), the second term represents an interference between the potential and the resonant scattering, and the last term gives pure resonant scattering with $\Gamma_0 = |\tau_{0a}|^2 k_a^2/k_0 x'_a$ being the width for entering the potential well u_a. $\Gamma_1 = |\tau_{a0}|^2(k_0/k_a)(k_a/x'_a)$ is the width for leaving the well to the left. In (38) the magnitude $\Gamma_2 = |\tau_{ac}|^2(k_c k_a)(k_c/x'_a)$ represents the width for leaving the well to the right. We see that $\Gamma_a = \Gamma_1 + \Gamma_2$, as it is for processes with two open channels. Here the two channels correspond to leaving the well to the left and to the right through the potentials V_1 and V_2, respectively.

4.2. Splitting of Two Resonances. To study splitting of the resonances let us suppose, that the potential V_2 also has a resonance inside it, i.e., that there is a constant potential level u_q of width x_q inside the potential V_2. Then ρ_{ac} in the denominators of (30) can be written as:

$$\rho_{ac} = \frac{\rho_{aq} - \exp(2ik_q x_q)\rho_{qc}(\rho_{aq}\rho_{qa} - \tau_{aq}\tau_{qa})}{1 - \exp(2ik_q x_q)\rho_{qc}\rho_{qa}}. \tag{39}$$

After substitution of (39) into (30) we find that the amplitudes $R_{0\to c}$ and $T_{0\to c}$ are expressed as fractions with the denominator:

$$D = [1 - \exp(2ik_q x_q)\rho_{qc}\rho_{qa}][1 - \exp(2ik_a x_a)\rho_{aq}\rho_{a0}] - \exp(2ik_q x_q + 2ik_a x_a)\rho_{qc}\rho_{a0}\tau_{aq}\tau_{qa}. \tag{40}$$

After extraction of the phase $\exp(i\xi_a + i\xi_q)$, where:

$$\xi_a = 2k_a x_a + 2\zeta_{qc} + 2\zeta_{qa}, \quad \xi_q = 2k_q x_q + 2\zeta_{aq} + 2\zeta_{a0},$$

we obtain

$$D = e^{i\xi_a + i\xi_q}\{[e^{-i\xi_a} - |\rho_{qc}\rho_{qa}|][e^{-i\xi_q} - |\rho_{aq}\rho_{a0}|] + |\rho_{qc}\rho_{a0}\tau_{aq}\tau_{qa}|\}, \tag{41}$$

where we have taken into account that $\tau_{aq}\tau_{qa} = -|\tau_{aq}\tau_{qa}|\exp(4i\phi_{Rqa})$ and $2\phi_{Rqa} = \zeta_{qa} + \zeta_{aq}$. After expansion of $\xi_a(k_0)$ and $\xi_q(k_0)$ near the points $k_0 = k_n$ and $k_0 = k'_n$, respectively we reduce formulas for $R_{0\to c}$ and $T_{0\to c}$ to fractions with the denominator equal to:

$$D' = [E_0 - E_n + i\Gamma_a][E_0 - E'_n + i\Gamma_q] - Q^2, \quad Q^2 = 4k_n k'_n \frac{|\rho_{qc}\rho_{a0}\tau_{aq}\tau_{qa}|}{d\xi_a(k_n)/dk_n d\xi_q(k'_n)/dk'_n}. \tag{42}$$

One can see that the denominator can be split into two BW-type denominators with modified position of the resonances and their widths. If both resonances are identical, i.e., $E'_n = E_n$, and $\Gamma_a = \Gamma_q \equiv \Gamma$, then

$$D' = [E_0 - E_n + Q + i\Gamma][E_0 - E_n - Q + i\Gamma], \tag{43}$$

which means that there is a splitting of the resonances. The splitting $2Q$ decreases as the transmission between wells a and q decreases.

There is an interesting case when we have two resonances with the same energy $E_n = E'_n$, but with different widths $\Gamma_a \neq \Gamma_q$. It may happen such that, if $|\Gamma_a - \Gamma_q| > 2Q$, then there will be no splitting, but only a modification of the widths. The difference of the widths in such a case decreases. It is interesting to investigate the physical meaning of this effect, and to see how such resonances do interfere with each other.

4.3. Reflection and Transmission Amplitudes of a Magnetic MS. If we take into account the neutron magnetic moment, then the neutron wave-function becomes a spinor one. The potential barrier is now a matrix $\hat{u}_a = u_a + \boldsymbol{\omega\sigma}$ as in section (2.1), where u_a is the nonmagnetic potential. The transmission and reflection amplitudes become operators or 2×2 matrices which do not commute if fields in ajacent layers are noncollinear.

For rectangular magnetic barrier the reflection and transmission amplitudes are determined in the same way as in (15,16), for nonmagnetic one, but the positions of different factors in formulas cannot be arbitrarily changed. Indeed, in the magnetic case the formulas (15,16) appear slightly more complicated:

$$\hat{R} = \hat{r} + \hat{t}'\hat{e}\hat{r}'\hat{e}[1 + \hat{r}'\hat{e}\hat{r}'\hat{e} + (\hat{r}'\hat{e}\hat{r}'\hat{e})^2 + \cdots]\hat{t} = \hat{r} + \hat{t}'\hat{e}\hat{r}'\hat{e}(1 - \hat{r}'\hat{e}\hat{r}'\hat{e})^{-1}\hat{t}, \tag{44}$$

where for simplicity we have omitted indices and have denoted $\hat{r} = \hat{r}^+_{0a}$, $\hat{r}' = \hat{r}^+_{a0}$, $\hat{t} = \hat{t}^+_{0a}$, $\hat{t}' = \hat{t}^+_{a0}$ for matrix reflection and transmission amplitudes of interfaces given by (9), and $\hat{e} = \exp(i\hat{k}^+_a x_a)$ for phase factor of propagation inside the potential.

The transmission matrix amplitude is obtained in a similar way:

$$\hat{T} = \hat{t}'\hat{e}[1 + \hat{r}'\hat{e}\hat{r}'\hat{e} + (\hat{r}'\hat{e}\hat{r}'\hat{e})^2 + \cdots]\hat{t} = \hat{t}'\hat{e}(1 - \hat{r}'\hat{e}\hat{r}'\hat{e})^{-1}\hat{t}. \tag{45}$$

Substitution of the operators gives the final expressions

$$\hat{T}^+_a = \hat{t}^+_{a0}\exp(i\hat{k}^+_a x_a)\frac{1}{1 - \hat{r}^+_{a0}\exp(i\hat{k}^+_a x_a)\hat{r}^+_{a0}\exp(i\hat{k}^+_a x_a)}\hat{t}^+_{0a} \tag{46}$$

and:

$$\hat{R}^+_a = \hat{r}^+_{0a} + \hat{t}^+_{a0}\exp(i\hat{k}^+_a x_a)\hat{r}^+_{a0}\exp(i\hat{k}^+_a x_a)\frac{1}{1 - \hat{r}^+_{a0}\exp(i\hat{k}^+_a x_a)\hat{r}^+_{a0}\exp(i\hat{k}^+_a x_a)}\hat{t}^+_{0a}. \tag{47}$$

For a more complicated potential, like the one shown in Fig. 6, the formulas with the magnetic field look similar to (46), (47) but contain more complicated matrices $\hat{t}$ and $\hat{r}$:

$$\hat{R}_{0\to c} = \hat{\rho}_{0a} + \hat{\tau}_{a0}\exp(i\hat{k}_a x_a)\hat{\rho}_{ar}\exp(i\hat{k}_a x_a)\frac{1}{1 - \hat{\rho}_{a0}\exp(i\hat{k}_a x_a)\hat{\rho}_{ar}\exp(i\hat{k}_a x_a)}\hat{\tau}_{0j}, \tag{48}$$

$$\hat{T}_{0\to c} = \hat{\tau}_{ac}\exp(i\hat{k}_a x_a)\frac{1}{1 - \hat{\rho}_{a0}\exp(i\hat{k}_a x_a)\hat{\rho}_{ac}\exp(i\hat{k}_a x_a)}\hat{\tau}_{0a}. \tag{49}$$

Let us consider the case when $u^-_a \equiv u_a - \omega_a < k_0^2 < u_a + \omega_a \equiv u^+_a$. In this case the neutron with one projection of the spin (say up, spinor ψ_u) propagates as a plane wave, and acquires the phase factor $e_1 = \exp(ik_a x_a)$ during propagation from one side of the well to another, where $k_a = \sqrt{k_0^2 - u^-_a}$. The other projection of spin (say down, spinor ψ_d) cannot propagate, because its phase factor becomes $e_2 = \exp(-\kappa_a x_a) \ll 1$, where $\kappa_a = \sqrt{u^+_a - k_0^2}$. To find the transmission it is necessary to find the eigenfunctions, ψ_Q, and the eigenvalues Q of the operator $\hat{Q} = 1 - \hat{\rho}_{a0}\exp(i\hat{k}_a x_a)\hat{\rho}_{ac}\exp(i\hat{k}_a x_a)$ in the denominators of (48,49).

One eigenfunction ψ^u_Q with $\hat{Q}\psi^u_Q = Q^u\psi^u_Q$ will correspond to the polarization close to up, and another one, ψ^d_Q with $\hat{Q}\psi^d_Q = Q^d\psi^d_Q$ — close to down.

Let us suppose that the neutron propagates from the left to the potential of Fig. 6 and has a polarization along the field and is described by spinor ψ^+, then the amplitudes $T^{++}_{0\to c}$, $T^{+-}_{0\to c}$ of transmission without and with reversal of the polarization are given:

$$T^{++,+-}_{0\to c} = [\hat{\tau}_{ac}\exp(i\hat{k}_a x_a)]^{+u}\frac{1}{Q^u}[\hat{\tau}_{0a}]^{u+,-}, \tag{50}$$

where $[\hat{A}]^{+u}$ represents the matrix element of the operator $\hat{A}$ between the states ψ^+ and ψ_Q^u.

If there is a resonance in the well in the state ψ_Q^u, then the transmission coefficients can be represented in BW form:

$$|T_{0\to r}^{++,+-}|\frac{k_r^{+,-}}{k_0^+} = \frac{\Gamma_{0a}^{+u}\Gamma^{u+}}{(E-E_n)^2+\Gamma^2/4}, \tag{51}$$

where $\Gamma = \Gamma_{a0}^{u+} + \Gamma_{a0}^{u-} + \Gamma_{ac}^{u+} + \Gamma_{ac}^{u-}$ is the total width, which is the sum of the widths for a neutron leaving the well to the left and to the right (lower indices $a0$ and ac, respectively) with the polarization $+$ or $-$ (upper indices $u+$ and $u-$, respectively). The width Γ_{0a}^{+u} describes penetration into the well in the propagating state u from the left, when the neutron is polarized along the external field.

It is interesting to note that if the neutron is polarized along the external field, which is parallel to the field inside the magnetic layer a (of high magnetic permeability), then the direct transmission of the neutron through the layer a is exponentially suppressed. However the neutron can transit the system via a nontunneling effect. This is possible if there is some noncollinearity of the internal and external fields inside of potentials V_1 and V_2 in Fig. 6. In that case there are matrix elements for the neutron to pass into the region a in the propagating mode, and, if the layer a is resonant, the transmission becomes high.

5. CONCLUSION

We have demonstrated the method for calculating reflection and transmission through magnetic and nonmagnetic multilayer systems (MS) without matching the wave function at interfaces, but using instead the multiple reflections approach. We also considered resonances in MS and showed how to find positions and widths of resonances describing scattering with the Breit–Wigner formula. We also found the amplitude of the wave function inside resonant layer, which is important for prediction of magnitudes of phenomena, which can take place at resonances.

We found an interesting phenomenon of resonant level splitting, when positions of resonances in two ajacent wells are the same but widths are different. In this case splitting will not really give two resonances with slightly different positions, but gives two resonances with the same position and with two different widths. It is very interesting to consider to what real phenomena can lead such a splitting.

We also have shown how to calculate nontunneling transmission of polarized neutrons through reflecting magnetic MS with noncollinear distribution of internal magnetization. It is not difficult to generalize the obtained formulas to look for splitting of magnetic resonances and study the analogous peculiarities of splitting as in nonmagnetic case.

We have considered only few examples in neutron optics, though the method is applicable to a wide variety of other problems which are manifest in wave and particle propagation through layered media.

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