T-ODD CORRELATION IN A NEUTRON REFLECTOMETRY EXPERIMENT

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Abstract

It is shown that transmission amplitude of a magnetic system with noncollinear magnetization contains T-odd correlation. Relation of this T-odd correlation to T-invariance and detailed balance is discussed.

1 Introduction

Let's consider reflection and transmission of the magnetic mirror shown in Fig. 1. The mirror of the total thickness d consists of two magnetic layers. Their magnetizations parallel to the coordinate plane x,y are at an angle φ to each other. The outside field is supposed to be zero. We will show that the neutron transmission matrix amplitude contains a term proportional to the time odd correlation

$$\boldsymbol{\sigma}\cdot[\boldsymbol{B}_1\times\boldsymbol{B}_2], \tag{1}$$

where $\boldsymbol{\sigma}$ is the vector of the Pauli matrices that represents direction of the neutron spin. Observation of such a correlation can be interpreted as a violation of the T-invariance.

The problem of T-odd correlations in cross sections of polarized neutrons in presence of corkscrew like magnetic fields and fluctuations was first discussed in works [1-4]. We will show that the T-odd term in the transmission matrix does not mean violation of the T-invariance even in presence of an absorption, which makes Hamiltonian to be noninvariant with respect to reverse of time.

In the next section we show how the correlation (1) does appear in transmission of the system, shown in Fig. 1. In section 3 reflection of the system shown in Fig. 1 is discussed. It is shown that reflection matrix does not contain T-odd terms, however it violates detailed balance principle. In section 4 we discuss T-odd correlation appearing in interaction of neutrons with a mirror having helicoidal magnetization, and show that violation of the detailed balance principle here is seen the most pronounced.

In section 5 we discuss the concept of the T-invariance as applied to neutron reflectometry, and show that this invariance is not violated notwithstanding of the appearance of T-odd terms, even if the system contains an absorption.

2 Derivation of (1)

Transmission matrix, T_t, of the system Fig. 1, if we neglect multiple reflections between layers[2], is represented [5, 6] as

$$T_t\approx T_2(\boldsymbol{\sigma}\boldsymbol{B}_2)T_1(\boldsymbol{\sigma}\boldsymbol{B}_1), \tag{2}$$

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[2]Inclusion of multiple reflections does not change the result, but complicates formulas.

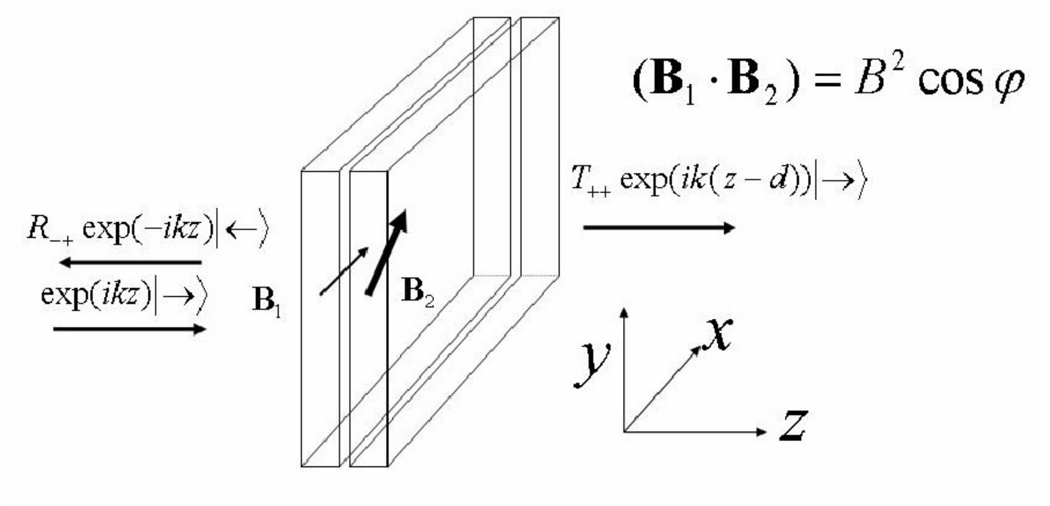

Figure 1: Reflection and transmission of a magnetic mirror of thickness d, consisting of 2 films magnetized within x, y coordinate plane, which is parallel to their interfaces. External magnetic field is zero. Magnetic fields $\boldsymbol{B}_{1,2}$ of the films are at an angle φ to each other. The incident neutron going from the left and polarized along the normal to the films (z-axis) can be reflected, say, with spin flip (R_{-+} is the reflection amplitude) or transmitted, say, without spin flip (T_{++} is the transmission amplitude).

where T_i ($i = 1, 2$) are transmission matrices of separate layers:

$$T_i(\boldsymbol{\sigma B}_i) = \exp(ik'(\boldsymbol{\sigma B}_i)l_i)\frac{1 - r^2(\boldsymbol{\sigma B}_i)}{1 - r^2(\boldsymbol{\sigma B}_i)\exp(2ik'(\boldsymbol{\sigma B}_i)l_i)}, \tag{3}$$

where l_i is the thickness of the i-th layer ($i = 1, 2$),

$$k'(\boldsymbol{\sigma B}_i) = \sqrt{k^2 - u_j - \boldsymbol{\sigma B}_i} \tag{4}$$

k is the wave number of the incident neutron, $u_i = \; - iu''$ is the optical potential of the i-th layer, and

$$r(\boldsymbol{\sigma B}_i) = \frac{k - k'(\boldsymbol{\sigma B}_i)}{k + k'(\boldsymbol{\sigma B}_i)} \tag{5}$$

is the reflection matrix at the interface between vacuum and i-th layer The potential u is defined with the factor $2m/\hbar^2$, and the field $\boldsymbol{B}$ is defined with the factor $2\mu m/\hbar^2$ (m and μ are the neutron mass and the absolute value of its magnetic moment respectively).

An arbitrary function $f(\boldsymbol{\sigma B})$ can be represented in the form

$$f(\boldsymbol{\sigma B}) = f^{(+)} + \boldsymbol{\sigma b} f^{(-)}, \tag{6}$$

where

$$f^{(\pm)} = \frac{f(B) \pm f(-B)}{2}, \qquad \boldsymbol{b} = \frac{\boldsymbol{B}}{B}. \tag{7}$$

Therefore

$$T_i(\boldsymbol{\sigma B}_i) = T_i^{(+)} + \boldsymbol{\sigma b}_i T_i^{(-)}, \tag{8}$$

and its substitution into (2) gives

$$T_t = \left[T_1^{(+)} + \boldsymbol{\sigma}\boldsymbol{b}_1 T_1^{(-)}\right]\left[T_2^{(+)} + \boldsymbol{\sigma}\boldsymbol{b}_2 T_2^{(-)}\right] =$$

$$= T_1^{(+)}T_2^{(+)} + T_1^{(-)}T_2^{(+)}\boldsymbol{\sigma}\cdot\boldsymbol{b}_1 + T_2^{(-)}T_1^{(+)}\boldsymbol{\sigma}\cdot\boldsymbol{b}_2 + T_1^{(-)}T_2^{(-)}(\boldsymbol{\sigma}\cdot\boldsymbol{b}_1)(\boldsymbol{\sigma}\cdot\boldsymbol{b}_2) =$$

$$= \left[T_1^{(+)}T_2^{(+)} + T_1^{(-)}T_2^{(-)}\cos\varphi\right] + T_1^{(-)}T_2^{(+)}\boldsymbol{\sigma}\cdot\boldsymbol{b}_1 + T_2^{(-)}T_1^{(+)}\boldsymbol{\sigma}\cdot\boldsymbol{b}_2 + iT_1^{(-)}T_2^{(-)}(\boldsymbol{\sigma}\cdot[\boldsymbol{b}_1\times\boldsymbol{b}_2]), \quad (9)$$

where the last term, which contains correlation (1), results from the well known relation

$$(\boldsymbol{\sigma}\cdot\boldsymbol{b}_1)(\boldsymbol{\sigma}\cdot\boldsymbol{b}_2) = (\boldsymbol{b}_1\cdot\boldsymbol{b}_2) + i(\boldsymbol{\sigma}\cdot[\boldsymbol{b}_1\times\boldsymbol{b}_2]). \quad (10)$$

Let's aline x-axis along the vector $\boldsymbol{B}_1$. Then

$$\boldsymbol{\sigma}\cdot\boldsymbol{b}_2 = \sigma_x \exp(i\varphi\sigma_z), \quad (11)$$

and the transmission matrix becomes of the form

$$T_t = A + C\sigma_x[1 + D\exp(i\varphi\sigma_z)] + iE(\boldsymbol{\sigma}\cdot[\boldsymbol{b}_1\times\boldsymbol{b}_2]), \quad (12)$$

where A, C, D, E are complex functions of the incident wave number k. From (12) it follows that the transmission probabilities without spin flip, for initial states $\sigma_z|\pm\rangle = \pm|\pm\rangle$ are

$$T(\pm\pm) = |\langle\pm|T_t|\pm\rangle|^2 = |A|^2 + |E|^2\sin^2\varphi \pm 2\mathrm{Im}(AE^*)\sin\varphi, \quad (13)$$

where $\mathrm{Im}(x)$ means imaginary part of x.

We see that because of the correlation (1) transmissions of neutrons polarized along and opposite z-axis are different. It can be interpreted as a violation of time-invariance. On the other hand, if we do not know about the presence of the fields $\boldsymbol{B}_i$, we can interpret the difference of non spin-flip transmissions as a result of correlation $\boldsymbol{k\sigma}$, which violates space parity-invariance. Such an interpretation looks plausible, because the term $\mathrm{Im}(AE^*)$ varies with change of the momentum k. So, we see that interpretation of an experiment is not unambiguous.

3 Neutron reflection from the two layer magnetic mirror

Though transmission of the two layer mirror contains T-odd term, reflectivity does not contain such terms, however spin-flip reflection probability violates detailed balance principle.

Reflection matrix amplitude (for simplicity we neglect multiple scattering) is

$$R_t \approx R_1(\boldsymbol{\sigma}\boldsymbol{B}_1) + T_1(\boldsymbol{\sigma}\boldsymbol{B}_1)R_2(\boldsymbol{\sigma}\boldsymbol{B}_2)T_1(\boldsymbol{\sigma}\boldsymbol{B}_1), \quad (14)$$

where

$$R(\boldsymbol{\sigma}\boldsymbol{B}_i) = r(\boldsymbol{\sigma}\boldsymbol{B}_i)\frac{1-\exp(2ik'(\boldsymbol{\sigma}\boldsymbol{B}_i)l_i)}{1-r^2(\boldsymbol{\sigma}\boldsymbol{B}_i)\exp(2ik'(\boldsymbol{\sigma}\boldsymbol{B}_i)l_i)}. \quad (15)$$

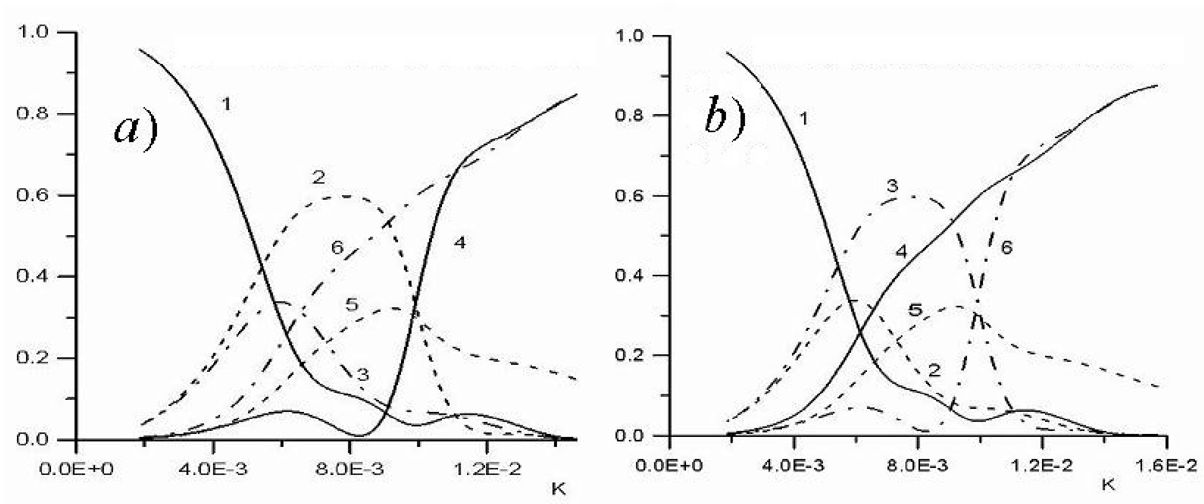

Figure 2: Calculated reflection, $R(ij) = |R_{ij}|^2$, and transmission, $T(ij) = |T_{ij}|^2$, $(i, j = \pm)$ coefficients of the two Co layers mirror of the same thickness 25 nm and magnetic induction $B = 1$ T, when the angle φ between magnetizations is a) $\pi/2$, and b) $-\pi/2$. The curves correspond to 1 — $R(++) = R(--)$, 2 — $R(-+)$, 3 — $R(+-)$, 4 — $T(++)$, 5 — $T(+-) = T(-+)$, 6 — $T(--)$. The change of sign of φ leads to exchange $R(\pm\mp) \to R(\mp\pm)$ of spin-flip curves in reflectivities and of non spin-flip $T(\omega\pm) \to T(\mp\mp)$ curves in transmissivities. The wave number k along horizontal axis is given in Å^{-1}.

Substitution of (15) and (3) into (14) with account of the representation (6) and choice of x-axis along vector $\boldsymbol{B}_1$ reduces (14) to the form

$$R_t = A + C\sigma_x[1 + D\exp(i\varphi\sigma_z) + E\exp(-i\varphi\sigma_z)], \tag{16}$$

where A, C, D, E are complex functions of the incident wave number k. From this expression we see that non spin-flip reflectivities for both incident polarizations are equal to each others:

$$R(++) = R(--) = |\langle\pm|R_t|\pm\rangle|^2, \tag{17}$$

while spin-flip reflectivities, $R(\pm\mp)$, are different and their dependence on the angle φ is such that

$$R(\pm\mp, \varphi) = R(\mp\pm, -\varphi), \tag{18}$$

which is clearly seen in Fig 2, where reflectivities and transmissivities calculated for two identical Co layers of thickness 25 nm with magnetizations $B_{1,2} = 1$ T, when angle between $\boldsymbol{B}_1$ and $\boldsymbol{B}_2$ is $\varphi = \pm\pi/2$, are shown.

We see that non spin-flip transmissivities are different and change with sign of φ according to the T-odd correlation (1). The spin-flip transmissivities are equal because according to (9) the factor D in (12) for two identical layers is equal to unity.

Difference of the two spin-flip reflectivities means violation of the detailed balance principle, because it creates a cycle current in phase space, which diminishes the entropy. We will discuss this effect in the next section, where violation of the detailed balance is seen more strikingly.

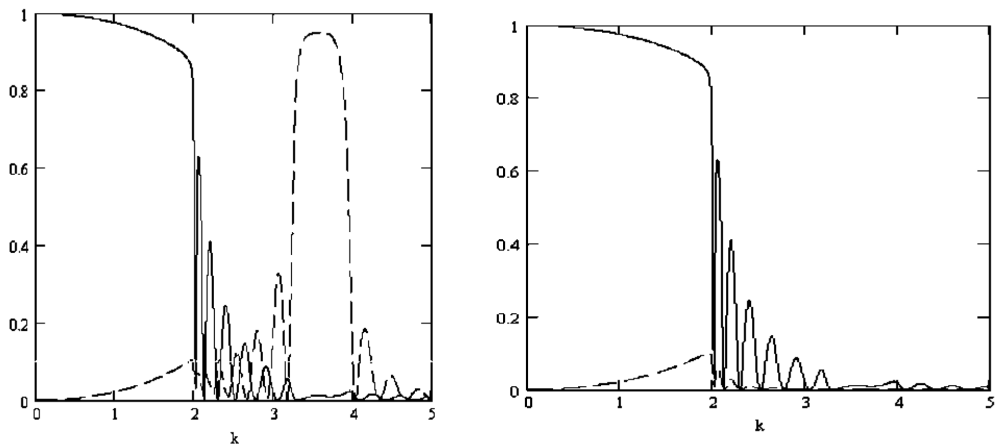

Figure 3: Reflectivity of a helicoidal magnetic mirror with (dashed line) and without spin flip (solid line) for the incident polarization opposite (left) and along (right) z-axis [9]. We see that above the range of the total reflection there is a well pronounced peak of almost total spin flip reflection, when the incident neutron is polarized against z-axis.

4 Neutron reflectometry for a magnetic mirror with helicoidal magnetization

The false effect of the time and parity violation is especially well seen in the case of the neutron reflection from a magnetic mirror magnetized helicoidally [9] around a vector $\boldsymbol{q}$ which is directed along z-axis parallel to the normal to the mirror interface. Neutron wave function in helicoidal field was found in [7], though reflection and transmission of helicoidal mirrors were calculated in [8, 9]. In Fig. 3 there are shown reflectivities with and without spin flip for polarizations of the incident neutron along and opposite z-axis. Outside of the mirror magnetic field is absent. The analogous transmission probabilities are shown in Fig. 4. We see that there is again a time-odd correlation $\boldsymbol{\sigma q}$, which can be also interpreted as a parity odd correlation with the incident neutron momentum $\boldsymbol{\sigma k}$. The resonant spin-flip reflectivity for $|-\rangle$ polarization increases with the mirror thickness, and becomes almost total. Such a reflectivity violates the detailed balance principle, and the violation in this example is especially well seen. Indeed, imagine that a vessel with ideal walls is homogeneously filled with a gas of unpolarized neutrons. If we split the vessel into two parts as shown in Fig. 5, inserting the helicoidal mirror, then all the neutrons from the left part I go through the mirror to the right part II, and become completely polarized along z-axis. Indeed, the neutrons in state $|+\rangle$ go directly through the mirror, and cannot go back, while the neutrons in the state $|-\rangle$ are reflected from the mirror with spin-flip, and after reflection from ideal walls of the vessel go again to the mirror and through it to the part II. Therefore it looks as if all the neutrons from the part I gather in the part II in the single state $|+\rangle$, which terribly decreases the entropy.

However in fact such a spilling over the mirror from left to right is compensated by the opposite flux from II to I, because in the right part neutrons in the state $|-\rangle$ can go through the mirror, while neutrons in the state $|+\rangle$ are reflected from the mirror with spin flip to the state $|-\rangle$ and at the second incidence go through the mirror to the part

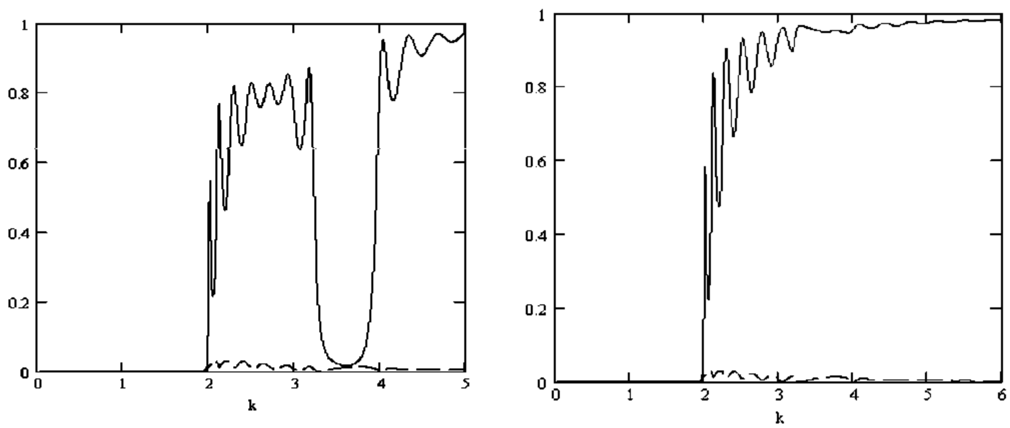

Figure 4: Transmission probabilities of a helicoidal magnetic mirror with (dashed line) and without spin flip (solid line) for the incident polarization opposite (left) and along (right) z-axis [9]. We see that above the range of total reflection there is a well pronounced dip in transmission of neutrons initially polarized against z-axis.

I. Therefore in both parts neutrons remain isotropic and in unpolarized state, however in the phase space there appear a cycle, which means a decrease of the entropy.

Decrease of the entropy is created by the rotation vector $\boldsymbol{q}$. Such a rotation makes the space into imbalance. Even two magnetic fields considered in previous section create an imbalance, though this imbalance is not so evident as in the considered case of the helicoidal mirror.

5 Analysis of the time invariance

Let's analyze the principle of T-invariance, in the simplest case of the neutron scattering on a nonmagnetic one-dimensional potential $u(x)$, which is nonzero in an interval $0 \le x \le d$.

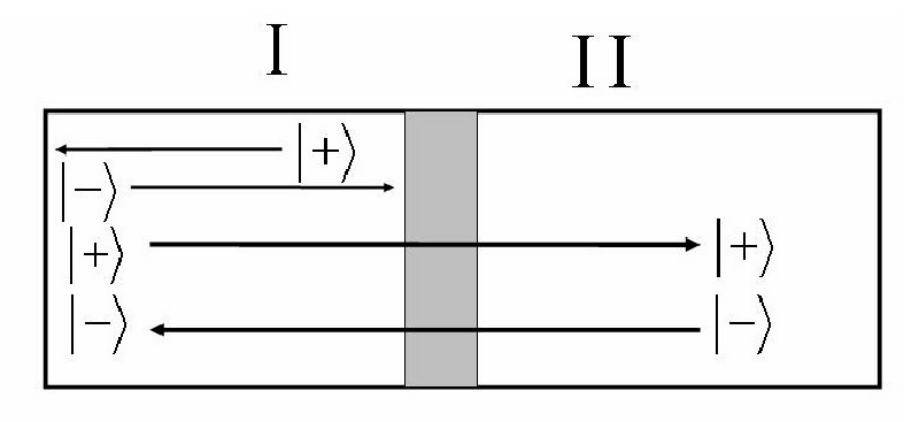

Figure 5: Illustration of violation of the detailed balance principle.

The neutron wave function outside of the potential is

$$\psi(x,t) = e^{-i\omega t}\left[\Theta(x<0)\Big(\exp(ikx) + R(k)\exp(-ikx)\Big) + \Theta(x>d)T(k)\exp(ik(x-d))\right], \tag{19}$$

where $\Theta(x)$ is a step function equal to unity when inequality in its argument is satisfied, and to zero otherwise, and $R(k)$ and $T(k)$ are reflection and transmission amplitudes, which are complex function of the incident wave number k. The wave function is a solution of the Schrödinger equation

$$\left(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial x^2} - u(x)\right)\psi(x,t) = 0. \tag{20}$$

If we make a transformation

$$t \to -t \tag{21}$$

the equation for $\psi(x,-t)$ will look differently comparing to (20). To restore its form we have to make complex conjugation, after which we get

$$\left(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial x^2} - u^*(x)\right)\psi^*(x,-t) = 0. \tag{22}$$

However we are to be careful here. The potential, if it has an imaginary part, changes after complex conjugation, therefore we cannot be sure that the function $\psi^*(x,-t)$ remains a solution of (22). Therefore, instead of (22) we should write

$$\left(i\frac{\partial}{\partial t} + \frac{\partial^2}{\partial x^2} - u^*(x)\right)\Psi(x,t) = 0, \tag{23}$$

and check, whether $\Psi(x,t) = \psi^*(x,-t)$ or not. We will prove that in the case of a rectangular potential this equality is true, and suggest that there are no reason to doubt its truth for other potentials.

In fact we can deal with stationary equations, representing $\Psi(x,t) = \exp(-i\omega t)\Phi(x)$ and $\psi(x,t) = \exp(-i\omega t)\phi(x)$, and our goal is to show that solution $\Phi(x)$ of the equation

$$\left(k^2 + \frac{\partial^2}{\partial x^2} - u^*(x)\right)\Phi(x) = 0, \tag{24}$$

coincides with $\phi^*(x)$.

In the case of a rectangular barrier potential of height $u = u' - iu''$ and width d the wave function on the full axis x is $\phi(x,u)$, where [10]

$$\phi(x,u) = \Theta(x<0)\Big(e^{ikx} + R(k,u)e^{-ikx}\Big) +$$
$$+\Theta(0<x<d)\frac{[1+r(k,u)]\exp(ik'(u)d)}{1-r^2(k,u)\exp(2ik'(u)d)}\left[e^{ik'(u)(x-d)} - r(k,u)e^{-ik'(u)(x-d)}\right] +$$
$$+\Theta(x>d)T(k,u)e^{ik(x-d)}, \tag{25}$$

where

$$R(k,u) = \frac{r(k,u)[1-\exp(2ik'(u)d)]}{1-r^2(k,u)\exp(2ik'(u)d)}, \qquad T(k,u) = \frac{\exp(ik'(u)d)[1-r^2(k,u)]}{1-r^2(k,u)\exp(2ik'(u)d)}, \tag{26}$$

$$r(k,u)=\frac{k-k'(u)}{k+k'(u)},\qquad k'(u)=\sqrt{k^2-u}, \tag{27}$$

and everywhere we explicitly pointed out dependence on the complex potential u.

The function $\phi^*(x,u)$ is

$$\phi^*(x,u)=\Theta(x<0)\Big(e^{-ikx}+R^*(k,u)e^{ikx}\Big)+$$

$$+\Theta(0<x<d)\frac{[1+r^*(k,u)]\exp(-ik'^*(u)d)}{1-r^{*2}(k,u)\exp(-2ik'^*(u)d)}\left[e^{-ik'^*(u)(x-d)}-r^*(k,u)e^{+ik'^*(u)(x-d)}\right]+$$

$$+\Theta(x>d)T^*(k,u)e^{-ik(x-d)}. \tag{28}$$

The function (28) describes interference of two waves incident from the left and right with relative amplitudes $R^*(k)$ and $T^*(k)$. We will show that it coincides with the solution $\Phi(x)$ of (24) containing these two incident waves. The wave incident from the left gives a solution $\Phi_l(x)$, the wave, incident from the right gives a solution $\Phi_r(x)$, and the total solution is $\Phi_l(x)+\Phi_r(x)$. With the help of general approach presented in [10, 11] we obtain

$$\Phi_l(x,u^*)=\Theta(x<0)R^*(k,u)\Big(e^{ikx}+R(k,u^*)e^{-ikx}\Big)+$$

$$+\Theta(0<x<d)R^*(k,u)\frac{[1+r(k,u^*)]\exp(ik'(u^*)d)}{1-r^2(k,u^*)\exp(2ik'(u^*)d)}\left[e^{ik'(u^*)(x-d)}-r(k,u^*)e^{-ik'(u^*)(x-d)}\right]+$$

$$+\Theta(x>d)R^*(k,u)T(k,u^*)e^{ik(x-d)} \tag{29}$$

is the wave function for the incident wave $R^*(k,u)\exp(ikx)$, and

$$\Phi_r(x,u^*)=\Theta(x<0)T^*(k,u)T(k,u^*)e^{-ikx}+$$

$$+\Theta(0<x<d)T^*(k,u)\frac{[1+r(k,u^*)]\exp(ik'(u^*)d)}{1-r^2(k,u^*)\exp(2ik'(u^*)d)}\left[e^{-ik'(u^*)x}-r(k,u^*)e^{ik'(u^*)x}\right]+$$

$$+\Theta(x>d)T^*(k,u)\left(T(k,u^*)e^{-ik(x-d)}+R(k,u^*)e^{ik(x-d)}\right) \tag{30}$$

is the wave function for the incident wave $T^*(k)e^{-ik(x-d)}$. From (27) and (26) it is seen, that $k'(u^*)=k'^*(u)$, and $r(u^*)=r^*(u)$, but $R(k,u^*)\neq R^*(k,u)$, and $T(k,u^*)\neq T^*(k,u)$.

It is easy to verify by simple algebra that the sum of terms in the interval $0<x<d$ from (29) and (30) is equal to the middle term in (28). This algebra is shown symbolically in the following 6 lines where K' denotes $k'(u^*)$, and in other terms dependence on k and u is omitted:

$$R^*\frac{[1+r^*]e^{iK'd}}{1-r^{*2}e^{2iK'd}}\left[e^{iK'(x-d)}-r^*e^{-iK'(x-d)}\right]+T^*\frac{[1+r^*]e^{iK'd}}{1-r^{*2}e^{2iK'd}}\left[e^{-iK'x}-re^{iK'x}\right]=$$

$$=\frac{r^*(1-e^{-2ik'^*d})}{1-r^{*2}e^{-2ik'^*d}}\frac{[1+r^*]e^{iK'd}}{1-r^{*2}e^{2iK'd}}\left[e^{iK'(x-d)}-r^*e^{-iK'(x-d)}\right]+$$

$$+\frac{e^{-ik'^*d}(1-r^{*2})}{1-r^{*2}e^{-2ik'^*d}}\frac{[1+r^*]}{1-r^{*2}e^{2iK'd}}\left[e^{-iK'(x-d)}-e^{2iK'd}r^*e^{iK'(x-d)}\right]=$$

$$e^{ik'^*(x-d)}\Big[r^*(1-e^{-2ik'^*d})[1+r^*]e^{ik'^*d}-e^{-ik'^*d}(1-r^{*2})[1+r^*]e^{2ik'^*d}r^*\Big]+$$
$$+e^{-ik'^*(x-d)}\Big[-r^*(1-e^{-2ik'^*d})[1+r^*]e^{ik'^*d}r^*+e^{-ik'^*d}(1-r^{*2})[1+r^*]\Big]=$$
$$=\frac{[1+r^*]e^{-ik'^*d}}{1-r^{*2}e^{-2ik'^*d}}\Big[e^{-ik'^*(x-d)}-r^*e^{ik'^*(x-d)}\Big] \tag{31}$$

In a similar way it is possible to verify that the sum of amplitudes of two outgoing waves at $x<0$ is equal to

$$R^*(k,u)R(k,u^*)+T^*(k,u)T(k,u^*)=1. \tag{32}$$

The right outgoing wave at $x>d$ vanishes. Its amplitude

$$R^*(k,u)T(k,u^*)+T^*(k,u)R(k,u^*)=2\mathrm{Re}(R^*(k,u)T(k,u^*))=0, \tag{33}$$

which shows that the phases of the amplitudes $R(k,u)$ and $T(k,u^*)$ differ by $\pi/2$. So, we see that the scattering of a scalar particle on a complex potential is time reversible. We have checked it for a simple rectangular potential, but there are no reason to think that for more complex potential the result will be different.

In a similar way it is possible to show that scattering of a spinor particle on an arbitrary magnetic potential will be reversible after transformation of (21), reverse of fields and spin and complex conjugation. The transformed wave function will describe the time reversed processes.

6 Conclusion

With the help of simple examples we have shown how in a simple neutron reflectometry experiment T-odd terms appear that can be interpreted as T- or P-parity violation though they do not violate neither T- nor P-invariance. At the same time, if the space contains even a couple of noncollinear magnetic fields, interaction of neutrons with this couple does not satisfy the principle of detailed balance.

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