Neutron reflection from condensed matter, the Goos-Hänchen effect and coherence.

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Abstract

The Goos-Hänchen (G-H) effect for neutron reflection from condensed matter is considered. An experiment to quantify the effect is proposed. The relation of G-H shift to the neutron coherence length is considered.

Key words: Neutron optics, Goos-Hänchen effect, quantum mechanics, wave packets.

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1 Introduction

Newton suggested first (see, for example [1,2]), that a beam of light at a specular reflection shifts some distance along the surface of a reflecting mirror, as shown in fig. 1. If the incident light is represented by a ray, then propagation of the ray in a mirror can be described by some trajectory, where exit point $B$ of the reflected ray does not coincide with entrance point $A$ of the incident one. The shift $AB$ is called G-H effect, because F. Goos and H. Hänchen [2,3] experimentally measured it.

The shift should exist not only for light but also for particles, because propagation of particles in quantum mechanics is described by wave functions similar to the wave field of the light.

The shift depends on interaction of particles with matter and investigation of it can be useful for applied [1,4] and fundamental research. In this article we consider G-H effect in neutron physics (see, for example, [5] and references there in).

We address several problems. First, we calculate longitudinal G-H shift at total reflection for restricted Gaussian beams (like in optics) and for wave packets. We believe that this approach is more general than the one (with the help of two plane waves) used in [5]. Second, we calculate deviation of reflected beam from specular direction for Gaussian beam (it is similar to [6] in x-ray optics) and for wave-packets. And third, we discuss the problem of enhanced G-H effect at reflection from a thin layer evaporated on a totally reflecting substrate. We believe that investigation of G-H effect in optics of neutrons can help to understand deeper the nature of the neutron wave function: whether it is a plane wave or a wave packet. If it is the wave packet then whether it is related to preparation of the neutron beam or it is an intrinsic property of the neutron.

Section 2 reminds the reader how the G-H effect is calculated. We consider plane waves, finite beams and wave packets reflection from a single interface and from a layer on a substrate. In section 3 we discuss how peculiarities related to the G-H effect can be measured, and what information on neutron wave packet can be obtained. We
Figure 1. Schematical explanation of the G-H shift

address there a question whether calculation of reflection amplitude from a layer with two interfaces, which uses coherent superposition of coherent multiple reflection of waves (see, for example [7,8,9,10]), is accurate, and justify the appropriateness of introduction in [11] of so called “coherence length”. This length determines such a length of the G-H shift, at which reflection coefficient contains a considerable contribution of incoherent reflection.

At the end of this paper, in conclusion, we shortly discuss applicability of our calculation of the neutron G-H effect to x-rays

2 Calculation of the G-H shift

Here we consider neutron reflection from an ideal surface of a semiinfinite mirror, which means that we have a single interface. Reflection takes place because interaction of neutron with matter. This interaction is characterized by an optical potential \( u/2 \), where \( u = 4\pi N_0 b \), \( N_0 \) is atomic density, \( b \) is coherent scattering amplitude on a single atom, and for convenience we set \( \hbar = m = 1 \). If normal component \( k_z \) of the incident neutron momentum \( \mathbf{k} \) is small \( (k_z^2 < u) \), the neutron is totally reflected from the interface, i.e. reflection coefficient \( |R|^2 = 1 \). If normal component \( k_z \) is large \( (k_z^2 > u) \), the reflection is not total (in the following we call it “nontotal”), and \( |R|^2 < 1 \). Here \( R \) denote reflection amplitude.

Reflection coefficient depends not only on \( \mathbf{k} \) and \( u \), but also on structure of the wave function of the incident particle. Below we consider three types of this function: plane wave, stationary beam, and a wave packet.

2.1 Plane wave

Let the incident particle be described by a plane wave

\[
\exp(i\mathbf{k}_0 \cdot \mathbf{r} - i\omega t),
\]

where \( \omega = k_0^2/2 \) is the energy of the neutron and \( \mathbf{k}_0 = (k_\parallel, -k_z) \) is a wave vector, with component \( k_\parallel \) parallel, and \( k_z \) — normal to the interface.

The reflected wave is

\[
R \exp(i k_z z + i k_\parallel \cdot \mathbf{r}_\parallel - i\omega t) = |R| \exp(-2i\phi(k_z) + i k_z z + i k_\parallel \cdot \mathbf{r}_\parallel - i\omega t),
\]

where the reflection amplitude

\[
R(k_z) = \frac{k_z - k_z'}{k_z + k_z'}
\]

\( (k_z' = \sqrt{k_z^2 - u}) \) is represented as \( R = |R| \exp(-2i\phi) \).

The phase \( \phi \) and the absolute value \( |R| \) depend only on \( k_z \). When \( k_z^2 > u \) and \( u/2 \) is purely real, i.e. there are no losses, then \( |R| < 1 \) (reflection is nontotal), and \( \phi = 0 \). Since there is no phase shift \( \phi = 0 \), the phase of the reflected wave at every points on the interface is equal to the phase of the incident wave.

When \( k_z^2 < u \) then \( |R| = 1 \), i.e. reflection is total, and the phase is nonzero: \( 0 \leq \phi = \arccos(k_z/\sqrt{u}) \leq \pi/2 \). It means that the phase of the reflected wave (1) is equal to the phase \( k_z z + k_\parallel \cdot \mathbf{r}_\parallel - \omega t \) of the incident wave at points \( \mathbf{r}_\parallel \) displaced along the interface by a distance \( \delta \mathbf{r}_\parallel = 2\phi/k_z \). This distance can be called the G-H shift, but a spatial displacement can be well defined only for finite size beams. In case of infinite plane waves we can talk only about the phase shift.
2.2 Two plane waves

In [5] the G-H shift was calculated with the help of two plane waves. The incident neutron was supposed to be described by the wave function

\[ \psi_i = \exp(ik_1r) + \exp(ik_2r) \]

consisting of two waves with wave vectors \( k_i = (k_{ix}, k_{i\perp}) \), where \( k_x \) is a component along surface, and \( k_{\perp} \) is perpendicular to it. This function can be also represented as

\[ \psi_i = 2 \exp(ikr) \cos(\delta kr), \] (2)

where \( k = (k_2 + k_1)/2, \delta k = (k_1 - k_2)/2 \). We see, that at the interface \( z = 0 \) we have a plane wave \( \exp(ikx) \) modulated by \( \cos(\delta kx) \).

After total reflection this wave function is transformed into

\[ \psi_r = R(k_{1\perp}) \exp(ik_1'r) + R(k_{2\perp}) \exp(ik_2'r) = \exp(ik_1'r + i\phi_1) + \exp(ik_2'r + i\phi_2), \]

where for total reflection we replaced reflection amplitudes \( R(k_{i\perp}) \), which depend only on normal components of the wave vectors by \( \exp(i\phi_i) \). Wave vectors of the reflected waves are \( k_i' = (k_{ix}, -k_{i\perp}) \). The sum of the reflected waves can be also represented as

\[ \psi_r = 2 \exp(ik'r + i\phi) \cos(\delta k'r + \delta \phi), \] (3)

where \( k' = (k_2' + k_1')/2, \phi = (\phi_1 + \phi_2)/2, \delta k = (k_1' - k_2')/2, \) and \( \delta \phi = (\phi_1 - \phi_2)/2 \). We see, that at the interface \( z = 0 \) we have a plane wave \( \exp(ikx + \phi) \) modulated by \( \cos(\delta kx + \delta \phi) \). If we represent \( \delta \phi \) as \( \delta kx \xi \) (why not?) we obtain that modulation of the reflected wave is shifted along \( x \) axis by \( \xi = \delta \phi/\delta k_x \), which can be considered and was accepted in [5] as the G-H shift.

2.3 Wave function of a beam

Imagine now that the wave function of a neutron is confined in space around a ray, i.e. it looks like a cylindrically symmetrical Gaussian [6]. Such a wave function can be stationary, and it creates an elliptical spot at the interface [6]. We will place an origin \( r = 0 \) of the coordinate system in the center of this spot and choose \( xz \) to be the plane of incidence. The beam at the interface is

\[ \psi(r||, z=0, t) = \exp(ik_x x - i\omega t) \times \exp \left( -s^2 \left[ \frac{x^2 \cos^2 \theta}{2} + \frac{y^2}{2} \right] \right), \] (4)

where \( r_\parallel = (x, y), \omega = k^2/2 = (k_x^2 + k_y^2)/2, 1/s \) is the beam’s width, and \( \cos \theta = k_z/k \equiv \sqrt{k^2 - k_x^2}/k \) is the effective angle of incidence.

Once we find the the wave function of the reflected beam at the interface, the position of the center of the reflected beam with respect to the origin will give the magnitude of the G-H shift.

To find the reflected wave function we need first to restore the complete incident one from its spot (4). In order to do that we represent (4) as a Fourier expansion

\[ \psi_0(r||, z = 0, t) = \int_{-\infty}^{\infty} \frac{d^2q_\parallel}{2\pi s^2 \cos \theta} \exp(\text{i}q_\parallel r_\parallel - \text{i}q_z z - \text{i}\omega t) \times \exp \left( -\frac{(q_x - k_x)^2}{2s^2 \cos^2 \theta} - \frac{q_y^2}{2s^2} \right), \] (5)

and multiply the integrand by a factor \( \exp(-\text{i}q_z z) \).

Then,

\[ \psi_0(r||, z, t) = \int_{-\infty}^{\infty} \frac{d^2q_\parallel}{2\pi s^2 \cos \theta} \text{e}^{\text{i}q_\parallel r_\parallel - \text{i}q_z z - \text{i}\omega t} \times \exp \left( -\frac{(q_x - k_x)^2}{2s^2 \cos^2 \theta} - \frac{q_y^2}{s^2} \right), \] (6)

where \( q_z \) must satisfy \( q_\parallel^2 + q_z^2 = 2\omega = k^2 \) so that the function (6) satisfies the free Schrödinger equation. Thus \( q_z = \sqrt{k^2 - q_\parallel^2} \).

The incident wave function can be represented as a superposition of plane waves, while the reflec-
tion of a plane wave is known. Thus, we can immediately find the wave function of the reflected particle:

\[ \psi_r(r_{||}, z, t) = \int_{-\infty}^{\infty} \frac{d^2q_{||}R(q_{||})}{2\pi s^2 \cos \theta} e^{iq_{||}r_{||} + iq_s z - i\omega t} \times \exp \left( -\frac{(q_x - k_x')^2}{2s^2 \cos^2 \theta} - \frac{q_y^2}{s^2} \right), \tag{7} \]

where \( R(q_{||}) \) is the reflection amplitude of the incident plane wave \( \exp(iq_{||}r_{||} - iq_s z) \). This amplitude is well known:

\[ R(q_{||}) = \frac{q_z - q_z'}{q_z + q_z'} = \exp(-2\chi), \tag{8} \]

where \( \chi = \text{arcch}(q_z/\sqrt{u}) = \text{arcch}(q_z'/\sqrt{u}) \), and \( q_z' = \sqrt{q_z^2 - u} \).

Since \( q_x \) is not an independent variable, \( q_x = \sqrt{k_x^2 - q_z^2} \), the amplitude \( R \) through \( q_x \) depends on \( q_{||} \): \( R(q_{||}) = \exp(-2\chi(q)) \), where \( q = |q_{||}| \), and

\[ \chi(q) = \text{arcch}(\sqrt{k_x^2 - q^2} - u/\sqrt{u}). \tag{9} \]

We assume for simplicity that \( s \) is small, i.e. the radius \( 1/s \) of the beam is large. In that case the integral (7) can be easily calculated asymptotically. The function \( 2\chi(q) \) in (7) is expanded around maximum point \( q = k_{||} = (k_x, 0) \) of the Gaussian up to the linear term \( 2\chi(q) = 2\chi_0 - (q - k_{||})\xi \), where \( \chi_0 = \text{arcsh}(k_x'/\sqrt{u}) \), \( \xi = (\xi_x, 0) \), and

\[ \xi_x = -2 \frac{d}{dq_x} \chi(q)|_{q=k_{||}} = 2 \frac{k_x}{k_z'k_{||}^2}. \tag{10} \]

When \( k_{||}^2 < u \) (total reflection) the wave-vector component \( k_x' \) and thus \( \xi_x \) become imaginary, \( k_x' = ik_x'' = i\sqrt{u - k_x^2} \) and \( \xi_x = -i\xi_x = -2ik_x/k_z'k_{||}^2 \).

\[ \text{2.3.1 Nontotal reflection} \]

At \( k_z^2 > u \) the cross-section of the reflected beam at the interface \( z = 0 \), according to (7), is

\[ \psi_r(r_{||}, z = 0) = \int_{-\infty}^{\infty} \frac{R(k_z)d^2q_{||}}{2\pi s^2 \cos \theta} \times \exp(iq_{||}r_{||} + (q_x - k_x)x)x \times \exp \left( -\frac{(q_x - k_x^{'})^2}{2s^2 \cos^2 \theta} - \frac{q_y^2}{s^2} \right), \tag{11} \]

where for simplicity we omitted the time factor \( \exp(-i\omega t) \). After integrating over \( d^2q_{||} \) we obtain

\[ \psi_r(r_{||}, z = 0) = R(k_z) \exp \left( \frac{s^2}{2}\xi_x^2 \cos^2 \theta \right) \times \exp \left( -\frac{s^2}{2}[x^2 \cos^2 \theta + y^2] \right) \times \exp(i(k_x + \xi s^2 \cos^2 \theta)x). \tag{12} \]

One can see that there is no G-H shift, since the reflected beam is centered at the same point as the incident beam. However the reflection amplitude is a little bit larger than for plane waves by the factor \( \exp \left( \frac{s^2}{2}\xi_x^2 \cos^2 \theta \right) \), and one can find that it is not specular. The wave vector component \( k_x \) of the reflected beam is larger than that of the incident beam by the amount

\[ \delta k_x = \xi s^2 \cos^2 \theta = 2\frac{k_x k_z s^2}{k^2 k_z'}, \tag{13} \]

and because of the energy conservation, the component \( k_z \) must be smaller than that of the incident wave. Thus the reflected beam slightly turns from specular direction toward the interface.

Deviation of the reflected beam from specular direction is easily understandable, if we take into account that the reflection coefficient is smaller for larger \( q_z \). Thus the reflected beam is enriched with smaller \( q_z \) (and larger \( q_x \) because of energy conservation). Thus the average \( \mathbf{q} \) of the reflected beam deviates from the specular \( \mathbf{k} \).
2.3.2 Total reflection

At $k_z^2 < u$ the section of the reflected beam by the interface according to (7) becomes

$$\psi_r(r\|, z = 0) = \int_{-\infty}^{\infty} \frac{R(k_z)}{2\pi s^2 \cos \theta} \times$$

$$\exp \left( -\frac{(q_x - k_x)^2}{2s^2 \cos^2 \theta} - \frac{q_y^2}{s^2} \right) \times$$

$$\exp \left( i q r\| - i(q_x - k_x)\xi_x \right), \quad \text{(14)}$$

where

$$\xi_x = 2 \frac{k_x}{k_z} k_z', \quad k_z'' = \sqrt{u - k_z^2}. \quad \text{(15)}$$

Integrating over $d^2q\|$ we obtain

$$\psi_r(r\|, z = 0) = R(k_z) \exp(ik_x x) \times$$

$$\exp \left( -\frac{s^2}{2} [(x - \xi_x)^2 \cos^2 \theta + y^2] \right). \quad \text{(16)}$$

We see that the spot center of the reflected beam is shifted with respect to that of the incident one by a distance $\xi_x$, which is the G-H shift. The reflection in this case is completely specular. However, the phase $k_x x$ is identical to that of the incident wave, i.e. it does not contain the correction $k_x \xi_x$, which we would expect because of the G-H shift.

Above, we limited ourselves to the linear term in the expansion of the exponent $\chi$ in (8). If we retain quadratic terms we can find the broadening of the reflected beam. This, however, does not bring any new insight because of the Gaussian beam own broadening.

Expansion of $\chi(q)$ is valid only when $|k_z'| > s$. It is no longer valid near $k_z' = 0$ because $\xi_x$ diverges at this point. If we want to find the reflected beam for the critical point $k_z' = 0$, we have to approximate exponent $\chi$ by a function

$$\chi(q) \approx \sqrt{\frac{2k_x(q_x - k_x)}{u}}, \quad \text{(17)}$$

and calculate the integral (7) using the steepest descent method. As a result the spot of the reflected beam at the interface is deformed, and the reflection is not exactly specular. This case will be analyzed elsewhere, when it will be clear how to study properties of the single neutron wave function experimentally.

2.4 The G-H shift for a wave packet

In the previous paragraph we consider the G-H shift for a particle represented by a stationary beam-like wave function. It is logical, however, to describe a particle by a moving wave packet. The wave packet is not a stationary wave function, and its Fourier representation is

$$\psi_0(r, t) = \int A(q) \exp(iqr - i\omega t)d^3q, \quad \text{(18)}$$

where all components of the vector $q = (q\//, q_z)$ are independent variables, and $\omega_q = q^2/2$. For coefficients $A(q)$ we use Gaussian function,

$$A(q) = \frac{1}{(2\pi s^2)^{3/2}} \exp(-(q - k)^2/2s^2), \quad \text{(19)}$$

where for incident particle $k = (k\//=, q_z)$

Integrating (18) over $q$ gives the Gaussian wave packet in space

$$\psi_0(r, t) = \frac{1}{(1 + is^2t)^{3/2}} \times$$

$$\exp \left( -\frac{s^2}{2(1 + is^2t)}(r - k_0 t)^2 + ik_0 r - i\omega t \right), \quad \text{(20)}$$

where $s^2t$ characterize spreading of the wave packet. We suppose that $s$ is small and neglect spreading.

Cross-section of the wave packet at the interface depends on time. We can choose the time when the wave packet center crosses the interface, $t =$
near and taking into account (19), we obtain
\[ \psi \approx R(z) \int A(q) \exp(\pm iqz - i\omega_q t) d^3q. \]

where \( q_r = (q_\parallel, q_z) \) (\( q_z \) is independent variable) and \( R(q_z) \) is given by (8).

2.4.1 Total reflection

First we consider the case of the total reflection \( k_z^2 < u \), when \( \chi \) in (8) is \( \phi = \arcsin(\sqrt{1 - q_z^2/u}) \). We assume that \( s \) is small and expand \( 2\phi(q_z) \) near \( q_z = k_z \) up to the linear term, \( 2\phi(q_z) = 2\phi(k_z - \zeta_z(q_z - k_z)) \), where
\[ \zeta_z = 2/k_z'' = 2/\sqrt{u - k_z^2}. \] (23)

Placing \( R(q_z) = R(k_z) \exp(i(q_z - k_z)\tilde{\zeta}_z) \) into (22) and taking into account (19), we obtain
\[ \psi_r(r, t) = R(k_z) \int A(q) \times \exp(iq_r \cdot r + i\tilde{\zeta}_z(q_z - k_z) - i\omega_q t) d^3q. \] (24)

Integrating over \( q \) (neglecting spreading) gives
\[ \psi_r(r, t) = R(k_z) \times \exp\left(-\frac{s^2}{2} (r + \zeta - k t)^2 + ikr - i\omega_k t \right), \] (25)

where \( k = (k_\parallel, k_z) \), and the vector \( \zeta \) has components \( \zeta = (0, 0, \zeta_z) \).

At the moment \( t = 0 \), when the incident wave packet crosses the interface, the center of the reflected wave packet is at the point \( z = -\zeta_z \) under the surface (depth \( C \) in fig. 1). Thus, the real shift is not in \( x \)-direction. It is in \( z \)-direction. However because of motion of the reflected wave packet its center crosses the interface. It happens at the moment \( t = \zeta_z/k_z \), and at this moment the center of the wave packet is located at \( r_\parallel = k_\parallel \zeta_z/k_z \). This location is shifted with respect to center of incident packet. So this shift well corresponds to the intuitive understanding illustrated in fig. 1, and can be called the G-H shift (15).

It is important to note that the cross-section of the wave packet at the interface has a circular form, not an elliptical form as in the case of a beam. Since the linear expansion is valid for \( k''_z \gg s \), the G-H shift is \( \zeta_z \ll 2/s \), and \( \zeta_\parallel = 2k_\parallel \zeta_z/k_z \ll 2k_\parallel/sk_z \) respectively.

2.4.2 Nontotal reflection

We consider now the case \( k_z^2 > u \), when \( \chi = \arcsin(q_z^2/u - 1) \) is real. Expanding \( 2\chi(q_z) \) near \( q_z = k_z \) up to the linear term gives \( 2\chi(q_z) = 2\chi(k_z) + \zeta_z(q_z - k_z) \), where \( \zeta_z = 2/k_z'' = 2/\sqrt{k_z^2 - u} \). Then we place \( R(q_z) = R(k_z) \exp(-(q_z - k_z)\zeta_z) \) into (22), take into account (19) and integrate the result over \( q \), while neglecting spreading of the wave packet. As a result, the wave function is
\[ \psi_r(r, t) = R(k_z)e^{i\tilde{\zeta}_z s^2/2} \times \exp\left(-\frac{s^2}{2}(r - k't)^2 + ikr - i\omega_{k't}t \right), \] (26)

where \( k' = (k_\parallel, k_z - \zeta_z s^2) \), and \( \omega_{k'} = k''/2 < k^2/2 \).

We see that the center of the reflected wave packet crosses the interface at the same moment \( t = 0 \) and at the same point \( r_\parallel = 0 \) as the incident wave packet, i.e. there are no G-H shift. However, the momentum of the reflected wave packet is less than that of the incident wave packet. The normal component of the momentum is less by the amount
\[ \delta k_z = -\zeta_z s^2, \] (27)
which means non-specular reflection. The energy \( \omega_{k'} \) of the reflected wave is less than that of the incident wave. However, since the total energy should conserve after the elastic interaction with the interface, the refracted wave has larger energy than the incident wave.

The change in energy is the result of the independent reflections of the different plane waves, and thus the result of the deformation of the wave packet at the reflection. The higher is the normal component of the component plane wave, the less is its reflection amplitude. To avoid such deformation we must assume that the wave packet is an intimate property of the particle as, for example, is in the case of the de Broglie wave packet [12]. For the de Broglie wave packet the energy after the reflection does not change, and the decrease of the normal component of the wave vector means that the direction of the reflected wave packet is different from specular one.

![Figure 2](image-url)

**Figure 2.** Reflection from a layer of thickness \( d \) with the potential \( u_1 \), placed on a substrate with the potential \( u_2 > u_1 \). For a sufficiently thick first layer the G-H shift \( AB \) can be arbitrary large.

Calculations of the shift for a beam-like wave function or for a wave packet for the mirror in fig. 2 are the same as before. The only difference is in the form of the reflection amplitude in (7). It can be calculated with the help of the method [10], which takes into account multiple reflection of plane waves from the two interfaces,

\[
R(q_z) = \frac{r_{01} + (1 - r_{01}^2) r_{12} \exp(2i q_z d)}{1 - r_{10} r_{12} \exp(2i q_z d)} =
\]

\[
r_{01} + r_{12} \exp(2i q_z d) \quad 1 - r_{10} r_{12} \exp(2i q_z d),
\]

where

\[
r_{01} = -r_{10} = \frac{q_z - q_{z1}}{q_z + q_{z1}}, \quad r_{12} = \frac{q_{z1} - q_{z2}}{q_{z1} + q_{z2}},
\]

\[
q_{z1,2} = \sqrt{q_z^2 - u_{1,2}}.
\]

We consider the case when \( q_z^2 - u_1 \gg s^2 \) and at the same time \( u_2 - q_z \gg s^2 \). In this case the reflection amplitudes from the substrate and from the whole mirror are unit complex numbers (the losses are neglected). If we denote \( r_{12} = \exp(-2i \phi_{12}) \), where \( \phi_{12} = \arcsin(q''_{z2}/\sqrt{u_2 - u_1}) \), \( q''_{z2} = \sqrt{u_2 - q_z^2} \), then

\[
R(q_z) =
\]

\[
e^{2i q_z d - 2i \phi_{12}} \frac{1 + r_{01} \exp(-2i q_z d + 2i \phi_{12})}{1 + r_{01} \exp(2i q_z d - 2i \phi_{12})} =
\]

\[
\exp(2i q_z d - 2i \phi_{12} - 2i \phi_{02})
\]
where \( \phi_{02} = \arcsin \left( \frac{r_{01} \sin(2q_z d - 2\phi_{12})}{\sqrt{1 + r_{01}^2 + 2r_{01} \cos(2q_z d - 2\phi_{12})}} \right) \).

(32)

In the case of a beam-like wave function, expanding the phase \( 2q_z d - 2\phi_{12} - 2\phi_{02} \) in (31) over \( q|| - k|| \), where \( k|| = (k_x, 0) \), up to the linear term gives the G-H shift,

\[
-\xi_x = \left[ \frac{2k_x d}{k_1} + \frac{2k_x}{k_1 k'_2} \right] \times \frac{1 + r_{01} \cos(2q_z d - 2\phi_{12})}{1 + 2r_{01} \cos(2q_z d - 2\phi_{12}) + r_{01}^2}.
\]

(33)

The first term of the expression in the brackets is \( k_z d \) times larger than the shift at a single interface. The factor outside the brackets depends on the neutron wave length and varies in the range from \( 1/(1 + r_{01}) \) to \( 1/(1 - r_{01}) \).

Same result can be obtained in the case of a wave-packet wave function.

3 Possible experiments to measure the neutron G-H effect

In this section we estimate the value of the G-H effect and look into perspectives of its measurement.

3.1 Nonspecular reflection from a single interface

In case of a nontotal reflection of a beam, the component \( k_x = k \sin \theta \) (\( \theta \) is the angle of incidence) of the wave vector in the reflection plane along the interface increases by \( 2k_x k_z s^2 / k^2 k'_z \) \((13)\). This is equivalent to rotating of the wave vector by a small angle \( \gamma \):

\[
k'_x \equiv k_x + \delta k_x = k_x + 2k_x s^2 / k_z k'_z = k \sin(\theta + \gamma) = k_x \cos \gamma + k_z \sin \gamma.
\]

(34)

From (34) follows that \( \delta k_x = k_z \gamma \), and when comparing the latter with (13) we find

\[
\gamma = 2k_x s^2 / k^2 k'_z.
\]

(35)

In order to estimate \( \gamma \) we need to find \( s \).

The width \( s \) of the wave packet was estimated in [13]. It was found that the anomalously high loss coefficient of ultracold neutrons in storage vessels can be explained, if the wave function of a neutron is represented by the de Broglie wave packet with the width \( s \approx 4 \cdot 10^{-5} k \), where \( k \) is the neutron wave number. We use this estimate in the rest of this article.

With the above estimate for \( s \), if we take \( k_z, k_x \approx \sqrt{u} = 4 \cdot 10^2 \) (which is typical for thermal neutrons) the angle is \( \gamma \approx 1.3 \cdot 10^{-6} \). This value is too small to measure. However, it is possible to design an experiment with \( k'_z \approx 0.1 \sqrt{u} \), then \( \gamma \approx 13 \cdot 10^{-6} \) rad, which can be measured.

In the case of the wave packets the change of the wave vector is determined by (27), \( \delta k_z = 2s^2 / k'_z \). If this change is the result of the rotation by the angle \( \gamma \), then \( \gamma = 2s^2 / k_z k'_z \). Thus, using the same estimates as in the previous paragraph we obtain the same number for the angle \( \gamma \).

We can check this result with the help of an experiment, schematic of which is shown in fig. 3. In the proposed experiment, the reflection of the monochromatic polarized neutrons from a magnetic mirror at a fixed angle is measured. After reflecting from the magnetic mirror, the polarized neutrons go to a single crystal where the Bragg condition is satisfied. After reflecting from the crystal, the neutrons are registered by a detector. When neutrons are polarized parallel to the magnetization of the mirror, they are totally and specularly reflected from it. If the polarization is opposite, the reflection is partial and not specular. The reflected beam from the mirror does not completely satisfy Bragg condition at the single crystal, so in order to restore the Bragg condition we need to rotate the crystal. Thus the experiment consists of measuring rocking curves of a
Figure 3. Scheme of experiment to check deviation of reflected neutrons from specular direction when reflection is partial. Monochromatic polarized neutrons (pn) go through spin flipper (SF) and are reflected from a magnetized mirror (MM). If SF is switched off then neutron polarization is parallel to the mirror magnetization, reflection is total and specular. The neutrons reflected from MM go to Si single crystal and after Bragg reflection to detector D. When SF is switched on, neutron polarization becomes opposite to magnetization of MM and the reflection is not total, thus the Bragg condition is not satisfied for neutrons going to Si crystal. In order to restore Bragg condition the Si crystal must be turned by an angle $\gamma$. The purpose of the experiment is to measure this angle.

Single crystal for two neutron polarizations. The centers of the two rocking curves will be shifted by $\gamma$. Of course, to achieve sufficient precision we need incident beam also monochromatized by an identical single crystal. More over, to avoid some false effects the analysis, may require reflection from two specially arranged single crystals. This can be discussed for a concrete reflectometer.

### 3.2 G-H shift at total reflection

Let us estimate the G-H shift (15) at the total reflection from a single interface. For thermal neutrons the ratio $k_x/k_z$ at the total reflection is about 400. Thus the G-H shift is 400 times larger than penetration depth $1/k''_z$, which can be estimated to be $1/\sqrt{u} \approx 10^{-6}$ cm. Therefore, for thermal neutrons the G-H shift is in the order of 8 $\mu$m.

For thermal neutrons with $\lambda = 2$ Å the spatial width of the wave packet is $< 1\mu$m, which is of the order of magnitude less than the G-H shift. However this changes, if the incident neutron instead of the wave packet is described by a beam of the same width. In this case we must compare the G-H shift to $1/s \cos \theta$, which is one order of magnitude more than the G-H shift.

In the case of the reflection from a layer of thickness, say 1 $\mu$m, on a substrate the G-H shift is in the order of 0.8 mm and is considerably larger even than $1/s \cos \theta$.

This shift is possible to measure in the experiment shown in fig. 4. If a Cadmium (Cd) plate restricts the area of the mirror enlightened by the incident beam, then the detector will detect only those particles, which can dive under the Cd plate.

It is possible that the beam which passed under the Cd plate will experience multiple reflections from the vacuum-layer interface and from the layer-substrate interface. In this case the distribution of the neutrons at the position sensitive detector (PSD in fig. 4) will look like a diffraction pattern. In reality, however, this pattern will be smeared by the non-monochromaticity and by scattering from the interface roughness and from the inhomogeneities of the film. However the contribution of scattering can be estimated and separated, if we can measure intensity of neutrons scattered outside of the incidence plane.

### 3.3 G-H effect and coherence

Reflection from two or more interfaces presents a problem, which is worth while to carefully investigate. In such a reflection we find coherence, incoherence and a transition between them.

Indeed, expression (31) is the result of a coherent superposition of plane waves instantaneously reflected multiple (infinite) times from two interfaces. This expression is obtained as a sum of
It is interesting to check whether different reflected wave packets interfere with each other, or the interference is present only when the spots of the consecutively reflected waves on the interface overlap (and is absent when they do not overlap). If they do not interfere when the spots do not overlap, then multiple reflections become incoherent. If we can measure the reflection with continuously changing overlapping, we can see how coherence transforms into incoherence.

To check the phenomenon mentioned in the previous paragraph, the experiment depicted in fig. 4 can be used. If the reflected beam is originated at one point close to the one of incidence, then it will be blocked by a cadmium shutter, and no neutrons will be detected by the PSD. It will prove the coherent summation of the reflected amplitudes. However, if the multiple reflections proceed according to (36), the distribution of the neutrons on the PSD will be similar to a diffraction pattern.

There is also a different way to check the transition of the coherence into the incoherence. Suppose the reflection from the substrate is not total, i.e. $r_{12}$ is a positive real number less than unity. In that case the full reflection amplitude (31) is not a unit complex number

$$R(q_z) = \frac{r_{01} + r_{12} \exp(2i q_z d)}{1 + r_{01} r_{12} \exp(2i q_z d)} = |R(q_z)| \exp(i \varphi(q_z)).$$

Here

$$|R| = \sqrt{\frac{r_{01}^2 + 2 r_{01} r_{12} \cos(2 q_z d) + r_{12}^2}{1 + 2 r_{01} r_{12} \cos(2 q_z d) + r_{01}^2 r_{12}^2}} < 1,$$

and $\varphi(q_z) = \arcsin \left( \frac{r_{12} \sin(2 q_z d)}{\sqrt{r_{01}^2 + 2 r_{01} r_{12} \cos(2 q_z d) + r_{12}^2}} \right) - \arcsin \left( \frac{r_{01} r_{12} \sin(2 q_z d)}{\sqrt{1 + 2 r_{01} r_{12} \cos(2 q_z d) + r_{01}^2 r_{12}^2}} \right).$
The fitting in the experiment [11] was done with the coherence length and without it, and it was found that \( \chi^2 \) of the fitting improves considerably, if the coherence length is included.

We show now how the coherence length, denoted \( \xi_0 \), was included in theoretical description of the reflection curve shown in fig. 5.

Let us introduce a function \( f(x) \), which monotonously increases from zero at \( x = 0 \) to one at \( x = \infty \), and represent the reflection coefficient as the sum

\[
|R|^2 = (1 - f(x))|R_c|^2 + f(x)R_i, \tag{40}
\]

where \( R_c \) is coherent reflection amplitude, and \( R_i \) is the incoherent reflection coefficient. If \( x = \frac{\xi_x}{\xi_0} \), then for small \( x \), i.e. for a small separation \( \xi_x \) compared to the coherence length \( \xi_0 \), the reflection is completely coherent. For a large separation \( \xi_x \) compared to the coherence length \( \xi_0 \), the reflection is completely incoherent. In [11] the error function \( \Phi(\xi_x/\sqrt{2}\xi_0) \) is chosen to be \( f(x) \).

Thus the reflection coefficient is defined as

\[
|R|^2(k_\perp) = |R_c|^2(k_\perp) \left(1 - \Phi\left(\frac{\xi_x(k_\perp)}{\sqrt{2}\xi_0}\right)\right) +
\]

\[
R_i(k_\perp)\Phi\left(\frac{\xi_x(k_\perp)}{\sqrt{2}\xi_0}\right),
\]

where \( k_\perp \) is the component of the incident wave vector normal to the mirror, \( R_c \) is given by (31), and \( R_i \) is the incoherent reflection coefficient

\[
R_i = \frac{R_1 + R_2 - 2R_1R_2}{1 - R_1R_2}.
\]

Here \( R_{1,2} \) are reflection coefficients from the two interfaces. In the case of ideal interfaces

\[
R_1 = \left|\frac{k_\perp - k_{1\perp}}{k_\perp + k_{1\perp}}\right|^2, \quad R_2 = \left|\frac{k_{1\perp} - k_{2\perp}}{k_{1\perp} + k_{2\perp}}\right|^2.
\]

In the case of smeared interfaces, when smearing is described by the Eckart potential [14],

\[
u(x) = \frac{u}{1 + \exp(x/\sigma)}
\]
with smearing parameter $\sigma$,

$$R_1 = \left| \frac{\sinh(\pi \sigma_1 (k_{\perp} - k_{1\perp}))}{\sinh(\pi \sigma_1 (k_{\perp} + k_{1\perp}))} \right|^2,$$

$$R_2 = \left| \frac{\sinh(\pi \sigma_2 (k_{\perp} - k_{2\perp}))}{\sinh(\pi \sigma_2 (k_{\perp} + k_{2\perp}))} \right|^2,$$

where $\sigma_{1,2}$ are smearing parameters of two interfaces.

The fitting of the experimental data revealed that the coherence parameter $\xi_0$ is equal to 1.5 mm. Further research has to be done to understand the meaning of this coherence parameter, and how it relates to the width of the neutron wave packet.

4 Conclusion

We discussed the G-H effect in case of neutrons, however almost everything said above is applicable also to x-rays. The most important difference is that we do not know how to estimate the wave packet width for x-rays. The experiments similar to those proposed in this article may give at least an upper limit of this very interesting parameter.

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