

# Scattering of scalar waves on a single crystalline plane

V.K.Ignatovich

*Frank Laboratory of Neutron Physics of Joint Institute for Nuclear Research, 141980,  
Dubna Moscow region, Russia*

## Abstract

Scattering of a scalar particle on a crystalline plane with quadratic cell and identical fixed scatterers is solved precisely. Contradiction of the standard scattering theory is pointed out.

## 1 Introduction

The standard dynamical diffraction theory was formulated many years ago (see, for instance [1, 2]) and since then enter all the textbooks almost without a change as is reflected, for instance in [3, 4]. I also did not like this theory as the Anonymous author of the epigraph and decided to reformulate it to see clearly all the physical processes that take place in the diffraction. After many years of lecturing on “Neutron optics” and many publications on this topic (see for instance [5]) I have understood that I reached a perfect level of understanding to expose some material for teachers of high school in clear and pedagogical manner. So I decided to submit a single part of this topic to Am.J.Phys. I should say that during my study of the subject I found some contradictions in present day scattering theory [6] and decided to disclose them on these pages in hope to initiate some thinking and discussion. The standard textbooks do not provide food for thinking. They provide only acquired knowledge that must be digested. And nobody does care whether the stuff is really digestible. A student who was feeded by the standard textbooks can become a scientist only, if he saved his curiosity, is brave enough to permit himself to doubt the acquired knowledge, and at the same time has a solid mathematical education. I hope the readers will agree with me.

Here I present my understanding of diffraction of an incident plane wave  $\exp(ik_0\mathbf{r})$  of a scalar particle on a single infinite crystalline plane perpendicular to  $z$ -axis, which crosses it at the point  $z = 0$ . The plane is inhabited by identical atoms firmly fixed at their positions and arranged in square lattice with an elementary cell having sides equal to  $a$  and directed along  $x$  and  $y$  axes, so that coordinates of atoms are at  $\mathbf{r}_n = a\mathbf{n}$ , where the vector  $\mathbf{n} = (n_x, n_y, 0)$  has integer components  $n_x$  and  $n_y$ . A single scatterers scatters as a point, and its scattering is characterized by the scattering amplitude  $b$ . So the problem is: how to find precisely diffraction of the incident wave on such a crystalline plane. This problem can be considered as a pure quantum or wave mechanical, however it has relation to real life because the plane wave can be imagined as a thermal neutron with wave length of  $1 \text{ \AA}$ , and crystalline plane as a plane inside a real crystal with  $a \approx 1 \text{ \AA}$ , and fixed atoms as real heavy atoms at zero temperature with scattering amplitude  $b \sim 10^{-12} \text{ cm}$ .

We start our story with description of wave function for scattering of the plane wave on a single atom taken alone. This wave function, as declared in all textbooks, is<sup>1</sup>

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}_0\mathbf{r}) - \frac{b}{r} \exp(ikr), \quad (1)$$

where  $b$  is the scattering amplitude and  $k = |\mathbf{k}_0|$ . To find diffraction on a whole plane we must take into account multiple wave scattering [7, 8, 9] between atoms in the plane.

## 2 Multiple wave scattering

In Eq. (1) the scattering atom is fixed at the point  $r = 0$ . If it is fixed at another point  $\mathbf{r}_1$  the wave function looks

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}_0\mathbf{r}) - \exp(i\mathbf{k}_0\mathbf{r}_1) \frac{b}{|\mathbf{r} - \mathbf{r}_1|} \exp(ik|\mathbf{r} - \mathbf{r}_1|) = \psi_0(\mathbf{r}) - \psi_0(\mathbf{r}_1) \frac{b}{|\mathbf{r} - \mathbf{r}_1|} \exp(ik|\mathbf{r} - \mathbf{r}_1|), \quad (2)$$

where  $\psi_0(\mathbf{r}) = \exp(i\mathbf{k}_0\mathbf{r})$ , and the factor  $\psi_0(\mathbf{r}_1)$  accounts for the field illuminating the scatterer.

If we have two scatterers at the points  $\mathbf{r}_{1,2}$ , then the total wave function becomes

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}_0\mathbf{r}) - \psi_1 \frac{b_1}{|\mathbf{r} - \mathbf{r}_1|} \exp(ik|\mathbf{r} - \mathbf{r}_1|) - \psi_2 \frac{b_2}{|\mathbf{r} - \mathbf{r}_2|} \exp(ik|\mathbf{r} - \mathbf{r}_2|), \quad (3)$$

where factors  $\psi_{1,2}$  should take into account rescattering between centers. This rescattering leads to equations

$$\psi_1 = \exp(i\mathbf{k}_0\mathbf{r}_1) - \psi_2 b_2 \eta, \quad \psi_2 = \exp(i\mathbf{k}_0\mathbf{r}_2) - \psi_1 b_1 \eta, \quad (4)$$

where  $\eta = \exp(ik\rho)/\rho$ , and  $\rho = |\boldsymbol{\rho}| = |\mathbf{r}_1 - \mathbf{r}_2|$ . Solution of this system of equations is

$$\psi_{1,2} = \frac{\exp(i\mathbf{k}_0\mathbf{r}_{1,2}) - b_{2,1}\eta \exp(i\mathbf{k}_0\mathbf{r}_{2,1})}{1 - b_1 b_2 \eta^2} = \exp(i\mathbf{k}_0\mathbf{r}_{1,2}) \frac{1 - b_{2,1}\eta \exp(\mp i\mathbf{k}_0\boldsymbol{\rho})}{1 - b_1 b_2 \eta^2}. \quad (5)$$

The wave function Eq. (3) at large  $r$  can be approximated as

$$\psi(\mathbf{r}) \approx \exp(i\mathbf{k}_0\mathbf{r}) - B \frac{\exp(ikr)}{r}. \quad (6)$$

Here we used approximation  $|\mathbf{r} - \mathbf{r}_i| \approx r - (\mathbf{r} \cdot \mathbf{r}_i)/r$ , and introduced the total scattering amplitude of both scatterers

$$B = \psi_1 b_1 \exp(-i\mathbf{k}\mathbf{r}_1) + \psi_2 b_2 \exp(-i\mathbf{k}\mathbf{r}_2), \quad (7)$$

where  $\mathbf{k} = k\mathbf{r}/r$ . Substitution of Eq. (5) into Eq. (7) gives

$$B = \frac{b_1 \exp(i\mathbf{q}\mathbf{r}_1) + b_2 \exp(i\mathbf{q}\mathbf{r}_2) - b_1 b_2 \eta [\exp(i\mathbf{q}\mathbf{r}_1 - i\mathbf{k}_0\boldsymbol{\rho}) + \exp(i\mathbf{q}\mathbf{r}_2 + i\mathbf{k}_0\boldsymbol{\rho})]}{1 - b_1 b_2 \eta^2}, \quad (8)$$

---

<sup>1</sup>It is common to write sign + before scattered spherical wave. I insist that it is more appropriate to write there minus, which means redefinition of the sign of the scattering amplitude  $b$ . With my choice positive  $b$  corresponds to positive optical potential of a medium  $u = 4\pi N_0 b$ , where  $N_0$  is atomic density of the medium. See [5].

where  $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}$  is the momentum transferred. From such a simple exercise one can see that scattering amplitude depends not solely on momentum transferred  $\mathbf{q}$ , but also on the other: incident,  $\mathbf{k}_0$ , or scattered momentum  $\mathbf{k}$ . Let's note the denominator in Eq. (8). At some  $\rho$  and  $k$  it can be small, and  $|B|$  can be much larger than  $b_{1,2}$ . There is a temptation to explain all the nuclear forces in this way.

The above simple exercise is easy to generalize to many scatterers. The generalization is called multiple wave scattering (MWS) theory. If we have  $N$  fixed scatterers with different amplitudes  $b_i$ , then the total wave function with account of scattering is

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}_0\mathbf{r}) - \sum_{n=1}^N \psi_n \frac{b_n}{|\mathbf{r} - \mathbf{r}_n|} \exp(ik|\mathbf{r} - \mathbf{r}_n|). \quad (9)$$

The field  $\psi_j$  illuminating  $j$ -th scatterer is determined from the equation

$$\psi_n = \exp(i\mathbf{k}_0\mathbf{r}_n) - \sum_{n' \neq n} \psi_{n'} b_{n'} \eta_{n'n}, \quad (10)$$

where  $\eta_{n'n} = \exp(ik|\mathbf{r}'_n - \mathbf{r}_n|)/|\mathbf{r}'_n - \mathbf{r}_n|$ . There are some sets of atoms for which the system Eq. (10) can be easily solved. One of them is a crystalline plane shown in fig.1 with identical  $b_n = b$  and  $\mathbf{r}_n = a\mathbf{n}$ , where vector  $\mathbf{n} = (n_x, n_y)$  has integer components  $n_{x,y}$ .

From symmetry considerations it follows that

$$\psi_n = C \exp(i\mathbf{k}_0\mathbf{r}_n). \quad (11)$$

Substitution of this expression into Eq. (10) gives  $C = 1 - CbS$ , and  $C = 1/(1 + bS)$ , where

$$S = \sum_{\mathbf{n} \neq 0} \exp(i(\mathbf{k}_0 \cdot \mathbf{n})a) \frac{\exp(ika|\mathbf{n}|)}{a|\mathbf{n}|}. \quad (12)$$

Now if we substitute Eq. (11) into Eq. (9) we obtain the full wave function with scattering on a crystalline plane to be

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}_0 \cdot \mathbf{r}) - bC \sum_{\mathbf{n}} \exp(ia\mathbf{k}_0 \cdot \mathbf{n}) \frac{\exp(ik|\mathbf{r} - a\mathbf{n}|)}{|\mathbf{r} - a\mathbf{n}|}, \quad (13)$$

where summation goes over infinite number of atoms in the crystalline plane [10]. It looks as if we use perturbation theory without multiple scattering, and all the multiple scattering is contained in the renormalization factor  $C$ . We will evaluate and discuss this factor later, but want to warn the reader here that it may happen that in rigorous standard scattering theory  $C = 0$ , i.e. the crystalline plane cannot scatter at all and is invisible for the incident plane wave. We know that the diffraction exists and will not believe such an extraordinary possible result  $C = 0$ .

### 3 Diffraction from a single crystalline plane

We found the total wave function Eq. (13) but it tells nothing. We need to know how to make a summation over all the atoms. However there is a simple recipe how to deal with arbitrary sums.

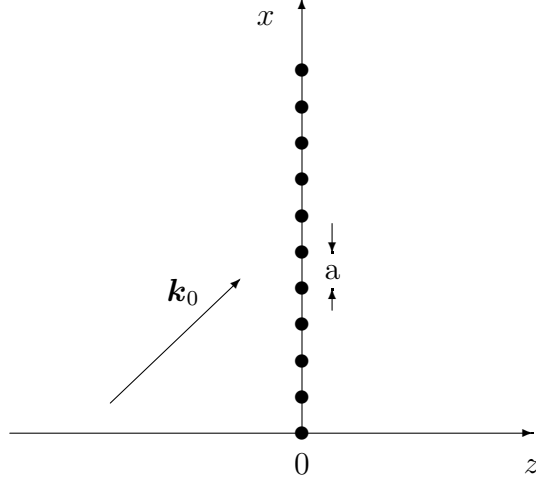


Figure 1: An infinite crystalline atomic plane perpendicular to the paper, and an incident plane wave with wave vector  $\mathbf{k}_0$ . Atoms are in the plane  $x, y$ , which crosses  $z$ -axis at the point  $z = 0$ . An elementary cell of the plane is a square with sides of length  $a$  along  $x$  and  $y$ -axes. The axis  $y$  is perpendicular to the figure plane and is directed toward the reader.

### 3.1 A recipe for summation

Let's consider a sum

$$S = \sum_{n=n_1}^{n_2} f(n) \quad (14)$$

for an arbitrary function  $f(n)$ . This sum can be represented in a different form

$$S = \sum_{N=-\infty}^{+\infty} F(N), \quad (15)$$

where

$$F(N) = \int_{n_1}^{n_2} f(n) \exp(2\pi i N n) dn, \quad (16)$$

and  $n$  is considered as a continuous variable.

The recipe can be easily checked. One can apply the same transformation to Eq. (15). As a result we obtain

$$\begin{aligned} S &= \sum_{M=-\infty}^{+\infty} \int_{-\infty}^{+\infty} dN \exp(2\pi i M N) \int_{n_1}^{n_2} f(n) \exp(2\pi i N n) dn = \\ &= \sum_{M=-\infty}^{+\infty} \int_{n_1}^{n_2} f(n) \exp(2\pi i N n) dn \delta(2\pi(M+n)) = \sum_{n=n_1}^{n_2} f(n). \end{aligned} \quad (17)$$

It looks like a trick, but can be rigorously proven. Indeed, the sum Eq. (14) can be represented as an integral

$$\sum_{n=n_1}^{n_2} f(n) = \oint_C dz \frac{f(z)}{1 - \exp(2\pi i z)} \quad (18)$$

over closed path in complex plane as is shown in fig. 2. Expansion of the function  $1/(1 - \exp(2\pi iz))$  over powers  $\exp(2\pi Niz)$  on upper half of the path, and over powers  $\exp(-2\pi Niz)$  on lower half of the path gives the sum Eq. (15) with definition Eq. (16).

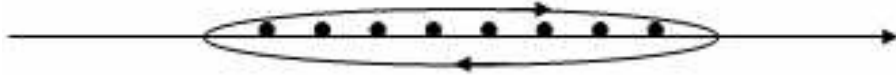


Figure 2: A closed path for integration Eq. (18) in the complex plane.

It looks not profitable to transform a final sum into an infinite one. However in our case of the infinite sum Eq. (13) it is profitable. Generalization of Eq. (16) to double sum is trivial, so we can represent Eq. (13) in the form

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}_0 \cdot \mathbf{r}) - bC \sum_{\mathbf{m}} \int d^2n \exp(2\pi i\mathbf{m}\mathbf{n}) \exp(i\mathbf{a}\mathbf{k}_0 \cdot \mathbf{n}) \frac{\exp(ik|\mathbf{r} - \mathbf{a}\mathbf{n}|)}{|\mathbf{r} - \mathbf{a}\mathbf{n}|}, \quad (19)$$

or

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}_0 \cdot \mathbf{r}) - b_C N_2 \sum_{\boldsymbol{\tau}} \int d^2r'_{\parallel} \exp(i(\boldsymbol{\tau} + \mathbf{k}_0) \cdot \mathbf{r}'_{\parallel}) \frac{\exp(ik|\mathbf{r} - \mathbf{r}'_{\parallel}|)}{|\mathbf{r} - \mathbf{r}'_{\parallel}|}, \quad (20)$$

where  $\mathbf{r}'_{\parallel}$  are coordinates in the plane,  $N_2 = 1/a^2$  is atomic density on the plane,  $b_C = bC$  is renormalized scattering amplitude of a single atom, and we introduced vectors  $\boldsymbol{\tau} = 2\pi\mathbf{m}/a$  of the reciprocal plane lattice. From Eq. (20) it follows that we need two-dimensional Fourier expansion of the spherical waves. Let's find it.

### 3.2 3-dimensional Fourier expansion of spherical waves

To find two-dimensional expansion we start with the well known 3-dimensional Fourier expansion of the spherical wave. It looks

$$\frac{\exp(ikr)}{r} = \frac{4\pi}{(2\pi)^3} \int d^3p \frac{\exp(i\mathbf{p}\mathbf{r})}{p^2 - k^2 - i\epsilon}. \quad (21)$$

To prove that the right side is equal to the left function, one represents  $d^3p = p^2 dp d\varphi d\cos\theta$ , integrates the right hand side over angles and obtains

$$\frac{1}{i\pi r} \int_0^{\infty} p dp \frac{\exp(ipr) - \exp(-ipr)}{p^2 - k^2 - i\epsilon} = \frac{1}{i\pi r} \int_{-\infty}^{\infty} p dp \frac{\exp(ipr)}{p^2 - k^2 - i\epsilon}. \quad (22)$$

Since  $r > 0$  the integration path can be closed in complex plane of the integration variable  $p$  by the infinite semicircle in the upper half part of the plane, and the result of the integration over closed path is the residual in the single pole at  $p = k + i\epsilon$ . This residual is  $2\pi ik \exp(ikr)/2k$ , and its substitution into Eq. (22) gives the left hand side of Eq. (21).

From Eq. (21) it is easy to deduce what equation does spherical wave satisfy. Indeed, if we apply to it the operator  $\Delta + k^2$ , we obtain

$$(\Delta + k^2) \frac{\exp(ikr)}{r} = \frac{4\pi}{(2\pi)^3} \int d^3p \frac{(k^2 - p^2) \exp(i\mathbf{p}\mathbf{r})}{p^2 - k^2 - i\epsilon} = -4\pi\delta(\mathbf{r}). \quad (23)$$

### 3.3 2-dimensional Fourier expansion of spherical waves

However we need not the 3-dimensional but 2-dimensional Fourier expansion of the spherical wave. It is obtained from Eq. (21) by representation  $d^3p = dp_z d^2p_{\parallel}$ , and  $p^2 - k^2 - i\varepsilon = p_z^2 - p_{\perp}^2 - i\varepsilon$ , where  $p_{\perp} = \sqrt{k^2 - p_{\parallel}^2}$  and vector  $\mathbf{p}_{\parallel}$  lies in the  $(x, y)$  plane. As a result we obtain

$$\frac{\exp(ikr)}{r} = \frac{4\pi}{(2\pi)^3} \int d^2p_{\parallel} \int_{-\infty}^{\infty} dp_z \frac{\exp(i\mathbf{p}_{\parallel}\mathbf{r}_{\parallel} + ip_z z)}{p_z^2 - p_{\perp}^2 - i\varepsilon}. \quad (24)$$

The integrand has two poles at  $p_z = \pm(p_{\perp} + i\varepsilon)$ . The integration path can be closed in complex plane of the integration variable  $p_z$  by an infinite semicircle in the upper half part of the plane, when  $z > 0$ , and in the lower half part of the plane, when  $z < 0$ . In both cases inside the closed path there is only one pole, so the result of the integration is

$$\frac{\exp(ikr)}{r} = \frac{i}{2\pi} \int \frac{d^2p_{\parallel}}{p_{\perp}} \exp(i\mathbf{p}_{\parallel}\mathbf{r}_{\parallel} + ip_{\perp}|z|). \quad (25)$$

One can directly integrate the right hand side to get spherical wave, if for every  $r$  one directs  $z$ -axis toward  $r$  so that  $\mathbf{r}_{\parallel} = 0$ , and then the integral in the right hand side of Eq. (25) is easily calculated.

### 3.4 Digression on contradictions in quantum scattering theory

Let's look at the wave function Eq. (1). It contains the incident wave. which satisfies free equation,

$$(\Delta + k^2) \exp(i\mathbf{k}_0\mathbf{r}) = 0, \quad (26)$$

and the scattered spherical wave, which satisfies Eq. (26). The last one is not free. It is inhomogeneous. So the spherical wave does not correspond to a free particle and should not be used. The standard objection to this claim is: we do not worry about the point  $r = 0$ , and outside this point the spherical wave satisfies the free Schrödinger equation. Therefore the spherical wave describes the free particle.

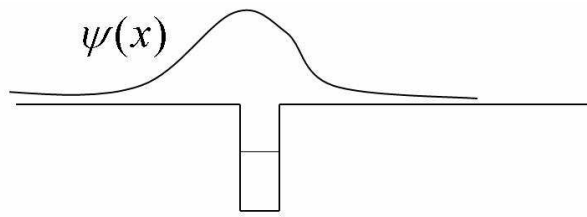


Figure 3: A particle in a bound state in a potential well has nonzero wave function outside of the well. The tails of this wave function satisfy the free Schrödinger equation  $(\Delta + k^2)\psi = 0$ . If potential well is one dimensional like a potential trough, the motion along the trough can be arbitrary, so the total energy  $k^2$  of the particle in Schrödinger equation outside of the well can be positive.

However this argument is not appropriate. Indeed, let's consider a potential well and a particle in a bound state in this well as shown in fig. 3. Outside of the well the particle

satisfies the free Schrödinger equation, however it is not free, and a distinguishing feature of the bound state is exponential decay of the wave function away from the well. In the case of a simple spherical potential the kinetic energy  $k^2$  in the Schrödinger equation outside the well is negative. But we can imagine a cylindrical potential well with arbitrary high movement along the cylinder. In that case the total kinetic energy  $k^2$  outside the well can be positive, nevertheless the wave function exponentially decays away from the potential.

The spherical wave, according to expansion Eq. (25), contains exponentially decaying part. It is the part of the integral with  $p_{\parallel} > k$ . If one excludes this part of the spherical wave, then the remaining integral will be

$$\frac{\exp(ikr)}{r} \implies \frac{i}{2\pi} \int_{p_{\parallel} < k} \frac{d^2 p_{\parallel}}{p_{\perp}} \exp(i\mathbf{p}_{\parallel} \cdot \mathbf{r}_{\parallel} + ip_{\perp}|z|) = \frac{i}{\pi} \int_{\mathbf{p} \cdot \mathbf{r} > 0} d^3 p \delta(p^2 - k^2) \exp(i\mathbf{p} \cdot \mathbf{r}), \quad (27)$$

where integration limit warrants that the integral contains only outgoing plane waves, so it cannot be reduced to imaginary part of the spherical function

$$i \frac{\sin(kr)}{r}, \quad (28)$$

which contains ingoing waves also.

With account of Eq. (27) the scattered waves after integration over  $dp$  can be represented as

$$\psi_{sc}(\mathbf{r}) = -\frac{ikb}{2\pi} \int_{\mathbf{k}_{\Omega} \cdot \mathbf{r} > 0} d\Omega \exp(i\mathbf{k}_{\Omega} \cdot \mathbf{r}), \quad (29)$$

where vector  $\mathbf{k}_{\Omega}$  has length  $k$  and direction determined by the solid angle  $\Omega$ . From this expression it follows, that probability of scattering in the direction  $\Omega$  is equal to

$$dw(\Omega) = |b/\lambda|^2 d\Omega. \quad (30)$$

It is dimensionless, and such a dimensional parameter as a cross section can be defined only artificially. To have a consistent theory one needs to work with wave packets and to introduce nonlinearity. Wave packet without nonlinear wave equation does not help.

In our diffraction problems we will deal only with probabilities, so no problem with definition of cross sections will arise.

### 3.5 Diffraction on the crystalline plane

Let's substitute Eq. (25) into Eq. (20), then, having in mind that all atoms in our crystalline plane have  $z_n = 0$  we get

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}_0 \cdot \mathbf{r}) - \frac{iN_2 b_c}{2\pi} \sum_{\tau} \int d^2 r'_{\parallel} \exp(i(\boldsymbol{\tau} + \mathbf{k}_0) \cdot \mathbf{r}'_{\parallel}) \int \frac{d^2 p_{\parallel}}{p_{\perp}} \exp(i\mathbf{p}_{\parallel} \cdot (\mathbf{r}_{\parallel} - \mathbf{r}'_{\parallel})) = \quad (31)$$

$$= \exp(i\mathbf{k}_0 \cdot \mathbf{r}) - \sum_{\tau} \frac{i\kappa}{k_{\tau\perp}} \exp(i\mathbf{k}_{\tau\parallel} \cdot \mathbf{r}_{\parallel} + ik_{\tau\perp}|z|), \quad (32)$$

where  $\mathbf{k}_{\tau\parallel} = \mathbf{k}_{0\parallel} + \boldsymbol{\tau}$ ,  $k_{\tau\perp} = \sqrt{k^2 - \mathbf{k}_{\tau\parallel}^2}$  and  $\kappa = 2\pi N_2 b_C$ . Let's note that for thermal neutrons  $\kappa/k_{\tau\perp} \approx b\lambda/a^2$  is of the order  $10^{-4} \ll 1$ , i.e. scattering on a single crystalline plane is very small.

Now we can sum up. We see that scattering creates a set of discrete diffracted plane waves going symmetrically on both sides of the crystalline plane. The diffracted waves propagate with wave vectors  $\mathbf{k}_\tau = (\mathbf{k}_{\tau\parallel}, k_{\tau\perp})$ , where  $\mathbf{k}_{\tau\parallel} = \mathbf{k}_{0\parallel} + \boldsymbol{\tau}$ ,  $k_{\tau\perp} = \sqrt{k^2 - \mathbf{k}_{\tau\parallel}^2}$ ,  $\boldsymbol{\tau} = \tau_1 \mathbf{n}$ ,  $\tau_1 = 2\pi/a$ , and  $\mathbf{n}$  is a 2-dimensional vector with integer components. The amplitudes of the waves are equal to

$$f_\tau = \frac{2\pi i N_2 b_C}{k_{\tau\perp}}. \quad (33)$$

It seems that the number of diffracted waves is infinite, however the real number of propagating plane waves is finite, because for sufficiently large  $\mathbf{n}$  the normal component of the wave vector  $k_{\tau\perp}$  becomes imaginary, and corresponding diffracted waves exponentially decay away from the crystalline plane. According to our consideration of the spherical wave we must exclude exponentially decaying waves from the integral in Eq. (31), then the exponentially decaying waves will not appear in Eq. (32) either. However sometimes we need exponentially decaying waves. If near our crystalline plane there is another plane, then an exponentially decaying wave from the first plane can reach the second one and in the process of diffraction it will create diffracted propagating waves. We will show it later.

It is worth also to discuss the amplitude Eq. (33) of the diffracted waves. Since wave vector  $\mathbf{k}_0$  of the incident wave can be arbitrary, it may happen that for some vector  $\boldsymbol{\tau}$  of the reciprocal lattice denominator  $k_{\tau\perp}$  of Eq. (33) becomes so small that  $|f_\tau| \gg 1$ . The question arises: what does it mean, and whether it is really possible? To answer this question it is now necessary to consider the role of the renormalization factor  $C$ , which is not a constant but depends on the incident wave vector  $\mathbf{k}_0$ . The role of  $C$  is to guard unitarity, which is a requirement equivalent to the law of energy conservation.

### 3.6 Unitarity for a single scatterer

First of all let's look at the simplest scattering wave function given by Eq. (1). It is easy to prove that to satisfy unitarity in absence of absorption the scattering amplitude must be of the form

$$b = \frac{b_0}{1 + ikb_0}, \quad (34)$$

where  $b_0$  is a real number. Let's prove it. Substitute Eq. (25) into Eq. (1), and choose  $z$ -axis in the direction of the incident wave propagation. Then the wave function becomes

$$\psi(\mathbf{r}) = \exp(ikz) - \frac{ib}{2\pi} \int \frac{d^2 p_\parallel}{p_\perp} \exp(i\mathbf{p}_\parallel \mathbf{r}_\parallel + ip_\perp |z|). \quad (35)$$

Let's choose two planes perpendicular to  $z$ -axis before,  $S_1$ , and behind,  $S_2$ , the scatterer. Unitarity means a requirement that flux density  $\overleftarrow{\mathcal{J}}_{S_1}$  of particles going after scattering to the left, plus the flux density  $\overrightarrow{\mathcal{J}}_{S_2}$  of particles going after scattering to the right should be equal to the flux density  $\overrightarrow{\mathcal{J}}_{0S_1}$  of the incident particles going toward the scattering center through the plane  $S_1$ . Let's calculate these fluxes.



### 3.6.1 The incident flux density

First of all let's remind definition of the flux density. For the wave function  $\psi(\mathbf{r})$  the flux density through a plane  $S$  with the normal along  $z$ -axis is

$$\vec{J} = \lim_{S \rightarrow \infty} \frac{1}{2iS} \int_S d^2x_{\parallel} \left[ \psi^*(\mathbf{r}) \left( \frac{\vec{d}}{dz} - \frac{\overleftarrow{d}}{dz} \right) \psi(\mathbf{r}) \right]_{z=0}, \quad (36)$$

where arrows over derivatives show which side should be differentiated. So, for  $\psi_0 = \exp(ikz)$  the incident flux is  $\vec{J}_0 = k$ .

### 3.6.2 Scattered flux density

Substitution of the wave function Eq. (35) into Eq. (36) gives the flux of the waves scattered to the left

$$\overleftarrow{J}_{sc} = \left( \frac{b}{2\pi} \right)^2 \int_{p_{\parallel} < k} \frac{d^2 p_{\parallel}}{p_{\perp}} \int_{p'_{\parallel} < k} \frac{d^2 p'_{\parallel}}{p'_{\perp}} \int d^2 r \frac{p_{\perp} p'_{\perp} + p_{\parallel} p'_{\parallel}}{2S} \exp(i(\mathbf{p}_{\parallel} - \mathbf{p}'_{\parallel})\mathbf{r}_{\parallel}) = \frac{2\pi|b|^2}{S}. \quad (37)$$

Since the scattering is symmetrical, the same flux will be obtained for the waves scattered to the right.

### 3.6.3 Interference flux density

Let's look carefully for the flux of particles going to the right plane  $S_2$  behind the scattering center. The wave function there is a superposition of the incident and scattered waves  $\psi = \psi_0 + \psi_{sc}$ . Therefore, substitution of it into Eq. (36) gives  $\vec{J}_0$ ,  $\vec{J}_{sc}$  and the interference flux

$$\begin{aligned} \vec{J}_{-int} &= \frac{1}{2iS} \int_S d^2x_{\parallel} \left\{ \left[ \psi_0^*(\mathbf{r}) \left( \frac{\vec{d}}{dz} - \frac{\overleftarrow{d}}{dz} \right) \psi_{sc}(\mathbf{r}) \right]_{z=0} + \left[ \psi_{sc}^*(\mathbf{r}) \left( \frac{\vec{d}}{dz} - \frac{\overleftarrow{d}}{dz} \right) \psi_0(\mathbf{r}) \right]_{z=0} \right\} = \\ &= -2\pi i \frac{b - b^*}{S}. \end{aligned} \quad (38)$$

Let's sum up. Requirement of unitarity is

$$\overleftarrow{J}_{sc} + \vec{J}_{sc} + \vec{J}_0 + \vec{J}_{int} = \vec{J}_0, \quad (39)$$

from which it follows

$$\overleftarrow{J}_{sc} + \vec{J}_{sc} + \vec{J}_{int} = 0, \quad (40)$$

or

$$4\pi|b|^2 k + 4\pi \text{Im}(b) = 0. \quad (41)$$

Finally we get the relation known as the optical theorem

$$\text{Im}(b) = -\frac{k\sigma}{4\pi}. \quad (42)$$

where  $\sigma = 4\pi|b|^2$  — cross section of elastic scattering. Now, if we look at Eq. (34), we see that it precisely satisfies optical theorem Eq. (42). We want also to add that removal of exponentially decaying part of the spherical wave does not spoil unitarity.

### 3.7 Unitarity for scattering on a single crystalline plane

Unitarity for crystalline plane is formulated with the same Eq. (40), however flux density with respect to the plane is determined by the normal component of the wave vector. For instance the flux of the incident wave  $\vec{J}_0 = k_{0\perp}$ .

From Eq. (32) it follows that

$$\overleftarrow{J}_{sc} = \vec{J}_{sc} = \sum_{\tau} \frac{|\kappa|^2}{k_{\tau\perp}}, \quad (43)$$

and

$$\vec{J}_{int} = i(\kappa^* - \kappa). \quad (44)$$

Therefore, the unitarity condition means

$$Im(\kappa) = - \sum_{\tau} \frac{|\kappa|^2}{k_{\tau\perp}}, \quad (45)$$

or

$$Im(bC) = 2\pi N_2 |bC|^2 \sum_{\tau} \frac{1}{k_{\tau\perp}}. \quad (46)$$

Let's note, that  $k_{\tau\perp}$  in sum are all real. Therefore exponentially decaying waves do not contribute to the unitarity.

#### 3.7.1 Calculation of the factor $C$

Now it is the time to calculate renormalization factor  $C$  to prove that it really helps to satisfy Eq. (46). To do that we can apply to Eq. (12) the sum rule Eq. (15)-(20). If there were not limitation  $n \neq 0$  in Eq. (12), we would obtain directly like in Eq. (32)

$$\begin{aligned} S &= \sum_{\mathbf{n}} \exp(i(\mathbf{k}_0 \cdot \mathbf{n})a) \frac{\exp(ika|\mathbf{n}|)}{a|\mathbf{n}|} = N_2 \sum_{\tau} \int d^2 r'_{\parallel} \exp(i(\boldsymbol{\tau} + \mathbf{k}_0) \cdot \mathbf{r}'_{\parallel}) \frac{\exp(ik|\mathbf{r}'_{\parallel}|)}{|\mathbf{r}'_{\parallel}|} = \\ &= \frac{iN_2}{2\pi} \sum_{\tau} \int d^2 r'_{\parallel} \exp(i(\boldsymbol{\tau} + \mathbf{k}_0) \cdot \mathbf{r}'_{\parallel}) \int \frac{d^2 p_{\parallel}}{p_{\perp}} \exp(ip_{\parallel} \cdot (\mathbf{r}_{\parallel} - \mathbf{r}'_{\parallel})) = \sum_{\tau} \frac{2\pi i N_2}{k_{\tau\perp}}. \end{aligned} \quad (47)$$

However the term with  $\mathbf{n} = 0$  in the left hand side is singular and unacceptable. Therefore it must be excluded. Exclusion can be made as shown in fig. 4. The integral over large closed loop gives the result in the right hand side of Eq. (47), and to exclude the point  $n = 0$  one adds to Eq. (47) the counter clockwise integral around this point along a small circle, which gives

$$I_0 = \oint \frac{dn}{1 - \exp(2\pi in)} \frac{\exp(ikan)}{an} = - \oint \frac{dn}{2\pi i a n^2} \exp(ikan) = -ik. \quad (48)$$

Let's note, that if we do not remove from the spherical wave the exponentially decaying part, then the sum in Eq. (47) contains real and imaginary  $k_{\tau\perp}$ . So, according to Eq. (12), (47), (48) and Eq. (34) the renormalized amplitude is

$$b_C = bC = \frac{b}{1 + b \left( -ik + \sum_{\tau} \frac{2\pi i N_2}{k_{\tau\perp}} \right)} = \frac{b_0}{1 + ikb_0 - ikb_0 + b_0 S' + ib_0 S''} = \frac{b_1}{1 + ib_1 S''}, \quad (49)$$

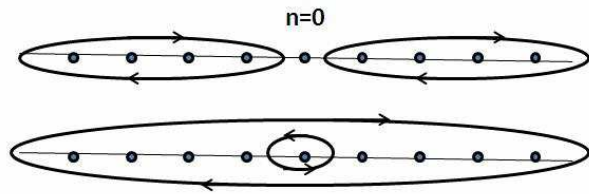


Figure 4: To exclude one point  $n = 0$  in summation, one can use two integrals of the type Eq. (18) over two closed loops as shown in the upper part of the figure. However it can be done as shown in lower part. It is possible to make the single integral Eq. (18) over large closed path without exclusion and to add an integral over closed loop around excluded point in the opposite direction.

where

$$S' = \sum_{k_{\tau\parallel} > k} \frac{2\pi N_2}{|k_{\tau\perp}|}, \quad S'' = \sum_{k_{\tau\parallel} < k} \frac{2\pi N_2}{k_{\tau\perp}}, \quad b_1 = \frac{b_0}{1 + b_0 S'}. \quad (50)$$

We see that normalization factor first of all cancels the term  $ikb_0$  in Eq. (34), which provides unitarity for a single scatterer, next, it changes the real value  $b_0$  to  $b_1$  and finally provides new imaginary part  $ib_1 S''$  in denominator, which is appropriate to satisfy unitarity for the crystalline plane. It is trivial to see that Eq. (49) does satisfy relation Eq. (46).

### 3.7.2 A problem of renormalization of the real part $b_0$ in Eq. (50)

The real part  $b_0$  of the amplitude  $b$  is renormalized, as follows from Eq. (50), only with that part of the sum, which contains imaginary  $k_{\tau\perp}$ . It stems from exponentially decaying part of the spherical wave. The sum

$$S' = \sum_{k_{\tau\parallel} > k} \frac{2\pi N_2}{|k_{\tau\perp}|}, \quad (51)$$

for large  $k_{\tau\parallel} = |\mathbf{k}_0| + (2\pi/a)\mathbf{n}$ , where  $\mathbf{n} = (n_x, n_y)$  has large integer components  $n_{x,y}$ , can be approximated as

$$S' = 2\pi N_2 a \sum_{n_x, n_y} \frac{1}{\sqrt{n_x^2 + n_y^2}}, \quad (52)$$

and such a sum is diverging. Therefore the renormalized value  $b_1$  becomes zero, the crystalline plane becomes invisible to incident waves and, contrary to our experience, creates no diffraction. It shows once again how contradictory is description of scattering with the help of spherical waves. If we exclude exponentially decaying part from spherical wave, the real part  $b_0$  of the scattering amplitude will not be renormalized.

### 3.7.3 Solution for singularity at $k_{\tau\perp} = 0$ in Eq. (32)

Now we can resolve the problem, which appears in Eq. (32) for some wave vectors  $\mathbf{k}_0$  of the incident wave, for which one of  $k_{\tau\perp}$  is close to zero. In that case the factor  $C$  goes to zero too because it contains  $1/k_{\tau\perp}$  in its denominator. Therefore the amplitudes of

all the diffracted waves go to zero except the wave, which amplitude contains the same factor  $1/k_{\tau\perp}$ . For this wave the divergent factors cancel, and the diffraction gives a single diffracted wave with unit amplitude, which propagates along the crystalline plane. It would be very interesting to observe such an effect, which can be seen not only for a single crystalline plane, but also for the whole crystal.

## 4 Conclusion

The story about crystalline plane and a scalar wave is over. However this story is only a beginning of many other stories, where one can deduce optical potential of media, diffraction of scalar waves on single crystals, diffraction of electromagnetic waves and many others, some of which possibly will be published in this journal. However one of the most important point of the finished story is the pinpointed contradiction of scattering theory. Without resolution or discussion of it quantum theory is doomed to stagnation.

## Acknowledgements

I am thankful to my students, who were patient, polite, and their eyes some times gave me an impression that they enjoyed my lectures. I am also grateful to the single referee of Am.J.Phys., who appreciated my paper. He is great, but his voice was drowned in between voices of those, who can only learn, but are not able to think.

## References

- [1] Paul Peter Ewald "Kristalle und Rntgenstrahlen" (Springer, 1923)
- [2] G.E. Bacon "Neutron Diffraction" Oxford University Press 1955.
- [3] R.T. Bush "The Ewald Construction and the Bragg Law of Diffraction in a First Course in Solid-State Physic." Am. J. Phys. 37, 669 (1969)
- [4] B. D. Hall "Introductory crystallography for solid-state physics: Computer simulations in two dimensions." Am. J. Phys. 66, 19 (1998).
- [5] M. Utsuro, V. K. Ignatovich, *Handbook of Neutron Optics* (Wiley-VCH, Weinheim, 2010).
- [6] Ignatovich VK. Contradictions in scattering theory. Concepts of Phys.2004;1:51-104.
- [7] Foldy L.L. "The multiple scatteling of waves." Phys.Rev. **67**(3) 107-19 (1945)
- [8] Lax M. "Multiple scattering of waves". Rev.Mod.Phys.**23**287-310 (1951).
- [9] Lax M. "Multiple scattering of waves II. The Effective Field in Dense Systems". Phys.Rev. **85**(4) 621-629 (1952).
- [10] Glasser M.L. "The evaluation of lattice sums. I. Analytic procedures." J.Math.Phys.**14**(3) 409-413 (1973).