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Scattering of scalar waves on a single crystalline plane

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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.

Keywords: neutron optics, diffraction, multiple waves scattering, spherical waves.

Introduction

I hate dynamical diffraction. Always had, always will.

Anonymous. (From a lecture by R.Golub)

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]. After many years of lecturing on ``Neutron optics'' and many publications (see for instance [5]) the author of this paper decided to submit a single part of this topic to Am.J.Phys, but submission was rejected, and the reasons of referees are presented here in the form of epigraphs.

During study of the subject it was found that there are some contradictions in present day scattering theory [6] and they become apparent in calculations of diffraction of neutrons from a single crystalline plane. The essence of the contradiction is: if one describes scattering on a fixed point scatterer by spherical waves then diffraction from a single crystalline plane, and therefore diffraction from any perfect crystal is absent. But in reality we see the diffraction; therefore nature does not use spherical waves. It is very interesting to find what does it really use. 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 is fed by the standard textbooks can become a real scientist only, if he saves his curiosity, is brave enough to permit himself to doubt the acquired knowledge, and at the same time has a solid mathematical education.

Here a precise theory of diffraction of an incident plane wave $\exp(i\mathbf{k}_0\mathbf{r})$ of a scalar particle (neutron) from a single infinite crystalline plane perpendicular to z-axis at the point z=0, is presented. 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 $\mathbf{r_n}=a\mathbf{n}$, where the vector $\mathbf{n}=(n_x,n_y,0)$ has integer components n_x and n_y. A single scatterer scatters as a fixed point, and its scattering is characterized by the scattering amplitude b. So the problem is: how to find precisely diffraction of the incident wave from such a crystalline plane. This problem can be considered as a pure theoretical, however it has relation to real life because the plane wave can be imagined as a thermal neutron with the wave length of 1Å, and the crystalline plane as a plane inside of a real crystal with a≈1Å. The fixed atoms are the real heavy atoms at zero temperature with scattering amplitude b of the order 10^{-12} cm.

The story starts with description of the wave function for scattering of the plane wave on a single atom taken alone. This wave function, as declared in all textbooks, is

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

b is the scattering amplitude [7] and $k=|\mathbf{k}_0|$. To find diffraction on a whole plane one must take into account multiple waves scattering [8-10] between atoms in the plane.

Multiple waves scattering

The article does not reach a major goal: to present a simplified and clear theoretical picture of the multiple scattering process. Textbooks and review articles, which are available in the current literature, explain well all effects considered in the present manuscript. (Referee of Am.J.Phys)

In (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

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

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

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

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

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

where $\eta=\exp(ik\rho)/\rho$, and $\rho=|\boldsymbol{\rho}|=|\mathbf{r}_1-\mathbf{r}_2|$.

Solution of this system of equations is

$$\psi_{1,2} = \frac{\exp(i\boldsymbol{k}_0\boldsymbol{r}_{1,2}) - b_{2,1}\eta\exp(i\boldsymbol{k}_0\boldsymbol{r}_{2,1})}{1-b_1b_2\eta^2} = \exp(i\boldsymbol{k}_0\boldsymbol{r}_{1,2})\frac{1-b_{2,1}\eta\exp(\mp i\boldsymbol{k}_0\boldsymbol{\rho})}{1-b_1b_2\eta^2}. \quad (5)$$

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

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

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

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

where **k**=k**r**/r. Substitution of (5) into (7) gives

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

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 **q**, but also on the incident, $\mathbf{k}_0$, or scattered momentum **k**. Let's look at the denominator in (8). At some ρ and k it can be small, and |B| can be much larger than $b_{1,2}$. It is interesting to look whether it is possible to explain all the nuclear forces this way.

The above simple exercise is easily generalized to many scatterers. If we have N fixed scatterers with different amplitudes b_i, then the total wave function with acco-unt of multiple scattering is

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

The field ψ_j illuminating j-th scatterer is determined from the equation

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

where $\eta_{n'n} = \exp(ik|\boldsymbol{r}'_n - \boldsymbol{r}_n|)/|\boldsymbol{r}'_n - \boldsymbol{r}_n|$. There are some sets of atoms, for which the system (10) can be solved analytically. One of them is the 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 $\mathbf{n}_{x,y}$. From symmetry considerations it follows that

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

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

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

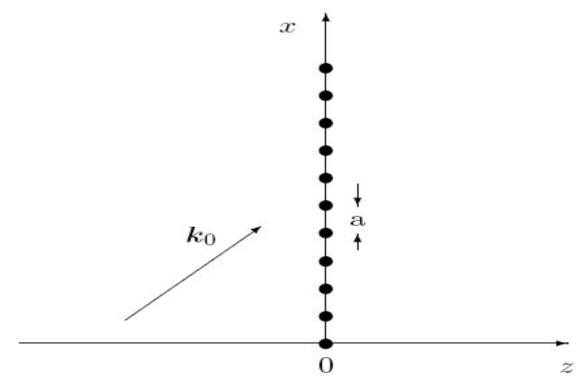


Fig.1. *An infinite crystalline atomic plane perpendicular to the paper, and an incident plane wave with wave vector* $\boldsymbol{k}_0$*. Atoms are in the plane x,y, which crosses z-axis at the point z=0. An elementary cell of the plane is a square with sides of length a along x and y-axes. The axis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

Substitution of (11) into (9) gives the full wave function for scattering on a crystalline plane to be

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

where summation goes over infinite number of atoms in the crystalline plane [11]. It looks as if the perturbation theory is used without multiple scattering, and all the multiple scattering is contained in the renormalization factor *C*, which will be evaluated and discussed later, but the reader is to be warned here 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. Therefore no diffraction is possible. However the diffraction exists, therefore such an extraordinary result *C*=0 looks impossible, but the standard scattering theory leads just to it.

Diffraction from a single crystalline plane

Most students in the West will not be equipped to understand this paper until they are in graduate school. High school teachers and their students are the paper's intended audience, but they are unlikely to have the knowledge or the interest in reading it.

(Referee of Am.J.Phys.)

The total wave function is found to be represented by (13), but it tells nothing about diffraction. It is necessary to know how to make a summation over all the atoms, and we are lucky that there is a good recipe how to deal with arbitrary sums.

A recipe for summation

Let's consider a sum

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

for an arbitrary function *f(n)*. This sum can be transformed to another one

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

where

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

and *n* is a continuous variable there. The recipe can be easily checked. One can apply the same transformation to (15). As a result one obtains

$$S = \sum_{M=-\infty}^{+\infty} \int_{-\infty}^{+\infty} dN \exp(2\pi MN) \int_{n_1}^{n_2} f(n) \exp(2\pi i N n) dn =$$

$$= \sum_{M=-\infty}^{+\infty} \int_{n_1}^{n_2} f(n) \exp(2\pi i N n) dn \delta(M+n) = \sum_{n=n_1}^{n_2} f(n). \qquad (17)$$

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

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

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

Fig.2. *A closed path for integration (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 (13) it is profitable. Generalization of (16) to double sums is trivial, so one can represent (13) in the form

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

or

$$\psi(\boldsymbol{r})=\exp(i\boldsymbol{k}_0\cdot\boldsymbol{r})-b_CN_2\sum_{\boldsymbol{\tau}}\int d^2r'_{||}\exp(i(\boldsymbol{\tau}+\boldsymbol{k}_0)\cdot\boldsymbol{r}'_{||})\frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}'_{||}|)}{|\boldsymbol{r}-\boldsymbol{r}'_{||}|}, \qquad (20)$$

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

3-dimensional Fourier expansion of the spherical wave

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

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

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

$$\frac{1}{i\pi r}\int\limits_0^\infty pdp\frac{\exp(ipr)-\exp(-ipr)}{p^2-k^2-i\varepsilon}=\frac{1}{i\pi r}\int\limits_{-\infty}^\infty pdp\frac{\exp(ipr)}{p^2-k^2-i\varepsilon}. \qquad (22)$$

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+iε. This residual is 2πikexp(ikr)/2k, and its substitution into (22) gives the left hand side of (21). From (21) it is easy to deduce what equation does spherical wave satisfy. Indeed, application of the operator $\Delta+k^2$ gives

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

2-dimensional Fourier expansion of the spherical wave

However one needs 2-dimensional Fourier expansion of the spherical wave. It is obtained from (21) by representation $d^3p=dp_zd^2p_{||}$, and $p^2-k^2-i\varepsilon=p_z^2-p_\perp^2-i\varepsilon$, where $p_\perp=\sqrt{k^2-p_\|^2}$ and vector $\mathbf{p}_{||}$ lies in the (x,y) plane. As a result one obtains

$$\frac{\exp(ikr)}{r} = \frac{4\pi}{(2\pi)^3}\int d^2p_\|\int\limits_{-\infty}^{\infty} dp_z\frac{\exp(i\boldsymbol{p}_\|\boldsymbol{r}_\| + ip_zz)}{p_z^2-p_\perp^2-i\varepsilon}. \qquad (24)$$

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

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

One can directly integrate the right hand side to get spherical wave, if for every *r* one directs *z*-axis toward *r* so that $\mathbf{r}_{||}=0$, and then the integral in the right hand side of

(25) is easily calculated.

Digression on contradictions in quantum scattering theory

Paradoxes and ":contradictions in present day scattering theory:" arise because of author's misleading interpretations of some fundamental results of the scattering theory. (Referee of Am.J.Phys)

I wonder:

which one?

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

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

and the scattered spherical wave, which satisfies (23). 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 free particles. 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.

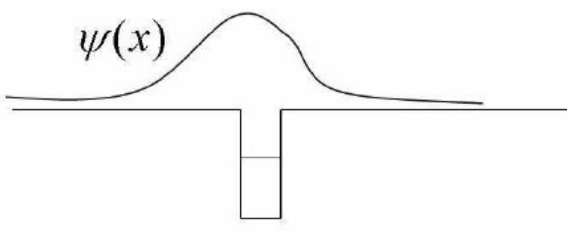


Fig.3. *A particle in a bound state in a potential well has nonzero wave function outside of the well. The tails of this wave function satisfy the free equation* $(\Delta+k^2)\psi=0$. *If potential well is one dimensional like a potential trough, the motion along the trough can be arbitrary, so the total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

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

$$\frac{\exp(ikr)}{r} \Longrightarrow \frac{i}{2\pi}\int\limits_{p_\parallel<k}\frac{d^2p_\parallel}{p_\perp}\exp(i\boldsymbol{p}_\parallel\boldsymbol{r}_\parallel + ip_\perp|z|) = \frac{i}{\pi}\int\limits_{\boldsymbol{p}\cdot\boldsymbol{r}>0} d^3p\delta(p^2-k^2)\exp(i\boldsymbol{p}\cdot\boldsymbol{r}), \tag{27}$$

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

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

which contains ingoing waves also.

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

$$\psi_{sc}(\boldsymbol{r}) = -\frac{ikb}{2\pi}\int\limits_{\boldsymbol{k}_\Omega\cdot\boldsymbol{r}>0} d\Omega\exp(i\boldsymbol{k}_\Omega\cdot\boldsymbol{r}), \tag{29}$$

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

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

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 diffractions one deals only with probabilities, so no problem with definition of cross sections do arise.

Diffraction from the crystalline plane

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

$$\psi(\boldsymbol{r}) = \exp(i\boldsymbol{k}_0\cdot\boldsymbol{r}) - \frac{iN_2b_c}{2\pi}\sum_{\boldsymbol{\tau}}\int d^2r'_\parallel\exp(i(\boldsymbol{\tau}+\boldsymbol{k}_0)\cdot\boldsymbol{r}'_\parallel)\int\frac{d^2p_\parallel}{p_\perp}\exp(i\boldsymbol{p}_\parallel\cdot(\boldsymbol{r}_\parallel-\boldsymbol{r}'_\parallel)) = \tag{31}$$

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

where $k_{\tau\|} = k_{0\|} + \tau$, $k_{\tau\perp} = \sqrt{k^2 - k_{\tau\|}^2}$ 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 and find 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 $\mathbf{k}_\tau=(\mathbf{k}_{\tau\|}, k_{\tau\perp})$, where $\mathbf{k}_{\tau\|}=\mathbf{k}_{0\|}+\boldsymbol{\tau}$, $k_{\tau\perp} = \sqrt{k^2 - k_{\tau\|}^2}$, $\boldsymbol{\tau}=\tau_1\mathbf{n}$, $\tau_1=2\pi/a$, and $\mathbf{n}$ is a 2-dimensional vector with integer components. The amplitudes of the waves are equal to

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

It is seen 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 above consideration of the spherical wave one must exclude exponentially decaying waves from the integral in (31), then the exponentially decaying waves will not appear in (32) either. However sometimes one needs 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, as will be shown later.

It is worth also to discuss the amplitude (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 (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.

Unitarity for a single scatterer

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

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

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

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

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 $\overleftarrow{J}_{S_1}$ of particles going after scattering to the left, plus the flux density $\overrightarrow{J}_{S_2}$ of particles going after scattering to the right should be equal to the flux density $\overrightarrow{J}_{0S_1}$ of the incident particles going toward the scattering center through the plane S_1. Let's calculate these fluxes.

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

$$\overrightarrow{J} = \lim_{S\to\infty} \frac{1}{2iS} \int_S d^2x_{\|} \left[\psi^*(\boldsymbol{r}) \left(\frac{\overrightarrow{d}}{dz} - \frac{\overleftarrow{d}}{dz}\right) \psi(\boldsymbol{r})\right]_{z=0}, \qquad (36)$$

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

Scattered flux density

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

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

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

Interference flux density

Let's look carefully for the flux of particles going to the right of the 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 (36) gives $\overrightarrow{J}_0, \overrightarrow{J}_{sc}$ and the interference flux density

$$\overrightarrow{J}_{int} = \frac{1}{2iS}\int\limits_S d^2x_{\|}\left\{\left[\psi_0^*(\boldsymbol{r})\left(\frac{\overrightarrow{d}}{dz}-\frac{\overleftarrow{d}}{dz}\right)\psi_{sc}(\boldsymbol{r})\right]_{z=0}+\left[\psi_{sc}^*(\boldsymbol{r})\left(\frac{\overrightarrow{d}}{dz}-\frac{\overleftarrow{d}}{dz}\right)\psi_0(\boldsymbol{r})\right]_{z=0}\right\} =$$

$$= -2\pi i\frac{b-b^*}{S}. \qquad (38)$$

Let's sum up. Requirement of unitarity is

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

from which it follows

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

or

$$4\pi|b|^2k+4\pi Im(b)=0. \qquad (41)$$

Finally we get the relation known as the optical theorem

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

where $\sigma=4\pi|b|^2$ --- cross section of elastic scattering. Expression (34) precisely satisfies the optical theorem (42). It is worth to point out that removal of exponen-tially decaying part of the spherical wave does not spoil unitarity.

Unitarity for scattering on a single crystalline plane

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

From (32) it follows that

$$\overleftarrow{J}_{sc} = \overrightarrow{J}_{sc} = \sum_{\boldsymbol{\tau}} \frac{|\kappa|^2}{k_{\tau\perp}}, \tag{43}$$

and

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

Therefore, the unitarity condition means

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

or

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

Let's note, that $k_{\tau\perp}$ in sum (46) are all real. Therefore exponentially decaying waves do not contribute to the unitarity.

Calculation of the factor *C*

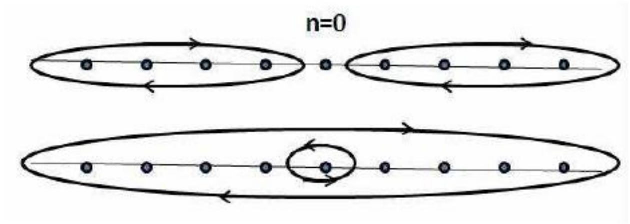
Now it is the time to calculate renormalization factor \$C\$ to prove that it really helps to satisfy (46). To do that one can apply to (12) the sum rule (15-20). If there were not limitation **n**≠0 in (12), we would obtain result directly like in (32)

$$S = \sum_{\boldsymbol{n}} \exp(i(\boldsymbol{k}_0 \cdot \boldsymbol{n})a) \frac{\exp(ika|\boldsymbol{n}|)}{a|\boldsymbol{n}|} = N_2 \sum_{\boldsymbol{\tau}} \int d^2r'_\| \exp(i(\boldsymbol{\tau} + \boldsymbol{k}_0) \cdot \boldsymbol{r}'_\|) \frac{\exp(ik|\boldsymbol{r}'_\||)}{|\boldsymbol{r}'_\||} =$$

$$= \frac{iN_2}{2\pi} \sum_{\boldsymbol{\tau}} \int d^2r'_\| \exp(i(\boldsymbol{\tau} + \boldsymbol{k}_0) \cdot \boldsymbol{r}'_\|) \int \frac{d^2p_\|}{p_\perp} \exp(i\boldsymbol{p}_\| \cdot (\boldsymbol{r}_\| - \boldsymbol{r}'_\|)) = \sum_{\boldsymbol{\tau}} \frac{2\pi i N_2}{k_{\tau\perp}}. \tag{47}$$

However the term with **n**≠0 in the left hand side is singular and unacceptable. There-fore 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 (47), and to exclude the point **n**=0 one adds to (47) the counter clockwise integral around this point along a small circle, which gives

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

 	**Fig. 4.** *To exclude one point n=0 in summation, one can use two Integrals of the type (18) over two closed loops as shown in the upper part of the figu-re. However they can be transformed as shown in lower part of the figure.*

Let's note that, if the exponentially decaying part is not removed from the spheri-cal wave, then the sum in (47) contains real and imaginary $k_{\tau\perp}$. So S in (47) is a complex value, and the renormalized scattering amplitude is

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

where

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

It is seen that normalization factor first of all cancels the term ikb_0 in (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_1S'' in the denominator, which is needed to satisfy unitarity for the scattering from the crystalline plane. It is trivial to see that (49) does satisfy relation (46).

A problem of renormalization of the real part b_0 in (50)

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

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

for large $k_{\tau\|} = |\boldsymbol{k}_{0\|} + (2\pi/a)\boldsymbol{n}|$, where $\mathbf{n}=(n_x,n_y)$ has large integer components $n_{x,y}$, can be approximated as

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

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

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

Now we can resolve the problem, which appears in (32): for some wave vectors $\mathbf{k}_0$ of the incident wave, one of $k_{\tau\perp}$ can happen to be 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 amplitu-des 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 crys-talline 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.

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. However one of the most important point of the finished story is the pinpointed contradiction of the quantum scattering theory. Without resolution or dis-cussion of it quantum theory is doomed to stagnation.

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in between voices of those, who can only learn, but are not able to think.

References

[1] Paul Peter Ewald ``Kristalle und Röntgenstrahlen'' (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 Physics." 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

[7] Phys. **1** 51-104 (2004).

[8] It is common to write sign + before scattered spherical wave, but it is more appropriate to write there minus, which means redefinition of the sign of the scattering amplitude b. With such a 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 [5].

[9] Foldy L.L. ``The multiple scatteling of waves.'' Phys.Rev. **67** (3) 107-19 (1945)

[10] Lax M. ``Multiple scattering of waves''. Rev.Mod.Phys. **23** 287-310 (1951).

[11] Lax M. ``Multiple scattering of waves II. The Effective Field in Dense Systems''. Phys.Rev. **85** (4) 621-629 (1952).

[12] Glasser M.L. ``The evaluation of lattice sums. I. Analytic procedures.'' J.Math. Phys. **14** (3) 409-413 (1973).