E901: Scattering of particles by a simple cubic lattice

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Problem:

Particles are scattered from 3D cubic lattice, with the characteristic distance between atoms a. The lattice contain $(2N+1)^3$ atoms, location of the i-atom:

$$\vec{a}_n = a(n_x\vec{e}_x + n_y\vec{e}_y + n_z\vec{e}_z) \qquad -N \leq n_x, n_y, n_z \leq N$$

the atoms are identical and their potentials $U(r)$ are identical as well.

a)find the differential cross section for the single atom in a first order Born Approximation.
b)find the scattering amplitude $f(\Omega)$ and differential cross section $\frac{d\sigma}{d\Omega}$ for finite N
c) find the differential cross section $\frac{d\sigma}{d\Omega}$ for infinite N

Solution:

The total potential could be written:

$$V(r) = \sum_{n_x n_y n_z} U(r - an) \tag{1}$$

We define:

$$\vec{q} = \vec{k}_\Omega - \vec{k}_0$$

$$\tilde{V}(q) = F.T.[V(r)]$$

$$\tilde{U}(q) = F.T.[U(r)]$$

Born approximation for the scattering amplitude:

$$f(\Omega) = -\frac{m}{2\pi\hbar^2}\int d^3r e^{iqr} V(r) = -\frac{m}{2\pi\hbar^2}\tilde{V}(q) \tag{2}$$

We may look at the total potential as a convolution of a single atom potential and an array of 2N+1 delta functions, which we call comb, then we have comb(x), comb(y) and comb(z):

$$V(r) = U(r)(*)comb(x)comb(y)comb(z) \tag{3}$$

According to the properties of F.T.:

$$\tilde{V}(q) = F.T.[V(r)] = F.T.[U(r)] \cdot F.T.[comb(x)] \cdot F.T.[comb(y)] \cdot F.T.[comb(z)] \tag{4}$$

a.

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2 = \frac{m^2}{4\pi^2\hbar^4}\tilde{U}^2(q) \tag{5}$$

b.

We find the F.T.[comb(x)] for finite N and then take it to infinity (see the Appendix), and the results are:

the scattering amplitude for a finite N (see Appendix 1):

$$f(\Omega) = -\frac{m}{2\pi\hbar^2}\tilde{U}(q)\frac{\sin q_x a(N+1/2)}{\sin\frac{q_x a}{2}}\frac{\sin q_y a(N+1/2)}{\sin\frac{q_y a}{2}}\frac{\sin q_z a(N+1/2)}{\sin\frac{q_z a}{2}}, \tag{6}$$

the differential cross section for a finite N:

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2 = \frac{m^2}{4\pi^2\hbar^4}\tilde{U}^2(q)\frac{\sin^2 q_x a(N+1/2)}{\sin^2\frac{q_x a}{2}}\frac{\sin^2 q_y a(N+1/2)}{\sin^2\frac{q_y a}{2}}\frac{\sin^2 q_z a(N+1/2)}{\sin^2\frac{q_z a}{2}}, \tag{7}$$

c.

Here we check the limit $N \to \infty$ and obtain the next result (see Appendix 2):

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2\hbar^4}\tilde{U}^2(q)\frac{(2\pi)^6}{a^6}\sum_{n_x}\delta(q_x - \frac{2\pi}{a}n_x)\sum_{n_y}\delta(q_y - \frac{2\pi}{a}n_y)\sum_{n_z}\delta(q_z - \frac{2\pi}{a}n_z) \tag{8}$$

From here we obtain the Bragg condition for scattering:

$q = \frac{2\pi n}{a}$ or $2k\sin\frac{\theta}{2} = \frac{2\pi}{a}n$

Definition: $\lambda = \frac{2\pi}{k}, \alpha = \frac{\theta}{2}$

we obtain the known formula:

$$2a\sin\alpha = n\lambda$$

The indexes n_x, n_y, n_z are called the Miller's Indices.

Appendix 1

Calculation of F.T.[comb(x)]:

$$comb(x) = \sum_{n_x=-N}^{N}\delta(x - na)$$

$$Comb(q) = F.T.[comb(x)] = e^{-iqaN} + e^{-iqa(N+1)} + .. + 1 + .. + e^{iqa(N-1)} + e^{iqaN}$$

we use the known formula for the sum of the geometric progression $S_n = b_1\frac{q^N-1}{q-1}$:

$$= |\alpha = qa| = e^{+i\alpha N}(\frac{e^{-i\alpha(2N+1)} - 1}{e^{-i\alpha} - 1}) = \frac{e^{-i\alpha(N+1)} - e^{+i\alpha N}}{e^{-i\alpha} - 1} = \frac{e^{-i\alpha(N+1)/2} - e^{+i\alpha(N+1)/2}}{e^{-i\alpha/2} - e^{+i\alpha/2}} =$$

$$= \frac{\sin\alpha(N+\frac{1}{2})}{\sin\frac{\alpha}{2}}$$

It is easy to show (basic trigo) that under transformation $\alpha \to \alpha - 2\pi\nu$ (ν is an integer)
The expression $\frac{\sin^2 \alpha(N+1/2)}{\sin^2 \alpha/2}$ does not change.

Appendix 2

We want to analyze the expression

$$\frac{\sin^2 \alpha(N+1/2)}{\sin^2 \frac{\alpha}{2}}$$

This expression has the poles at $\alpha = 2\pi n$ and the limit at $\alpha \to 2\pi n$ is
(according to L'Hopitals Rule):

$$\lim_{\alpha\to 2\pi n} \frac{\sin^2 \alpha(N+1/2)}{\sin^2 \frac{\alpha}{2}} = \lim_{\alpha\to 2\pi n} \frac{(N+\frac{1}{2})2\sin\alpha(N+1/2)\cos\alpha(N+\frac{1}{2})}{\sin\frac{\alpha}{2}\cos\frac{\alpha}{2}} =$$

$$\lim_{\alpha\to 2\pi n} \frac{(N+\frac{1}{2})\sin 2\alpha(N+\frac{1}{2})}{\frac{1}{2}\sin\alpha} = \lim_{\alpha\to 2\pi n} \frac{4(N+\frac{1}{2})^2\cos 2\alpha(N+\frac{1}{2})}{\cos\alpha} = 4(N+\frac{1}{2})^2 = (2N+1)^2$$

If we have a large number of atoms ($N \to \infty$) and making the use of the fact

$$\frac{1}{2\pi N}\int_{-\infty}^{\infty} \frac{\sin^2 Nx}{x^2} = 1$$

We come to the conclusion that under this conditions ($\alpha \to 2\pi n, N \to \infty$) we get an array of delta functions.

Then

$$F.T.[comb(x)] = Comb(q) = \frac{2\pi}{a}\sum_n \delta(q - \frac{2\pi}{a}n)$$

As it was expected from the direct F.T. of infinite array of delta functions