Scattering of a photon by a Bloch function

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Introduction

In a periodic crystal, electrons are described by specific states called *Bloch functions*. These wavefunctions take account of the periodicity of the crystal. In this short note we shall have a look at scattering processes for which an incoming photon is scattered of a Bloch function, into a different outgoing photon. This should enlighten us on the ways to probe experimentally the state by which the electron is described, as well as the crystal structure.

1 Hamiltonian, initial and final states

We wish to study the interaction of a Bloch electron with a photon. In order to do so, we first need to understand the Hamiltonian of the system. As we shall use a perturbative approach in the following, we might as well describe the initial and final states of the electron and the photon independently.

1.1 Electron

Let us start by focusing on the electron. The electron we want to study is prepared in a Bloch state. We quickly recall what is a Bloch state and how it can arise from a physical context below.

The most obvious case of apparition of a Bloch function is in a periodic structure (*e.g* a crystal). In such a structure, the Hamiltonian is typically given by,

$$H_{e^-} = \frac{p^2}{2m} + V(\mathbf{r}) \tag{1.1}$$

where V is periodic with periods L_i for each three direction $i = x, y, z$ (or $1, 2, 3$).

In what follows we offer a very simple derivation of Bloch's theorem (see [4] and [6]).

Let us define the translation group as the transaltions that leaves V invariant, that is to say, we consider the translation $T_{\mathbf{a}} : \mathbf{r} \to \mathbf{r} + \mathbf{a}$, such that

$$V(\mathbf{r}) = V(T_{\mathbf{a}}\mathbf{r})$$

(this equation is written in the classical sense, that is to say witout considering that V is a quantum mechanical operator).

This group (easy to check) acts naturally on the position states with the representation $|\mathbf{r}\rangle \to |\mathbf{r} + \mathbf{a}\rangle$. This way, one can easily show that V (now considered as a quantum mechanical operator) is invariant under the action of $T_{\mathbf{a}}$, that is to say,

$$T_{\mathbf{a}} V T_{\mathbf{a}}^{-1} = V$$

This in turn implies that the Hamiltonian is also invariant under the action of $T_{\mathbf{a}}$,

$$T_{\mathbf{a}} H_{e^-} T_{\mathbf{a}}^{-1} = H_{e^-}$$

which can also be cast in the form,

$$T H_{e^-} = H_{e^-} T$$

One can also show by expanding a general state $|\psi\rangle$ on the position basis, that $T_{\mathbf{a}}$ acts on wavefunctions as $T_{\mathbf{a}}\psi(\mathbf{r}) = \psi(\mathbf{r} - \mathbf{a})$.

Let us now consider an eigenfunction ψ of the system, that is to say,

$$H_{e^-}\psi(\mathbf{r}) = E\psi$$

Then $\psi'(\mathbf{r}) = T\psi(\mathbf{r}) = \psi(\mathbf{r} - \mathbf{a})$ must also be an eigenfunction with the same energy since,

$$H_{e^-}\psi'(\mathbf{r}) = H_{e^-} T\psi(\mathbf{r}) = T H_{e^-}\psi(\mathbf{r}) = E\psi'(\mathbf{r}) \tag{1.2}$$

Since the group of translations is abelian, it can only admit 1-dimensional irreducible representation which in turn implies that,

$$\psi'(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{a}}\psi(\mathbf{r})$$

This could have been deduced directly from Schur's lemma and the decomposition of representations into irreducible representations, see for instance [1]. (The argument may seem a bit concise and blurry as we shall not expose the whole mathematical theory behind. In fact, it may seem that it doesn't work for degenerate states (it does). A simpler derivation, using only basic linear algebra is proposed in the footnotes of [4].)

Taking $\mathbf{a} = \mathbf{L}$ to be the smallest period in each direction $i = x, y, z$, one shows that we can always choose,

$$-\frac{\pi}{L_i} \leq k_i \leq \frac{\pi}{L_i} \tag{1.3}$$

Imposing periodic boundary conditions, we could also constrain the values taken by $\mathbf{k}$, but that won't really matter for our purposes.

We now write $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$. It is straightforward to show that $u_{\mathbf{k}}(\mathbf{r}+\mathbf{a}) = u_{\mathbf{k}}(\mathbf{r})$. This statement is known as Bloch's theorem, *in a periodic crystal, the wavefunction describing the electrons can be cast in the form*,

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r}) \tag{1.4}$$

where $u_{\mathbf{k}}$ has the periodicity of the crystal. Since $u_{\mathbf{k}}$ is periodic we can also expand it as a Fourier series on the reciprocal lattice,

$$u_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}\in\Lambda^*} C(\mathbf{k}+\mathbf{G})e^{i\mathbf{G}\cdot\mathbf{r}} \tag{1.5}$$

The uptake of this discussion is that any electron can be described by a state $|\psi_{\mathbf{k}}\rangle$, such that,

$$\langle\mathbf{r}|\psi_{\mathbf{k}}\rangle = \psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r}) \tag{1.6}$$

This means that if there is only a single electron in the target, it should have an initial state $\left|\psi_{\mathbf{k}_i}\right\rangle$ and a final state $\left|\psi_{\mathbf{k}_f}\right\rangle$.

1.2 Photons

We now need to talk about radiation. In order to treat radiation quantum mechanically it is nice to resolve to a second quantization description of the potential vector $\mathbf{A}$. We shall work in Coulomb gauge such that $\partial_\mu A^\mu = 0$ and $A^0 = \phi = 0$ where $A^\mu = (\phi, \mathbf{A})$. This way, one can show that quantification of the potential 3−vector $\mathbf{A}$ in a box of volume V leads to,

$$\mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{q},\alpha}\sqrt{\frac{\hbar}{2V\varepsilon_0\omega_{\mathbf{q}}}}\left[a_{\mathbf{q},\alpha}\vec{\sigma}_\alpha e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_{\mathbf{q}}t)} + h.c.\right] \tag{1.7}$$

where $\mathbf{q}$ ranges over all wavevectors and α ranges over possible polarization. The associated Hamiltonian is just given by

$$H_\gamma = \sum_{\mathbf{q},\alpha}\hbar\omega_{\mathbf{q}}\left(a^\dagger_{\mathbf{q},\alpha}a_{\mathbf{q},\alpha} + \frac{1}{2}\right) \tag{1.8}$$

This is sufficient to described any kind of free photons, namely photons are boring without matter or relativity...

The process we are interested in is the scattering of a single photon by the previously described electron. We prepare a single photon in the state $|\mathbf{q}_i,\alpha_i\rangle$ and shoot it towards a target that is in some state $|\psi_{\mathbf{k}}\rangle$. The scattered photon is detected in a different state $\left|\mathbf{q}_f,\alpha_f\right\rangle$. Eventhough only one photon is interacting, it is nice to suppose that we are actually shooting a number n_i of photons towards the target. This shall allow us to check that our calculations don't depend on the number n_i and so easily check if our results make sense. The initial state of the system can then be described as $|n_i,0\rangle$ in the occupation number representation. The first slot refers to the number of photons in the initial state while the second slot is for the number of photons in the scattered state. The final state for the photons shall then be $|n_i-1,1\rangle$. All the other photon states are not indicated since they are not involved in the process under study (we could simply put all other photon modes with an occupation number 0).

1.3 Interactions

The interesting stuff happens only when the interaction are turned on. The general Hamiltonian in Coulomb gauge ($\phi = 0, \partial_\mu A^\mu = 0$) reads,

$$H = H_{e^-} + H_\gamma - q\frac{\mathbf{p}\cdot\mathbf{A}}{m} + \frac{q^2\mathbf{A}^2}{2m} \tag{1.9}$$

To derive this expression, the Coulomb gauge has been used to commute $\mathbf{p}$ and $\mathbf{A}$. Thus, the interaction is described by the last two terms that we denote,

$$H_I = -q\frac{\mathbf{p}\cdot\mathbf{A}}{m} \qquad 1\ \gamma \text{ term} \tag{1.10}$$

$$H_{II} = \frac{q^2\mathbf{A}^2}{2m} \qquad 2\ \gamma \text{ term} \tag{1.11}$$

In perturbation theory we always assume that the interaction are turned on adiabatically, that is to say the initial and final states are eigenstates of the free theory. In our case, these are given by,

$$|i\rangle = \left|\psi_{\mathbf{k}_i}\right\rangle \otimes |n_i, 0\rangle \tag{1.12}$$

$$|f\rangle = \left|\psi_{\mathbf{k}_f}\right\rangle \otimes |n_i - 1, 1\rangle \tag{1.13}$$

They have respective energy,

$$E_i = \mathcal{E}_i + \hbar\omega_i n_i \tag{1.14}$$

$$E_f = \mathcal{E}_f + \hbar\omega_i(n_i - 1) + \hbar\omega_f \tag{1.15}$$

where $\mathcal{E}$ refers to the energy of the electron. Note that we have not included vaccum energies since they irrelevant for our purposes. [Not to mention we don't want to deal with infinities and Casimir effect in this simple note.]

2 Cross section

In an experimental setup, one shall use a detector covering a solid angle $\delta\Omega$ to detect the scattered photons. Then, the detector can be moved around in space to probe the full 4π solid angle. For now we consider covering only the elementary solid angle $\delta\Omega$.

Let us now compute the cross section of the process. To achieve this we will naturally resolve to Fermi's golden rule. However, before diving deeper in the computations we should study in greater depth our interaction potential to understand which terms are relevant for our purposes.

2.1 Interaction potential

In time dependent perturbation theory, one needs to compute matrix elements of the form,

$$\langle f|\, W\, |i\rangle$$

where W denotes the interaction potential, which is $W = H_I + H_{II}$ in our case.

First, let us take a look at $H_I = -q\frac{\mathbf{p}\cdot A}{m}$. Schematically, this term reads

$$H_I \sim \sum_{\mathbf{G},\beta} \left[a_{\mathbf{G},\beta} + a^\dagger_{\mathbf{G},\beta} \right]$$

So that, when acting on a single photon state $|\mathbf{q},\alpha\rangle \sim a^\dagger_{\mathbf{q},\alpha}|0\rangle$, it yields

$$\langle f| H_I |i\rangle \sim \langle n_i - 1, 0| a_{\mathbf{q}_f,\alpha_f} \sum_{\mathbf{G},\beta} \left[a_{\mathbf{G},\beta} + a^\dagger_{\mathbf{G},\beta} \right] a^\dagger_{\mathbf{q}_i,\alpha_i} |n_i - 1, 0\rangle = 0$$

since a sequence of three operator a or $a^\dagger$ must change the total number of photons between the initial and final states. This proves that we only have to deal with the second term,

$$H_{II} = \frac{q^2\mathbf{A}^2}{2m}$$

Actually taking a closer look at this term, we notice that only the terms going as $a^\dagger a$ and $aa^\dagger$ will allow a transition $\gamma_i \to \gamma_f$. Let us describe schematically how this goes. Dropping all unnecessary terms and the terms $a^\dagger a^\dagger$ and aa (which cancels as explained above), $\mathbf{A}^2$ reads schematically,

$$\mathbf{A}^2 \sim \sum_{\lambda_1,\lambda_2} \left[a_{\lambda_1} a^\dagger_{\lambda_2} + a^\dagger_{\lambda_1} a_{\lambda_2} \right]$$

where λ_i should be understood as a double index over the wave vector and the polarization. Then,

$$\langle f| \mathbf{A}^2 |i\rangle \sim \langle n_i - 1, 0| \sum_{\lambda_1,\lambda_2} \left[a_{\lambda_f} a_{\lambda_1} a^\dagger_{\lambda_2} a^\dagger_{\lambda_i} + a_{\lambda_f} a^\dagger_{\lambda_1} a_{\lambda_2} a^\dagger_{\lambda_i} \right] |n_i - 1, 0\rangle$$

Using the commutation relations,

$$\left[a_\lambda, a^\dagger_{\lambda'} \right] = \delta_{\lambda\lambda'} \tag{2.1}$$

one easily gets,

$$\langle f| \mathbf{A}^2 |i\rangle \sim \sum_{\lambda_1\lambda_2} \langle n_i - 1, 0| \left[\delta_{\lambda_1\lambda_f}\delta_{\lambda_2\lambda_i} + \delta_{\lambda_1\lambda_i}\delta_{\lambda_2\lambda_f} \right] |n_i - 1, 0\rangle$$

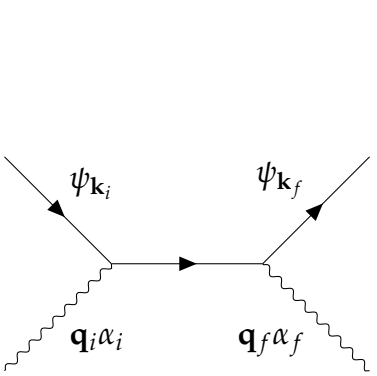
where we've used the fact that $|i\rangle \neq |f\rangle$. Using a Feynman diagram approach might be more insightful. The two diagrams to be taken into account to compute the scattering amplitude are shown in Figure 1.

The point of this is that when we will need to compute precisely the matrix element, we won't need to expand it and we will directly know that only two terms contribute, which correspond to either first creating the final state and annihilating the initial state or the other way around. If these schematic calculations allow us to understand which terms will disappear, we will still need to restore all the multiplicative terms that we dropped in order to get the precise result. We shall do that later.

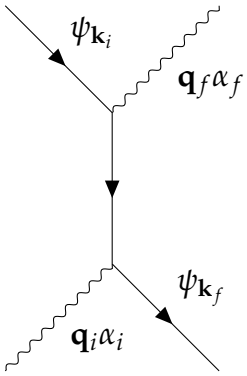
2.2 Fermi's golden rule

What we are interested in, is the number of photons hitting the detector per second, in the solid angle $\delta\Omega$, with energy in an interval δE_γ. This is denote by, $\frac{\delta^2 N_\gamma}{\delta\Omega\delta E_\gamma}$. The differential cross section is then simply defined by this number divide by the incoming flux,

$$\frac{\delta^2\sigma}{\delta\Omega\delta E_\gamma} = \frac{1}{\phi_i}\frac{\delta^2 N_\gamma}{\delta\Omega\delta E_\gamma} \tag{2.2}$$



(a) Absorption followed by emission



(b) Emission followed by absorption

Figure 1: The two processes involved in the scattering

Let us now focus on the quantity $\frac{\delta^2 N_\gamma}{\delta\Omega\delta E_\gamma}$. This is related to the transition rate from the initial state to the final state for photons with wavevector in a solid angle $\delta\Omega$ and energy in δE_γ. We denote it $\delta^2\mathcal{W}_{i\to f}$. It is given by,

$$\frac{\delta^2 N_\gamma}{\delta\Omega\delta E_\gamma} = \frac{\delta^2\mathcal{W}_{i\to f}}{\delta\Omega\delta E_\gamma} \tag{2.3}$$

By Fermi's golden rule,

$$\delta^2\mathcal{W}_{i\to f} = \frac{2\pi}{\hbar}\left|\langle f|\,\frac{q^2\mathbf{A}^2}{2m}\,|i\rangle\right|^2 \delta(E_f - E_i)g^{\alpha_f}(E_\gamma)\delta E_\gamma$$

where $g^{\alpha_f}(E_\gamma)$ is the density of states with wavevector $\delta\Omega$ for the outgoing photon. We compute it in the following section.

2.2.1 Density of states

The density of states is a classical computation. The first thing we do is compute the number of states with energy smaller than E per photon polarization. We denote it $\Phi(E)$. The dispersion relation for photons is $E = \hbar c\|\mathbf{k}\|$.

Using periodic boundary conditions in a box of volume V, one gets

$$\Phi(E) = \frac{V}{(2\pi)^3}\int_{\|\mathbf{k}\|<E/\hbar c}^{\delta\Omega} \mathrm{d}^3\mathbf{k} = \frac{V}{3(2\pi)^3}\delta\Omega\left(\frac{E}{\hbar c}\right)^3$$

so that for a single polarization the density of state is,

$$g^\alpha(E) = \frac{\mathrm{d}\Phi}{\mathrm{d}E} = \frac{V}{(2\pi)^3}\delta\Omega E^2\frac{1}{\hbar^3c^3}$$

This way we get,

$$\frac{\delta^2\sigma}{\delta\Omega\delta E_\gamma} = \frac{1}{\phi_i}\frac{2\pi}{\hbar}\left|\langle f|\,\frac{q^2\mathbf{A}^2}{2m}\,|i\rangle\right|^2 \delta(E_f - E_i)\frac{2V}{h^3c^3}E_\gamma^2$$

that we can already integrate over all energies E_γ to get only the angular differential cross section. To do so, we use the fact that

$$E_f - E_i = \mathcal{E}_f - \mathcal{E}_i + E_\gamma - \hbar\omega_i$$

So that upon integrating over E_γ, one finds,

$$\frac{\delta\sigma}{\delta\Omega} = \frac{1}{\phi_i}\frac{2\pi}{\hbar}\left|\langle f|\,\frac{q^2\mathbf{A}^2}{2m}\,|i\rangle\right|^2 \frac{V}{h^3c^3}E_\gamma^2$$

where in this last equation E_γ is not a variable anymore but fixed to

$$E_\gamma = \mathcal{E}_i + \hbar\omega_i - \mathcal{E}_f \tag{2.4}$$

Let us go one step further before computing the matrix element and replace ϕ_i by its value,

$$\phi_i = \frac{n_i c}{V} \tag{2.5}$$

This yields,

$$\frac{\delta\sigma}{\delta\Omega} = \frac{(2\pi)^2V^2}{n_i h^4c^4}\left|\langle f|\,\frac{q^2\mathbf{A}^2}{2m}\,|i\rangle\right|^2 E_\gamma^2 \tag{2.6}$$

2.2.2 Matrix element

Now we come to the nasty bits of these calculations as we should evaluate the matrix element involved. It's actually not as bad as it seems since our previous discussions already provided most of the work. In fact, as previously stated, there are only two terms contributing to the matrix element with equal weight, this allows us to write

$$\langle f|\,\frac{q^2\mathbf{A}^2}{2m}\,|i\rangle = 2\cdot\frac{q^2}{2m}\left\langle\psi_{\mathbf{k}_f}\right|\otimes\langle n_i-1,1|\,\frac{\hbar}{2V\varepsilon_0\sqrt{\omega_i\omega_f}}a_i a_f^\dagger e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\vec{\sigma}_f^*\cdot\vec{\sigma}_i\,|n_i,0\rangle\otimes\left|\psi_{\mathbf{k}_i}\right\rangle$$

We should be very careful with this notation as the operator betwen the *bra* and *ket* is not hermitean anymore. We just keep in mind that we apply it to the state on the right first. Using,

$$a_\lambda\,|n_\lambda\rangle = \sqrt{n_\lambda}\,|n_\lambda-1\rangle \quad \text{and} \quad a_\lambda^\dagger\,|n_\lambda\rangle = \sqrt{n_\lambda+1}\,|n_\lambda+1\rangle \tag{2.7}$$

the matrix element reads,

$$\langle f|\,\frac{q^2\mathbf{A}^2}{2m}\,|i\rangle = \frac{1}{\sqrt{\omega_i\omega_f}}2\cdot\frac{q^2\hbar}{4V\varepsilon_0 m}\sqrt{n_i}\vec{\sigma}_f^*\cdot\vec{\sigma}_i\left\langle\psi_{\mathbf{k}_f}\right|e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\left|\psi_{\mathbf{k}_i}\right\rangle$$

We only need to compute the remaining matrix element as an integral over space,

$$\left\langle\psi_{\mathbf{k}_f}\right|e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\left|\psi_{\mathbf{k}_i}\right\rangle = \int \mathrm{d}\mathbf{r}\psi_{\mathbf{k}_f}^*(\mathbf{r})e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\psi_{\mathbf{k}_i}(\mathbf{r}) \tag{2.8}$$

Packing up all these results, we can finally compute the differential cross section. It reads,

$$\frac{\delta\sigma}{\delta\Omega} = \frac{(2\pi)^2V^2}{n_i h^4c^4}E_\gamma^2\frac{q^4\hbar^2 n_i}{4V^2\varepsilon_0^2 m^2\omega_i\omega_f}\left|\vec{\sigma}_f^*\cdot\vec{\sigma}_i\right|^2\left|\int \mathrm{d}\mathbf{r}\psi_{\mathbf{k}_f}^*(\mathbf{r})e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\psi_{\mathbf{k}_i}(\mathbf{r})\right|^2$$

Replacing the electron by its charge $q=-e$ and using $E_\gamma=\hbar\omega_f$, we simplify the above expression to find,

$$\frac{\delta\sigma}{\delta\Omega} = \frac{1}{(2\pi)^2}\alpha^2\lambda_c^2\frac{\omega_f}{\omega_i}\left|\vec{\sigma}_f^*\cdot\vec{\sigma}_i\right|^2\left|\int \mathrm{d}\mathbf{r}\psi_{\mathbf{k}_f}^*(\mathbf{r})e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\psi_{\mathbf{k}_i}(\mathbf{r})\right|^2 \tag{2.9}$$

where we introduced the fine structure constant,

$$\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \tag{2.10}$$

and the electron Compton wavelength,

$$\lambda_c = \frac{h}{mc} \tag{2.11}$$

We are glad to find that the process is depending on the fine sturcture constant squared. This makes perfect sense since the fine sturcture constant is the relevant coupling constant for electromagnetism. Since we computed matrix element at tree level, they should depend on α and the cross section should depend on α^2. The apparition of the Compton wavelength is also understandable since it characterizes the scattering of a photon by an electron. This also proves that the above expression has the right units.

We should also notice how the polarization of the incoming and outgoing photon should be *overlapping* otherwise the scalar product of the polarization vectors would be 0.

Finally, let us take a closer look at the integral involving the Bloch functions. It reads, with V_c the colume of the crystal,

$$\begin{aligned}
\int_{V_c} \mathrm{d}\mathbf{r}\psi^*_{\mathbf{k}_f}(\mathbf{r})e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\psi_{\mathbf{k}_i}(\mathbf{r}) &= \sum_{\mathbf{r}_j\in\Lambda}\int_{v_j}\mathrm{d}\mathbf{x}u^*_{\mathbf{k}_f}(\mathbf{r}_i+\mathbf{x})u^*_{\mathbf{k}_j}(\mathbf{r}_j+\mathbf{x})e^{i(\mathbf{q}_i+\mathbf{k}_i-\mathbf{q}_f-\mathbf{k}_f)\cdot(\mathbf{r}_j+\mathbf{x})} \\
&= \sum_{\mathbf{r}_j\in\Lambda} e^{i(\mathbf{q}_i+\mathbf{k}_i-\mathbf{q}_f-\mathbf{k}_f)\cdot\mathbf{r}_j}\int_v \mathrm{d}\mathbf{x}u^*_{\mathbf{k}_f}(\mathbf{x})u_{\mathbf{k}_i}(\mathbf{x})e^{i(\mathbf{q}_i+\mathbf{k}_i-\mathbf{q}_f-\mathbf{k}_f)\cdot\mathbf{x}} \\
&= \sum_{\mathbf{r}_j\in\Lambda} e^{i(\mathbf{q}_i+\mathbf{k}_i-\mathbf{q}_f-\mathbf{k}_f)\cdot\mathbf{r}_j}F_{fi}(\mathbf{q}_f+\mathbf{k}_f-\mathbf{q}_i-\mathbf{k}_i)
\end{aligned}$$

where in the first line we summed over every unit cell with volume $v_i = v$ and in the second line we used the periodicity of u in the lattice Λ. Finally, we denote the structure factor as,

$$F_{fi}(\mathbf{q}_1-\mathbf{q}_2) = \int_v \mathrm{d}\mathbf{x}u^*_{\mathbf{k}_f}(\mathbf{x})u_{\mathbf{k}_i}(\mathbf{x})e^{-i(\mathbf{q}_1-\mathbf{q}_2)\cdot\mathbf{x}} \tag{2.12}$$

Taking the modulus squared of this quantity, one finds,

$$\left|\int \mathrm{d}\mathbf{r}\psi^*_{\mathbf{k}_f}(\mathbf{r})e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\psi_{\mathbf{k}_i}(\mathbf{r})\right|^2 = \sum_{\mathbf{r}_j,\mathbf{r}'_j\in\Lambda} e^{i(\mathbf{q}_i+\mathbf{k}_i-\mathbf{q}_f-\mathbf{k}_f)\cdot(\mathbf{r}_j-\mathbf{r}'_j)}\left|F_{fi}(\mathbf{q}_f+\mathbf{k}_f-\mathbf{q}_i-\mathbf{k}_i)\right|^2$$

The sum in this last equation reads, with N the number of nodes in the lattice,

$$\sum_{\mathbf{r}_j,\mathbf{r}'_j\in\Lambda} e^{i(\mathbf{q}_i+\mathbf{k}_i-\mathbf{q}_f-\mathbf{k}_f)\cdot(\mathbf{r}_j-\mathbf{r}'_j)} = N\sum_{\mathbf{r}_j\in\Lambda} e^{i(\mathbf{q}_i+\mathbf{k}_i-\mathbf{q}_f-\mathbf{k}_f)\cdot\mathbf{r}_j}$$

one can use the relation (for a proof see [3]),

$$\sum_{\mathbf{r}\in\Lambda} e^{-i\mathbf{k}\cdot\mathbf{r}} = v^*\sum_{\mathbf{Q}\in\Lambda^*}\delta(\mathbf{k}-\mathbf{Q}) \tag{2.13}$$

so that finally, one finds,

$$\begin{aligned}
\left|\int \mathrm{d}\mathbf{r}\psi^*_{\mathbf{k}_f}(\mathbf{r})e^{i(\mathbf{q}_i-\mathbf{q}_f)\cdot\mathbf{r}}\psi_{\mathbf{k}_i}(\mathbf{r})\right|^2 = Nv^*\sum_{\mathbf{G}\in\Lambda^*}&\delta(\mathbf{q}_i+\mathbf{k}_i-\mathbf{q}_f-\mathbf{k}_f-\mathbf{G}) \\
&\times\left|F_{fi}(\mathbf{q}_f+\mathbf{k}_f-\mathbf{q}_i-\mathbf{k}_i)\right|^2
\end{aligned}$$

which reads just like a Bragg's law or momentum conservation.

2.3 Elastic scattering

The case of elastic scattering, or *diffraction*, is particularly interesting. In this case the incoming and outgoing photons have the same energy, which in turn forces the electron to have the same energy before and after the scattering process. Let us suppose that the ground state for the electron is non degenerate. This can appear as a rather bold claim since there are many lattices and crystal for which this shouldn't be true. In fact, any rotational invariance would force the appearance of degenerate states. However, in a general crystal there are impurities which break translational and rotational invariance. This way, one can convince himself that these impurities will enforce the appearance of a single ground state. Then, as the Bloch states are defined only by a wavevector, this enforces $\mathbf{k}_f = \mathbf{k}_i$.

This can actually help us simplify greatly our last computation and now the cross section becomes (because $\omega_i = \omega_f$),

$$\frac{\delta\sigma}{\delta\Omega} = \frac{1}{(2\pi)^2}\alpha^2\lambda_c^2\left|\vec{\sigma}_f^* \cdot \vec{\sigma}_i\right|^2 N v^* \sum_{\mathbf{G}\in\Lambda^*} |F_{ii}(\mathbf{G})|^2 \delta(\mathbf{q}_i - \mathbf{q}_f + \mathbf{G}) \tag{2.14}$$

The first thing that appears is that the cross section follows Bragg's law, in the sense that the two photons momenta really are related by some reciprocal lattice vectors.

However, it's not quite clear what $Nv^*|F_{ii}(\mathbf{G})|^2$ really represents physically. In order to interpret this we first prove a very short lemma which states that for any function f periodical in the Bravais lattice, one has,

$$f(\mathbf{r}) = \frac{v^*}{(2\pi)^3} \sum_{\mathbf{G}\in\Lambda^*} e^{i\mathbf{G}\cdot\mathbf{r}} \int_v \mathrm{d}\mathbf{x} e^{-i\mathbf{G}\cdot\mathbf{x}} f(\mathbf{x}) \tag{2.15}$$

We've actually alsmot done all the work to prove this. Let us just introduce the Fourier transform of f and denote it by $\tilde{f}$. By definition,

$$\begin{aligned}\tilde{f}(\mathbf{k}) &= \int \mathrm{d}\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r}) \\ &= \sum_{\mathbf{R}\in\Lambda} e^{-i\mathbf{k}\cdot\mathbf{r}} \int_v \mathrm{d}\mathbf{x} f(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}}\end{aligned}$$

where we used the periodicity of f. Using a previous claim for the first sum, one can inject this form for the Fourier transform $\tilde{f}$ into the expression of f to prove the claim.

Let us use this lemma for the probability density, which is in fact periodic in Λ,

$$\rho(\mathbf{r}) = \left|\psi_{\mathbf{k}_i}(\mathbf{r})\right|^2 = \left|u_{\mathbf{k}_i}(\mathbf{r})\right|^2 \tag{2.16}$$

so that,

$$\rho(\mathbf{r}) = \frac{v^*}{(2\pi)^3} \sum_{\mathbf{G}\in\Lambda^*} e^{i\mathbf{G}\cdot\mathbf{r}} F_{ii}(\mathbf{G}) \tag{2.17}$$

We can also expand ρ on the reciprocal lattice using the expansion of u,

$$\rho(\mathbf{r}) = \sum_{\mathbf{K},\mathbf{G}\in\Lambda^*} C^*(\mathbf{k}_i + \mathbf{K}) C(\mathbf{k}_i + \mathbf{K} + \mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}$$

that we denote simply finally,

$$\rho(\mathbf{r}) = \sum_{\mathbf{G}\in\Lambda^*} S_{ii}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}} \tag{2.18}$$

where

$$S_{ii}(\mathbf{G}) = \sum_{\mathbf{K}\in\Lambda^*} C^*(\mathbf{k}_i + \mathbf{K})C(\mathbf{k}_i + \mathbf{K} + \mathbf{G}) \tag{2.19}$$

This in turn proves that,

$$S_{ii}(\mathbf{G}) = \frac{v^*}{(2\pi)^3} F_{ii}(\mathbf{G}) \tag{2.20}$$

Inputting this result back into the cross section and using $vv^* = (2\pi)^3$, one gets

$$\frac{\delta\sigma}{\delta\Omega} = 2\pi\alpha^2\lambda_c^2 \left|\vec{\sigma}_f^* \cdot \vec{\sigma}_i\right|^2 Nv \sum_{\mathbf{G}\in\Lambda^*} |S_{ii}(\mathbf{G})|^2 \delta(\mathbf{q}_i - \mathbf{q}_f + \mathbf{G}) \tag{2.21}$$

We can now fully interpret the result. At first sight, the cross section seems proportionnal to the crystal volume, $V_c = Nv$. However, we now know that S_{ii} are the Fourier components of the probability density and so we would expect them to decrease as V_c increases. This is quite a relief since a cross section increasing forever with V_c would break unitarity at some point.

The cross section not only follows Bragg's law but allow us to probe the probability density Fourier coefficients and so the ground state of the system. In fact, by measuring the number of incoming photons for different reciprocal lattice vectors, one gets access to the coefficients S_{ii}. The bigger the S_{ii}, the bigger the number of incoming photon should be.

3 Spin effects

To take account of the spin effects, one would classically just add a term $\mathbf{J}\cdot\mathbf{B}$, where $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$ and $\mathbf{J} = \mathbf{L} + g\mathbf{S}$. One can wonder where this term really comes from and if there are no other terms that are left out when we treat the photon quantum mechanically rather than like a classical electromagnetic field. To achieve so we resolve to quantum field theory and the so called Dirac equations, which reads,

$$\left(i\gamma^\mu\left[\partial_\mu - ieA_\mu\right] - m\right)\psi \tag{3.1}$$

where ψ is a Dirac spinor (a 4 component mathematical object that changes sign under the action of a rotation by 2π). The computations are quite heavy and require some knowledge about quantum field theory. However, the result really is the one stated above. The interested reader can have a look at [5] and [2].

The uptake of all of this that we can really treat the spin dependent processe as adding a contribution $\mathbf{J}\cdot\mathbf{B}$ to the interaction Hamiltonian. This term is linear in $\mathbf{A}$ so, similarly to previous arguments, it won't contribute to the scattering process at first order in perturbation theory. Obviously, going to higher orders will yield terms as $\sim H_{int}^2$ which may involve contributions from the spin dependent interaction of the Hamiltonian.

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