The Bragg law with radiative corrections

Miroslav Pardy

Department of Physical Electronics,
and
The Laboratory of the Plasma Physics,
Masaryk University,
Kotlářská 2, 611 37 Brno, Czech Republic
e-mail:pamir@physics.muni.cz

June 26, 2025

Abstract

The one-loop radiative correction to the photon propagator, called vacuum polarization, can be represented by the Feynman diagram of the second order. The physical meaning of this diagram is the virtual process $\gamma \to (e^- + e^+) \to \gamma$, where γ is denotation for photon, and e^-, e^+ is the electron-positron pair. It means that photon can exist in the intermediate state with the e^+, e^- being the virtual particles. The photon propagation function based on such process is determined in the framework of he Schwinger source QED methods. Then, the modification of the Brag equation is defined.

1 Introduction

Bragg's law, or, Bragg's condition, or, Laue-Bragg interference is a special case of Laue diffraction that gives the angles for coherent scattering of waves from a large crystal lattice. It describes relation between the wavelength and scattering angle. This law was initially formulated for X-rays, but it also applies to all types of matter waves including neutron and electron waves.

Bragg diffraction occurs when radiation of a wavelength comparable to atomic spacings is scattered in mirror-like reflection by planes of atoms in a crystalline material, and undergoes constructive interference (Ashcroft et al., 1976). When the scattered waves are incident at a specific angle, they remain in phase and constructively interfere. The glancing angle θ, the wavelength , and the "grating constant" d of the crystal are connected by the relation $n\lambda = 2d \sin\theta$ (Ashcroft et al., 1976), where n is the diffraction order (n = 1 is the first order, n = 2 is the second order, an so on . This equation, so called Bragg's law, describes the condition on θ for constructive interference (Ashcroft et al., 1976). The derivation of eq. (1) performed with the pedagogical clarity was realized by Ashcroft et al. (1976).

2 Radiative corrections in QED

Radiative corrections are of the fundamental importance for modern high-precision, sub-atomic physics experiments. In the experiments with percent precision, radiative corrections on the experimental observables need to be known to sub-percent precision. These corrections are a subject of active research in modern QED experiments.

Typical probes are leptons or photons. In modern experiments, the muon serves as an attractive alternative to the electron, as its higher mass typically leads to smaller radiative corrections.

The calculation of one-loop radiative corrections in atomic physics has played a central role in QED since the first evaluation of the Lamb shift. In the case of highly charged ions, the Lamb shift is enhanced by some a factor of Z and can affect energy shifts. Its calculations at high Z is complicated by the need for an exact treatment of the electron propagator. These calculations have been confirmed by experiment.

The radiative corrections to the Bragg equation follow from the quantum electrodynamics and cannot be determined by the classical mathematical procedures of the classical electromagnetism. We explain, in the next section, the determination of the Green function of photon with the radiative corrections. Then, we determine the radiative corrections to the photon wave function and to the Bragg equation.

3 The modified propagation function of photon

It is well known from the traditional theory of the Feynman propagator of photon that the one-loop radiative correction to the photon propagator can be graphically represented by the Feynman diagram of the second order. The physical meaning of this diagram is the virtual process $\gamma \to (e^- + e^+) \to \gamma$, where γ is denotation for photon, and e^-, e^+ is the electron-positron pair. It means that photon can exist in the intermediate state with e^+, e^- being the virtual particles.

The modified photon propagation function involving only the two-particle exchange process between sources is then diagrammatic expressed by the analogical way in the Schwinger source theory of QED.

Now, let us determine the photon propagator corresponding to the intermediate electron-positron pair (Schwinger, 1969). The emission photon source emits by manner of the intermediate virtual photon the electron-positron pair which is absorbed by the detection source. Such process is possible when a source emits too much energy to produce only a photon. For the virtual photon, we have the relation $k^2 \neq 0$ and the excitation cannot propagate very far because the balance of energy and momentum is broken.

We can split the process into two parts. The lower part and the upper part. The lower part is the emission part and the upper one is the absorption part. The emission part corresponds to the emission effective source. The effective two-particle source is here the electromagnetic vector potential.

There is no renormalization procedure necessary, neither for the mass, nor for the charge. Here is the way from free traveling photon ($k^2 = 0$) to the modified effective photon propagator which experiences from the source an excess of energy ($k^2 = -M^2$), so that after an extremely short time, it can produce an electron-positron pair. Everything happens between the "vacua" $< 0_-|$ and $|0_+ >$. These are not the vacuum with particle-antiparticle pairs, etc. They are absolutely empty until an external source delivers or takes the necessary attributes of energy, momentum, spin, etc. to, or, from the particles to be produced or annihilated (Dittrich, 1978).

The vacuum amplitude corresponding to the primitive interaction that occurs is involved in the vacuum to vacuum amplitude with $i/\hbar = i$, for $\hbar = 1$ (Dittrich, 1978)

$$\langle 0_+|0_-\rangle = e^{iW_{int}}, \tag{1}$$

where

$$W_{int} = \int (dx) j^\mu(x) A_\mu(x) \tag{2}$$

with

$$j^\mu(x) = \frac{1}{2}\psi(x)\gamma^0 eq\gamma^\mu\psi(x) \tag{3}$$

and the vacuum amplitude corresponding to the considered process is

$$\langle 0_+|0_-\rangle = i\int (dx)\psi(x)\gamma^0 eq\gamma^\mu\psi(x)A_\mu(x), \tag{4}$$

where q is the charge matrix: $q = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

The vacuum amplitude for the non-interacting spin 1/2 particle is involved in the general formula (Dittrich, 1978)

$$\langle 0_+|0_-\rangle = \langle 0_+|0_-\rangle^\eta \langle 0_+|0_-\rangle^\eta = e^{iW(\eta)}e^{iW(\eta)} \tag{5}$$

with

$$W(\eta) = \int \psi\gamma^0\eta, \tag{6}$$

from which we extract the vacuum amplitude for the two non-interacting spin 1/2 particles in the form (Schwinger, 1970; 2018)

$$\langle 0_+|0_-\rangle = \frac{1}{2}\left[i\int (dx)\psi(x)\gamma^0\eta(x)\right]^2 = -\frac{1}{2}\int (dx)(dx')\psi(x)\gamma^0\eta(x)\eta(x')\gamma^0\psi(x') \quad \rightarrow$$

$$-\frac{1}{2}\int \psi_1(x)\gamma^0\eta_2(x)\eta_2(x')\gamma^0\psi_1(x'). \tag{7}$$

The comparison of eq. (7) with eq. (4) supplies the matrix

$$i\eta_2(x)\eta_2(x')|_{eff\ emiss} = eq\gamma^\mu\gamma^0 A_{2\mu}\delta(x-x'), \tag{8}$$

or, in the momentum representation

$$i\eta_2(p)\eta_2(p')|_{eff\ emiss} = eq\gamma^\mu\gamma^0 A_{2\mu}(k) \tag{9}$$

with $k = p + p'$.

By the same procedure just performed we get for the absorption effective source the following formula:

$$i\eta_1(p)\eta_1(p')|_{eff\ abs} = eq\gamma^\mu\gamma^0 A_{1\mu}(-k) \tag{10}$$

with $k = p + p'$.

Let us remark that the antisymmetry of the left side of eq. (8) for all indices expressing the Fermi-Dirac statistics is involved in the charge matrix q.

The amplitude which describes emission and absorption of the two non-interacting particles which propagate freely between the effective sources can be separated from the vacuum amplitude

$$\langle 0_+|0_-\rangle = \exp\left\{\int (dx)(dx')\eta_1(x)\gamma^0 G_+(x-x')\eta_2(x')\right\} \tag{11}$$

as its quadratic term of its expansion. Here

$$G_+(x-x') = i\int d\omega_p e^{ip(x-x')}(m-\gamma p); \quad d\omega_p = \frac{d(\mathbf{p})}{2\pi^3}\frac{1}{2p^0}, \tag{12}$$

where $p^0 = +\sqrt{\mathbf{p}^2+m^2}$ (Dittrich, 1978).

Then,

$$\langle 0_+|0_-\rangle = \frac{1}{2}\int d\omega_p \int d\omega_{p'} \left[\eta_1(-p)\gamma^0(m-\gamma p)\eta_2(p)\eta_2(p')\gamma^0(m+\gamma p')\eta_1(p')\right]. \tag{13}$$

Using relation

$$\eta_{1a}(-p)M_{ab}\eta_{1b}(-p') = -M_{ab}\eta_{1b}(-p')\eta_{1a}(-p) \quad = -\mathrm{tr}[M\eta_1(-p')\eta_1(-p)], \tag{14}$$

where a and b are indexes for the eight-dimensional mathematical object η and symbol tr denotes the eight-dimensional trace.

Using eq. (14) we can write

$$\langle 0_+|0_-\rangle = \frac{1}{2}\int d\omega_p \int d\omega_{p'}\mathrm{tr}\left[(m-\gamma p)\eta_2(p)\eta_2(p')\gamma^0(-m-\gamma p')\eta_1(-p)\eta_1(-p)\gamma^0\right]. \tag{15}$$

After inserting of the effective emission and absorption sources with $k = p + p'$

$$i\eta_2(p)\eta_2(p')|_{eff\ emiss} = eq\gamma^\mu\gamma^0 A_{2\mu}(k) \tag{16}$$

$$i\eta_1(-p')\eta_1(-p)|_{eff\ abs} = eq\gamma^\mu\gamma^0 A_{1\mu}(-k) \tag{17}$$

into eq. (13) we get with $(\gamma^0)^2 = 1$,

$$\langle 0_+|0_-\rangle = -\frac{1}{2}\int d\omega_p \int d\omega_{p'} \mathrm{tr}\left[(m-\gamma p)eq\gamma A_2(k)(-m-\gamma p')eq\gamma A_1(-k)\right]. \tag{18}$$

Substituting the unit factor

$$1 = (2\pi)^3 \int dM^2 d\omega_k \delta(k - p - p'), \tag{19}$$

we find

$$\langle 0_+|0_-\rangle = -e^2 \int dM^2 d\omega_k A_1^\mu(-k) I_{\mu\nu}(k) A_2^\nu(k), \tag{20}$$

where

$$I_{\mu\nu}(k) = I_{\nu\mu}(k) = (2\pi)^3 \int d\omega_p d\omega_{p'} \delta(k-p-p') \mathrm{tr}[\gamma_\mu(m-\gamma p)\gamma_\nu(-m-\gamma p')]. \tag{21}$$

Using relations $p^2 + m^2 = 0$, $p'^2 + m^2 = 0$ we find

$$\mathrm{tr}[\gamma_\mu(m-\gamma p)\gamma_\nu(-m-\gamma p')] = \mathrm{tr}[(\gamma p + m)\gamma_\mu(\gamma p' - m)(m-\gamma p)\gamma_\nu(-m-\gamma p')]. \tag{22}$$

It may be easily seen that

$$k^\mu I_{\mu\nu}(k) = 0, \tag{23}$$

which implies the gauge invariance of $\langle 0_+|0_-\rangle$ in the form

$$A_\mu(k) \to A_\mu(k) + ik_\mu \lambda(k). \tag{24}$$

The symmetrical tensor constructed from the vector k_μ is

$$I_{\mu\nu} = \left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right) I(M^2), \tag{25}$$

where $I(M^2)$ can be calculated from relation

$$3I(M^2) = (2\pi)^3 \int d\omega_p d\omega_{p'} \delta(p + p' - k) \mathrm{tr}[\gamma^\mu(m-\gamma p)\gamma_\nu(-m-\gamma p')]. \tag{26}$$

Then, using (Dittrich, 1978)

$$\gamma^\mu\gamma_\mu = -4; \quad \gamma^\mu\gamma p\gamma_\mu = 2\gamma p \tag{27}$$

$$\mathrm{tr}[\gamma_\mu\gamma_\nu] = -4g_{\mu\nu}; \quad \mathrm{tr}\gamma_\mu = 0 \tag{28}$$

$$-M^2 = k^2 = (p+p')^2 = -2m^2 + 2pp' \tag{29}$$

and

$$(2\pi)^3 \int d\omega_p d\omega_{p'}\delta(p+p'-k) = \frac{1}{(4\pi)^2}\left(1-\frac{4m^2}{M^2}\right)^{1/2}, \tag{30}$$

we obtain

$$I(M^2) = \frac{4}{3}\left(M^2+2m^2\right)\frac{1}{(4\pi)^2}\left(1-\frac{4m^2}{M^2}\right)^{1/2}. \tag{31}$$

Now, we can write the vacuum amplitude in the form

$$\langle 0_+|0_-\rangle = -e^2\int dM^2 d\omega_k A_1^\mu(-k) \quad \times$$

$$\left(g_{\mu\nu}+\frac{k_\mu k_\nu}{M^2}\right)\frac{4}{3}\left(M^2+2m^2\right)\frac{1}{(4\pi)^2}\left(1-\frac{4m^2}{M^2}\right)^{1/2} A_2^\nu(k). \tag{32}$$

Since $k^2A^\mu(k) = J^m$ and $k^2 = -M^2$, we have for the effective sources $J_{1,2}(\mp k)$:

$$A_2^\mu(k) = -\frac{1}{M^2}J_2^\mu(k); \quad A_1^\mu(-k) = -\frac{1}{M^2}J_1^\mu(-k) \tag{33}$$

and after substitution of eq. (33) into vacuum amplitude (32) we get

$$\langle 0_+|0_-\rangle \quad = \quad i\frac{\alpha}{3\pi}\int\frac{dM^2}{M^2}\left(1+\frac{2m^2}{M^2}\right)\left(1-\frac{4m^2}{M^2}\right)^{1/2} id\omega_k J_1^\mu(-k)J_{2\mu}(k). \tag{34}$$

Now, we substitute for the momentum representation of $J^\mu(k)$

$$J_1^\mu(-k) = \int (dx) J_1^\mu(x)e^{ikx} \tag{35}$$

$$J_2^\mu(-k) = \int (dx') J_2^\mu(x')e^{ikx'} \tag{36}$$

and put

$$\Delta_+(x-x';M^2) = i\int d\omega_k e^{ik(x-x')}. \tag{37}$$

Then,

$$\langle 0_+|0_-\rangle = i\frac{\alpha}{3\pi}\int\frac{dM^2}{M^2}\left(1+\frac{2m^2}{M^2}\right)\left(1-\frac{4m^2}{M^2}\right)^{1/2} \quad \times$$

$$\int (dx)(dx')J_1^\mu(x)\Delta_+(x-x';M^2)J_{2\mu}(x'). \tag{38}$$

The amplitude (38) involves the electron-positron pair production and the complete radiation process is described by the amplitude

$$\langle 0_+|0_-\rangle = \int (dx)(dx')J_1^\mu(x)\tilde{D}_+(x-x';M^2)J_{2\mu}(x'), \tag{39}$$

where the momentum representation of $\tilde{D}_+(x-x')$ can be now written with the regard to eq. (38) in the form:

$$\tilde{D}_+(k) = \frac{1}{k^2-i\varepsilon} \quad +$$

$$\frac{\alpha}{3\pi}\int_{4m^2}^{\infty}\frac{dM^2}{M^2}\left(1+\frac{2m^2}{M^2}\right)\left(1-\frac{4m^2}{M^2}\right)^{1/2}\frac{1}{k^2+M^2-i\varepsilon}, \tag{40}$$

or,

$$\tilde{D}_+(k) = \frac{1}{k^2-i\varepsilon} \quad + \int_{4m^2}^{\infty} dM^2 a(M^2)\frac{1}{k^2+M^2-i\varepsilon}, \tag{41}$$

where

$$a(M^2) = \frac{\alpha}{3\pi}\frac{1}{M^2}\left(1+\frac{2m^2}{M^2}\right)\left(1-\frac{4m^2}{M^2}\right)^{1/2}. \tag{42}$$

is the weight function of the e^+e^- - particle production. Let us remark that for $M \gg 2m$ the radiative corrections to the Green function of the free photon $\tilde{D}_+$ behave like

$$\int_{4m^2}^{\infty}\frac{dM^2}{M^2}\frac{1}{k^2+M^2} \tag{43}$$

and therefore there is no convergence problem of integral in eq. (41).

4 Interference of light

The waves may be produced in such a way that a definite relation between their phases is maintained at all times. Such waves are called coherent.

At this situation the maximum of one wave occurs always at the same instant as the maximum of the other wave, the waves are coherent and in phase. Or, their phase difference remains equal to zero. Similarly, if the maximum of one wave always occurs at the same instant as the minimum of the other wave, the waves are coherent and half a cycle out of phase. Or, their phase difference remains equal to one-half cycle.

Let us consider two wave intensities:

$$\mathbf{E}_1 = \mathbf{E}_{10}\cos(\omega t + \alpha_1), \tag{44a}$$

$$\mathbf{E}_2 = \mathbf{E}_{20} \cos(\omega t + \alpha_2). \tag{44b}$$

Then, the total intensity is as follows:

$$\mathbf{E} = \mathbf{E}_1 + \mathbf{E}_2 = \mathbf{E}_0 \cos(\omega t + \alpha), \tag{45}$$

where

$$E_0^2 = E_{01}^2 + E_{02}^2 + 2E_{01}E_{02} \cos\alpha, \tag{46}$$

with

$$\tan\alpha = \tan(\alpha_2 - \alpha_1) = \frac{E_{01}\sin\alpha_1 + E_{02}\sin\alpha_2}{E_{01}\cos\alpha_1 + E_{02}\cos\alpha_2}. \tag{47}$$

5 The wave function of photon

We can see from eq. (41) that the wave $\exp(ikx)$ corresponds to the component $1/k^2$ with $k = (\mathbf{k}, k^0)$, of the propagator (41). It means that the additional wave in the propagator in eq. (41) is

$$\int_{4m^2}^{\infty} dM^2 a(M^2) e^{\kappa x}, \tag{48}$$

where

$$\kappa = (\mathbf{k}, K^0); \quad K^0 = \sqrt{(k^{02}) + M^2} \tag{49}$$

and the total wave function of photon with radiative corrections is as follows

$$\psi(k, x) = e^{ikx} + \int_{4m^2}^{\infty} dM^2 a(M^2) e^{i\kappa x}. \tag{50}$$

The real part of this function, which we use for the derivation of the generalized Bragg law with radiative correction is

$$\varphi(k, x) = \cos kx + \int_{4m^2}^{\infty} dM^2 a(M^2) \cos\kappa x. \tag{51}$$

6 Radiative correction to the Bragg law

We have seen how to calculate the Green function of photon with the radiative corrections and the photon with radiative correction according to formula (50).

Bragg diffraction occurs when radiation of a wavelength comparable to atomic spacings is scattered in mirror-like reflection by planes of atoms in a crystalline material, and undergoes constructive interference (Ashcroft et al., 1976). When the scattered waves are incident at a specific angle, they remain in phase and constructively interfere. The glancing angle θ, the wavelength , and the "grating constant" d of the crystal are connected by the relation $n\lambda = 2d \sin\theta$, where n is the diffraction order (n = 1 is the first order, n = 2 is the second order, an so on . This equation, so called Bragg's law, describes the condition on θ for constructive interference (Ashcroft et al., 1976).

In our situation with the photon with the radiative corrections we have for two such photons 1 and 2 the two wave function instead of eqs. (44a) and (44b):

$$\psi_1(k,\kappa,x) = e^{i(kx+\alpha_1)} + \int_{4m^2}^{\infty} dM^2 a(M^2) e^{i(\kappa x+\alpha_1)}, \tag{52}$$

$$\psi_2(k,\kappa,x) = e^{i(kx+\alpha_2)} + \int_{4m^2}^{\infty} dM^2 a(M^2) e^{i(\kappa x+\alpha_2)}. \tag{53}$$

Or, in the cosine-form of eq. (50)

$$\varphi_1(\omega,t) = \cos(\omega t + \alpha_1) + \int_{4m^2}^{\infty} dM^2 a(M^2)\cos(\omega t + \alpha_1), \tag{54a}$$

$$\varphi_2(\omega,t) = \cos(\omega t + \alpha_2) + \int_{4m^2}^{\infty} dM^2 a(M^2)\cos(\omega t + \alpha_2). \tag{54b}$$

Or, in the vector form

$$\mathbf{E}_1(\omega,t) = \mathbf{E}_{10}\left(\cos(\omega t + \alpha_1) + \int_{4m^2}^{\infty} dM^2 a(M^2)\cos(\omega t + \alpha_1)\right), \tag{55a}$$

$$\mathbf{E}_2(\omega,t) = \mathbf{E}_{20}\left(\cos(\omega t + \alpha_2) + \int_{4m^2}^{\infty} dM^2 a(M^2)\cos(\omega t + \alpha_2)\right). \tag{55b}$$

The process of the interference is involved in the summation of the two photon wave function, in the Bragg situation. Or, the result is the superposition expressed as

$$\Sigma(\omega,t) = \varphi_1(\omega,t) + \varphi_2(\omega,t). \tag{56}$$

The maximal values of the function Σ is evidently given by the derivation condition $(d/dt)\Sigma(\omega,t) = 0$. So, we see that the radiative corrections, or, so called polarization of vacuum, leads to the very complex wave function of photon and it is easy to see that the maximal constructive interference cannot be expressed by the Brag law $n\lambda = 2d\sin\theta$. Or, in other words, the original Brag law is broken.

7 Discussion

We have used te momentum representation of the propagator of photon expressed by the eq. (41). Let us remark that the coordinate representation of eq. (41) is as it follows:

$$\tilde{D}_+(x-x';M^2) = D_+(x-x') + \int_{4m^2}^{\infty} dM^2 a(M^2)\Delta_+(x-x';M^2), \tag{57}$$

where

$$\Delta_+(x-x';M^2) = i\int d\omega_k e^{ik(x-x')}. \tag{58}$$

is solution of the differential equation

$$\Delta_+(M^2 - \partial^2)\Delta_+(x - x'; M^2) = \delta(x - x'). \tag{59}$$

in the form

$$\Delta_+(x - x'; M^2) = \int \frac{(dp)}{(2\pi)^4} \frac{e^{ip(x-x')}}{p^2 + M^2 - i\varepsilon}. \tag{60}$$

So, we can use also the coordinate representation for the derivation of the photon propagator with the radiative corrections.

The radiative corrections in the form of so called polarization vacuum lead to the very complex wave function of photon and it means that the maximal constructive interference cannot be expressed by the Brag law. Or, the original Brag law must be perfectionized.

Let us remark, that the radiative corrections follow from the quantum electrodynamics and cannot be determined by the classical mathematical procedures of the classical electromagnetism. QED vacuum polarization effects are measurable at the present level of experimental technique. The most elementary situation is that of hydrogen atoms where the strengthened attraction between electron and nucleus depresses the energy values of zero orbital angular momentum states (Schwinger, 1973; 2018).

The vacuum polarization effects applied to the Bragg equation is considered here for the first time and it is not excluded that the application will be the starting point of the new deal of the Brag experimental and theoretical physics.

References

Ashcroft, N. W. and Mermin, N. D. *Solid State Physics* (Harcourt: Orlando, 1976).

Dittrich, W. (1978). Source methods in quantum field theory, Fortschritte der Physik **26**, 289.

Schwinger, J. *Particles and Sources*, (Gordon and Breach Science Publishers, 1969). Schwinger, J. *Particles, Sources and Fields*, Vol. I, (Addison-Wesley, Reading, Mass., 1970). (Or, Published 2018 by CRC Press Taylor & Francis Group 6000 Broken Sound Parkway NW, Suite 300 Boca Raton, FL 33487-2742).

Schwinger, J. *Particles, Sources and Fields* Vol. II, (Addison-Wesley, Reading, Mass., 1973). (Or, Published 2018 by CRC Press Taylor & Francis Group 6000 Broken Sound Parkway NW, Suite 300 Boca Raton, FL 33487-2742).