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Scattering of non-relativistic quantum charge in electromagnetic radiation M. Apostol Department of Theoretical Physics, Institute of Atomic Physics, Magurele-Bucharest MG-6, POBox MG-35, Romania

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We consider a non-relativistic quantum electric charge e and mass m in the electromagnetic radiation described by the vector potential $\mathbf{A} = \mathbf{A}_0 \cos(\omega t - \mathbf{kr})$ (linear polarization), where \mathbf{A}_0 is the amplitude and ω and \mathbf{k} are the radiation frequency and, respectively, the wavevector; t and \mathbf{r} denote the time and, respectively, the position. Since the phase velocity of the non-relativistic charge is much smaller than the speed of light c in vacuum ($\omega = ck$), we may neglect the spatial phase \mathbf{kr} in comparison with the temporal phase ωt ; consequently, the vector potential may be approximated by $\mathbf{A} \simeq \mathbf{A}_0 \cos \omega t$. There exist two forms of the non-relativistic hamiltonian of the charge in radiation; one is the standard non-relativistic hamiltonian

$$H = \frac{1}{2m} (\mathbf{p} - \frac{e}{c} \mathbf{A})^2 + V(\mathbf{r})$$
(1)

and another is the dipole hamiltonian

$$H = \frac{1}{2m}p^2 - e\mathbf{r}\mathbf{E} + V(\mathbf{r}) \quad , \tag{2}$$

where $V(\mathbf{r})$ is a potential which does not depend on the time and $\mathbf{E} = \mathbf{E}_0 \sin \omega t$, $\mathbf{E}_0 = \omega \mathbf{A}_0/c$, is the electric field. These two hamiltonians lead to the same classical equations of motion and are related by a gauge transformation. They differ from each other by the momentum \mathbf{p} , which in equation (1) includes the radiation contribution ($\mathbf{p} = m\mathbf{v} + q\mathbf{A}/c$, where \mathbf{v} is the velocity), while in equation (2) it reduces to the mechanical contribution ($\mathbf{p} = m\mathbf{v}$). This difference generates two distinct scattering processes.

First, we consider the scattering process immersed in radiation; the Schrödinger equation corresponding to the hamiltonian given by equation (1) reads

$$i\hbar\frac{\partial\psi}{\partial t} = \left[H_0 - \frac{e}{mc}\mathbf{A}\mathbf{p} + \frac{e^2}{2mc^2}A^2 + V(\mathbf{r})\right]\psi \quad , \tag{3}$$

where $H_0 = p^2/2m$.¹ For $t \to \infty$ the potential $V(\mathbf{r})$ is vanishing and we set the final "free" wavefunction of the charge in radiation field

$$\psi_f = \frac{1}{\sqrt{V}} e^{-\frac{ie^2 A_0^2}{8\hbar m c^2 \omega} (\sin 2\omega t + 2\omega t) + \frac{ie}{\hbar m c \omega} \mathbf{A}_0 \mathbf{p}_f \sin \omega t} e^{-\frac{i}{\hbar} E_f t + \frac{i}{\hbar} \mathbf{p}_f \mathbf{r}} \quad , \tag{4}$$

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¹If we start with the dipole hamiltonian given by equation (2) we arrive at the Schrodinger equation (3) by the Goeppert-Mayer transform[1] $\tilde{\psi} = e^{-\frac{ier\mathbf{E}_0}{\hbar\omega}\cos\omega t}\psi$, where $\tilde{\psi}$ is the wavefunction of the dipole hamiltonian and ψ is the wavefunction of the standard non-relativistic hamiltonian; this phase factor is immaterial in the subsequent calculations.

where \mathbf{p}_f and $E_f = p_f^2/2m$ are the momentum and, respectively, the energy of the final state and V denotes the normalization volume. The state of the incident particle is the solution

$$\psi_i = \psi_i^0 - \frac{i}{\hbar} e^{-\frac{i}{\hbar}H_0 t} \int_{-\infty}^t dt' V(\mathbf{r}) \psi_i \tag{5}$$

of the Schrodinger equation (3) with interaction with the initial condition

$$\psi_i^0 = \frac{1}{\sqrt{V}} e^{-\frac{ie^2 A_0^2}{8\hbar mc^2 \omega} (\sin 2\omega t + 2\omega t) + \frac{ie}{\hbar mc\omega} \mathbf{A}_0 \mathbf{p}_i \sin \omega t} e^{-\frac{i}{\hbar} E_i t + \frac{i}{\hbar} \mathbf{p}_i \mathbf{r}} \tag{6}$$

for $t \to -\infty$; \mathbf{p}_i and $E_i = p_i^2/2m$ are the initial momentum and, respectively, energy. Making use of the interaction representation we get the transition amplitude

$$a_{fi} = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt(\psi_f, V(\mathbf{r})\psi_i) \quad .$$
(7)

In the Born approximation we may limit ourselves to $\psi_i = \psi_i^0$; we get

$$a_{fi} = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt e^{\frac{ie}{\hbar m c \omega} \mathbf{A}_0 \mathbf{p} \sin \omega t - \frac{i}{\hbar} (E_i - E_f) t} \cdot \frac{1}{V} \int d\mathbf{r} V(\mathbf{r}) e^{\frac{i}{\hbar} \mathbf{p} \mathbf{r}} \quad , \tag{8}$$

where $\mathbf{p} = \mathbf{p}_i - \mathbf{p}_f$ is the transfer momentum (a_{fi} is the matrix element of the S-matrix). Making use of the decomposition

$$e^{iz\sin\varphi} = \sum_{n=-\infty}^{+\infty} J_n(z)e^{in\varphi}$$
(9)

the transition amplitude becomes

$$a_{fi} = -2\pi i \sum_{n=-\infty}^{+\infty} J_n (e\mathbf{A}_0 \mathbf{p}/\hbar m c\omega) \delta(E_f - E_i + n\hbar\omega) \cdot \frac{1}{V} \int d\mathbf{r} V(\mathbf{r}) e^{\frac{i}{\hbar} \mathbf{p} \mathbf{r}}$$
(10)

and the transition probability per unit time

$$w_{fi} = \frac{2\pi}{\hbar} \sum_{n=-\infty}^{+\infty} J_n^2 (e\mathbf{A}_0 \mathbf{p}/\hbar m c\omega) \delta(E_f - E_i + n\hbar\omega) \left| \frac{1}{V} \int d\mathbf{r} V(\mathbf{r}) e^{\frac{i}{\hbar} \mathbf{p} \mathbf{r}} \right|^2 \tag{11}$$

(by replacing $\delta^2(E_f - E_i + n\hbar\omega)$ by $(t/2\pi\hbar)\delta(E_f - E_i + n\hbar\omega)$, where t is the duration of the process). The differential cross-section $d\sigma$ is obtained by dividing $w_{fi}d\nu_f$, where $d\nu_f = d\mathbf{p}_f V/(2\pi\hbar)^3$ is the number of final states, to the incident current density $v_i |\psi_i^0|^2 = v_i/V$, where $\mathbf{v}_i = \mathbf{p}_i/m$ is the velocity of the incident particle; for the n-photon exchange process we get

$$d\sigma = \frac{2\pi}{\hbar v_i} J_n^2 (e\mathbf{A}_0 \mathbf{p}/\hbar m c\omega) \delta(E_f - E_i + n\hbar\omega) \left| \int d\mathbf{r} V(\mathbf{r}) e^{\frac{i}{\hbar} \mathbf{p} \mathbf{r}} \right|^2 \frac{d^3 \mathbf{p}_f}{(2\pi\hbar)^3} \tag{12}$$

and, after integration with respect to p_f ,

$$d\sigma = \frac{p_f}{p_i} J_n^2 (e\mathbf{A}_0 \mathbf{p}/\hbar m c\omega) d\sigma_B \quad , \tag{13}$$

where

$$d\sigma_B = \left| \frac{m}{2\pi\hbar^2} \int d\mathbf{r} V(\mathbf{r}) e^{\frac{i}{\hbar}\mathbf{p}\mathbf{r}} \right|^2 d\Omega$$
(14)

is the Born cross-section; $d\Omega = 4\pi \sin \theta d\theta$ is the solid angle and θ is the scattering angle. Equation (13) is known as the Kroll-Watson formula.[1, 2] We note that the cross-section includes both emission (n > 0) and absoption (n < 0) of photons. The squared Bessel function $J_n^2(x)$ has a maximum for $x \simeq n$ (Debye approximation[4, 5]); i.e. for

$$\theta^2 \simeq n \frac{\hbar\omega}{E_i} \left(\frac{2mcE_i}{e\mathbf{A}_0 \mathbf{p}_i} - 1 \right) \tag{15}$$

(for small angles θ).

In the scattering experiments with focused laser beams the radiation is confined to a region Fand the asymptotic scattering states correspond to particles free of radiation. Therefore, in this case it is convenient to start with the dipole hamiltonian given by equation (2); the final state is described by the wavefunction

$$\psi_f = \frac{1}{\sqrt{V}} e^{-\frac{i}{\hbar}E_f t + \frac{i}{\hbar}\mathbf{p}_f \mathbf{r}} \tag{16}$$

and the state of the incident particle is described by the wavefunction given by

$$\psi_{i} = \psi_{i}^{0} - \frac{i}{\hbar} e^{-\frac{i}{\hbar}H_{0}t} \int_{-\infty}^{t} dt' \left[-e\mathbf{r}\mathbf{E}_{0}\sin\omega t' + V(\mathbf{r}) \right] \psi_{i} \quad , \tag{17}$$

where

$$\psi_i^0 = \frac{1}{\sqrt{V}} e^{-\frac{i}{\hbar}E_i t + \frac{i}{\hbar}\mathbf{p}_i \mathbf{r}} ; \qquad (18)$$

the transition amplitude reads

$$a_{fi} = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \left[-e \sin \omega t(\psi_f, \mathbf{r} \mathbf{E}_0 \psi_i) + (\psi_f, V(\mathbf{r}) \psi_i) \right] \quad . \tag{19}$$

We limit ourselves to the Born approximation, which, for the radiation term is valid provided $edE_0/(\hbar^2/md^2) \ll 1$, where d is the dimension of the region where the radiation is confined to; the cross-section is given by

$$d\sigma = \frac{p_f}{2p_i} \left| \frac{me}{2\pi\hbar^2} \int d\mathbf{r} \cdot \mathbf{r} \mathbf{E}_0 e^{\frac{i}{\hbar}\mathbf{p}\mathbf{r}} \right|^2 d\Omega + d\sigma_B \quad , \tag{20}$$

where p_f is given by $p_f^2/2m = p_i^2/2m \pm \hbar\omega$; we can see that the first term in equation (20) gives the cross-section of the scattering with emission or absorption of one photon; higher-orders of the Born approximation give cross-sections with emission or absorption of multiple photons. For a large integration volume in equation (20) the cross-section has a maximum for $\cos \theta = p_i/p_f$, *i.e.* $\theta \simeq \pm \sqrt{n\hbar\omega/E_i}$, where *n* is the number of absorbed or emitted photons.

It is worth noting a comment upon the S-matrix related to the potential $U = -e\mathbf{r}\mathbf{E}_0 \sin \omega t$; the S-matrix is

$$a_{fi} = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt(\chi_f, e^{\frac{i}{\hbar}H_0 t} U e^{-\frac{i}{\hbar}H_0 t} \chi_i) = \frac{ie}{\hbar} \int_{-\infty}^{+\infty} dt \sin \omega t(\chi_f, e^{\frac{i}{\hbar}H_0 t} \mathbf{r} \mathbf{E}_0 e^{-\frac{i}{\hbar}H_0 t} \chi_i) \quad , \qquad (21)$$

where $\chi_f = e^{\frac{i}{\hbar} \mathbf{p}_f \mathbf{r}}$ and χ_i is the incoming wavefunction depending only on time; in the Born approximation $\chi_i = e^{\frac{i}{\hbar} \mathbf{p}_i \mathbf{r}}$. The scalar product can be computed in two ways; one by applying the operator $e^{-\frac{i}{\hbar}H_0 t}$ to the wavefunctions $\chi_{i,f}$,

$$(\chi_f, e^{\frac{i}{\hbar}H_0 t} \mathbf{r} \mathbf{E}_0 e^{-\frac{i}{\hbar}H_0 t} \chi_i) = e^{\frac{i}{\hbar}(E_f - E_i)t} (\chi_f, \mathbf{r} \mathbf{E}_0 \chi_i) \quad , \tag{22}$$

another by using

$$e^{\frac{i}{\hbar}H_0t}\mathbf{r}\mathbf{E}_0e^{-\frac{i}{\hbar}H_0t} = \mathbf{r}\mathbf{E}_0 + \frac{t}{m}\mathbf{p}\mathbf{E}_0 \quad ; \tag{23}$$

this second way leads to

$$(\chi_f, e^{\frac{i}{\hbar}H_0 t} \mathbf{r} \mathbf{E}_0 e^{-\frac{i}{\hbar}H_0 t} \chi_i) = (\chi_f, \mathbf{r} \mathbf{E}_0 \chi_i) + \frac{t}{m} (\chi_f, \mathbf{p} \mathbf{E}_0 \chi_i) \quad ,$$
(24)

which, in the Born approximation gives

$$\left(\chi_f, e^{\frac{i}{\hbar}H_0 t} \mathbf{r} \mathbf{E}_0 e^{-\frac{i}{\hbar}H_0 t} \chi_i\right) = \left(\chi_f, \mathbf{r} \mathbf{E}_0 \chi_i\right) \ . \tag{25}$$

Equation (22) gives a transition amplitude

$$a_{fi} = \frac{ie}{\hbar} \int_{-\infty}^{+\infty} dt \sin \omega t e^{\frac{i}{\hbar} (E_f - E_i) t} (\chi_f, \mathbf{r} \mathbf{E}_0 \chi_i) \quad , \tag{26}$$

while equation (25) gives a vanishing transition amplitude

$$a_{fi} = \frac{ie}{\hbar} \int_{-\infty}^{+\infty} dt \sin \omega t(\chi_f, \mathbf{r} \mathbf{E}_0 \chi_i) = 0 \quad .$$
⁽²⁷⁾

For $\chi_i = e^{\frac{i}{\hbar} \mathbf{p}_i \mathbf{r}}$ and an infinite **r**-domain of integration equation (26) produces a derivative of a delta function with the final result zero, as in equation (27). For a finite range of **r**-integration, the results given by equations (26) and (27) differ. However, for a finite range of **r**-integration the potential U should be continuously and differentiably continued outside the integration domain (in particular for ensuring the self-adjointness of the operators), which makes equation (23) invalid and, consequently, equation (25) too. In particular, we can see that the behaviour of the potential U at the border of its definition domain is important for the scattering amplitude. Consequently, the first procedure given by equation (22), is the correct one for computing the scattering amplitude (for a finite domain of **r**-integration).

If $edE_0/(\hbar^2/md^2) > 1$ the Born approximation is not valid anymore, though the quantummechanical behaviour of the particle may be preserved in the scattering region, even for high incident energies. The transition amplitude is

$$a_{fi} = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt (\psi_f, (U+V)\psi_i) \quad , \tag{28}$$

where

$$\psi_f = \frac{1}{\sqrt{V}} e^{-\frac{i}{\hbar} E_f t + \frac{i}{\hbar} \mathbf{p}_f \mathbf{r}}$$
(29)

and ψ_i is the solution of the Schrodinger equation

$$i\hbar \frac{\partial \psi_i}{\partial t} = (H_0 + U + V)\psi_i , \ U = -e\mathbf{r}\mathbf{E}_0\sin\omega t$$
 (30)

with the initial condition

$$\psi_i^0 = \frac{1}{\sqrt{V}} e^{-\frac{i}{\hbar}E_i t + \frac{i}{\hbar}\mathbf{p}_i \mathbf{r}} \ . \tag{31}$$

The interaction U can be removed from the hamiltonian by using the Goeppert-Mayer transform

$$\psi_i = e^{-\frac{i}{\hbar} \int_{-\infty}^t dt' U(t')} \phi_i = e^{-\frac{ie}{\hbar\omega} \mathbf{r} \mathbf{E}_0 \cos \omega t} \phi_i \quad , \tag{32}$$

where the wavefunction ϕ_i satisfies the Schrödinger equation

$$i\hbar \frac{\partial \phi_i}{\partial t} = \left[\frac{1}{2m} (\mathbf{p} - \frac{e}{c} \mathbf{A})^2 + V\right] \phi_i \quad ; \tag{33}$$

The momentum **p** in equation (33) includes the radiation contribution ($\mathbf{p} = m\mathbf{v}_i + e\mathbf{A}/c$); for an energetic particle $mv_i \gg eA/c$, or $E_i \gg e^2 A^2/2mc^2$; in addition we should have also $2mc^2 \gg E_i$ (non-relativistic particles); in these conditions, we may neglect the contribution of the radiation terms in equation (33); in addition we restrict ourselves to the first-order contribution in powers of the potential V, such that we may use the approximation $\phi_i \simeq \psi_i^0$. The transition amplitude given by equation (28) becomes

$$a_{fi} = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt e^{\frac{i}{\hbar}(E_f - E_i)t} \cdot \frac{1}{V} \int d\mathbf{r} e^{\frac{i}{\hbar}\mathbf{pr}} (U + V) e^{-\frac{i}{\hbar} \int_{-\infty}^{t} dt' U(t')} =$$

$$= \int_{-\infty}^{+\infty} dt e^{\frac{i}{\hbar}(E_f - E_i)t} \cdot \frac{1}{V} \int d\mathbf{r} e^{\frac{i}{\hbar}\mathbf{pr}} \frac{\partial}{\partial t} e^{-\frac{ie}{\hbar\omega}\mathbf{r}\mathbf{E}_0 \cos\omega t} +$$

$$-\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt e^{\frac{i}{\hbar}(E_f - E_i)t} \cdot \frac{1}{V} \int d\mathbf{r} e^{\frac{i}{\hbar}\mathbf{pr}} V e^{-\frac{ie}{\hbar\omega}\mathbf{r}\mathbf{E}_0 \cos\omega t} ;$$
(34)

at this point we use the decomposition

$$e^{iz\cos\varphi} = \sum_{n=-\infty}^{+\infty} i^n J_n(z) e^{in\varphi}$$
(35)

and get

$$a_{fi} = -2\pi \sum_{n=-\infty}^{+\infty} (-i)^{n+1} \delta(E_f - E_i + n\hbar\omega) \cdot \frac{1}{V} \left[n\hbar\omega \int d\mathbf{r} e^{\frac{i}{\hbar}\mathbf{pr}} J_n(e\mathbf{r}\mathbf{E}_0/\hbar\omega) - \int d\mathbf{r} e^{\frac{i}{\hbar}\mathbf{pr}} V(\mathbf{r}) J_n(e\mathbf{r}\mathbf{E}_0/\hbar\omega) \right]$$
(36)

the cross-section is

$$d\sigma = \sum_{n=-\infty}^{+\infty} \frac{p_f}{p_i} \left(\frac{m}{2\pi\hbar^2}\right)^2 \left[n\hbar\omega \int d\mathbf{r} e^{\frac{i}{\hbar}\mathbf{pr}} J_n(e\mathbf{r}\mathbf{E}_0/\hbar\omega) - \int d\mathbf{r} e^{\frac{i}{\hbar}\mathbf{pr}} V(\mathbf{r}) J_n(e\mathbf{r}\mathbf{E}_0/\hbar\omega)\right]^2 d\Omega \quad , \quad (37)$$

where for each n the final momentum is given by $p_f^2/2m = p_i^2/2m - n\hbar\omega$. We can see in equation (37) the multiple-photon scattering by the radiation field (first term in the bracket), the modification of the Born scattering cross-section for the potential $V(\mathbf{r})$ due to the presence of the radiation and interference terms between radiation and potential scattering.

The argument of the Bessel functions in equation (37) varies rapidly over the domain of integration; consequently, we may use the asymptotic behaviour of the Bessel functions for large values of the argument. It is easy to see that the main contribution comes from $\mathbf{p} = \pm e\mathbf{E}_0/\omega$, *i.e.* $p_i - p_f \cos \theta = \pm eE_0 \cos \alpha/\omega$, where α is the angle between \mathbf{p}_i and \mathbf{E}_0 . It is convenient to introduce the parameter $\xi = eE_0/\omega p_i = eA_0/cp_i \ll 1$; we get $1 - (p_f/p_i) \cos \theta = \pm \xi \cos \alpha$ and, from the energy conservation, $p_f = p_i(1 - n\hbar\omega/2E_i)$; it follows that the cross-section has maxima for $\theta_n^2 \simeq \pm 2\xi \cos \alpha - n\hbar\omega/E_i > 0$. The order of magnitude of the **r**-integrals in equation (37) is $\simeq \sqrt{\hbar\omega d^5/eE_0}$. We can see that in the limit $\xi \to 0$, when the particle is quasi-classical, the maxima occur at $\theta_n = \pm \sqrt{n\hbar\omega/E_i}$, which is the diffraction result (the magnitudes of the cross-section differ).[6]

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