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Quantum theory of Thomson scattering

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ABSTRACT

The general theory of the scattering of electromagnetic radiation in atomic plasmas and metals, in the non-relativistic regime, in which account is taken of the Kramers–Heisenberg polarization terms in the Hamiltonian, is described from a quantum mechanical viewpoint. As well as deriving the general formula for the double differential Thomson scattering cross section in an isotropic finite temperature multi-component system, this work also considers closely related phenomena such as absorption, refraction, Raman scattering, resonant (Rayleigh) scattering and Bragg scattering, and derives many essential relationships between these quantities. In particular, the work introduces the concept of scattering strength and the strength-density field which replaces the normal particle density field in the standard treatment of scattering by a collection of similar particles and it is the decomposition of the strength-density correlation function into more familiar-looking components that leads to the final result. Comparisons are made with previous work, in particular that of Chihara [1].

1. Introduction

Thomson scattering is the scattering of electromagnetic radiation by electrons in matter, in the non-relativistic or near-relativistic regime. Two key features of Thomson scattering are that it is sensitive to correlations between electrons and that the polarization of the scattered radiation is entirely determined by the initial polarization and the scattering geometry. This is unlike Compton scattering, which is incoherent scattering by individual electrons and which contains a polarization-independent contribution. Nevertheless Compton and Thomson scattering are descriptions of the same phenomenon to the extent that incoherent Thomson scattering and Compton scattering are interchangeable descriptions of scattering by effectively free and uncorrelated non-relativistic electrons. In matter, electrons are correlated via their mutual interactions, collective motions, exchange and degeneracy, and interactions with other particles (ions). These correlations are directly probed by X-ray Thomson scattering (XRTS) measurements, making the technique an important emerging diagnostic tool for studying the equation-of-state properties of cold and warm dense matter [2–8]. Understanding these correlation effects allows quantities such as temperature and density to be deduced directly from measurements. A baseline description of Thomson scattering from ideal plasmas is provided by the Random Phase Approximation (RPA) which ignores short-range correlations between electrons, with only large-scale collective motion taken into account. For dense plasmas and plasmas in which bound electrons contribute to the scattering, a more general treatment is required both to provide more accurate modelling and to be able to extract meaningful information from scattering measurements.

Coherent X-ray Thomson back-scattering is also a potentially useful spectroscopic tool for carrying out material assays as the cross-sections depend strongly on atomic spectra as well as being amplified by an underlying proportionality of the cross-sections to the square of the number of bound electrons.

This report presents a quantum mechanical derivation of the general Thomson differential scattering cross-section for scattering of electromagnetic radiation in a fully or partially ionised plasma comprising one or more nuclear species. The work generalizes the work of Chihara [1] who applies a fundamentally classical approach to a two component system comprising electrons and ions. While the current method and the results yielded have clear parallels to the earlier work, they provide a different perspective while incorporating a proper quantal treatment of the electrons as well as a more consistent treatment of the polarization terms in the interaction. A second-quantized approach is used to treat the electrons thus including the effects of antisymmetry and the Pauli principle from the outset. However a classical approach is maintained for the nuclear ions, as is justified by their large masses and extremely

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short deBroglie wavelengths. The new work is generally important for extending existing detailed methodologies for treating Thomson scattering by warm dense matter, e.g. Ref. [9], to heavier elements.

This work also generalizes our previous work [10] which introduces, in the context of a simplified form of the Hamiltonian, the basic quantum mechanical approach employed here.

At a fundamental level, the scattering process is represented by the non-relativistic Hamiltonian

$$\mathbf{H} = \frac{1}{2m_e}(\mathbf{p} - e\mathbf{A})^2 + \mathbf{H}_{\text{field}} + \ldots = \mathbf{H}_0 + \mathbf{H}' + \mathbf{H}_{\text{field}} \tag{1}$$

where m_e, e and $\mathbf{p}$ are respectively the mass, charge and canonical momentum of the electron, $\mathbf{A}$ is the electromagnetic vector potential of the incident (probe) radiation and $\mathbf{H}_{\text{field}}$ is the Hamiltonian for the *in vacuo* electromagnetic field, which comprises the probe radiation and any ambient radiation field. The electron interacts with the field through the perturbation,

$$\mathbf{H}' = \frac{e}{m_e}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}) + \frac{e^2}{2m_e}\mathbf{A}^2 \tag{2}$$

which comprises two terms, the first of which is the Kramers–Heisenberg (KH) polarization, which represents absorption and emission of photons by the electron, while the second is the quiver energy. The quiver motion gives rise to point scattering in the first order (Born) approximation and tends to dominate the scattering of high energy photons in the non-relativistic regime, while the KH part gives rise to scattering only in second order via transition operators of the form $\mathbf{A}\cdot\mathbf{p}\,\mathbf{G}\,\mathbf{A}\cdot\mathbf{p}$ in which the propagator $\mathbf{G}$ represents an intermediate virtual state of the electron. Although the two scattering processes occur in different orders of perturbation theory, they are of the same order in the electromagnetic coupling constant and therefore must be considered together. It is noteworthy that the $\mathbf{A}^2$ term does not arise in the linearized Dirac Hamiltonian and so is not treated as a separate term in a fully relativistic QED theory of Compton scattering. The fully relativistic formulations of the theory are discussed elsewhere [10–12].

For transverse waves, $[\mathbf{p},\mathbf{A}]=\mathbf{p}\cdot\mathbf{A} - \mathbf{A}\cdot\mathbf{p} = 0$ and a second-quantized representation of the electromagnetic field experienced by an electron at position $\mathbf{r}$, in terms of photon (boson) creation and annihilation field operators, $\mathbf{b}_{\mathbf{k},\mathbf{e}}$, $\mathbf{b}^\dagger_{\mathbf{k},\mathbf{e}}$, is represented in terms of the Hermitian operator $\mathbf{A} = \tilde{\mathbf{A}} + \tilde{\mathbf{A}}^\dagger$ where [10]

$$\tilde{\mathbf{A}}(\mathbf{r}) = \sum_{\mathbf{k},\mathbf{e}} \frac{-\mathrm{i}}{\sqrt{2V\varepsilon_0\omega}}\mathbf{e}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\mathbf{b}_{\mathbf{k},\mathbf{e}},\quad \tilde{\mathbf{A}}^\dagger(\mathbf{r}) = \sum_{\mathbf{k},\mathbf{e}} \frac{\mathrm{i}}{\sqrt{2V\varepsilon_0\omega}}\mathbf{e}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\mathbf{b}^\dagger_{\mathbf{k},\mathbf{e}} \tag{3}$$

where $\mathbf{k}$ and $\mathbf{e}$ are respectively the wavenumber and direction of polarization ($\mathbf{e}\cdot\mathbf{e} = 1, \mathbf{e}\cdot\mathbf{k} = 0$) of the photon modes present, $\omega = k\,c$ is the frequency, V is the volume and ε_0 is the permittivity of free space. The operators $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{A}}^\dagger$ therefore represent the absorption and emission of a photon respectively while the terms in the transition operator representing scattering are those involving the operator pairs $\tilde{\mathbf{A}}^\dagger, \tilde{\mathbf{A}}$, in either order.

2. Scattering by a single electron: the Kramers, Heisenberg, Waller formula

In lowest-order perturbation theory, without making any other approximations, the above yields the differential cross-section for the angular distribution of scattering of photons, from the channel $\mathbf{e},\mathbf{k}$ into the channel $\mathbf{e}',\mathbf{k}'$, by a single electron initially in the state β, according to the formula

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega'} = r_e^2 \sum_\alpha \left(\frac{\omega'}{\omega}\right)^2 \left|\langle\alpha|\mathbf{F}(\mathbf{e},\mathbf{k},z;\mathbf{e}',\mathbf{k}',z';E_\beta)|\beta\rangle\right|^2 (1 + n_{\mathbf{k}'} - \delta_{\mathbf{k}\mathbf{k}'}) \tag{4}$$

where $r_e = e^2/4\pi\,\varepsilon_0 m_e c^2$ is the *classical electron radius*,

$$\begin{aligned} z &= \omega + \mathrm{i}0^+ \\ z' &= \omega' + \mathrm{i}0^+ \\ E_\beta + \omega &= E_\alpha + \omega' \end{aligned} \tag{5}$$

$$\begin{aligned} \mathbf{F}(\mathbf{e},\mathbf{k};\mathbf{e}',\mathbf{k}',z,z';E) = -\frac{1}{m_e}\Big(&\mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{r}}\mathbf{e}'\cdot\mathbf{p}G(E+z)\mathbf{e}\cdot\mathbf{p}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \\ &+\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\mathbf{e}\cdot\mathbf{p}G(E-z')\mathbf{e}'\cdot\mathbf{p}\mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{r}}\Big) \\ &-\mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{r}}\mathbf{e}'\cdot\mathbf{e}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \end{aligned} \tag{6}$$

$$\mathbf{G}(E) = (E - \mathbf{H}_0)^{-1} \tag{7}$$

α denotes an electron state in the final channel, and the factor $(1 + n_{\mathbf{k}'} - \delta_{\mathbf{k}\mathbf{k}'})$ accounts for the effect of *stimulated scattering* in the presence of $n_{\mathbf{k}'} - \delta_{\mathbf{k}\mathbf{k}'}$ spectator photons in the exit channel. Eqs. (4)–(7) constitute the Kramers, Heisenberg, Waller formula [11].

3. Scattering from a many-electron system

3.1. Effective photon scattering operator

Our previous work [10] describes a general quantum-mechanical treatment of Thomson scattering, but considers only the $\mathbf{A}^2$ term in the Hamiltonian, which corresponds to the right-most term on the right-hand side of Eq. (6). In the present work, we generalize this to include the remaining polarization term in the case of a system of electrons that is initially isotropic and unpolarized. In order to simplify the ensuing formalism, it is convenient to carry out the average over the directions of the electron motions at this stage. The scattering depends on the average of an expression like $|a(\mathbf{e}'\cdot\mathbf{p})(\mathbf{e}\cdot\mathbf{p}) + b(\mathbf{e}'\cdot\mathbf{e})|^2$, where a and b are constant coefficients, over the direction of the vector $\mathbf{p}$. Expanding and applying the average yields

$$\begin{aligned} \overline{|a(\mathbf{e}'\cdot\mathbf{p})(\mathbf{e}\cdot\mathbf{p}) + b(\mathbf{e}'\cdot\mathbf{e})|^2} = {}& |a|^2\overline{(\mathbf{e}'\cdot\mathbf{p})^2(\mathbf{e}\cdot\mathbf{p})^2} \\ &+ (a^*b + b^*a)(\mathbf{e}'\cdot\mathbf{e})\overline{(\mathbf{e}'\cdot\mathbf{p})(\mathbf{e}\cdot\mathbf{p})} \\ &+ |b|^2(\mathbf{e}'\cdot\mathbf{e})^2 \end{aligned} \tag{8}$$

where the average is defined as $\overline{X(\mathbf{p})} = (4\pi)^{-1}\int X(\mathbf{p})\mathrm{d}\Omega_{\mathbf{p}}$.

and

$$\begin{aligned} \overline{(\mathbf{e}'\cdot\mathbf{p})(\mathbf{e}\cdot\mathbf{p})} &= \frac{1}{3}\mathbf{p}^2(\mathbf{e}'\cdot\mathbf{e}) \\ \overline{(\mathbf{e}'\cdot\mathbf{p})^2(\mathbf{e}\cdot\mathbf{p})^2} &= \frac{1}{9}\mathbf{p}^4(\mathbf{e}'\cdot\mathbf{e})^2 \end{aligned} \tag{9}$$

Hence

$$\begin{aligned} \overline{|a(\mathbf{e}'\cdot\mathbf{p})(\mathbf{e}\cdot\mathbf{p}) + b(\mathbf{e}'\cdot\mathbf{e})|^2} &= \left(\frac{1}{9}|a|^2\mathbf{p}^4 + \frac{1}{3}(a^*b + b^*a)\mathbf{p}^2 + |b|^2\right) \\ &\quad\times(\mathbf{e}'\cdot\mathbf{e})^2 \\ &= \left|\frac{1}{3}a\mathbf{p}^2 + b\right|^2(\mathbf{e}'\cdot\mathbf{e})^2 \\ &= |ap_\sigma p_\sigma + b|^2(\mathbf{e}'\cdot\mathbf{e})^2 \end{aligned} \tag{10}$$