X-ray scattering by many-particle systems

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\textbf{Abstract.} This paper reviews the treatment of high-frequency Thomson scattering in the non-relativistic and near-relativistic regimes with the primary purpose of understanding the nature of the frequency redistribution correction to the differential cross-section. This correction is generally represented by a factor involving the ratio $\omega_\alpha/\omega_\beta$ of the scattered ($\alpha$) to primary ($\beta$) frequencies of the radiation. In some formulae given in the literature, the ratio appears squared, in others it does not. In Compton scattering, the frequency change is generally understood to be due to the recoil of the particle as a result of energy and momentum conservation in the photon–electron system. In this case, the Klein–Nishina formula gives the redistribution factor as $(\omega_\alpha/\omega_\beta)^2$. In the case of scattering by a many-particle system, however, the frequency and momentum changes are no longer directly interdependent but depend also upon the properties of the medium, which are encoded in the dynamic structure factor. We show that the redistribution factor explicit in the quantum cross-section (that seen by a photon) is $\omega_\alpha/\omega_\beta$, which is not squared. Formulae for the many-body cross-section given in the literature, in which the factor is squared, can often be attributed to a different (classical) definition of the cross-section, though not all authors are explicit about which definition they are using. What is shown not to be true is that the structure factor simply gives the ratio of the many-electron to one-electron differential cross-sections, as is sometimes supposed. Mixing up the cross-section definitions can lead to errors when describing x-ray scattering. We illustrate the nature of the discrepancy by deriving the energy-integrated angular

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distributions, with first-order relativistic corrections, for classical and quantum scattering measurements, as well as the radiative opacity for photon diffusion in a Thomson-scattering medium, which is generally considered to be governed by quantum processes.

Contents

1. Introduction 2
2. Photon scattering—the quantum cross-section 3
   2.1. Low-energy Compton scattering 3
   2.2. Thomson scattering by a system of many electrons 4
   2.3. Thomson scattering by individual electrons 7
   2.4. Photon angular distribution for scattering by a many-electron system 9
3. Scattering of energy—the classical cross-section 11
4. Radiation transport—the Rosseland scattering opacity 13
   4.1. The Rosseland scattering opacity 13
5. Conclusions 15
Acknowledgments 15
Appendix. Scattering theory 16
References 22

1. Introduction

The scattering of electromagnetic radiation in complex many-electron systems is of great interest both for understanding and modelling the transport of high frequency radiation in plasmas [1–6] and as a diagnostic tool for probing states of matter [7–11]. In this paper, we address, in some detail, the formal derivation of the general formulae for the scattering of high frequency x-ray photons by non-relativistic electrons. We show that generalizing from the single-particle formula to the many-body formula, is not straightforward and can readily lead to an incorrect result. In the following, we derive the general formula for the many-body Thomson cross-section from first principles and then deduce the one particle cross-section deduced from it. In this way it is possible to gain an understanding of the cause(s) of the apparent discrepancies in the literature.

The regime considered is one in which the frequency of the scattered radiation is well above the (electron) plasma frequency, \( \Omega_e \), and the electron motions are non-relativistic both before and after scattering. For scattering from systems in near-thermodynamic-equilibrium, the prevailing assumptions are therefore that

\[
\Omega_e \ll \omega \ll mc^2, \\
T_e \ll mc^2,
\]

where \( \omega \) is the frequency of the radiation, \( m \) is the mass of an electron, \( c \) is the velocity of light and \( T_e \) is the electron temperature, and where units used are such that \( k_B = 1, \hbar = 1 \). The theory presented, in which first-order relativistic terms are retained, would be expected to be applicable, for example, to scattering of x-rays in the energy range 0.1–50 keV in matter at solid densities and below and temperatures \( \lesssim 10 \text{ keV} \).
While the electrons are assumed to remain non-relativistic, the Compton recoil is generally not negligible being readily measurable and of importance in respect of the residual effects on the scatterer for which the recoil energy can be very significant, as well as the coherence and interference between temporally and spatially separated scattering events. It is important to bear in mind that the energy scales for the probe radiation (keV) and the scatterer system may be quite different, making it necessary to keep track of (at least) first-order recoil corrections. The underlying process is therefore Compton scattering by electrons, but in the non-relativistic regime. However, the interactions between the component particles of the scatterer system can mean that the recoil is taken up, not by a single electron, but by many particles, such as whole atoms (Rayleigh scattering) or even whole crystals (Bragg scattering, Mossbauer effect). In these regimes, the distinction between Compton and Thomson scattering is somewhat blurred. Nowadays, the term Thomson scattering is commonly used to describe scattering of electromagnetic radiation in the non-relativistic limit when many-body correlations between the particles in the scatterer play a significant role, while Compton scattering is generally reserved for a fully relativistic description of incoherent scattering by individual uncorrelated electrons. Another feature of Thomson scattering is that the polarization of the scattered radiation is completely determined by the polarization of the primary radiation and the scattering geometry while Compton scattering features an unpolarized component in the relativistic regime. According to these definitions, the treatment that follows is of Thomson scattering.

2. Photon scattering—the quantum cross-section

2.1. Low-energy Compton scattering

The Klein–Nishina differential cross-section \(d\sigma_\beta/d\Omega_\alpha\) for the Compton scattering of a photon into the solid angle element \(d\Omega_\alpha\) by an electron that is initially at rest is \([12, 13]\)

\[
\frac{d\sigma_\beta}{d\Omega_\alpha} = \frac{1}{4} r_e^2 \left(\frac{\omega_\alpha}{\omega_\beta}\right)^2 \left(\frac{\omega_\alpha}{\omega_\beta} + \frac{\omega_\beta}{\omega_\alpha} - 2 + 4 (e_\alpha \cdot e_\beta)^2\right),
\]

in which \(\alpha\) and \(\beta\) denote the final and initial photon states respectively; \(e_\alpha, e_\beta\) is the photon polarization unit vector, which, for transverse waves, is orthogonal to the photon wavevector, \(k_\alpha, k_\beta\); \(\omega_\alpha, \omega_\beta\) is the photon frequency and \(r_e = e^2/4\pi\epsilon_0mc^2\) is the classical electron radius; and where \(\omega_\alpha\) and \(\omega_\beta\) are related by the Compton condition

\[
\omega_\beta - \omega_\alpha = \frac{\omega_\alpha \omega_\beta}{mc^2} (1 - \mu),
\]

where \(m\) is the electron mass and \(\mu\) is the cosine of the scattering angle. Combining (2) and (3) yields the Klein–Nishina equation in the form

\[
\frac{d\sigma_\beta}{d\Omega_\alpha} = r_e^2 \left(\frac{\omega_\alpha}{\omega_\beta}\right)^2 \left((e_\alpha \cdot e_\beta)^2 + \frac{\omega_\alpha \omega_\beta}{(2mc^2)^2} (1 - \mu)^2\right).
\]

At low photon energies, that is when \(\omega_\alpha, \omega_\beta \ll mc^2\), this can be approximated by

\[
\frac{d\sigma_\beta}{d\Omega_\alpha} \simeq r_e^2 \left(\frac{\omega_\alpha}{\omega_\beta}\right)^2 (e_\alpha \cdot e_\beta)^2 \equiv \left.\frac{d\sigma_\beta}{d\Omega_\alpha}\right|_T,
\]

in which \(\left.\frac{d\sigma_\beta}{d\Omega_\alpha}\right|_T\) is the quantum Thomson one-electron cross-section as we define it here. Note that only terms of second and higher order in \(\omega/mc^2\) have been neglected. By quantum, we mean...
that it is the cross-section seen by a quantum of the radiation field, i.e. a photon. Equation (5), in which \( \omega_e \) is given by the Compton condition (3), provides a reasonably accurate description of Compton-scattering into all angles at sub ~50 keV photon energies, and at considerably higher energies in the case of small angle scattering.

The approximation (5) picks out only the polarization-dependent component of the cross-section, which then vanishes if \( \mathbf{e}_\alpha \cdot \mathbf{e}_\beta = 0 \). Since \( \hat{\mathbf{k}}_\alpha \cdot \mathbf{e}_\alpha = \mathbf{k}_\beta \cdot \mathbf{e}_\beta = 0 \), it follows that \( \mathbf{e}_\alpha \cdot \mathbf{e}_\beta \neq 0 \) only if \( \mathbf{e}_\beta \times \hat{\mathbf{k}}_\alpha \neq \mathbf{0} \) and \( (\mathbf{e}_\alpha \times \mathbf{e}_\beta) \cdot \hat{\mathbf{k}}_\alpha = 0 \), which are the classical non-relativistic selection rules, and which are applicable to the polarized scattering component in the relativistic regime. These relations are sufficient to determine the outgoing polarization

\[
\mathbf{e}_\alpha = \frac{\hat{\mathbf{k}}_\alpha \times (\mathbf{e}_\beta \times \hat{\mathbf{k}}_\alpha)}{|\hat{\mathbf{k}}_\alpha \times (\mathbf{e}_\beta \times \hat{\mathbf{k}}_\alpha)|} = \frac{\mathbf{e}_\beta - \hat{\mathbf{k}}_\alpha (\mathbf{e}_\beta \cdot \hat{\mathbf{k}}_\alpha)}{\sqrt{1 - (\mathbf{e}_\beta \cdot \hat{\mathbf{k}}_\alpha)^2}}.
\]

(6)

If the scattering angle is \( \theta \), and \( \phi \) is the angle between the initial plane of polarization and the scattering plane, then

\[
(\hat{\mathbf{k}}_\alpha \times \hat{\mathbf{k}}_\beta) \cdot (\mathbf{e}_\beta \times \hat{\mathbf{k}}_\beta) \equiv \mathbf{e}_\beta \cdot \hat{\mathbf{k}}_\alpha = \cos \phi \sin \theta
\]

and hence

\[
(\mathbf{e}_\alpha \cdot \mathbf{e}_\beta)^2 = 1 - (\mathbf{e}_\beta \cdot \hat{\mathbf{k}}_\alpha)^2 = 1 - \cos^2 \phi \sin^2 \theta,
\]

(8)

which is the Thomson scattering angular distribution, and in terms of which \( d\Omega_\alpha = \sin \theta d\theta d\phi \).

One might naïvely generalize this formula to a system containing \( N_e \) electrons according to \( \partial^2 \sigma / \partial \omega_d \partial \omega_a \approx N_e S^2 (\omega_a / \omega_\beta)^3 (\mathbf{e}_\alpha \cdot \mathbf{e}_\beta)^2 S(\mathbf{k}_\alpha - \mathbf{k}_\beta, \omega_a - \omega_\beta) \), where \( S(q, \omega) \) is the Van Hove dynamic structure factor, which encodes the correlations between the electrons, and \( \mathbf{k} \) denotes the photon wavevector. However, despite formulae apparently supporting this generalization appearing in the literature e.g. [9], this would be wrong. In the following, we resolve the issue of differing powers of \( \omega_a / \omega_\beta \) appearing in various published cross-section formulae, which although largely attributable to differing definitions of the cross-section, can sometimes be due to, or result in, misunderstanding.

At this stage it is worth remarking that equation (2) applies specifically to Dirac particles. In the case of Compton scattering by a Klein–Gordon particle (meson) initially at rest, the corresponding (fully relativistic) cross-section [13] is given exactly by the quantum Thomson cross-section (5) in conjunction with (3) without the need for any further approximation. The neglected polarization-independent term in the Klein–Nishina cross-section is therefore peculiar to Dirac (fermion) particles.

2.2. Thomson scattering by a system of many electrons

We proceed by analysing the problem of Thomson scattering by a non-relativistic many-electron system from first principles. The interaction of electromagnetic radiation with a non-relativistic particle of mass \( m \) and charge \( e \) is described, in the first instance, by the classical Hamiltonian

\[
\mathcal{H}(\mathbf{p}, \mathbf{r}) = mc^2 + \frac{(\mathbf{p} - eA(\mathbf{r}))^2}{2m} + \cdots,
\]

(9)

where \( A \) is the vector potential. The terms \( e^2A^2/2m \) and \( -(e/2m)(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) \) comprise the principal perturbation terms that give rise to scattering of the radiation. We consider
only the term proportional to \( A^2 \), which is the principal source of high frequency scattering. The remaining \( A \cdot p \) term is the Kramers–Heisenberg polarization contribution \([12]\), which contributes to scattering in second order, and gives rise to Raman scattering, by bound electrons for example. In general, this term makes a relatively small contribution to the scattering of photons whose frequencies are much greater than the plasma frequency and which are not subject to significant dispersion \([12, 14]\). It is neglected for the purpose of the discussion presented here. To describe the interaction of radiation with a many-body system, we move to a second-quantized formulation. The effective interaction term in the Hamiltonian operator for the scattering of high-frequency radiation, by a many-body system confined to a volume \( V \), is then

\[
\mathcal{H}' = \frac{e^2}{2m} \int_V A^\dagger (r) \cdot A (r) \rho (r) \, d^3r
\]

which is given at an arbitrary time \( t = 0 \), where \( \rho (r) \) is the particle density operator and the electromagnetic vector potential operator at is represented by the modal expansion \([15]\)

\[
A (r) = -\frac{i}{\sqrt{V} \epsilon_0} \sum_{|k,e\rangle} e^{i k \cdot r} a_{k,e}.
\]

where \( \epsilon_0 \) is the vacuum permittivity, \( a_{k,e} \) is a boson annihilation operator for a photon in state \( k, e \) where \( k \) is the wavenumber, \( e \) is a unit vector in the direction of polarization (such that \( e \cdot k = 0 \)); and \( \omega = k c \) is the corresponding frequency. Note that, although \((9)\) describes a non-relativistic particle, for Klein–Gordon particles, the interaction \((10)\) represents the lowest order perturbation, even in the relativistic regime. For electrons, when the elementary scattering is described by the Klein–Nishina formula, the additional Dirac contribution is second order in \( \omega_{\alpha,\beta}/mc^2 \). This means that, despite \((9)\) being non-relativistic, we can expect the following to have validity in the near-relativistic regime, as least as far as first-order relativistic corrections.

Substituting \((11)\) into \((10)\) yields

\[
\mathcal{H}' = \frac{e^2}{2mV \epsilon_0} \sum_{|k,e\rangle} \sum_{|k',e'\rangle} \frac{e' \cdot e}{\sqrt{\omega' \omega}} a_{k',e'}^\dagger a_{k,e} \int_V e^{-i(k'-k) \cdot r} \rho (r) \, d^3r
\]

\[
= \frac{e^2}{2mV \epsilon_0} \sum_{|k,e\rangle} \sum_{|k',e'\rangle} \frac{e' \cdot e}{\sqrt{\omega' \omega}} a_{k',e'}^\dagger a_{k,e} \rho_{k' \rightarrow (-k)},
\]

where

\[
\rho_k = \int_V e^{-i k \cdot r} \rho (r) \, d^3r
\]

is the density operator in reciprocal \((k)\) space. Taking matrix elements between the states \((i, \beta)\), denoting the initial state of the system, and \((f, \alpha)\), denoting a possible final state, in which the labels \( \alpha, \beta \) denote the states of the scattered photon and \( i, f \) denote the states of the scatterer system, yields

\[
\langle \alpha f | \mathcal{H}' | \beta i \rangle = \frac{e^2}{2mV \epsilon_0} \frac{e_{\alpha \cdot e_{\beta}}}{\sqrt{\omega_{\alpha} \omega_{\beta}}} \langle f | \rho_{-q} | i \rangle,
\]

where \( q = k_\beta - k_\alpha \) and \( e_{\alpha} \) is given by \((6)\).

The matrix element given by \((14)\) does not depend upon time and, for a system in a steady state, gives the matrix element at an arbitrary time \( t = 0 \). Even for scattering from systems in...
equilibrium, the density exhibits time-dependent fluctuations, which influence the scattering. For other times, \( t \neq 0 \), the matrix element, in the interaction picture, is

\[
\langle \alpha f | \mathcal{H}_i(t) | \beta i \rangle = \frac{e^2}{2MV_{e0}m_{\omega}m_{\beta}} \left( f | \rho_{-q}(0) | i \right) \exp(-i(E_{\beta i} - E_{\alpha f})t)
\]

\[
= \frac{e^2}{2MV_{e0}m_{\omega}m_{\beta}} \exp(i(\omega_{\alpha} - \omega_{\beta})t) \langle f | \rho_{-q}(t) | i \rangle ,
\]

(15)

where \( \mathcal{H}_i \) is the perturbation Hamiltonian in the interaction picture, i.e. as given by (A.5), and \( E_{\beta i} = \omega_{\beta} + \varepsilon_{i} \), \( E_{\alpha f} = \omega_{\alpha} + \varepsilon_{f} \). Equation (15) yields the \( t \)-matrix in the Born approximation, equation (A.42), in terms of which, according (A.43), the corresponding differential cross section for scattering into the photon channel \( d\Phi_{\alpha} = d\omega_{\alpha}d\Omega_{\alpha} \) is

\[
\frac{\partial^2 \sigma_{\beta}}{\partial \Omega_{\alpha} \partial \omega_{\alpha}} = \frac{V}{c} \sum_{q} \int_{-\infty}^{+\infty} \left( \langle \beta i | \mathcal{H}_i \left( \frac{1}{2} t \right) | \alpha f \rangle \langle \alpha f | \mathcal{H}_i' \left( -\frac{1}{2} t \right) | \beta i \rangle \right) dt ,
\]

(16)

in which \( \langle \ldots \rangle \) denotes the average over the initial states of the scatterer and where the density of final states is defined by

\[
\sum_{\alpha, f} = \sum_{f} \int \omega_{\alpha} d\omega_{\alpha} d\Omega_{\alpha} .
\]

(17)

We choose to give (16) in the ‘time-symmetric’ form [15], which is generalizable to non-equilibrium systems (see the appendix) rather than in the more usual time-asymmetric form, (A.36), to which it is entirely equivalent for systems in equilibrium.

Substituting (15) into (16) yields

\[
\frac{\partial \sigma_{\beta}}{\partial \Omega_{\alpha} \partial \omega_{\alpha}} = r_{e}^{2} \frac{4\pi^{2}c^{3}}{V} \left( e_{\alpha} \cdot e_{\beta} \right)^{2} \sum_{f} \int_{-\infty}^{+\infty} \left( \langle i | \rho_{q} \left( \frac{1}{2} t \right) | f \rangle \langle f | \rho_{-q} \left( -\frac{1}{2} t \right) | i \rangle \right) \exp(i(\omega_{\beta} - \omega_{\alpha})t) dt
\]

\[
= r_{e}^{2} \frac{4\pi^{2}c^{3}}{V} \left( e_{\alpha} \cdot e_{\beta} \right)^{2} \sum_{f} \int_{-\infty}^{+\infty} \rho_{q} \left( \frac{1}{2} t \right) \rho_{-q} \left( -\frac{1}{2} t \right) \exp(i(\omega_{\beta} - \omega_{\alpha})t) dt
\]

\[
= n_{e}r_{e}^{2} \frac{2\pi c}{V} \omega_{\alpha} \omega_{\beta} \left( e_{\alpha} \cdot e_{\beta} \right)^{2} \sum_{f} \int_{-\infty}^{+\infty} \rho_{q} \left( \frac{1}{2} t \right) \rho_{-q} \left( -\frac{1}{2} t \right) \exp(i\omega_{\beta} t) dt
\]

(18)

where

\[
S \left( q, \omega \right) = \frac{1}{2\pi N_{e}} \sum_{q} \int_{-\infty}^{+\infty} \rho_{q} \left( \frac{1}{2} t \right) \rho_{-q} \left( -\frac{1}{2} t \right) \exp(i\omega_{\beta} t) dt
\]

(19)

is the Van Hove dynamic structure factor [16–19], which is a real quantity for real \( q, \omega \).

The density of final states \( \omega_{\alpha} \) follows from

\[
\sum_{\alpha, f} = \frac{V}{(2\pi)^{3}} \int d^{3}k_{\alpha} = \frac{V}{(2\pi)^{3}} \sum_{f} \int \omega_{\alpha}^{2} d\omega_{\alpha} d\Omega_{\alpha} ,
\]

(20)

whereby the definition (17) yields

\[
\omega_{\alpha} = \frac{V\omega_{\alpha}^{2}}{2\pi c^{3}}.
\]

(21)
Combining (18) and (21) yields finally
\[
\frac{\partial^2 \sigma_{\beta}}{\partial \Omega_{\alpha} \partial \omega_{\alpha}} = N_e r_c^2 (e_{\alpha} \cdot e_{\beta})^2 \frac{\omega_{\alpha}}{\omega_{\beta}} S(k_{\beta} - k_{\alpha}, \omega_{\beta} - \omega_{\alpha}) \\
= \frac{3}{8\pi} N_e \sigma_T (1 - \cos^2 \phi \sin^2 \theta) \frac{\omega_{\alpha}}{\omega_{\beta}} S(k_{\beta} - k_{\alpha}, \omega_{\beta} - \omega_{\alpha}),
\]
(22)
where \(\sigma_T = 8\pi r_c^2/3\) is the Thomson cross-section, which is presented as the general quantum-mechanical formula for Thomson scattering of photons from a many-particle system. It is relativistically accurate as far as terms of order \(\omega/mc^2\). The formula for the scattering by a single particle follows from this and is considered below. An important feature of this formula is that it explicitly allows for an exchange of energy between the radiation and the particles with an associated change in the photon frequency. As well as the argument of the structure factor, this energy exchange also appears in the factor \(\omega_{\alpha}/\omega_{\beta}\), which, note, does not appear squared, as it does in the single-particle formula (5).

Equation (22) agrees with formulae given by some authors, e.g. [9, 10], but is apparently contradicted by formulae given by others, e.g. [11], which differ by the factor of \(\omega_{\alpha}/\omega_{\beta}\) being replaced by \((\omega_{\alpha}/\omega_{\beta})^2\).

As an aside, before proceeding further, we should caution against interpreting \(k_{\beta} - k_{\alpha}\) as a momentum exchange, since, as the \(k\)s actually represent reciprocal vectors, this is, strictly speaking, a pseudomomentum [20]. This is related to the fact that, in an extended system, the continuous translational symmetry, which gives rise to momentum conservation, is replaced by a discrete topological symmetry, that of a three-torus, resulting from the imposition of cyclic boundary conditions. For electromagnetic radiation, this becomes an issue only when the refractive index differs significantly from unity. However, for x-rays, the refractive index is typically sufficiently close to unity for \(k_{\beta} - k_{\alpha}\) to be considered as a real momentum exchange due to the scattering. In the following, we shall be concerned only with regimes in which the refractive index is effectively unity.

2.3. Thomson scattering by individual electrons

Equation (22) gives the double differential cross-section for Thomson scattering of photons by a many-particle system. The details of the individual scatterings, and the correlations on which they depend, are hidden in the structure factor, which is a property of the scattering system. By reversing (18), and substituting for \(g_{\alpha}\) from (21), we can rewrite the differential cross section in the form
\[
\frac{\partial^2 \sigma_{\beta}}{\partial \Omega_{\alpha} \partial \omega_{\alpha}} = r_c^2 \frac{4\pi^2 c^3}{V} (e_{\alpha} \cdot e_{\beta})^2 \frac{\omega_{\alpha}}{\omega_{\beta}} g_{\alpha} \sum_f \int_{-\infty}^{+\infty} \left\langle |i| \rho_{-q}^\dagger \left( \frac{1}{2} t \right) |f\right\rangle \\
\times \left\langle f | \rho_{-q} \left( -\frac{1}{2} t \right) |i\right\rangle \exp(i(\omega_{\beta} - \omega_{\alpha})t)dt \\
= r_c^2 (e_{\alpha} \cdot e_{\beta})^2 \frac{\omega_{\alpha}}{\omega_{\beta}} \sum_f \left\langle |i| \rho_{-q}^\dagger (0) |f\right\rangle \left\langle f | \rho_{-q} (0) |i\right\rangle \delta(\varepsilon_i + \omega_{\beta} - \varepsilon_f - \omega_{\alpha})],
\]
(23)
which we apply to the scattering of high energy photons from free electrons in the non-collective regime, i.e. to incoherent scattering. Integrating both sides over \(\omega_{\alpha}\), noting that, for a given
scattering direction, \( \omega_\alpha \) and \( \epsilon_f \) are not independent, but are related through the Compton condition, yields the differential cross-section for the angular distribution

\[
\frac{d\sigma_\beta}{d\Omega_\alpha} = r_c^2 (e_\alpha \cdot e_\beta)^2 \sum_f \left\langle \left( \frac{\omega_\beta + \epsilon_i - \epsilon_f}{\omega_\beta} \right) \left| \langle f \mid \rho_{-q} (0) \mid i \rangle \right|^2 \delta(\epsilon_i + \omega_\beta - E_f) \frac{\partial \omega_\alpha}{\partial E_f} dE_f \right\rangle,
\]

where \( E_i = \epsilon_i + \omega_\beta \) and \( E_f = \epsilon_f + \omega_\alpha \) denote the initial and final state energies respectively and where the derivative \( \frac{\partial \omega_\alpha}{\partial E_f} \) is calculated for fixed initial conditions and fixed scattering geometry, and subsequently evaluated on the energy shell. The density operator for a single free particle in a finite volume is \( \rho_q (0) = e^{-iq \cdot r} \), which leads to

\[
\frac{d\sigma_\beta}{d\Omega_\alpha} = r_c^2 (e_\alpha \cdot e_\beta)^2 \sum_f \left\langle \left( \frac{\omega_\alpha}{\omega_\beta} \right) \left( \frac{\partial \omega_\alpha}{\partial E_f} \right) \delta_{p_i, p_f} \right\rangle_{E_i = E_f},
\]

in which \( P_i = p_i + k_\beta \) and \( P_f = p_f + k_\alpha \) now denote the initial and final total momenta respectively, and where \( \omega_\alpha = k_\alpha c, \omega_\beta = k_\beta c, \epsilon_i = \epsilon(p_i), \epsilon_f = \epsilon(p_f) \) with

\[
\epsilon(p) = \sqrt{m^2 c^4 + p^2 c^2} \approx mc^2 + \frac{p^2}{2m}.
\]

Now \( \epsilon_f^2 = p_f^2 c^2 + m^2 c^4 \) and \( p_f = p_i + k_\beta - k_\alpha \equiv P - k_\alpha \) where \( P \equiv p_i + k_\beta = p_f + k_\alpha \) is the total momentum of the system, from which

\[
\epsilon_f^2 = m^2 c^4 + \omega_\alpha^2 + P^2 c^2 - 2P \cdot \hat{k}_\alpha \omega_\alpha c,
\]

\[
P \cdot k_\alpha c = \omega_\alpha - \frac{\epsilon_f^2 + \omega_\alpha^2 - P^2 c^2 - m^2 c^4}{2\omega_\alpha}.
\]

Differentiation of (27) with respect to \( \omega_\alpha \), for fixed \( p_i, \ k_\beta, \ \hat{k}_\alpha \), and subsequently eliminating \( P \cdot k_\alpha c \) using (28), yields

\[
\frac{\partial \epsilon_f}{\partial \omega_\alpha} = \frac{\omega_\alpha - P \cdot \hat{k}_\alpha c}{
\epsilon_f} = \frac{\epsilon_f^2 + \omega_\alpha^2 - P^2 c^2 - m^2 c^4}{2\omega_\alpha \epsilon_f}
\]

and hence

\[
\frac{\partial E_f}{\partial \omega_\alpha} = 1 + \frac{\epsilon_f}{\omega_\alpha} = \frac{E^2 - P^2 c^2 - m^2 c^4}{2\omega_\alpha \epsilon_f},
\]

where \( E = \epsilon_f + \omega_\alpha = \epsilon_i + \omega_\beta \) is the total energy. Upon substituting \( P^2 = (p_i + k_\beta)^2 \), we get

\[
\frac{\partial E_f}{\partial \omega_\alpha} = \frac{\omega_\beta \epsilon_i}{\omega_\alpha \epsilon_f} \left( 1 - \frac{\hat{k}_\beta \cdot p_i c}{\epsilon_i} \right)
\]

which is the relativistically exact result. Combining this with (25) now yields

\[
\frac{d\sigma_\beta}{d\Omega_\alpha} = r_c^2 (e_\alpha \cdot e_\beta)^2 \left( \frac{\omega_\alpha}{\omega_\beta} \right)^2 \frac{\epsilon_f}{\epsilon_i} \left( 1 - \frac{\hat{k}_\beta \cdot p_i c}{\epsilon_i} \right)^{-1} \bigg|_{E_i = E_f, \ P_i = P_f}
\]
(in which the stray \( \varepsilon f/\varepsilon i \) factor is due to not using relativistically normalized wavefunctions). If the electron is initially stationary, then, neglecting terms of order \((\omega/mc^2)^2\) as previously, this becomes

\[
\frac{d\sigma_\beta}{d\Omega_\alpha} \simeq r_e^2 (e_\alpha \cdot e_\beta)^2 \left( \frac{\omega_\alpha}{\omega_\beta} \right)^2 E_i = E_f \quad P_i = P_f
\]

which is in agreement with one-electron Thomson formula (5) which also applies to an electron initially at rest. Recoil and quantum-relativistic corrections are included as far as \(O(\omega/mc^2)\) as represented by the factor \((\omega_\alpha/\omega_\beta)^2 \simeq 1 + 2\omega_\alpha - \omega_\beta \omega_\beta\). As has thus been shown, this is consistent with the more general many-body formula (22) involving the dynamic structure factor where the correction factor appears as \(\omega_\alpha/\omega_\beta = 1 + \omega_\alpha - \omega_\beta\omega_\beta\), the missing factor of \(\omega_\alpha/\omega_\beta\) having effectively been subsumed into the structure factor.

2.4. Photon angular distribution for scattering by a many-electron system

The energy-integrated photon angular distribution for scattering from a many-electron system that follows from (22) is

\[
\frac{d\sigma_\beta}{d\Omega_\alpha} = \int_0^\infty \frac{\partial^2 \sigma_\beta}{\partial \omega_\alpha \partial \omega_\beta} d\omega_\alpha = N_e r_e^2 (e_\alpha \cdot e_\beta)^2 \int_0^\infty \frac{\omega_\alpha}{\omega_\beta} S(q, \omega_\beta - \omega_\alpha) d\omega_\alpha
\]

\[
= N_e r_e^2 (e_\alpha \cdot e_\beta)^2 \int_0^{\omega_\beta} \left( 1 - \frac{\omega}{\omega_\beta} \right) S(q, \omega) d\omega,
\]

where \(q = k_\beta - k_\alpha\). There are two things to note about the integral in the rightmost expression in (34): firstly, the integral over \(\omega\) does not extend all the way to \(\infty\); and secondly, the integration must be carried out for fixed scattering geometry, as expressed by \(\Omega_\alpha = (\theta, \phi)\) in which case \(q\) is not independent of \(\omega = \omega_\beta - \omega_\alpha\). Since, by definition, \(q_c = \omega_\beta \hat{k}_\beta - \omega_\alpha \hat{k}_\alpha\) which yields,

\[
q^2 \simeq q_0^2 \left( 1 - \frac{\omega}{\omega_\beta} \right),
\]

where

\[
q_0 \equiv \frac{\omega_\beta}{c} (\hat{k}_\beta - \hat{k}_\alpha),
\]

\[
q_0^2 = 2\frac{\omega_\beta^2}{c^2} (1 - \mu),
\]

and \(\mu = \hat{k}_\alpha \cdot \hat{k}_\beta\) is the cosine of the scattering angle. Using that \(S(q, \omega)\) is generally a function of \(q^2\), then, by means of Taylor series expansions around \(q^2 = q_0^2\), one obtains

\[
S(q, \omega) \approx 1 - D_1 \frac{\omega}{\omega_\beta} + D_2 \left( \frac{\omega}{\omega_\beta} \right)^2 - D_3 \left( \frac{\omega}{\omega_\beta} \right)^3 + \cdots \approx S(q_0, \omega),
\]

\[
\left( 1 - \frac{\omega}{\omega_\beta} \right) S(q, \omega) \approx 1 - \left( 1 + D_1 \right) \frac{\omega}{\omega_\beta} + \left( D_1 + D_2 \right) \left( \frac{\omega}{\omega_\beta} \right)^2 - \left( D_2 + D_3 \right) \left( \frac{\omega}{\omega_\beta} \right)^3 + \cdots \approx S(q_0, \omega),
\]

New Journal of Physics 15 (2013) 015014 (http://www.njp.org/)
\[
\left(1 - \frac{\omega}{\omega_\beta}\right)^2 S(\mathbf{q}, \omega) \approx \left(1 - (2 + D^1) \frac{\omega}{\omega_\beta} + (1 + 2D^1 + D^2) \left(\frac{\omega}{\omega_\beta}\right)^2 \right.
\]
\[
\left. - (D^1 + 2D^2 + D^3) \left(\frac{\omega}{\omega_\beta}\right)^3 + \cdots \right) S(\mathbf{q}_0, \omega),
\]

where \(D^j = \frac{1}{j!}(q_0^2)^j \left(\frac{\omega}{\omega_\beta}\right)^j\). The next thing we need to consider is the residual integration over \(\omega_\beta < \omega < \infty\). The high-frequency part of the structure factor is considered to be dominated by quasi-free particle motions, with resonant and collective behaviour confined to much lower frequencies.

We therefore deem it appropriate to use the high-frequency limit of the random phase approximation (RPA), which, for arbitrary electron degeneracy, is

\[
S(\mathbf{q}, \omega) \sim \frac{e^\eta}{4I_{1/2}(\eta)} \frac{1}{\sqrt{T_e v_q}} \exp \left(-\frac{(\omega - v_q)^2}{4T_e v_q}\right),
\]

where \(\eta = \mu_e/T_e\) is the degeneracy parameter, \(I_j(x) = \int_0^\infty y^j (1 + \exp(y - x))^{-1} \, dy\) is the standard Fermi integral, and \(v_q = q^2/2m\). Using (38) together with the asymptotic form [21]

\[
\int_{\Omega \to \infty} x^n \exp(-x^2) dx \sim \Omega^n \frac{\sqrt{\pi}}{2} \text{erfc}(\Omega) \sim \frac{1}{2} \Omega^{n-1} \exp(-\Omega^2),
\]

it follows straightforwardly that, for large \(\Omega = (\omega_\beta - v_q)/\sqrt{4T_e v_q}\),

\[
\int_{\omega_\beta}^\infty (\omega - v_q)^n S(\mathbf{q}, \omega) \, d\omega \approx \frac{e^\eta}{4I_{1/2}(\eta)} \sqrt{4T_e v_q} (\omega_\beta - v_q)^{n-1} \exp\left(-\frac{(\omega_\beta - v_q)^2}{4T_e v_q}\right),
\]

in which, ignoring the minor difference between \(\mathbf{q}\) and \(\mathbf{q}_0\),

\[
\frac{v_q}{\omega_\beta} = \frac{q^2}{2m\omega_\beta} < \frac{2k_\beta^2}{m\omega_\beta} = \frac{2\omega_\beta}{mc^2} \ll 1
\]

and

\[
\frac{v_q T_e}{\omega_\beta^2} = \frac{q^2 T_e}{2m\omega_\beta^2} < \frac{2k_\beta^2 T_e}{m\omega_\beta^2} = \frac{2T_e}{mc^2} \ll 1.
\]

The exponential factor in (40) is therefore \(\ll \exp(-mc^2/8T_e)\) which means that, at low enough temperatures, certainly those below \(\sim 10\) keV, the residual contribution to the integral over \(\omega\) is negligible, allowing the limit to be extended to infinity. Combining the above results then yields the photon angular distribution according to

\[
\frac{d\sigma_\beta}{d\Omega_e} \approx N e^2 \left(\mathbf{e}_e \cdot \mathbf{e}_\beta\right)^2 \int_{-\infty}^{+\infty} \left(1 - (1 + D^1) \frac{\omega}{\omega_\beta} + (D^1 + D^2) \left(\frac{\omega}{\omega_\beta}\right)^2 \right.
\]
\[
\left. - (D^2 + D^3) \left(\frac{\omega}{\omega_\beta}\right)^3 + \cdots \right) S(\mathbf{q}_0, \omega) \, d\omega.
\]

Now, from the elastic and f-sum rules [17–19]

\[
\int_{-\infty}^{+\infty} S(\mathbf{q}, \omega) d\omega = S(\mathbf{q}),
\]

\[\text{New Journal of Physics 15 (2013) 015014 (http://www.njp.org/)}\]
\[ \int_{-\infty}^{+\infty} \omega S(q, \omega) d\omega = \frac{q^2}{2m}, \] (45)

where \( S(q) \) is the static structure factor, while, for hot (classical) plasmas, those for which \( T_e \gg \Omega_e, q^2/2m \), the second moment is given by \[ \int_{-\infty}^{+\infty} \omega^2 S(q, \omega) d\omega \simeq \frac{q^2 T_e}{m}. \] (46)

The higher moments depend upon more detailed properties of the scatterer. Explicit formulae for the fourth moment, for example, are given in [22]. The odd moments vanish in the classical limit. For electrons in a hot plasma, for which \( T_e \gg \Omega_e \), we assume the general semiclassical forms

\[ \frac{1}{S(q)} \int_{-\infty}^{+\infty} \omega^{2n-1} S(q, \omega) d\omega \equiv \langle \omega^{2n-1} \rangle_q = \frac{1}{2T_e} \left( \frac{q^2 T_e}{m S(q)} \right)^n F_n(q), \]

\[ \frac{1}{S(q)} \int_{-\infty}^{+\infty} \omega^{2n} S(q, \omega) d\omega \equiv \langle \omega^{2n} \rangle_q = \left( \frac{q^2 T_e}{m S(q)} \right)^n F_n(q), \] (47)

where \( \langle \omega^n \rangle_q \) denotes the nth frequency moment of the dynamic structure factor and where, for \( n \geq 0 \), the functions \( F_n(q) \) are relatively slowly varying \( O(1) \) functions of \( q \) whose derivatives will be ignored. For the first few values of \( n \) we find \( F_0(q) = 1 \), \( F_1(q) = 1 \) and for small-\( q \) and large-\( q \) respectively, \( F_2(q) \sim 1 + O(q^2 D_e^2) \), \( F_2(q) \sim 3 + O(1/q^2 D_e^2) \), where \( D_e = \sqrt{T_e/m \Omega_e} \) is the electron screening length. Equations (47) yield the leading order dependences on \( q^2 T_e/m \) and \( \Omega_e/T_e \). Carrying out the integrals in (43) according to these formulæ and making reference to (36), yields the angular distribution

\[ \frac{d\sigma_\beta}{d\Omega_\alpha} \simeq N_e r_e^2 (e_\alpha \cdot e_\beta)^2 \left( \frac{S(q_0)}{m \omega_\beta} \left( 1 - \frac{T_e}{\omega_\beta} \right) \right), \] (48)

in which only the lowest order recoil correction terms of order \( \omega_\beta/mc^2 \) and \( T_e/mc^2 \) have been retained. In the classical limit, (48) becomes

\[ \frac{d\sigma_\beta}{d\Omega_\alpha} \simeq N_e r_e^2 (e_\alpha \cdot e_\beta)^2 \left( \frac{S(q_0) + \frac{q^2 T_e}{m \omega_\beta}}{m \omega_\beta} \right) \]

\[ = N_e r_e^2 (e_\alpha \cdot e_\beta)^2 \left( \frac{S(q_0) + \frac{2T_e}{mc^2} (1 - \mu)}{m \omega_\beta} \right), \] (49)

where \( q_0 \) is defined by (36).

3. Scattering of energy—the classical cross-section

The above defines the differential cross-section \( \partial^2 \sigma_\beta/\partial \omega_\alpha \partial \Omega_\alpha \) as being the ratio of the number of scattered photons per unit time in \( d\omega_\alpha \), \( d\Omega_\alpha \) to the photon flux in a collimated monochromatic incident beam (the incident channel). This is the quantum cross-section. It describes scattering in terms of discrete processes involving a quantized electromagnetic field in which the number of energy quanta (photons) is conserved.

However, in classical systems, the concept of a photon is not recognized and the differential cross-section \( \partial^2 \Sigma_\beta/\partial \omega_\alpha \partial \Omega_\alpha \) is defined differently to be the ratio of the scattered energy (or power) in \( d\omega_\alpha \), \( d\Omega_\alpha \) to the energy (or power) incident per unit area in the form of a collimated
monochromatic beam. Since the energy of a photon is proportional to the frequency, the relationship between the classical and quantum cross-sections is readily found to be given by

\[ d\Sigma_\beta = \frac{\omega_\alpha}{\omega_\beta} d\sigma_\beta. \tag{50} \]

This yields, from (22),

\[ \frac{\partial^2 \Sigma_\beta}{\partial \Omega_\alpha \partial \omega_\alpha} = N_c r_\epsilon^2 (e_\alpha \cdot e_\beta)^2 \left( \frac{\omega_\alpha}{\omega_\beta} \right)^2 S(k_\beta - k_\alpha, \omega_\beta - \omega_\alpha), \tag{51} \]

in which the factor of \( \omega_\alpha/\omega_\beta \) now does appear squared. Equation (51) agrees with formulae in the literature that are derived classically in accordance with this definition, e.g. [10]. Moreover, in the same way, referring to (5) and applying (50), the classical one-electron Thomson cross-section is

\[ d\Sigma_\beta \bigg|_{\Omega_T} = r_\epsilon^2 \left( \frac{\omega_\alpha}{\omega_\beta} \right)^3 (e_\alpha \cdot e_\beta)^2. \tag{52} \]

The relationship between the double differential cross section of a many electron system and the corresponding one-electron Thomson cross-section is thus expressed by [24]

\[ \frac{\partial \tilde{\sigma}}{\partial \Omega_\alpha \partial \omega_\alpha} = \frac{\omega_\beta}{\omega_\alpha} \frac{d\tilde{\sigma}}{d\Omega_\alpha} \bigg|_{\Omega_T} S(q, \omega), \]

\[ q = k_\beta - k_\alpha, \]

\[ \omega = \omega_\beta - \omega_\alpha, \tag{53} \]

which holds generally for both the classical, \( \tilde{\sigma} = \Sigma_\beta \), and quantum, \( \tilde{\sigma} = \sigma_\beta \), cross-sections.

The angular distribution of the scattered energy is given by

\[ \frac{d\Sigma_\beta}{d\Omega_\alpha} = N_c r_\epsilon^2 (e_\alpha \cdot e_\beta)^2 \int_{-\infty}^{+\infty} \left( 1 - \frac{2 + D^1}{\omega_\beta} + \left( 1 + 2D^1 + D^2 \right) \left( \frac{\omega_\alpha}{\omega_\beta} \right)^2 \right) \]

\[ \times S(q_0, \omega) d\omega, \tag{54} \]

which is the formula for the classical angular distribution that replaces (43). Evaluating (54) in the same manner as that leading to (48) then yields

\[ \frac{d\Sigma_\beta}{d\Omega_\alpha} \approx N_c r_\epsilon^2 (e_\alpha \cdot e_\beta)^2 \left( S(q_0) \left( 1 - \frac{(\omega^3 q_0)}{\omega_\beta^3} \right) - \frac{3q_0^2}{m \omega_\beta} \left( \frac{1}{2} - \frac{T_e}{\omega_\beta} \right) \right) \]

\[ = N_c r_\epsilon^2 (e_\alpha \cdot e_\beta)^2 \left( S(q_0) \left( 1 - \frac{\omega_\beta (\omega^3 q_0)}{2T_e \omega_\beta^3} \right) - \frac{3q_0^2}{m \omega_\beta} \left( \frac{1}{2} - \frac{T_e}{\omega_\beta} \right) \right). \tag{55} \]

in which the term proportional to \( (\omega^3 q_0)/\omega_\beta^3 \) contributes only in the small-\( q \) regime as defined above. Equation (55) is still a fully quantal expression for the angular distribution of the scattered energy. It is similar, but not identical, to the photon angular distribution (48). Which of these two forms may be applicable depends upon the particular experimental setup, whether envisaged or actual. If the detectors measuring the scattered radiation at each angle respond proportionally to the number of photons, then (48) is the appropriate formula, while, if, as is more widely the case, they respond proportionally to the energy, then (55) is the appropriate form to use.

New Journal of Physics 15 (2013) 015014 (http://www.njp.org/)
Equation (55) also defines the classical angular distribution. However, a fully classical description generally requires \( \omega_\beta \ll T_e \) (which does not hold for x-ray scattering in cold and warm matter) while only the even moments of the structure factor are classically finite quantities. Eliminating \( \mathcal{O}(\hbar) \) terms from (55) with reference to (47) yields

\[
\frac{d \Sigma_\beta}{d \Omega_\alpha} \simeq N_e r_c^2 (e_\alpha \cdot e_\beta)^2 \left( S(q_0) + \frac{3 q_0^2 T_e}{m \omega_\beta^2} \right) \\
= N_e r_c^2 (e_\alpha \cdot e_\beta)^2 \left( S(q_0) + \frac{3 T_e}{mc^2} (1 - \mu) \right)
\]

(cf (48)). Equation (56) gives the angular distribution of the scattered energy in a classical system. We observe that, in both (49) and (56), the retained terms involving \( q_0^2 T_e / mc^2 = (2T_e/mc^2)(1 - \mu) \) are first-order relativistic corrections involving the temperature that vanish in the non-relativistic limit when \( T_e \ll mc^2 \).

4. Radiation transport—the Rosseland scattering opacity

4.1. The Rosseland scattering opacity

An example of a process that is governed, at the microscopic level, by quantum processes is the transport of thermal radiation in dense matter. Thermal radiation transport involves the absorption, emission and scattering of photons by the constitutive atoms and electrons. In the case of transport in systems in local thermodynamic equilibrium (LTE), these processes can be represented by the frequency-dependent or monochromatic opacity \( \kappa(\omega) \) which is essentially the effective photon absorption cross-section per unit mass, taking account of all relevant processes and their inverses. In the diffusion limit, radiative energy transport is governed by the Rosseland opacity, which is related to an appropriate average over frequency of the monochromatic mean free path \( \lambda(\omega) = 1/\rho \kappa(\omega) \) taken over a black body distribution. In this context, the scattering contribution to \( \kappa(\omega) \) is quite complicated, as it not only needs to take account of the change of direction of the photon, but also the effect of any frequency change of the emergent photon on its subsequent transport, as well as stimulated scattering due to the presence of a background (e.g. black-body) radiation field. These corrections are likely to be of the same order as the above corrections to the angular distribution and therefore need to be considered at the same time.

The scattering contribution to the monochromatic opacity governing the diffusion of radiative energy, in matter that is in LTE at temperature \( T \), is given by [4, 5]

\[
\frac{1}{\lambda_s(\omega_\beta)} = \frac{1}{V} \int \left[ \frac{1 - \exp(-\omega_\beta/T)}{1 - \exp(-\omega_\alpha/T)} \right] \left( 1 - \frac{\omega_\alpha \lambda(\omega_\alpha)}{\omega_\beta \lambda(\omega_\beta)} \right) \frac{\partial^2 \sigma_\beta}{\partial \Omega_\alpha \partial \omega_\alpha} d\Omega_\alpha d\omega_\alpha.
\]

As well as the differential cross-section, the integrand contains two additional factors. The factor \( \frac{1 - \exp(-\omega_\beta/T)}{1 - \exp(-\omega_\alpha/T)} \) represents the effect of stimulated scattering in the presence of a background black-body radiation field. The other factor represents the effect of the change in photon frequency on its ability to transport energy in the exit (\( \alpha \)) channel and involves the total photon mean free path \( \lambda(\omega) \) due to all processes. In a purely scattering medium, \( \lambda = \lambda_s \) and, in general, \( \lambda(\omega) \) depends on \( \lambda_s \), via \( \lambda^{-1} = \lambda_s^{-1} + \lambda_m^{-1} \) where \( \lambda_m \) is the mean free path due to non-scattering processes, such as absorption and stimulated emission, so equation (57) is not closed and needs to be solved iteratively. Two circumstances in which this is not necessary are when the
scattering contribution to $\lambda(\omega)$ is small, i.e. $\lambda_s \gg \lambda_{ns}$, or when $\lambda$ does not depend (strongly) on the frequency. The first case is unlikely to be of much interest simply because scattering is then of low importance. In the case of a system dominated by Thomson scattering, a frequency independent mean free path is a reasonable first approximation, which, using (22) and (8) and extending the integration over $\omega$ to infinity, becomes, for non-relativistic electrons,

$$\frac{1}{\lambda_s(\omega_\beta)} = \frac{3}{8} n_e \sigma_T \int_{-\infty}^{\infty} d\omega \int_{-1}^{1} d\mu \left( 1 + \mu^2 \right) \left( 1 - \mu + \frac{\omega_\alpha}{\omega_\beta} \right) \omega_\alpha \frac{1 - \exp(-\omega_\beta/T)}{\omega_\beta} \frac{1 - \exp(-\omega_\alpha/T)}{\omega_\alpha} S(q, \omega),$$

(58)

where $\omega_\alpha = \omega_\beta - \omega$. Expanding about $\omega = 0$ yields

$$\frac{1 - \exp(-\omega_\beta/T)}{1 - \exp(-\omega_\alpha/T)} \approx 1 + \frac{\omega}{\omega_\beta} \xi_\beta + \left( \frac{\omega}{\omega_\beta} \right)^2 \left( \frac{1}{2} \frac{\omega_\beta}{T} + \xi_\beta \right) \xi_\beta,$$

(59)

where

$$\xi_\beta = \frac{\omega_\beta / T}{\exp(\omega_\beta / T) - 1} < 1, \quad \omega_\beta, \quad T > 0,$$

(60)

whereupon (58) becomes

$$\frac{1}{\lambda_s(\omega_\beta)} \approx \frac{3}{8} n_e \sigma_T \int_{-\infty}^{\infty} d\omega \int_{-1}^{1} d\mu \left( 1 + \mu^2 \right) \left( 1 - \mu + \frac{\omega}{\omega_\beta} \right) \left( 1 - \frac{\omega}{\omega_\beta} \right) \times \left( 1 + \frac{\omega}{\omega_\beta} \xi_\beta + \left( \frac{\omega}{\omega_\beta} \right)^2 \left( \frac{1}{2} \frac{\omega_\beta}{T} + \xi_\beta \right) \xi_\beta \right) S(q, \omega).$$

(61)

Using the expansion (37) and carrying out the integrations in accordance with (44)–(46) yields, after some algebra,

$$\frac{1}{\lambda_s(\omega_\beta)} \approx n_e \sigma_T \left( \frac{3}{8} \right) \int_{-1}^{1} S(q_0)(1 + \mu^2)(1 - \mu) d\mu + \frac{2}{5} \frac{\omega_\beta}{mc^2} \left( 7\xi_\beta - 8 + \frac{T}{\omega_\beta} (11 - 16\xi_\beta + 7\xi_\beta^2) \right),$$

(62)

where $q_0$ is given by (36) and in which relativistic corrections only as far as $O(\omega_\beta/mc^2)$ or $O(T/mc^2)$ have been retained. In the fully non-relativistic low-photon-energy limit we recover the Thomson opacity [6, 25]

$$\frac{1}{\lambda_s(\omega_\beta)} \approx n_e \sigma_T \int_{-1}^{1} S(q_0)(1 + \mu^2)(1 - \mu) d\mu$$

(63)

which incorporates, through the static structure factor $S(q_0)$, the effect of electron correlations, including exchange and the direct effect of degeneracy, which can be important at very high densities such as occur in stellar cores [26]. The correction terms in (62) become important at the 10% level at temperatures $T \gtrsim 6$ keV. In the highly relativistic regime, in addition to including the additional relativistic terms from the Klein–Nishina formula (2), it is necessary to account for extra electron–positron pairs in the equilibrium state. A somewhat different approach [5] is then required.
5. Conclusions

We have presented derivations of the high-frequency Thomson differential scattering cross-sections for the scattering of photons by a many-electron system (22) and by a single electron (33). In the case of a many-electron system, the direction and energy of the outgoing photon are treatable as independent parameters and the result is expressed as a double differential cross-section. In the case of scattering by one electron, however, momentum and energy conservation mean that the change in energy is determined by the scattering angle. The key feature to note is that the index $\nu$ of the overall factor $(\omega_\alpha/\omega_\beta)^\nu$ differs between the two formulae, with $\nu = 1$ for the many-electron formula and $\nu = 2$ for one electron.

In the calculation of the angular distribution of photons scattered from a many-body system, it is necessary to take account of the lack of independence between $\omega$ and $q$ in the argument of the dynamic structure factor when integrating over the final state energy for fixed initial energy and scattering geometry. This yields a formula (48) that contains additional $O(\omega_\beta/mc^2)$ and $O(T_e/mc^2)$ terms compared with the result when this interdependence is ignored.

However, when the cross-section is defined classically in terms of the energy in each channel, then the cross-section formula acquires an extra factor of $\omega_\alpha/\omega_\beta$. It is important to be aware of the difference between these two forms of the cross-section. Which choice of cross-section is employed will depend on how the scattering is envisaged as being measured, in particular whether the detectors respond to photon number (quantum detectors) or to the energy (classical detectors). The formulae for the angular distributions differ in respect of the coefficients of higher order relativistic correction terms of $O(\omega_\beta/mc^2)$ and $O(T_e/mc^2)$ as well as, in the small-$q$/forward-angle regime, terms involving the fourth moment of the dynamic structure factor, which we estimate to be $O(\Omega_\omega^2/\omega_\beta T_e)$.

The differences between the classical and quantum formulae can lead to confusion if the reader is not at pains to establish which cross-section a particular author is referring to. Authors do not help by simply referring to the Compton or Thomson cross section as if this were uniquely defined. However the cited texts [8–10] generally give correct formulae in their respective contexts, with the exception of reference [9], where the one-electron Thomson cross-section, $d\sigma_\beta/d\Omega_\alpha|_T$ is incorrectly deduced from a correct many-electron formula, thus yielding the cross-section as $r_e^2(\omega_\alpha/\omega_\beta)(\mathbf{e}_\alpha \cdot \mathbf{e}_\beta)^2$ instead of as given by (5). A guiding principle is that, whichever way the cross-section is defined, the relationship, between the one-electron cross-section and the double differential cross-section for scattering by a many-body system, is always expressed by equation (53).

We also consider the implications for the radiative opacity as used in modelling the diffusion of thermal radiation. The scattering opacity is generally formulated in terms of the photon cross-sections with additional corrections due to photon transport and stimulated scattering. These corrections lead to additional relativistic corrections that are of the same order as those arising from the $\omega_\alpha/\omega_\beta$ factor and which therefore need to be considered at the same time.

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Appendix. Scattering theory

A.1. General S-matrix formulation of scattering cross-section

The following outlines the quantum theory of scattering by complex systems close to, but not necessarily in equilibrium, starting with the general theory of scattering in a time-dependent potential and progressing to standard stationary scattering theory.

We consider a general system governed by some Hamiltonian $H(t) = H_0 + H'(t)$ where $H_0$ is the time-independent unperturbed Hamiltonian in the Schrödinger and interaction pictures, whose eigenstates are the states of the unperturbed system in which scattering is deemed not to occur; and $H'(t)$, which generally depends on time, vanishes at times in the distant past ($t = -\infty$) and in the distant future ($t = +\infty$).

Denoting the orthonormal eigenstates of $H_0$ by $|\alpha\rangle$, $|\beta\rangle$, ... such that $H_0|\alpha\rangle = E_\alpha|\alpha\rangle$, $\langle\alpha|\beta\rangle = \delta_{\alpha\beta}$, $\sum_\alpha |\alpha\rangle \langle\alpha| = 1$ etc, and, working in the interaction picture, we define the wave operator $\Omega_1(t)$ to be the operator that generates the physical state $|\beta^+(t)\rangle$ that evolves from an arbitrary initial state $|\beta\rangle$, which is the specified state of the system at $t = -\infty$, i.e.

$$|\beta^+(t)\rangle = \Omega(t)|\beta\rangle. \quad (A.1)$$

For processes that conserve the number(s) of particles, $\langle\beta^+(t)|\beta^+(t)\rangle = \langle\beta|\beta\rangle \forall \beta$ which implies that

$$\Omega^\dagger(t)\Omega(t) = 1, \quad (A.2)$$

which is a statement of the fact that $\Omega(t)$ is unitary.

By definition, the state $\exp(-iH_0t)|\beta^+(t)\rangle = \exp(-iH_0t)\Omega(t)|\beta\rangle$ satisfies the Schrödinger equation $(H - i\frac{d}{dt})\psi = 0$, which implies that $|\beta^+(t)\rangle$ satisfies

$$\left(\mathcal{H}'_{\text{int}}(t) - i\frac{d}{dt}\right)|\beta^+(t)\rangle = 0 \quad (A.3)$$

and hence

$$\frac{d}{dt} \Omega(t) = -i\mathcal{H}'_{\text{int}}(t)\Omega(t), \quad (A.4)$$

where

$$\mathcal{H}'_{\text{int}}(t) = \exp(iH_0t)\mathcal{H}'(t)\exp(-iH_0t) \quad (A.5)$$

is the perturbation in the interaction picture. Let the generalized transition operator be defined by

$$T(t) \equiv i\frac{d}{dt}\Omega(t) = \mathcal{H}'_{\text{int}}(t)\Omega(t). \quad (A.6)$$

From the conditions imposed at $t = \pm\infty$,

$$\mathcal{H}'_{\text{int}}(-\infty) = \mathcal{H}'_{\text{int}}(+\infty) = 0, \quad \Omega(-\infty) = 1, \quad \Omega(+\infty) = 1, \quad T(-\infty) = T(+\infty) = 0. \quad (A.7)$$

Now define the time-dependent matrix

$$S_{\alpha\beta}(t) = \langle\alpha|\beta^+(t)\rangle = \langle\alpha|\Omega(t)|\beta\rangle, \quad S^\dagger_{\beta\alpha}(t) = \langle\beta^+(t)|\alpha\rangle = \langle\beta|\Omega^\dagger(t)|\alpha\rangle = S^\ast_{\alpha\beta}(t). \quad (A.8)$$

New Journal of Physics 15 (2013) 015014 (http://www.njp.org/)
the second of which expresses the matrix \( \mathbf{S}^\dagger(t) = ||S_{\alpha\beta}(t)|| \) as the Hermitian adjoint of \( \mathbf{S}(t) = ||S_{\alpha\beta}(t)|| \).

The property
\[
\sum_a S_{\gamma\alpha}^\dagger(t)S_{\alpha\beta}(t) = \delta_{\gamma\beta}; \quad \forall t
\]
(A.9)

follows from the unitary property of \( \Omega(t) \) given at (A.2). \( \mathbf{S}(t) \) is a time-dependent generalization of the standard \( \mathbf{S} \)-matrix, \( S_{\alpha\beta}^0 \), to which it reduces when \( t = \infty \).

Using (A.6), the time derivative of the generalized \( \mathbf{S} \)-matrix is
\[
\frac{\partial}{\partial t}S_{\alpha\beta}(t) = \left( \alpha \left| \frac{d}{dt} \Omega(t) \right| \beta \right) = -i \langle \alpha | T(t) | \beta \rangle \equiv -iT_{\alpha\beta}(t),
\]
(A.10)
where \( T_{\alpha\beta}(t) \) is the time-dependent generalization of the \( t \)-matrix. Integrating equations (A.10), using that \( S_{\alpha\beta}(-\infty) = \delta_{\alpha\beta} \), yields
\[
S_{\alpha\beta}(t) = \delta_{\alpha\beta} - i \int_{-\infty}^t T_{\alpha\beta}(t')dt'.
\]
(A.11)

The time-dependence of the \( t \)-matrix can be expressed, in the interaction picture, by
\[
T(t) = \exp(i\mathcal{H}_0 t)T^0(t)\exp(-i\mathcal{H}_0 t),
\]
(A.12)
where \( T^0(t) \) is the transition operator in the Schrödinger picture, which, from (A.6), is given by
\[
T^0(t) \equiv \exp(-i\mathcal{H}_0 t) \left[ \frac{d}{dt} \left( \exp(i\mathcal{H}_0 t) \Omega^0(t)\exp(-i\mathcal{H}_0 t) \right) \right] \exp(i\mathcal{H}_0 t)
\equiv \left[ \Omega^0, \mathcal{H}_0 \right] + i \frac{\partial \Omega^0}{\partial t} = \mathcal{H}'(t)\Omega^0(t),
\]
(A.13)
where
\[
\Omega^0(t) = \exp(-i\mathcal{H}_0 t)\Omega(t)\exp(i\mathcal{H}_0 t)
\]
is the wave operator in the Schrödinger picture.

Using (A.12), the \( t \)-matrix becomes
\[
T_{\alpha\beta}(t) = \langle \alpha | T^0(t) | \beta \rangle \exp(i(E_\alpha - E_\beta) t)
\equiv T_{\alpha\beta}^0(t) \exp(i(E_\alpha - E_\beta) t),
\]
(A.15)
where
\[
T_{\alpha\beta}^0(t) = \langle \alpha | T^0(t) | \beta \rangle.
\]
(A.16)

Substitution of (A.15) into (A.11) yields
\[
S_{\alpha\beta}(t) = \delta_{\alpha\beta} - i \int_{-\infty}^t T_{\alpha\beta}^0(t')\exp(i(E_\alpha - E_\beta)t')dt'
\]
\[
= \delta_{\alpha\beta} - i \int_{-\infty}^{t+\infty} \theta(t-t')T_{\alpha\beta}^0(t')\exp(i(E_\alpha - E_\beta)t')dt'
\]
\[
= \delta_{\alpha\beta} + i \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega + i0^+} \tilde{T}_{\alpha\beta}^0(\omega + E_\alpha - E_\beta)d\omega.
\]
(A.17)
where
\[ \tilde{T}_{\alpha \beta}^0(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} T_{\alpha \beta}^0(t) \, dt \]  \hspace{1cm} (A.18)

and where use has been made of the following representation of the step function:
\[ \theta(\tau) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\omega \tau}}{\omega + i0^+} d\omega. \]  \hspace{1cm} (A.19)

For \( t \to \infty \), the first of equations (A.17) yields
\[ S_{\alpha \beta}(\infty) = \delta_{\alpha \beta} - 2\pi i \tilde{T}_{\alpha \beta}^0(E_\alpha - E_\beta). \]  \hspace{1cm} (A.20)

For finite \( t \), by making use of the Cauchy identity,
\[ \frac{1}{\omega + i0^+} = -\pi i \delta(\omega) + \mathcal{P} \left( \frac{1}{\omega} \right) \]  \hspace{1cm} (A.21)
in conjunction with the third of equations (A.17), leads to
\[ S_{\alpha \beta}(t) = \delta_{\alpha \beta} - \pi i \tilde{T}_{\alpha \beta}^0(E_\alpha - E_\beta) + \mathcal{P} \int_{-\infty}^{\infty} e^{-i\omega t} \tilde{T}_{\alpha \beta}^0(\omega + E_\alpha - E_\beta) \frac{d\omega}{\omega}. \]  \hspace{1cm} (A.22)

Furthermore, by Fourier transforming (A.17)
\[ \tilde{S}_{\alpha \beta}(\omega) = \delta_{\alpha \beta} \delta(\omega) + \frac{\tilde{T}_{\alpha \beta}^0(E_\alpha - E_\beta + \omega)}{\omega + i0^+}, \]  \hspace{1cm} (A.23)
where \( \tilde{S}_{\alpha \beta}(\omega) \) is defined in terms of \( S_{\alpha \beta}(t) \) analogously to (A.18).

A.2. Stationary scattering theory

The special case when the perturbation \( \mathcal{H}' \) does not depend on time, and energy is conserved, is known as stationary scattering theory. However we still have the prevailing requirement that \( \mathcal{H}'(-\infty) = \mathcal{H}'(\infty) = 0 \). This is formally dealt with by allowing \( \mathcal{H}' \) to depend on time for \( t < -t_1 \) and \( t > t_2 \) during which times, the time dependent processes are adiabatic so as to maintain the system in a pure state, and then taking the limit \( t_1, t_2 \to \infty \). This is sometimes described as adiabatic switching of the perturbation on and off in the distant past and the distant future respectively.

In the special case when \( \mathcal{H}' \) is, for all finite times, independent of time, energy is conserved and so
\[ (\mathcal{H}_0 + \mathcal{H}'_{\text{int}}) \Omega(t) = \Omega(t) \mathcal{H}_0, \]  \hspace{1cm} (A.24)
\[ (\mathcal{H}_0 + \mathcal{H}') \Omega^0(t) = \Omega^0(t) \mathcal{H}_0, \]  \hspace{1cm} (A.25)
whereupon
\[ [\Omega^0, \mathcal{H}_0] = \mathcal{H}'_0 \Omega^0 \]  \hspace{1cm} (A.25)
which, when combined with (A.13), implies that the operators \( \Omega^0 \) and \( \mathcal{T}^0 \) are time-independent, i.e.
\[ \frac{\partial \Omega^0}{\partial t} = 0, \]  \hspace{1cm} (A.26)
\[ \frac{\partial \mathcal{T}^0}{\partial t} = 0. \]  \hspace{1cm} (A.26)
The $t$-matrix (A.15) then becomes
\[ T_{αβ}(t) = T_{αβ}^0 \exp(-i(E_β - E_α + i0^+)t), \]  
(A.27)
in which $T_{αβ}^0$ does not depend on time. Equation (A.18) then yields
\[ \tilde{T}^0_{αβ}(ω) = T^0_{αβ} \delta(ω). \]  
(A.28)
The $S$-matrix, from (A.11), is then
\[ S_{αβ}(t) = \delta_{αβ} - i \int_{-∞}^{t} T^0_{αβ} \exp(-i(E_β - E_α + i0^+)t) dt', \]
\[ = \delta_{αβ} + T^0_{αβ} \exp(-i(E_β - E_α + i0^+)t), \]  
(A.29)
the limit of which for $t \to ∞$ is given, using (A.20) and (A.8), by
\[ S_{αβ}(∞) = S_{αβ}^0 = \delta_{αβ} - 2πi T^0_{αβ} δ(E_β - E_α) \]  
(A.30)
which is the standard relationship between the $S$-matrix and the $t$-matrix for conservative systems.

A.3. Transition rate

The $S$-matrix element $S_{αβ}$, as defined by (A.8), expresses by how much the state (A.1) has evolved into the ‘final’ state $|α⟩$. The total transition probability at time $t$ is therefore $|S_{αβ}|^2 = S_{βα}^+(t) S_{αβ}(t)$. The instantaneous transition rate is therefore
\[ ν_{αβ} = \frac{∂}{∂t} S_{βα}^+(t) S_{αβ}(t) \]  
(A.31)
which, using (A.10) and (A.11), becomes, for $α ≠ β$,
\[ ν_{αβ}(t) = -i(T^+_βα(t) S_{αβ}(t) - S^+_βα(t) T_{αβ}(t)) \]
\[ = \int_{-τ/2}^{τ/2} (T^+_βα(t) T_{αβ}(t') + T^+_βα(t') T_{αβ}(t)) dt' \]
\[ = \int_{-τ/2}^{τ/2} \theta(t - t') (T^+_βα(t) T_{αβ}(t') + T^+_βα(t') T_{αβ}(t)) dt', \]  
(A.32)
where $H(t)$, and hence $T_{αβ}(t)$ etc., are presumed to vanish for $t < -τ/2$ and $t > +τ/2$. (The formula (A.32) is therefore unchanged by taking the limit $τ → ∞$. However, for the moment, we retain the assumption that $τ$ is finite.)

The transition rate defined by (A.32) includes the effect of the time-dependent fluctuations of the system. Real measurements however are taken over finite time intervals, and what one generally wants is a time-averaged transition rate. Any average over a finite time interval will itself remain subject to fluctuations. However, in the case of a system that is undergoing steady-state fluctuations, by which it is meant that, in the limit of $τ → ∞$, the functions $T^0_{βα}(t)$ are non-square-integrable functions of time, for which the expectations
\[ E_τ[T] = \lim_{τ→∞} \frac{1}{τ} \int_{τ/2}^{τ+τ/2} T(t') dt', \]
\[ E_τ[|T|^2] = \lim_{τ→∞} \frac{1}{τ} \int_{τ/2}^{τ+τ/2} |T(t')|^2 dt'. \]
exist and are independent of \( t \), it is appropriate to carry out the average over the interval \((-\tau/2, +\tau/2)\) in the limit of \( \tau \to \infty \). This yields

\[
\bar{v}_{\alpha\beta} \equiv \lim_{\tau \to \infty} \frac{1}{\tau} \int_{-\tau/2}^{+\tau/2} v_{\alpha\beta}(t) \, dt
\]

\[
eq \lim_{\tau \to \infty} \frac{1}{\tau} \int_{-\tau/2}^{+\tau/2} \int_{-\tau/2}^{+\tau/2} \theta(t - t')(T^{\dagger}_{\beta\alpha}(t)T_{\alpha\beta}(t') + T^{\dagger}_{\beta\alpha}(t')T_{\alpha\beta}(t)) \, dt' \, dt
\]

\[
eq \lim_{\tau \to \infty} \frac{1}{\tau} \int_{-\tau/2}^{+\tau/2} T_{\alpha\beta}(t) \, dt \bigg|_{t=0}^2.
\]  

(A.33)

The transition rate defined by (A.33) is a well-defined non-fluctuating quantity.

The quantity \( \bar{v}_{\alpha\beta} \) is the zero-frequency power spectral density \( \bar{v}_{\alpha\beta}(0) \) of the time-dependent \( t \)-matrix (A.10) as defined by

\[
\bar{v}_{\alpha\beta}(\omega) = \lim_{\tau \to \infty} \frac{1}{\tau} \left| \int_{-\tau/2}^{+\tau/2} T_{\alpha\beta}(t)e^{-i\omega t} \, dt \right|^2.
\]  

(A.34)

Expanding (A.34) yields

\[
\bar{v}_{\alpha\beta}(\omega) = \lim_{\tau \to \infty} \frac{1}{\tau} \int_{-\tau/2}^{+\tau/2} \int_{-\tau/2}^{+\tau/2} T^{\dagger}_{\beta\alpha}(t)T_{\alpha\beta}(t')e^{i\omega(t-t')} \, dt \, dt'
\]

\[
eq \lim_{\tau \to \infty} \frac{1}{\tau} \int_{-\tau/2}^{+\tau/2} \int_{-\tau}^{+\tau} T^{\dagger}_{\beta\alpha} \left( t' + \frac{1}{2} t \right) T_{\alpha\beta} \left( t' - \frac{1}{2} t \right) e^{i\omega t} \, dt \, dt'
\]

\[
eq \int_{-\tau}^{+\tau} \left( T^{\dagger}_{\beta\alpha} \left( \frac{1}{2} t \right) T_{\alpha\beta} \left( -\frac{1}{2} t \right) \right) e^{i\omega t} \, dt
\]  

(A.35)

in which the notation \( \langle f \rangle \) denotes the time-average according to

\[
\lim_{\tau \to \infty} \frac{1}{\tau} \int_{-\tau/2}^{+\tau/2} \langle f(t') \rangle \, dt' = \langle f(0) \rangle
\]

and where the scattering event is considered to be centred about \( t = 0 \).

For equilibrium systems, time \( t = 0 \) in (A.35) represents an arbitrary finite time, of which the result is then independent, and it can then be written in the more usual form

\[
\bar{v}_{\alpha\beta}(\omega) = \int_{-\tau}^{+\tau} \langle T^{\dagger}_{\beta\alpha}(t)T_{\alpha\beta}(0) \rangle e^{i\omega t} \, dt.
\]  

(A.36)

For systems in equilibrium or in LTE, the time average can generally replaced by the ensemble average, in accordance with the ergodic hypothesis, and where the ensemble average is effectively taken over a subset of initial states \( \Gamma_\beta \) around \( \beta \), comprising the entrance channel, also labelled by \( \beta \). i.e.

\[
\langle f \rangle = \text{trace}(\rho_\beta f),
\]

\[
\rho_\beta = \mathbf{P}_\beta \rho / \text{trace}(\mathbf{P}_\beta \rho),
\]

\[
\mathbf{P}_\beta = \sum_{\gamma \in \Gamma_\beta} |\gamma\rangle \langle \gamma|,
\]

(A.37)

in which \( \rho \) denotes the statistical operator. This formulation is appropriate when the projectile, in this case the photon, is in a definite state, while the scatterer, in this case a many-body system of electrons, is in a statistical state.

*New Journal of Physics* **15** (2013) 015014 (http://www.njp.org/)
A.4. Total cross section

The total cross-section for scattering of a single photon from the entrance channel $\beta$ is defined by

\[ \sigma_\beta = \frac{V}{v_\beta} \sum_{\alpha \neq \beta} \tilde{v}_{\alpha\beta}(0), \]

(A.38)

where $v_\beta$ is the relative incident velocity. This expression includes a sum over final states, which can be transformed into integrals over the phase space \{\Phi_\alpha\} of the final states, according to

\[ \sum_{\alpha} = \int g_f(\Phi_\alpha) \, d\Phi_\alpha, \]

(A.39)

which leads to the general definition of the differential cross section

\[ \frac{d\sigma_\beta}{d\Phi_\alpha} = \frac{V}{v_\beta} \tilde{v}_{\alpha\beta}(0) g_f(\Phi_\alpha), \]

\[ = \frac{V}{v_\beta} g_f(\Phi_\alpha) \int_{-\infty}^{+\infty} \left( T_{\beta\alpha}^0 \left( \frac{1}{2} t \right) T_{\alpha\beta}^0 \left( -\frac{1}{2} t \right) \right) dt \]

(A.40)

where $g_f(\Phi_\alpha)$ is the density of final states. For the special case of a time-independent interaction potential, (A.40) reduces to

\[ \frac{d\sigma_\beta}{d\Phi_\alpha} = \frac{2\pi V}{v_\beta} |T_{\alpha\beta}^0|^2 \delta(E_\beta - E_\alpha) g_f(\Phi_\alpha), \]

(A.41)

which is the exact form of the Fermi Golden Rule [27].

A.5. Born approximation

The lowest order solutions for $\Omega(t)$ and $\mathcal{T}(t)$ are

\[ \Omega(t) = 1 - i \int_{-\infty}^{t} \mathcal{H}'_{\text{int}}(t') dt', \]

\[ \mathcal{T}(t) = \mathcal{H}'_{\text{int}}, \]

(A.42)

which constitute the Born approximation whereby

\[ \frac{d\sigma_\beta}{d\Phi_\alpha} = \frac{V}{v_\beta} g_f(\Phi_\alpha) \int_{-\infty}^{+\infty} \left( \mathcal{H}'_{\beta\alpha} \left( \frac{1}{2} t' \right) \mathcal{H}'_{\alpha\beta} \left( -\frac{1}{2} t' \right) \right) \exp(i(E_\beta - E_\alpha)t') dt', \]

(A.43)

where $\mathcal{H}'_{\beta\alpha}(t) = \langle \beta | \mathcal{H}'(t) | \alpha \rangle$ and use has been made of the fact that $\mathcal{H}'(t)$ is Hermitian and where

\[ \left\langle \mathcal{H}'_{\beta\alpha}(t_1) \mathcal{H}'_{\alpha\beta}(t_2) \right\rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_{-\tau/2}^{+\tau/2} \left\langle \mathcal{H}'_{\beta\alpha}(t') \mathcal{H}'_{\alpha\beta}(t') \right\rangle dt'. \]

(A.44)

Equation (A.43) gives the differential cross-section for a scattering process centred around $t = 0$. In the event that the non-equilibrium time-dependence of the system is slow on the timescale of the scattering, then, by the ergodic hypothesis, the time average becomes replaced by a local-time ensemble average.

New Journal of Physics 15 (2013) 015014 (http://www.njp.org/)
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