INCOHERENT X-RAY SCATTERING BY ATOMS IN SEMICLASSICAL APPROXIMATION

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The Fourier transform is used for the evaluation of the semiclassical wavefunction in momentum representation. As a consequence of this approach, the incoherent scattering function is obtained.

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1. Introduction

The Thomas-Fermi calculations of the incoherent scattering function are well known [1, 2]. This model gives satisfactory results in the description of the incoherent X-ray scattering by atoms in the region of large values of the momentum transfer $k$. In the region of small and intermediate $k$, the Thomas-Fermi results lie substantially higher than the results of the self-consistent-field Hartree-Fock method. Essential improvements were not obtained with the use of the Thomas-Fermi-Dirac model of the atom [3, 4]. In statistical calculations, the situation is incorrigible for the range of small $k$ [3]. The improvement is possible for the range of intermediate $k$. It follows from the fact that the incoherent scattering cross-section is sensitive to a choice of an atomic potential model. From this point of view, it is interesting to calculate the incoherent scattering cross-section using the semiclassical approximation. The application of the semiclassical atomic models [5, 6] is more correct in this approximation. Although this task has not been discussed in literature, it has independent significance for several applied problems.

2. The calculation method

One starting point of this calculation, and an useful one here, is the impulse approximation in which the double differential cross section $d^2\sigma/d\omega d\Omega$ for the incoherent X-ray scattering is given by [7]

$$\frac{d^2\sigma}{d\omega d\Omega} = 2 \left(\frac{d\sigma}{d\Omega}\right)_0 \frac{\omega_1}{\omega_2} \frac{m}{k} \sum_n J_{n\mu}(q)$$

(1)

where $(d\sigma/d\Omega)_0$ is the Thomson cross-section, $h\omega_1$ and $h\omega_2$ are the initial and final energies of the photon, $\omega = \omega_1 - \omega_2$, $k = 2(\omega_1/c) \sin(\theta/2)$, $\theta$ is the scattering angle, $q = \hbar k/2 - m\omega/k$, $m$ is the mass of an electron, $c$ is the velocity of light and

$$J_{n\mu}(q) = \frac{2\pi}{\hbar} \int_{|q|/\hbar}^\infty \left|\chi_{n\mu}(\kappa)\right|^2 \kappa d\kappa .$$

(2)
The quantity $\chi_{nl\mu}(\mathbf{x})$ is the momentum representation of the atomic wave function $\psi_{nl\mu}(r)$

$$
\chi_{nl\mu}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\mathbf{x}\cdot\mathbf{r}} \psi_{nl\mu}(r) \, d^3r .
$$

The coefficient 2 in (1) is the spin factor.

The basic distinction of the present work from other models [1, 3, 4, 7] is the use of the semiclassical approximation with radial wave function $u_{nl}(r)$ defined by

$$
u_{nl}(r) = \frac{a_{nl}}{k_{nl}^{1/2}} \cos \left( \int_{r_1}^r k_{nl} \, dr - \pi/4 \right) .
$$

where

$$
k_{nl}(r) = \frac{1}{\hbar} \left[ 2m(E_{nl} - U(r) - \hbar^2(l + 1/2)^2/2mr^2) \right]^{1/2} .
$$

Here, $U(r)$ is the potential energy of an atomic electron, $E_{nl}$ is the eigenvalue of the energy, $a_{nl}$ is the normalization constant, $r_1$ is the left turning point, and $l$ is the orbital quantum number.

Our aim now is to calculate the Fourier transform (3) of the semiclassical atomic wave function

$$
\psi_{nl\mu}(r) = \frac{u_{nl}(r)}{r} \, Y_{l\mu}(\theta, \varphi) .
$$

It will be seen that in this approach the incoherent scattering cross-section may be expressed in analytical form.

3. The semiclassical wavefunction in momentum representation

The central problem now is to compute the Fourier transform

$$
\chi_{nl\mu}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\mathbf{x}\cdot\mathbf{r}} \frac{1}{r} u_{nl}(r) \, Y_{l\mu}(\theta, \varphi) \, dV .
$$

For isotropic or spherically averaged system this integral equals zero if $\mu \neq 0$, therefore taking into account that in the semiclassical approximation [8]

$$
Y_{l0} = \frac{i^l \cos \left[ (l + 1/2) \theta - \pi/4 \right]}{\pi \left( \sin \theta \right)^{1/2}}
$$

it is easy to see that

$$
\chi_{n00}(\mathbf{x}) = \frac{1}{(2\pi)^{1/2}} \int I(\mathbf{x}, r) \, u_{nl}(r) \, r \, dr
$$