Chapter 7

Structure and Electronic Properties of Liquid Semiconductors

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J. Tauc (ed.), *Amorphous and Liquid Semiconductors* © Plenum Publishing Company Ltd 1974
7.1 THE STRUCTURE OF PURE LIQUIDS

7.1.1 The Interference Function

It is now quite clear that a good knowledge of \( a(q) \), the interference function, is necessary for a fundamental understanding of the electronic properties of liquid conductors. The purpose of this section is to describe the use of neutron and X-ray diffraction techniques in determining this quantity. In most scattering experiments the measured intensities are proportional to differential scattering cross sections. Let \( b_c \) and \( b_i \) represent respectively the bound atom scattering lengths for coherent and incoherent scattering. Then the differential scattering cross section for coherent scattering is \( N b_c^2 a(q) \) whilst that for incoherent scattering is \( N b_i^2 \), provided the scattering is perfectly elastic (see, for example, Bacon (1962)), \( a(q) \) here is defined in the usual way as the expectation value of \( N S(q) S^*(q) \) where

\[
S(q) = \sum_i e^{-iq \cdot r_i}
\]

\( N \) is the number of scatterers, \( q \) is a wave number and \( r_i \) refers to the positions of the nuclei.

Contrary to what is frequently supposed, \( a(q) \) is not directly accessible through X-ray or neutron diffraction experiments either in principle or in practice. Indeed, until comparatively recently marked discrepancies existed between \( a(q) \) data derived by different techniques and these in part can be traced to a failure to recognize the inherent limitations of neutron or X-ray diffraction methods.

In a conventional diffraction experiment an integrated intensity \( J \) is measured at a given angle of scattering \( \theta \). The integration over the energy is performed by the detector so that an effective differential scattering cross section \( (d\sigma/d\Omega)_{\text{eff}} \) rather than a true static cross section is measured. In terms of the generalized quantity \( S(q, \omega) \) which measures the probability that the radiation absorbs energy \( \hbar \omega \) from the liquid and imparts momentum \( \hbar q \) to it, Placzek (1952) showed that

\[
\left( \frac{d\sigma}{d\Omega} \right)_{\text{eff}} \propto \int_{-E_0/\hbar}^{\infty} \frac{\kappa}{\kappa_0} S(q, \omega) f(\omega) \, d\omega
\]

(7.1)

where \( E_0 \) is the incident energy of the neutron, \( \kappa_0 \) and \( \kappa \) are the incident and final wave numbers, and \( f(\omega) \) measures the energy dependence of the detection system. If \( E_0 \) greatly exceeds the energy transfers, the integral on