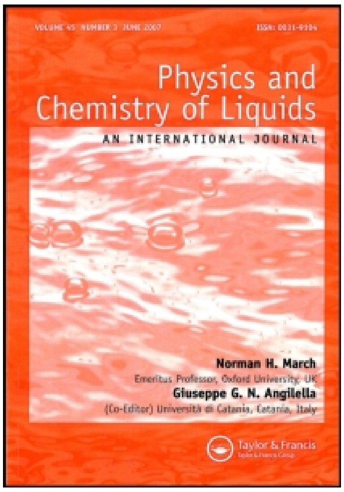

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On the placzek correction for simple liquids and gases

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On the Placzek Correction for Simple Liquids and Gases

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The "inelasticity correction" (IC) due to deviations from the static approximation in structure measurements using neutrons for liquid aluminium at 1000 K and liquid copper at 1393 K has been calculated. The dynamical scattering function $S(Q, \omega)$ has been approximated by the viscoelastic model and by the result of MD-calculations. Incoming neutron wavelengths ranging from 0.7 up to 2.4 Å have been investigated. The results are compared with the usual Placzek correction in the form as derived by Yarnell *et al.* In analogy to the ideal gas model and the model of Ascarelli and Caglioti (AC) approximate ways of allowing for recoil and detailed balance when calculating the correction using a classical model of $S(Q, \omega)$ are proposed. It is shown that AC can be useful to obtain a first estimate of IC in cases where no models of $S(Q, \omega)$ are available. As a demonstration IC has been calculated for liquid rubidium and krypton gas at several densities.

1 INTRODUCTION AND THEORY

In neutron diffraction experiments the structure factor $S(Q)$ can be directly measured only if the static approximation holds.[1] In order to correct for deviations several methods all implying a series expansion of the exact double differential scattering cross section have been proposed.[2-4] Molecular fluids have been extensively discussed by Powles and coworkers,[5] by Egelstaff and coworkers[6] and also by others.[7,8] The ideal gas was also recently treated.[9] For simple systems the most widely used method to correct for inelastic scattering is the one proposed by Placzek[2] in the form as extended by Yarnell *et al.*[10] to arbitrary counter efficiencies.

In this paper the applicability of this so called Placzek correction in neutron diffraction measurements on simple liquid metals is discussed using as examples aluminium and copper. In the case of aluminium recent molecular dynamics (MD)[11] calculations as well as experimental data[12] on the dynamical structure factor $S(Q, \hbar\omega)$ become available over a wide (Q, ω) range. Because of the small mass and high melting temperature of aluminium the Placzek correction is comparatively large. Copper has been chosen, because its scattering law can be fitted by the same analytical model as aluminium[13] with good accuracy, its mass, however, is about twice as large. Because of the rapidly growing interest in the structure of dense gases[14] we have also included the gas case into our discussion.

In the next few paragraphs we write down the formulae which are necessary for the further discussion, closely following the work of Yarnell *et al.*[10]

The structure factor $S(Q)$ is defined by

$$S(Q) = \int_{\substack{-\infty \\ Q=\text{const.}}}^{+\infty} S(Q, \hbar\omega)\, \mathrm{d}(\hbar\omega) \tag{1}$$

The integration over the dynamical structure factor $S(Q, \hbar\omega)$ (the dimension of which will be inverse energy units throughout this paper) has to be performed keeping the wavevector transfer Q constant. $\hbar\omega$ is the energy transfer to the target.

The "experimental" structure factor can be written[2]

$$S(Q_0)_{\text{exp}} = \frac{1}{\varepsilon(k_0)} \int_{\substack{-\infty \\ 2\theta=\text{const.}}}^{E_0} \frac{k}{k_0} S(Q, \hbar\omega)\varepsilon(k)\, \mathrm{d}(\hbar\omega) \tag{2}$$

as in a diffraction experiment the intensity is summed over $\hbar\omega$ at a constant scattering angle 2θ. $\hbar Q_0$ is the elastic momentum transfer. $\mathbf{k}_0$ and $\mathbf{k}$ are the wavevectors of the incident and scattered neutron, respectively. E_0 is the energy of the incident neutron. The counter efficiency is approximated by

$$\varepsilon(k) = 1 - \exp(-Ck_0/k) \tag{3}$$

with C being a counter parameter.

An approximate relation between the experimental and theoretical structure factors

$$S(Q_0)_{\text{exp}} = S(Q) + f(Q) \tag{4}$$

is obtained by expanding the terms in the integral (2) in a power series in $\hbar\omega/E_0$ and calculating their respective derivatives at Q_0 and k_0.[2] $\varepsilon(k)$ in full generality was taken into account later.[10]

The Placzek correction terms $f^{r}(Q)$ and $f^{cl}(Q)$ are defined by

$$f^{r}(Q) = \frac{m}{2M}\frac{k_B T}{E_0} - \frac{m}{M}\left(C_1 + C_3\frac{k_B T}{E_0}\right)\left(\frac{Q}{k_0}\right)^2 + \frac{1}{2}\left(\frac{m}{M}\right)^2\left(1 + 2C_2\frac{Q^2}{k_0^2}\right)\left(\frac{Q}{k_0}\right)^2 \tag{5}$$

and

$$f^{cl}(Q) = \frac{m}{2M}\frac{k_B T}{E_0}\left[1 - 2C_3\left(\frac{Q}{k_0}\right)^2\right]. \tag{6}$$

Here m and M are the masses of the neutron and the scatterer, respectively. k_B is the Boltzmann constant, T is the sample temperature. C_1, C_2 and C_3 are constants depending on the counter efficiency (for details see ref. 10). Equation (5) was arrived at by using the moments of $S(Q, \hbar\omega)$ and assuming the scatterer was an ideal gas of atoms with the mass M at the temperature T. Equation (6) is obtained by the same approximation but with the classical moments (i.e. $\langle\omega^1\rangle = 0$ and $\langle\omega^2\rangle = Q^2 k_B T/M$). We introduce $f^{cl}(Q)$ because theoretical models for $S(Q, \hbar\omega)$ are developed usually for classical systems, the moments of which correspond to $f^{cl}(Q)$ rather than to $f^{r}(Q)$. As will be shown in the next section, there is, however, a way of including recoil and detailed balance into classical models of $S(Q, \hbar\omega)$ sufficient for our purposes.

In our calculations we evaluate (2) numerically for a number of scattering kernels $S(Q, \hbar\omega)$ and compare the results with PC. We shall call the correction obtained by numerical integration of (2) "inelasticity correction" (IC) and denote it by $\phi(Q)$ in contrast to $f(Q)$. $\phi(Q)$ is therefore defined by the "exact equation" (see footnote)

$$S(Q_0)_{\text{exp}} = S(Q) + \phi(Q) \tag{7}$$

This equation is exact if one uses the correct scattering kernel or experimental inelastic data. In this paper we calculate $\phi(Q)$ using theoretical models and MD results for $S(Q, \hbar\omega)$. An attempt to calculate $\phi(Q)$ from experimental time-of-flight data is under way.[14]

II THE PLACZEK CORRECTION FOR SIMPLE LIQUIDS

As already mentioned, we have approximated the symmetrical scattering law $\tilde{S}(Q, \hbar\omega)$ which is defined by

$$\tilde{S}(Q, \hbar\omega) = S(Q, \hbar\omega)\exp(-\hbar\omega/2k_B T) \tag{8}$$

Note: $\phi(Q)$ is different from $IN(Q)$ as defined by Copley.[9]

TABLE I

Numerical values of the parameters of VEL for liquid aluminium and copper.

	T	ω_E	σ	τ_0	Q_1	ν	$S(Q)$
dimension	K	$\sec^{-1}$	Å	sec	$Å^{-1}$		
Al	1000	$5.19 \cdot 10^{13}$	2.56	$0.421 \cdot 10^{-13}$	2	$\frac{1}{3}$	From ref. 16
Cu	1393	$4.16 \cdot 10^{13}$	2.29	$0.821 \cdot 10^{-13}$	2	$\frac{1}{3}$	From ref. 13

using the viscoelastic model (VEL).[15,12,13] Thus

$$\tilde{S}(Q, \hbar\omega) = \frac{1}{\hbar}\frac{1}{\pi}\frac{S(Q)\omega_0^2(\omega_l^2 - \omega_0^2)\tau(Q)}{[\omega\tau(Q)(\omega^2 - \omega_l^2)]^2 + (\omega^2 - \omega_0^2)^2} \tag{9}$$

The notations are

$$\omega_0^2 = Q^2 k_B T / M S(Q) \tag{10}$$

$$\omega_l^2 = 3\frac{Q^2 k_B T}{M} + \omega_E^2\left[1 - 3\frac{\sin Q\sigma}{Q\sigma} - 6\frac{\cos Q\sigma}{(Q\sigma)^2} + 6\frac{\sin Q\sigma}{(Q\sigma)^3}\right] \tag{11}$$

$$\begin{aligned}\tau^{-2}(Q) = S^{2\nu}(Q)\Bigg\{&\frac{8}{3}\left(\omega_l^2 - \omega_0^2 - \frac{Q^2 k_B T}{M}\right) + \frac{1}{\tau_0^2} \\ &- \frac{8}{3}\left(\omega_l^2 - \omega_0^2 - 2\frac{Q^2 k_B T}{M}\right)\left(1 + \frac{Q^2}{Q_1^2}\right)^{-1}\Bigg\}\end{aligned} \tag{12}$$

In Table I we list the values of the parameters used in our calculations. We have approximated $S(Q)$ for Al at 1000 K by the X-ray data at 943 K by Ruppersberg and Wehr.[16]

The approximation VEL as given in eq. (9) is correct up to the fourth classical moment of $S(Q, \hbar\omega)$.

The reason why VEL is used in the calculations is that it has been found to fit the measured $\tilde{S}(Q, \hbar\omega)$ for liquid aluminium. Thus, in this respect, *no* approximation of the scattering cross section is involved. Following Schofield[17] one can include detailed balance into this model via relation (8). The corresponding IC's are denoted $\phi_{\mathrm{VEL}}^{\tilde{S}}(Q)$ and $\phi_{\mathrm{VEL}}^{S}(Q)$, respectively. Three pairs of incident neutron energies and counter parameters have been selected for the calculation of IC as given in Table II.

The cases I and II correspond to experiments on liquid aluminium as described by Eder and coworkers[18] and approximately to the ones by Dahlborg and Olsson,[19] respectively. Further, case II corresponds to recent structure measurements on liquid copper.[13] Case III is included because Stallard and Davies[20] used three neutron wavelengths (2.38, 1.0, 0.72 Å) to measure $S(Q)$ of liquid aluminium over the Q range $0.8 < Q < 14.5$ $Å^{-1}$.

TABLE II

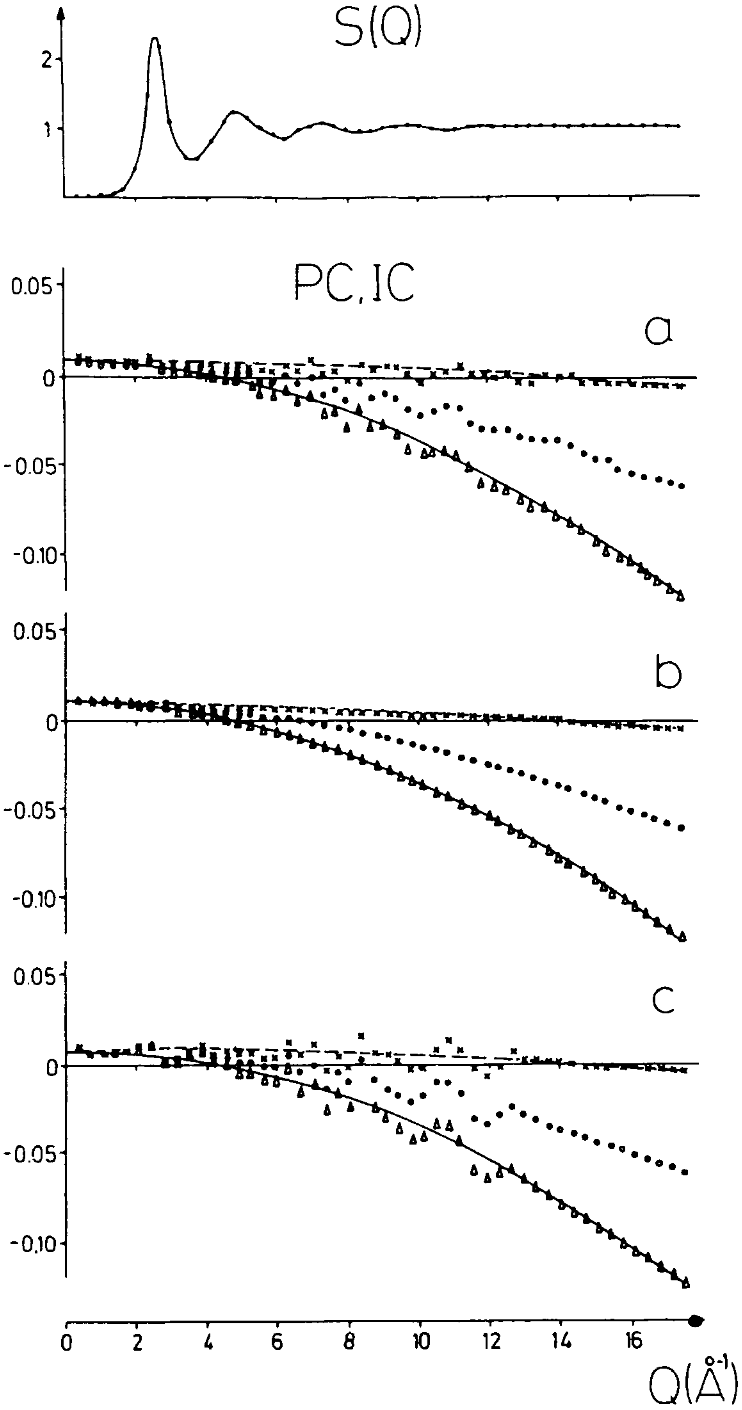
Pairs of incident neutron wavelengths λ_0 and counter parameters C for which IC has been calculated.

	λ_0	C
case I	0.7	2.8
case II	1.0	1.3
case III	2.4	4.26

A similar experiment using the wavelengths 2.51, 1.17 and 0.72 Å was performed by Jovic *et al.*[21] In both these experiments $S(Q)$ was not determined absolutely meaning that the data were not normalized by a vanadium calibration measurement. Instead other known properties of $S(Q)$ were used for normalization purposes[1,22]

In Figure 1a the PC's $f^{cl}(Q)$ and $f^{r}(Q)$ are compared to the IC's $\phi_{\text{VEL}}(Q)$, $\phi^{S}_{\text{VEL}}(Q)$ and $\phi^{r}_{\text{VEL}}(Q)$. ($\phi^{r}_{\text{VEL}}(Q)$ will be discussed below). Also shown is $\phi^{S}_{\text{MD}}(Q)$ calculated from eqs. (2), (7) and (8) using molecular dynamics results. The MD data did not cover a Q region large enough. This was circumvented by making least squares fits of a theoretical model to the MD data and then using the predictions of the model in the Q region where no data were available. The detailed balance was included according to the Schofield prescription. Although the IC's are smooth curves we have chosen to represent them by a number of points only for reasons of computational economy. The number has been chosen requiring that the main features if IC should show up clearly (lines through the points are meant as guides for the eye only). The difference between ϕ^{S}_{VEL} and ϕ^{S}_{MD} is small as is expected from the relatively good agreement between the VEL, MD-data and experimental data.[12] $\phi_{\text{VEL}}(Q)$ oscillates around $f^{cl}(Q)$ with amplitudes which cease at around $Q = 12.5$ Å^{-1}. This vanishing is due to the limited Q-range of the used $S(Q)$. For $Q > 12.5$ Å$^{-1}S(Q)$ has been put equal to 1. The oscillations are of the order of the statistical error in a careful scattering experiment performed under favourable conditions (negligible container scattering and background, etc.). ϕ^{S}_{VEL} (Q) deviates from $f^{r}(Q)$ as expected because only the detailed balance condition has been included into the scattering kernel whereas the difference between $f^{cl}(Q)$ and $f^{r}(Q)$ mainly comes from recoil.

To proceed, we studied two simple models having scattering laws corresponding to $f^{cl}(Q)$. These are i) the ideal gas model and ii) the model constructed by Ascarelli and Caglioti,[4] further denoted by IG and AC, respectively. The ideal gas was recently discussed by Copley.[9] The classical models can be easily extended to include recoil and to obey the detailed balance condition. We shall denote the extended models IGR and ACR.


S(Q)
2
1
PC, IC
a
0.05
0
-0.05
-0.10
b
0.05
0
-0.05
-0.10
c
0.05
0
-0.05
-0.10
0
2
4
6
8
10
12
14
16
$Q(\mathring{A}^{-1})$

These are obtained from IG and AC, respectively, by multiplying with $K(Q, \omega)$ defined by

$$K(Q, \omega) = \exp\left(\frac{\hbar\omega}{2k_B T} - \frac{\hbar^2 Q^2}{8k_B TM}\right) \tag{13}$$

where, in the case of AC, M has to be replaced by $M^* = M \cdot S(Q)$. The scattering laws have the following form:

i) IG:

$$\tilde{S}(Q, \hbar\omega) = \frac{1}{\hbar}\left[\frac{M}{2\pi Q^2 k_B T}\right]^{1/2} \exp\left(-\frac{M\omega^2}{2Q^2 k_B T}\right) \tag{14}$$

IGR:

$$S(Q, \hbar\omega) = \frac{1}{\hbar}\left[\frac{M}{2\pi Q^2 k_B T}\right]^{1/2} \exp\left[-\frac{M}{2Q^2 k_B T}\left(\omega - \frac{\hbar Q^2}{2M}\right)^2\right] \tag{15}$$

ii) AC:

$$\tilde{S}(Q, \hbar\omega) = \frac{1}{\hbar} S(Q)\left[\frac{MS(Q)}{2\pi Q^2 k_B T}\right]^{1/2} \exp\left(-\frac{MS(Q)\omega^2}{2Q^2 k_B T}\right) \tag{16}$$

ACR:

$$S(Q, \hbar\omega) = \frac{1}{\hbar} S(Q)\left[\frac{MS(Q)}{2\pi Q^2 k_B T}\right]^{1/2} \exp\left[-\frac{MS(Q)}{2Q^2 k_B T}\left(\omega - \frac{\hbar Q^2}{2MS(Q)}\right)^2\right] \tag{17}$$

As IG and AC are classical models their energy moments equal those corresponding to $f^{cl}(Q)$. The same holds to a good approximation for IGR and ACR with respect to $f^r(Q)$. (Because of the presence of $S(Q)$ ACR has a second moment $\langle\omega^2\rangle$ slightly different from the ideal gas value at Q values where $S(Q) \neq 1$; the moments differ, however, in our case less than 2%). In Figure 1b the PC's and IC's are plotted for the ideal gas and case I assuming the gas consisting of aluminium atoms at 1000 K. $f^{cl}(Q)$ and $\phi_{\mathrm{IG}}(Q)$ nearly coincide as well as $f^r(Q)$ and $\phi_{\mathrm{IGR}}(Q)$ showing that the expansion method of Placzek is valid at this incoming neutron wavelength. We have included in Figure 1b $\phi^S_{\mathrm{IG}}(Q)$, which was calculated using the Schofield prescription (8) and IG to obtain $S(Q, \hbar\omega)$. $\phi^S_{\mathrm{IG}}(Q)$ deviates from $\phi_{\mathrm{IGR}}(Q)$ in the same way as $\phi^S_{\mathrm{VEL}}(Q)$ does from $f^r(Q)$. The effect can qualitatively be simulated using AC and ACR as shown in Figure 1c. Comparison of Figure 1a and Figure 1c reveals that $\phi_{\mathrm{AC}}(Q)$ exaggerates the oscillations as compared to $\phi_{\mathrm{VEL}}(Q)$. As the ideal gas model is accurate in the limit of high Q values for any monatomic

FIGURE 1 Placzek corrections (PC) and inelasticity corrections (IC) for liquid aluminium. Top curve is measured $S(Q)^{16}$. Parameters correspond to case I. a) VEL model. Notations: dashed line: $f^{cl}(Q)$, full line: $f^r(Q)$, crosses: $\phi_{\mathrm{VEL}}(Q)$, open circles: $\phi^S_{\mathrm{VEL}}(Q)$, triangles: $\phi^r_{\mathrm{VEL}}(Q)$, squares: $\phi^S_{\mathrm{MD}}(Q)$. b) Ideal gas models. Notations: dashed line: $f^{cl}(Q)$, full line: $f^r(Q)$, crosses: $\phi_{\mathrm{IG}}(Q)$, circles: $\phi^S_{\mathrm{IG}}(Q)$, triangles: $\phi_{\mathrm{IGR}}(Q)$. c) AC and ACR models. Notations: dashed line: $f^{cl}(Q)$, full line: $f^r(Q)$, crosses: $\phi_{\mathrm{AC}}(Q)$, open circles: $\phi^S_{\mathrm{AC}}(Q)$, triangles: $\phi_{\mathrm{ACR}}(Q)$.

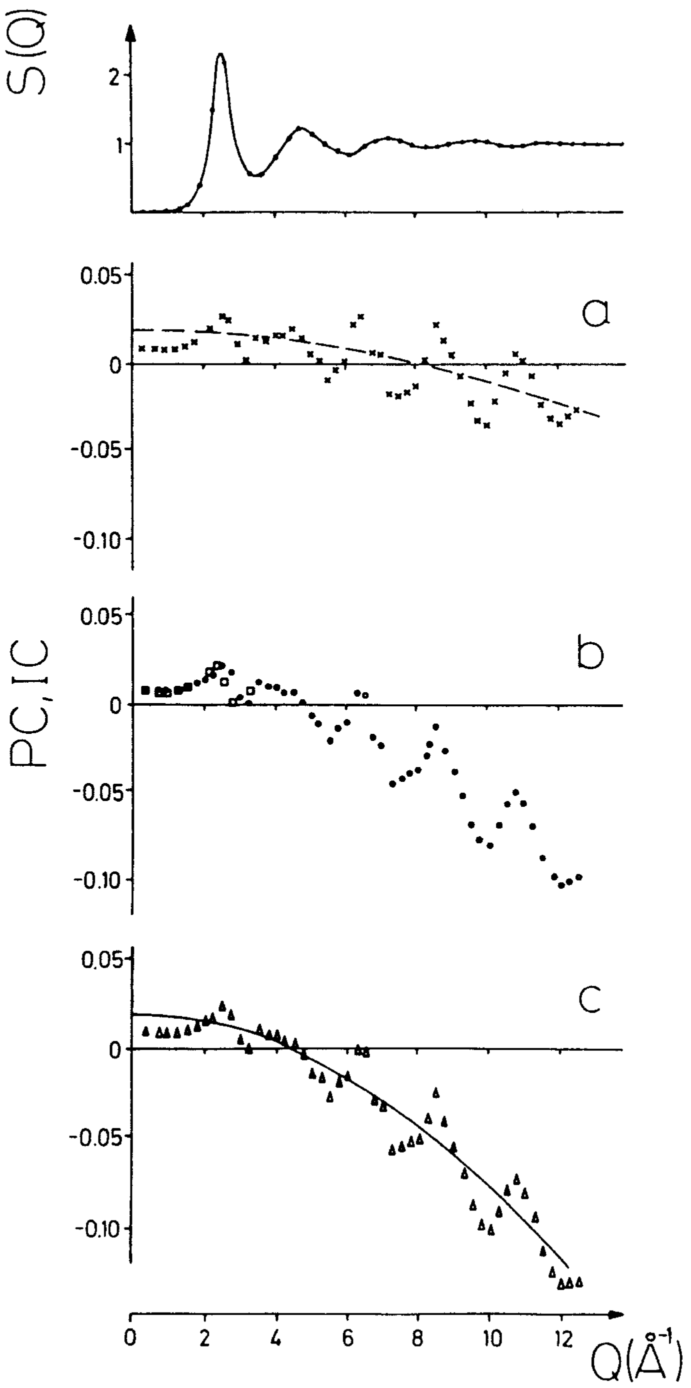


FIGURE 2 Same as Figure 1a with parameters corresponding to case II.

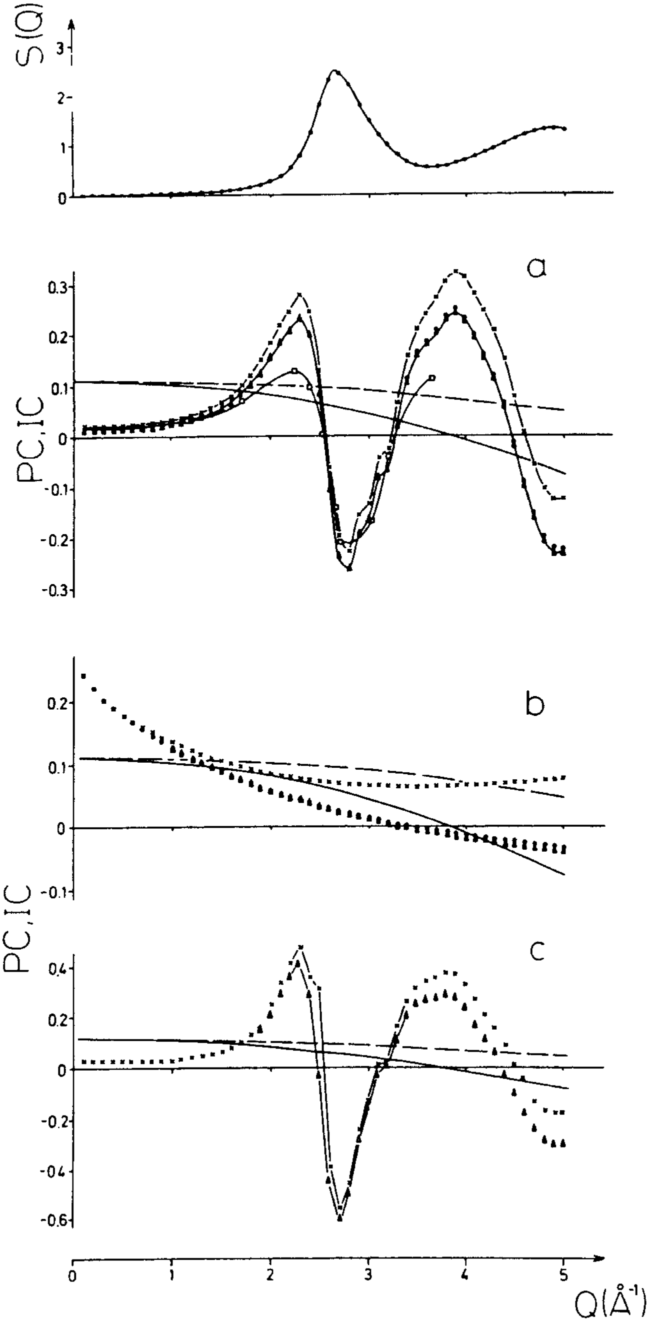


FIGURE 3 Same as Figure 1 with parameters corresponding to case III.

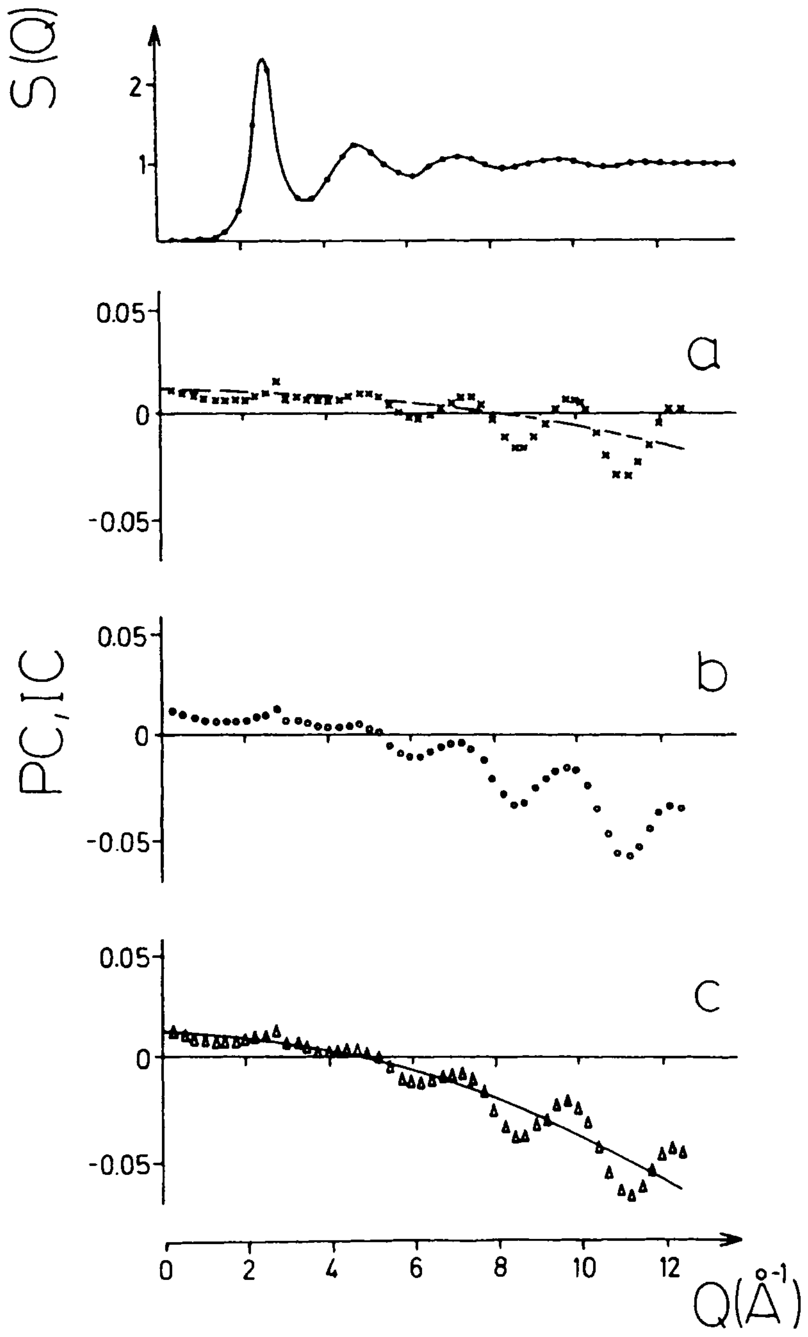


FIGURE 4 PC and IC for liquid copper at 1393 K. Parameters correspond to case II. Notations see Figure 1a.

system we have extended VEL by multiplying with $K(Q, \omega)$. The resulting IC is denoted by $\phi^r_{\mathrm{VEL}}(Q)$ and is also given in Figure 1.

Figures 2 and 3 show the PC's and IC's for liquid aluminium for the cases II and III, respectively. For convenience the structure factor is also given. It is seen that the expansion method is increasingly worse as the neutron wavelength increases. This is expected as then the detailed shape of $S(Q, \hbar\omega)$ is more and more important. The model of Ascarelli and Caglioti[4] gives an IC having considerably too large oscillations. It gives, however, correctly the qualitative behaviour of IC.

Figure 3 shows that the structure factor for aluminium as obtained in a neutron scattering experiment using a neutron wavelength of 2.4 Å is strongly distorted (amplitude of main peak is reduced by about 10%) and that it is seriously affected at the leading edge of the main peak. Correction of the experimental data in the usual way[22] using $f^r(Q)$ instead of $\phi^r_{\mathrm{VEL}}(Q)$ means that multiple and (in cases where applicable) incoherent scattering will be underestimated, because of the large difference between PC and IC at very low Q-values. It is also obvious that if the height of the measured main peak of $S(Q)$ is used for normalization purposes and not a vanadium calibration measurement the resulting $S(Q)$ will be seriously distorted.

This holds also for copper, the PC's and IC's of which are displayed in Figures 4 and 5 (cases II and III). It is interesting to note that $\phi^r_{\mathrm{VEL}}(Q)$ for copper and aluminium are of similar magnitude for $\lambda = 2.4$ Å, irrespective of the mass difference.

VEL is a convenient model to study the influence of the magnitude of the quasielastic scattering $S(Q, 0)$ on $\phi(Q)$. We can exploit the fact, that the lower moments of VEL are not affected by the choice of v. Figure 6 compares the IC for liquid aluminium for $v = 0$ and $v = \frac{1}{3}$, where $v = 0$ implies an increase of $S(Q, 0)$ of 34% at the main peak when compared to $v = \frac{1}{3}$. As expected the increase of $S(Q, 0)$ leads to a reduction of $\phi^r_{\mathrm{VEL}}(Q)$. This $\phi^r_{\mathrm{VEL}}(Q)$ is in better agreement with the MD-result ϕ^S_{MD} except in the Q-region around the main peak.

Recently, a number of experiments has been published, aiming at measuring $S(Q)$ over a wide range of densities and temperatures for liquid rubidium.[14,23,24] As PC does not depend on the density and IC is dominated by the topography of $S(Q, \hbar\omega)$ at large neutron wavelengths a systematic error will be introduced when correcting the experimental data by the conventional Placzek method. Fully aware of the fact that ACR will reflect this only qualitatively we have calculated $\phi_{\mathrm{ACR}}(Q)$ using the parameters of the experiment of Block *et al.*[23] on expanded liquid rubidium (See Table III). The hard core parameter σ has been taken from their fit of the Percus-Yevick hard core structure factors $S_{\mathrm{PY}}(Q)$[25] to the experimental data. $S_{\mathrm{PY}}(Q)$ has been used as input to ACR. Figure 7 shows the resulting $\phi_{\mathrm{ACR}}(Q)$ for the two temperatures

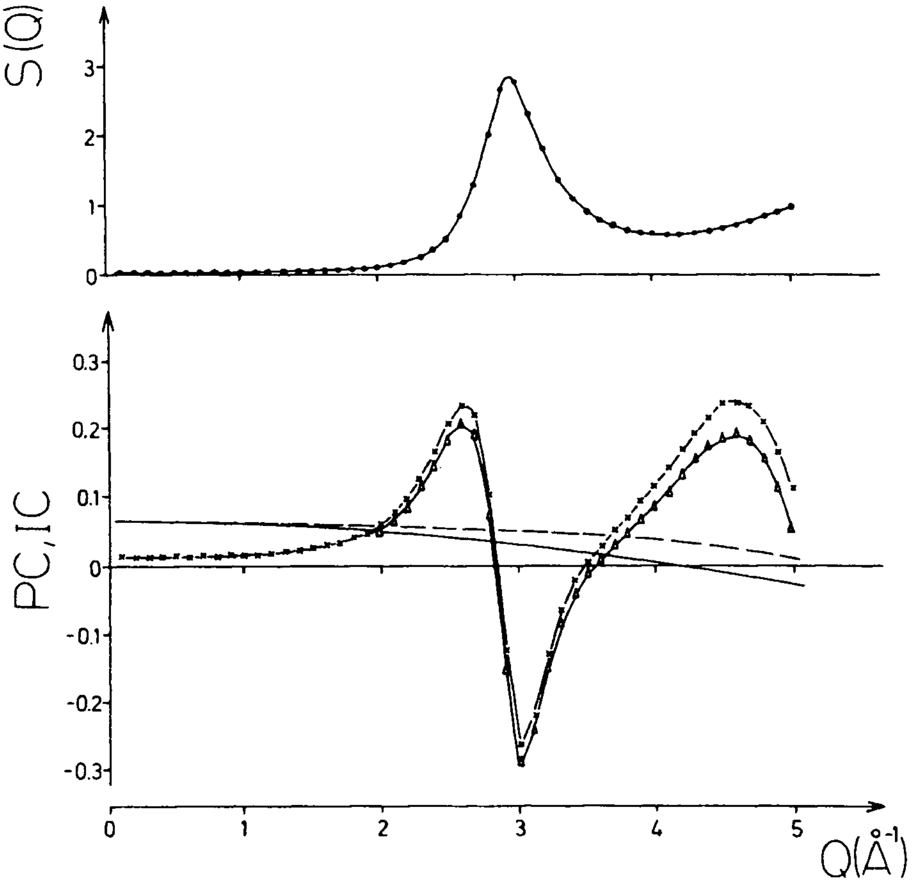


FIGURE 5 PC and IC for liquid copper at 1393 K. Parameters correspond to case III. Notations see Figure 1a.

together with the corresponding $f'(Q)$. For convenience the two $S_{PY}(Q)$ are also included in Figure 7. Despite of the qualitative nature of the IC obtained via ACR, there is a clear indication, that PC is not adequate at this long neutron wavelength and that a model for $S(Q, \hbar\omega)$ is needed to correct $S(Q)$. It is interesting to note that $\phi_{ACR}(Q)$ increases for $Q \to 0$ in qualitative agreement with the measured structure factor (See Figure 1 in ref. 23). Further, at this large neutron wavelength the normalization to vanadium may be in error if the vanadium data are corrected using PC. To obtain an estimate of this we used IGR as the simplest assumption possible for the scattering law of vanadium. A calculation of IC then gives that $0.11 < \phi_{IGR}(Q) < -0.03$ while $0.7 < f'(Q) < -0.05$ for $0 < Q < 2.5$ Å^{-1}. This corresponds to a possible calibration error up to 4%.

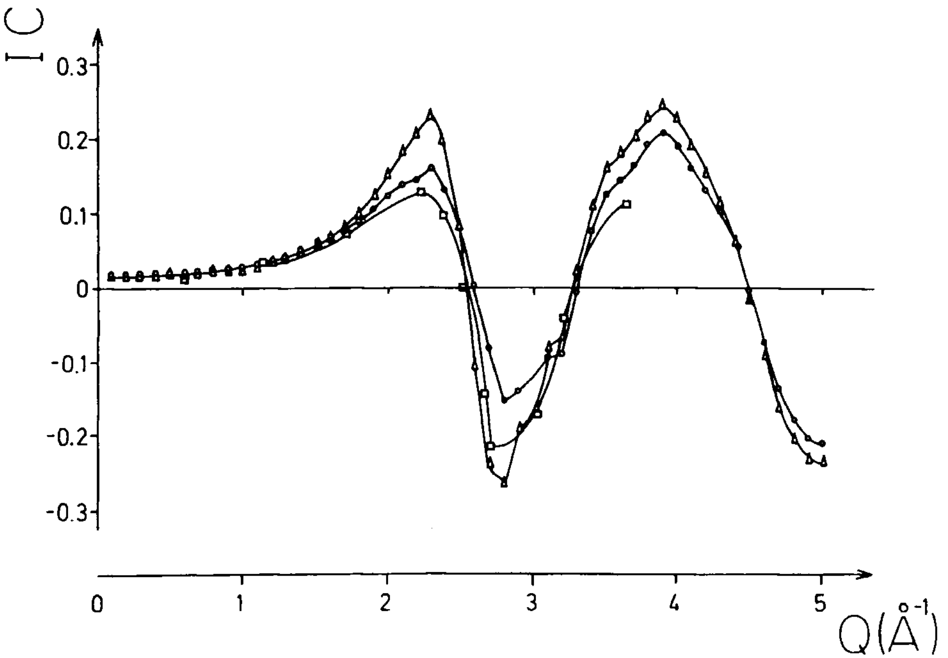


FIGURE 6 Influence of magnitude of $S(Q, 0)$ on $\phi^{c}_{\mathrm{VEL}}(Q)$. Parameters correspond to case III. Triangles: $\phi^{c}_{\mathrm{VEL}}(Q)$ obtained with $\nu = \frac{1}{3}$, circles: $\phi^{c}_{\mathrm{VEL}}(Q)$ with $\nu = 0$. For VEL the parameters of liquid aluminium (Table 1) have been used. For convenience, $\phi^{S}_{\mathrm{MD}}(Q)$ (see Figure 3) also has been included (squares).

TABLE III

Numerical values of the parameters of the experiment on liquid rubidium, as used in the calculations of $\phi_{\mathrm{ACR}}(Q)$. Notations: T = temperature, ρ = number density, σ = hard core diameter. The value of C has been chosen as no value is given in reference 23.

T	ρ	σ	λ	C
K	Å^{-3}	Å	Å	
450	0.0100	4.2	4.9	4.0
1300	0.00735	3.8		

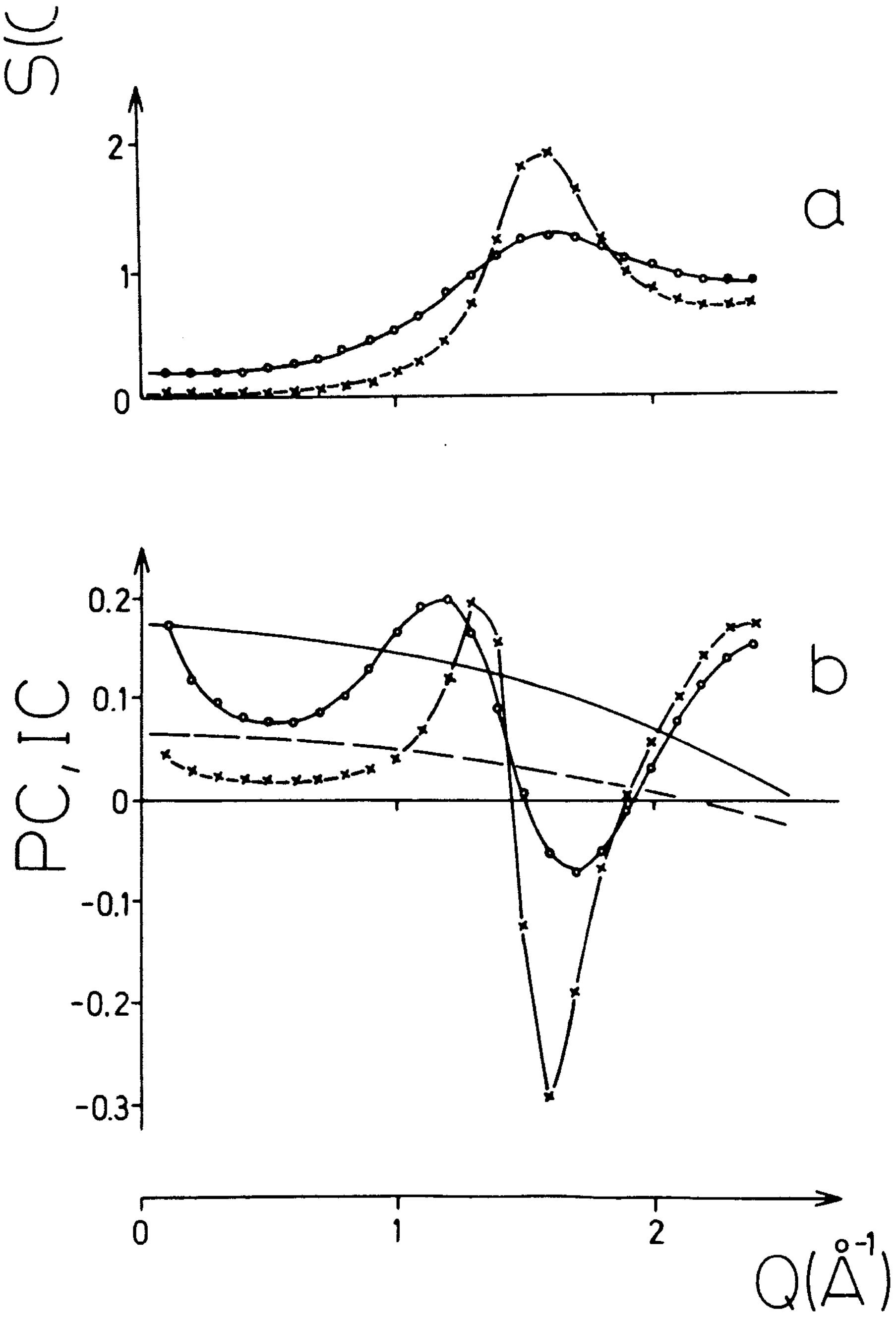


FIGURE 7 PC and IC for liquid rubidium at 1300 K and 450 K. a) $S_{PY}(Q)$ at 1300 K (circles) and at 450 K (crosses) b) full line: $f'(Q)$ at 1200 K, dashed line: $f'(Q)$ at 450 K, circles: $\phi_{ACR}(Q)$ at 1200 K, crosses: $\phi_{ACR}(Q)$ at 450 K.

From the calculated results displayed in Figures 1–7 the following conclusions regarding the correction for inelastic scattering in a neutron diffraction experiment can be drawn:

i) The differences between IC and PC are not negligible especially not for neutron wavelengths of the order of 1 Å and larger.

ii) $K(Q, \omega)$ takes satisfactorily quantummechanical effects into account.

iii) The Schofield prescription (8) is valid for large incoming neutron wavelengths.

iv) There is no general prediction whether the structure of $S(Q)_{exp}$ is reduced or enhanced due to IC in a diffraction experiment. This depends both on the neutron wavelength used and the Q-range under investigation.

v) $\phi^r_{VEL}(Q)$ which we regard as the exact IC can be approximated by

$$\phi^r_{VEL}(Q) = f^r(Q) + \phi_{VEL}(Q) - f^{cl}(Q) \qquad (18)$$

as an alternative to using $K(Q, \omega)$.

It is expected that i)–v) hold generally, not only for the VEL model (see also section III).

III THE PLACZEK CORRECTION FOR SIMPLE DENSE GASES

Gases are particularly well suited to reveal the dependence of IC to the topography of $S(Q, \hbar\omega)$ as the IC's obtained for different densities at the same temperature all correspond to the same PC. The study of the structure of gases at different densities gives the opportunity to gain information about the triplet potential.[14]

Here we obtain IC from two models: i) ACR and ii) the Q-dependent triple relaxation time model (QTRT).[26] Both models are calculated for hard spheres. The QTRT is extended by applying $K(Q, \omega)$ and thus the IC is denoted $\phi^r_{QTRT}(Q)$. The parameters have been chosen to agree with those of the experiment on krypton gas[14] (see Table IV).

TABLE IV

Numerical values of the parameters of the experiment on krypton gas as used in the calculations. For notations see Table III.

λ_0	C	T	σ	ρ
Å		K	Å	$Å^{-3}$
2.39	1.51	295	4.0	0.000258
2.39	1.51	295	4.0	0.00288
2.39	1.51	295	4.0	0.00619

Figure 8a shows the result for ACR. The PC for a black counter is also included as this was the correction used in reference 24. Figure 8b shows the correction obtained using the QTRT-model. $\phi^{r}_{QTRT}(Q)$ was calculated for the highest and lowest density in Table IV. Corresponding to scattering laws having the same zeroth moment $\phi^{r}_{QTRT}(Q)$ and $\phi_{ACR}(Q)$ are in good qualitative agreement. The difference reflects the influence of the higher moments.

We have also calculated IC using ACR but instead of $S_{PY}(Q)$ the experimental $S(Q)$ of krypton was inserted. Except for small anomalies close to the upper limit of the experimental Q-range, caused by the limited Q-range over which data for $S(Q)$ were available, there are only small differences as compared to the hard sphere case. Especially there is no increase of $\phi_{ACR}(Q)$ for

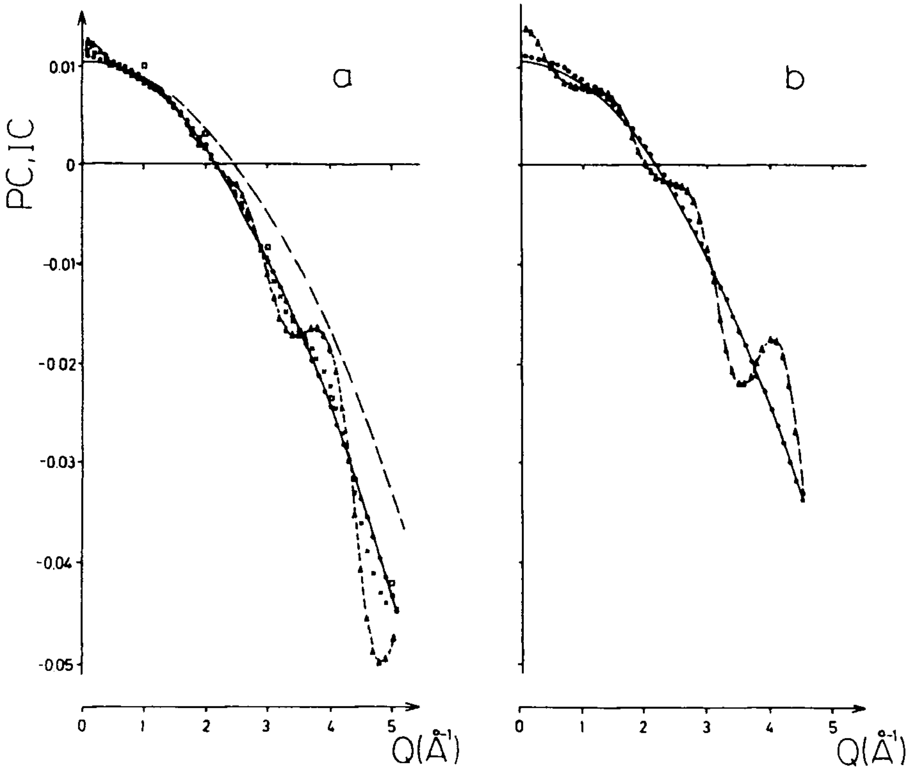


FIGURE 8 PC and IC for krypton gas. Parameters correspond to the ones given in Table IV. Notations: a) dashed line: Placzek correction assuming black counter, full line: $f^{r}(Q)$, circles: $\phi_{ACR}(Q)$ for $\rho = 0.000258$ Å^{-3}, crosses: $\phi_{ACR}(Q)$ for $\rho = 0.00288$ Å^{-3}, triangles: $\phi_{ACR}(Q)$ for $\rho = 0.00619$ Å^{-3}, open squares: $\phi_{IGR}(Q)$.
b) full line: $f^{r}(Q)$, circles: $\phi^{r}_{QTRT}(Q)$ for $\rho = 0.000258$ Å^{-3}, triangles: $\phi^{r}_{QTRT}(Q)$ for $\rho 0.00619$ Å^{-3}.

$Q \to 0$ and also the oscillations of $\phi_{ACR}(Q)$ are more damped than in the hard sphere case, as expected. Thus a correction using $f^{r}(Q)$ seems to be adequate to about ±0.5% in the range $0.2 < Q < 4.3$ Å^{-1}. It should be noted, however, that the angular dependence of IC may introduce an error in the calibration procedure.

IV SUMMARY AND CONCLUSIONS

We have calculated IC and PC for liquid aluminium and liquid copper for a number of neutron wavelengths covering the full range of energies used in neutron structure work. It has been shown that the deviations of IC from PC exceed the statistical errors which are associated with such experiments for neutron wavelengths above 1 Å. As the extension of the expansion of Placzek[2] to include higher order moments does not seem feasible, one should avoid measurements using larger wavelengths when measuring the structure of liquid metals in cases where no appropriate models for $S(Q, \hbar\omega)$ are available. However, as there is a number of good reasons for using high neutron wavelengths we believe that ACR is a useful model to calculate a first estimate of IC, having the correct qualitative behaviour and giving an upper limit for the magnitude of IC. The structure factor required in ACR may be approximated by $S_{exp}(Q)$ or by $S_{PY}(Q)$. In cases, where models are available either from a fit to inelastic experimental data or from molecular dynamics calculations, they are usually constructed to fit the first classical moments of $\tilde{S}(Q, \hbar\omega)$. In order to allow for quantummechanical effects as detailed balance and recoil in an approximate way, we propose either of two methods as described in section II.

As example on estimates of IC we have included into our discussion liquid rubidium and krypton gas, both at several densities. The parameters have been chosen to represent actual experiments.[14,23] There are strong indications that the correction using PC is not accurate enough for the liquid rubidium experiment, whereas it may be appropriate for the krypton case.

Finally it should be stressed once again that a brief knowledge of $S(Q, \hbar\omega)$ is necessary if a measurement of $S(Q)$ is to be properly corrected for inelasticity effects. This conclusion should also be applicable to molecular system but a discussion on this point is outside the scope of this paper. A series expansion of the scattering cross section including only the terms corresponding to the first three energy moments is not appropriate for today's demands of measured $S(Q)$ accurate within 1%. This is a fact which has been mentioned before but it has not been demonstrated so clearly as in our calculations.

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