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STRUCTURE FACTOR AND n,e-SCATTERING

1.Introduction

For more than twenty years a considerable interest has been focused on the structure factors $S(q)$ of noble gases as a source of information on interactions between atoms. Meanwhile, the corresponding research can light up the fundamental problem of the neutron mean squared charge radius $<r_n^2>$, which is determined by other fundamental constant of the n,e-scattering length b_{ne}. As for the last one, the best 10 – 12 results on b_{ne} with errors $\leq 0.05 \cdot 10^{-3}$ fm are spread in the interval $-(1.30 \div 1.60) \cdot 10^{-3}$ fm (see, for example, [1,2]). It means that many of them are mistaken.

The b_{ne} value together with other corrections appears when the transition from the raw neutron intensity $I(q)$ or $I(\vartheta)$ (ϑ is scattering angle, $q = 4\pi \sin(\vartheta/2)/\lambda$, λ is the neutron wavelength) to $S(q)$ is made. Due to the n,e-interaction, the scattering cross section for an atom is

$$\sigma_s^{atom}(q) = \sigma(q) + 8\pi \bar{a} b_{ne} Z f(q),$$

where $\sigma(q)$ is the nuclear part of it, $\bar{a}$ is the length of nuclear coherent scattering, Z and $f(q)$ are number of electrons and their form factor in atom, the term with b_{ne}^2 is small and neglected. Therefore, a factor

$$E(q) = 1 + 8\pi \bar{a} b_{ne} Z f(q)/\sigma(q) \qquad (1)$$

is used as a correction to the nuclear scattering cross section.

2.Diffraction as hindrance for n,e-scattering research

One of the first accurate results on b_{ne} [3] was obtained by means of measuring the scattering intensities ratio 45^0 / 135^0 for noble gases. As it is shown in [4], a diffraction contribution in those ratios for krypton and xenon is very probable and the obtained value b_{ne} has to be corrected in this case. Although now there are a lot of data on $S(q)$ for these gases, the adequate correcting is impossible due to the absence of the precise data on the product of neutron spectrum and detector efficiency in the experiments of [3]. Authors of [3] had such data but they had no $S(q)$, and they should be reproached only with that they did not take into consideration the visible scattering ratio dependence on the gas pressure [4]. In the case of argon, we have a possibility to compare in Fig.1 the b_{ne} contribution to the ratio 30^0 /150^0 with the diffraction contribution, which is obtained in the experiment [5] at pressure 50 atm and weakened by 50 times. It is obviously, that diffraction could essentially change the obtained result of [3].

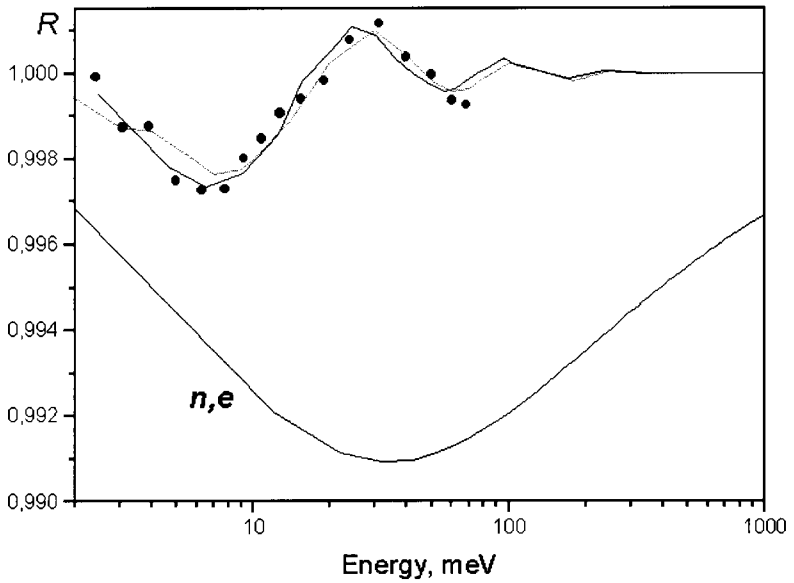

Fig.1. Comparison of the intensity ratios $30^0/150^0$ due to the diffraction in argon at 1 atm with the ratio (in the c.m.s.) due to the n,e-scattering. The points are the results of [5], the thin and thick lines are rough estimates from $S(q)$ [6,7].

Much worse situation with neutron diffraction takes place in liquid lead and bismuth in the last work on b_{ne} [1] considered as one of the best works. An attempt to derive b_{ne} with a high accuracy from the energy behavior of total cross section seems doubtful from the very beginning. In fact, the oscillating diffraction contribution to cross section at small q ($|S(q)-1| \sim 1$) exceeds the b_{ne} contribution by hundreds times, and only due to $S(q)$ oscillating around a middle line diffraction contribution to the total cross section is suppressed and becomes comparable with b_{ne} contribution at small q. Authors of [1] calculated the diffraction correction up to the neutron energy $E \cong 800$ eV employing as the asymptotic function for $S(q)$ the solution of a simplest hard core model up to $q \cong 1200\,\text{Å}^{-1}$, but $S(q)$ are measured only for $q \cong 1 \div 6.5\,\text{Å}^{-1}$ and their accuracy is worse than $\sim 10^{-4}$ what is necessary to obtain b_{ne} with the accuracy $\sim 10^{-2}$. That is why the systematic error of b_{ne} can prove to be higher, for example, because of some shift of the middle line from unity. The diffraction and n,e-interaction contributions from [1] are compared in Fig.2. Similar energy behavior (except for residual diffraction oscillations) does not allow to distinguish these contributions. The diffraction contribution could be distinguished (at least at neutron energy E<1 eV) by oscillations, but they were not observed exactly by authors of [1]. So, the result of [1]

should be interpreted as follows: the obtained value of b_{ne} and the known $S(q)$ at low q are in accordance with the used theoretical model for $S(q)$ at the accuracy ~3%.

Thus, the best works [1,3] by declared accuracy of b_{ne} have essential defects. The similar thing takes place, apparently, in other works and this is the reason for a large (up to 5 – 10 errors) scatter of the b_{ne} values. Such situation induced our proposal to measure b_{ne} by a new method.

Returning to diffraction and Fig.1, it is possible to see that diffraction and n,e-scattering effects can be separated at precise measurement of $S(q)$ (accuracy 10^{-4}). But it is more preferable to make this using almost linear dependence of diffraction on the gas pressure (see for example [8]). The goal of the present work is to demonstrate such possibility.

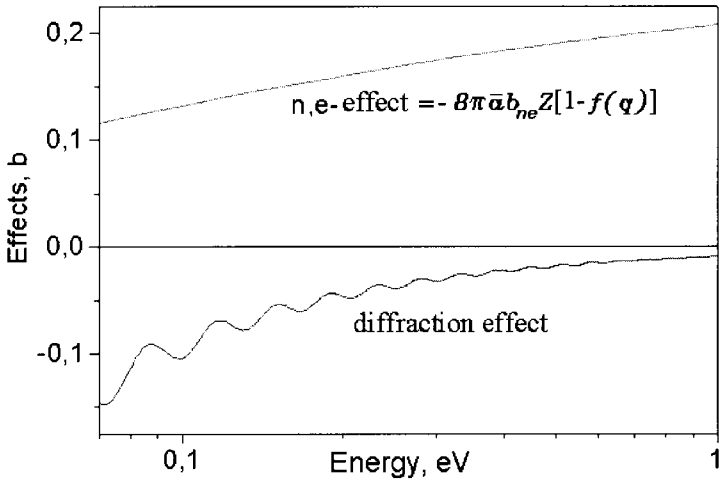

Fig.2. Comparison of the diffraction contribution and the n,e-contribution (with taking into account the nucleus charge) to the total cross section in experiment of [1].

3. The new method demonstration

For analysis, we chose a very detailed article [8] containing the table of $S(q)$ values and also all necessary formulae used in data reduction. Neutrons of $\lambda = 2.39$ Å were scattered at $\vartheta \cong 6^0 \div 109^0$ in turn by gaseous krypton in aluminum container, by empty container and by vanadium sample. After a background subtraction the scattering intensities for each angle per unit of neutron flux were expressed by formulae, which are analogous to the one for the empty container:

$$I_c(\vartheta) = N_c A_c(\vartheta)\{\sigma_c^{coh}[S_c(\vartheta) - 1] + \sigma_c^{tot}[1 + P_c(\vartheta) + \Delta_c(\vartheta)]\}\varepsilon(\vartheta) \qquad (2)$$

where N_c is number of atoms in the beam, $A_c(\vartheta)$ is the absorption factor, $P_c(\vartheta)$ is the correction for scattering angle dependence, $\Delta_c(\vartheta)$ is the ratio of multiple and single

scattering, $\varepsilon(\vartheta)$ is the detection efficiency, subscripts *coh* and *tot* mean the coherent and the total scattering cross section, subscript *c* means container. The expression for vanadium (subscript *v*) is simpler because $\sigma_v^{coh} \cong 0$ and the scattering by the sample in container is described by two parts like (2) with subscripts *s* (sample), *c*, *sc* (sample in container).

Three equations (one of them is (2)) have three unknowns: $\varepsilon(\vartheta)$, $S_c(\vartheta)$ and the interesting one for us $S_s(\vartheta)-1$, which we have found as

$$S_s(\vartheta)-1=\frac{N_v A_v(\vartheta)\sigma_v^{tot}[1+P_v(\vartheta)+\Delta_v(\vartheta)]}{N_s A_{s,sc}(\vartheta)\sigma_s^{coh}E_s(\vartheta)}\cdot\left[\frac{I_{sc}}{I_v}-\frac{A_{c,sc}(\vartheta)}{A_c(\vartheta)}\cdot\frac{I_c}{I_v}\right]-$$

$$-\frac{\sigma_s^{tot}}{\sigma_s^{coh}}\cdot\left[1+P_s(\vartheta)+\Delta_{sc}(\vartheta)\right]-\frac{N_c A_{c,sc}(\vartheta)\sigma_c^{tot}}{N_s A_{s,sc}(\vartheta)\sigma_s^{coh}E_s(\vartheta)}\cdot\left[\Delta_{sc}(\vartheta)-\Delta_c(\vartheta)\right]. \qquad (3)$$

And now, our task is to obtain initial scattering data of [8] from the table of $S_s(q)$ and to use our new method to extract the b_{ne} value and $S_s(q)$ again.

With this aim, we separated a function from (3)

$$Y(\vartheta)=\frac{N_v A_v(\vartheta)\sigma_v^{tot}}{N_s A_{s,sc}(\vartheta)\sigma_s^{tot}}\left[\frac{I_{sc}}{I_v}-\frac{A_{c,sc}(\vartheta)}{A_c(\vartheta)}\cdot\frac{I_c}{I_v}\right] \qquad (4)$$

and calculated it for all $q=(0.25\div 4.0)$ Å^{-1} at krypton densities $n=(0.258\div 6.19)\cdot 10^{21}$ cm^{-3} using the $S_s(q)$ and some information, which is, unfortunately, far from being complete, on other parameters. Nevertheless, $Y(\vartheta)$ has to be close to the observed ratio of the scattering intensities by krypton and vanadium and we solve the problem of b_{ne} by an expression

$$Y^{theor}(q,n)=\frac{1+\Delta_{sc}}{1+Q_v(q)+\Delta_v}\times$$

$$\times\left\{\left[1+f(q)B\right]\left[1+Q_s(q)\right]+\frac{nC}{1-nC}\left[\frac{4\pi\bar{a}^2}{\sigma_s^{tot}}+f(q)B\right]\left[1+Q_{2s}(q)\right]\right\}, \qquad (5)$$

because B does not depend on n and the diffraction does. Here $B=8\pi\bar{a}b_{ne}Z/\sigma_s^{tot}$ and $C(q)=[S(q)-1]/nS(q)$ are two parameters to be fitted at each q to the "experimental" values $Y(\vartheta)$ after (4). Instead of functions P_s and P_v, we use more adequate corrections in (5)

$$Q_s(q)=0.036-0.00174q^2, \qquad (6)$$

$$Q_{2s}(q)=0.018-0.00087q^2, \qquad (7)$$

$$Q_v(q)=0.0045-0.00116q^2. \qquad (8)$$

The function $1+Q_s(q)$ gives the angular distribution (in laboratory system) of neutrons with $\lambda=2.39$ Å scattered in the monatomic gas with $A=83.8$ at $T=293K$. It is calculated taking into account the center of mass motion by integration over atom velocities (as in [2,3]). $Q_{2s}(q)$ differs from $Q_s(q)$ only in that it contains $A=167.6$ (a

pair of atoms scatters the neutrons coherently). The function $Q_v(q)$ is obtained from the theory [9] confirmed by the experiment [5]. It is worth to note, that $Q_s(q)$ is very close to $P_s(\vartheta)$ but $Q_v(q)$ decreases with q more slowly (by ~2.5 times) than $P_v(\vartheta)$.

The results of fitting are shown in Fig.3 where the points with a curve are $C(q)$ and the points approximately along the horizontal line are B values. From all experimental $S(q)-1$, we chose those points only, which satisfactorily lie on a direct line as a function of n. The lower part is the main fit when the whole available information about all parameters of (3) – (5) given in [8] and functions (6) – (8) are used. To our puzzle, the average over q quantity $\overline{B}$

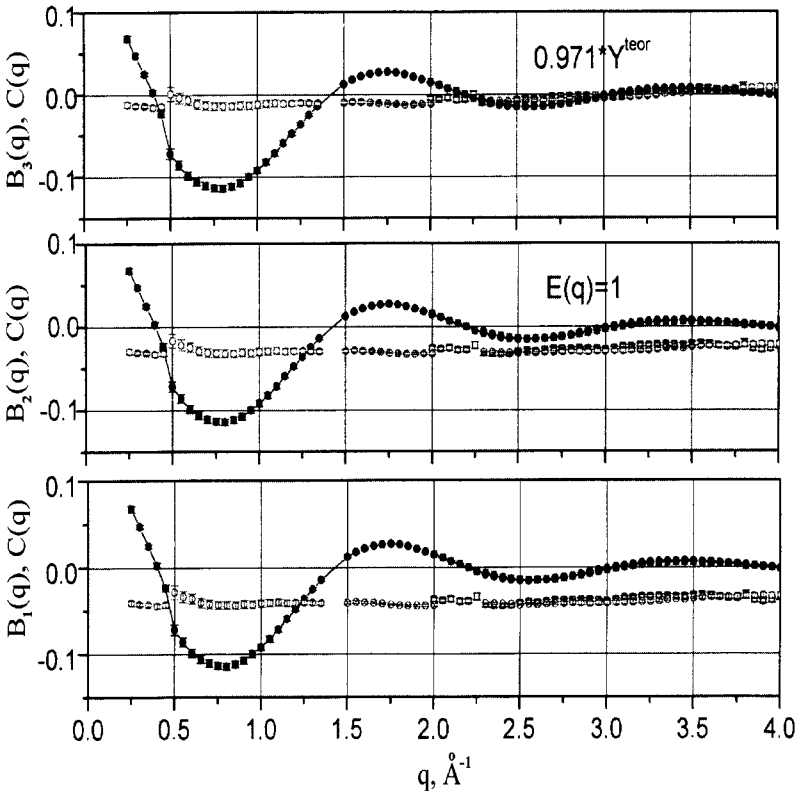

Fig.3. The results of fitting parameters B and C of the function (5) to the values (4).

proved to be not $\overline{B}_0 \cong -0.012$, corresponding to $b_{ne} = -1.34 \cdot 10^{-3}$ fm, but $\overline{B}_1 \cong -0.041$. To check the method, a fit was made when instead of (1) $E(q) \equiv 1$ was taken in (3), and this fit is shown in the middle of Fig.3. We obtained the new $\overline{B}_2 \cong -0.029$, and we have $\overline{B}_1 - \overline{B}_2 = \overline{B}_0$ how it should be. Such situation most probably means that a

normalizing factor in (4) or (and) (5) is wrong and has to be additionally multiplied just by $1+\overline{B}_2$. And indeed, such fit resulted in $\overline{B}_3 \cong \overline{B}_0$ (the upper part of Fig.3).

It is worth to note that the approximate constancy of parameter B with changing q demonstrates a success of separating (B and C do not correlate) the n,e-scattering contribution $Bf(q)$ at $f(q)$ changing from 1 to ~0.7. As for $S(q)$, any of three fit variants gives value $nC/(1-nC)+1$ very close to the initial $S(q)$ in [8].

4. Conclusion

We performed all above calculations to demonstrate how the neutron scattering data on a noble gas intended for the structure factor $S(q)$ finding can be used for n,e-scattering length b_{ne} deriving. Instead of correction for the "known" n,e-scattering length b_{ne}, this value should be derived from these data at obtaining the structure factor. Unfortunately, the data [8] together with numerous parameters turned out to be not enough accurate to give a correct value B corresponding to the real b_{ne} value. So, in order to succeed, precise data at q in more wide range from ~0.5 $Å^{-1}$ to 10 – 20 $Å^{-1}$ (in order to "see" the n,e- effect as $B=const$ from $f(q)$~0.9 up to $f(q)=0.4-0.3$) together with precise quantities of all corrections are required. The accuracy of values $\Delta(q)$ and $Q(q)$ is especially important. Absolute error of each of them $\sim 10^{-4}$ gives the contribution to systematic error of $b_{ne} \sim 0.01 \cdot 10^{-3}$ fm, i.e. less than 1%.

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Мицына Л. В. и др. Е3-2003-183
Структурный фактор и n,e-рассеяние

Предлагается принципиально новый метод извлечения длины нейтрон-электронного рассеяния b_{ne} из прецизионных данных по рассеянию нейтронов в благородном газе при нескольких различных плотностях n. Суть метода заключается в разделении экспериментальных данных на две части: пропорциональную плотности атомов n дифракционную часть и малый вклад n,e-рассеяния, который от n не зависит. Предложенный метод продемонстрирован при получении величины b_{ne} с помощью структурного фактора $S(q)$ для газообразного криптона. В расчетах использованы более точные кинематические поправки на угловую зависимость рассеяния.

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Structure Factor and n,e-Scattering

A principally new method to extract the neutron-electron scattering length b_{ne} from the precise neutron scattering data measured for a noble gas at several different densities n is proposed. The main point of this method is separation of the experimental data into two parts: diffraction part proportional to n, and small contribution of n,e-scattering which does not depend on n. Such a new method to obtain the b_{ne} value is demonstrated using structure factor $S(q)$ for gaseous krypton. More exact kinematic corrections for the angular dependence of scattering have been used in calculations.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

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