

# Neutron-electron scattering length extraction from the neutron diffraction data measured on noble gases

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## Abstract

The proposed new method for extraction of the neutron-electron scattering length  $b_{ne}$ , which is connected directly with the fundamental physical value of neutron mean squared charge radius, from the slow neutron diffraction on noble gases was developed and performed by analysis of literature data on structure factors for gases Kr,  $^{36}\text{Ar}$  and liquid Kr.

For the most part, different variants of analysis of these experimental data allow us to obtain  $b_{ne}$  value with the statistical accuracy 10–20 %, but in some of them the real possibility for the accessible accuracy no worse than 2–3% was shown. In order to remove some systematical errors and to reach such good accuracy the execution of the comparative diffraction measurements is proposed with a pair of gases having close atomic properties and different n,e-scattering contributions, such as Ar –  $^{36}\text{Ar}$  or Xe – Kr.

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## 1. Introduction

History of the n,e-interaction investigations began nearly 70 years ago, the first mention of this effect was made by D.Ivanenko in 1941 [1]. However, in spite of existence of a dozen of the most precise experimental  $b_{ne}$  values with errors  $< 0.05 \cdot 10^{-3}$  fm obtained by different methods (see, for example [2]) there were doubts about the validity of their declared accuracy, as they differed by  $\sim 5$  standard errors. In all methods there are principal troubles connected with the necessity of introducing large corrections, whose size of order of the investigated effect. Thus, further investigations of this problem with the aim to adjust  $b_{ne}$  value are desired and required as before.

The intrigue is that in the interval about  $\pm 10\%$  all  $b_{ne}$  values were scattered around the so-called Foldy scattering length

$$b_F = -\frac{\mu e^2}{Mc^2} = -1.468 \cdot 10^{-3} \text{ fm} ,$$

which, according to the Dirac generalized equation for neutron, is connected with the interaction between the neutron anomalous magnetic momentum and electric field. One may note that the terms attached to  $\text{div}\vec{E}$  in the Dirac generalized equation for neutron and in the Dirac equation for electron have the same structure

$$[\varepsilon + \frac{\hbar}{4Mc} (\frac{e\hbar}{2Mc} + 2\mu)] \text{div}\vec{E}$$

and depend on the particle magnetic momentum  $\mu$  only, and parameter  $\varepsilon$  appears just in the equation for neutron. In case of  $b_{ne}$  and  $b_F$  values the coincidence parameter  $\varepsilon$  must be equal to zero. Possible equality of  $b_{ne}$  and  $b_F$  values would be surprising, as it signifies that

the charge distribution of a neutron scattered on the outside charge becomes displayed through magnetic momentum only. So closeness of  $b_{ne}$  and  $b_F$  values will confirm this non-trivial phenomenon.

From the point of view of comprehension of all corrections introduced into the experimental data for masking effects the simplest experiment to obtain  $b_{ne}$  value is the slow neutron scattering by noble gas. Nevertheless, in these experiments it is impossible to ignore the diffraction on nuclei of neighboring atoms even at low gas densities. So, weak dependence of  $b_{ne}$  value obtained from the data of [3] on the gas pressure was noticed and taken into account in [4], whereupon the extracted  $|b_{ne}|$  values were decremented by  $\sim 10\%$  for Kr and by  $\sim 5\%$  for Xe.

Seemingly, the negative role of neutron diffraction at the observation of n,e-interaction effect was noticed first by A.I.Akhieser and I.J.Pomeranchuk [5] soon after appearance of the classical paper by E.Fermi and L.Marshall [6], which was one of the pioneering attempts to discover n,e-scattering. The warning [5] was evidently known to the authors of one of the most accurate results for the n,e-scattering length obtained in [3]. The authors of [3] used gases at low pressures 0.33 – 1.68 atm just to detect possible diffraction distorting the result.

The new method to obtain  $b_{ne}$  value proposed in Dubna [7] permits to use much more dense gases, inasmuch as the diffraction can be taken into account with satisfactory accuracy when extracting the n,e-effect. Our method is based on two facts:

- 1) diffraction and n,e-interaction contributions to scattering cross section have very different dependences on the momentum transfer  $\hbar q$  (oscillating and monotonous);
- 2) diffraction contribution to the scattering is proportional to a gas density  $n$  (or even has a term with  $n^2$ ), but the nuclear and n,e-scatterings do not depend on  $n$ .

Investigations of the neutron diffraction in monatomic gases in quest of interatomic interaction potentials are progressing in the last decades. As for gas densities, the pressures up to hundreds atmospheres are used in these experiments. So, the effect of n,e-scattering in them is essentially more than in the researches like [3].

## 2. Basic relations

According to conceptions accepted in literature we describe the neutron scattering intensity per one target atom and unity neutron flux with the accuracy enough for our purposes by the following expression

$$\frac{dI(q)}{d\Omega} = \frac{\sigma_s}{4\pi} \left\{ F_s(V_0, q, A)(1+B) + \frac{nC(q)}{1-nC(q)} F_s(V_0, q, 2A) \left( \frac{\sigma_{coh}}{\sigma_s} + B \right) \right\}, \quad (1)$$

where  $B = \frac{8\pi a_{coh} b_{ne} Z f(q)}{\sigma_s}$ ,  $q$  is the wave number of momentum transfer,  $\sigma_s$  and  $\sigma_{coh}$  are the total and coherent nuclear cross sections,  $a_{coh}$  is the length of coherent nuclear scattering,  $Z$  is the number of electrons in atom,  $f(q) = [1 + 3(q/q_0)^2]^{-1/2}$  is the electron form factor of an atom,  $q_0$  is the Hartree-Fock's constant, which characterizes atomic properties (see [8]). For taking into account the influence of the atoms thermal motion on the neutron scattering distribution in expression (1) we did not use the Placzek corrections, which are generally applied in the works for diffraction investigations, but more correct (see [9]) kinematic description. It was used in [3] and set out in detail in V.Turchin's book [10]. The thermal motion effect is described by function  $F_s$

$$F_s(V_0, \theta, A) = \frac{(A+1)^2}{A^2 \sqrt{\pi} V_0 U_0} \int_0^\infty \frac{V^2}{\sqrt{V_0^2 + V^2 - 2V_0 V \cos \theta}} \times$$

$$\times \exp \left\{ - \frac{(V^2 - V_0^2 \frac{A-1}{A+1} - \frac{2V_0 V \cos \theta}{A+1})^2}{4(\frac{A}{A+1})^2 U_0 (V_0^2 + V^2 - 2V_0 V \cos \theta)} \right\} dV. \quad (2)$$

In expression (2)  $\theta$  is the scattering angle of neutron in the laboratory reference frame,  $V_0$  and  $V$  are the initial neutron velocity and its velocity after scattering,  $A$  is the atom mass number,  $U_0 = \sqrt{\frac{2kT}{mA}} = 128.9 \sqrt{\frac{T}{A}}$  [m/s],  $T$  is the gas temperature in K.

Function  $C(q)$  is connected with the structure factor  $S(q)$  by formula

$$S(q) - 1 = \frac{nC(q)}{1 - nC(q)}. \quad (3)$$

The peculiarity of expression (1) applied by us is the use of the function  $F_s$  attached to diffraction term with doubled atom mass, as the diffraction, first of all, is connected with the interaction between the neutron and pair of atoms having coincident velocity vectors.

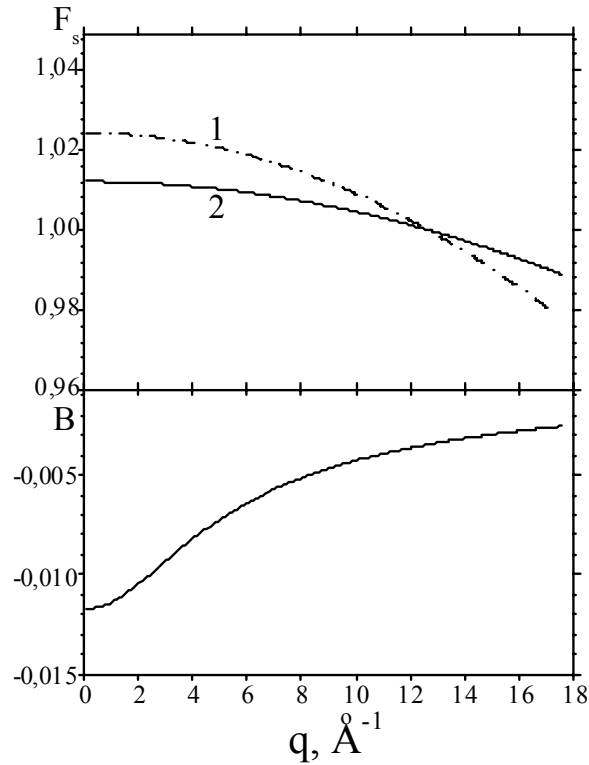


Fig.1. Contributions of thermal motion corrections to the neutron scattering intensity for Kr calculated for neutron diffraction scattering on single atom (curve 1) and on two atoms (curve 2) and calculation of n,e-contribution.

The values of separate effects for gaseous krypton are shown in Fig.1 and Fig.2. It is seen, that n,e-contribution to nuclear scattering is  $\sim 1\%$  or less and does not depend on the

gas density. And the diffraction amplitudes rise strongly with the gas density increase at preserving positions of their maximums and minimums.

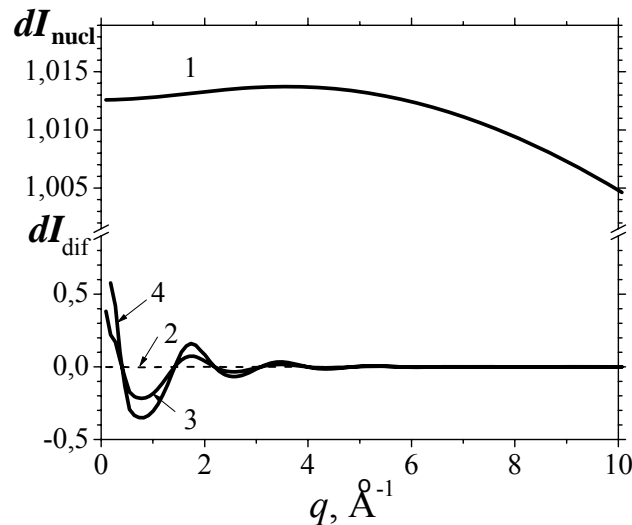


Fig.2. Calculation for Kr of the nuclear and n,e-scattering term contribution to the neutron intensity, which does not depend on the gas density – curve 1 and diffraction term dependent on the gas density: curve 2 – at the pressure 1 atm., curve 3 – at 100 atm., curve 4 – at 200 atm.

The problem of  $b_{ne}$  value determination comes to accurate separating the n,e-contribution from the diffraction waves with taking into account the thermal motion of atoms.

Unfortunately, for diffraction description there is no strict theory yet, so in our analysis we used different expressions describing relaxing oscillations of the correlation function  $C(q)$ , such as

$$C(q) = (A_1 - A_2 n) \exp(-A_3 q) \sin\left(\frac{2\pi q}{A_4} + A_5\right), \quad (4)$$

where one or two out of five parameters  $A_1 - A_5$  are sometimes fixed.

Testing the different phenomenological formulas for  $C(q)$  description including hard-core model approach (as in [2]) adjudicated that all considered variants with the exception of the last one fit to the experimental data satisfactorily.

### 3. Results

The experimental data of [11–13] were used, where the  $S(q)$  values were obtained for gaseous Kr, isotope  $^{36}\text{Ar}$  and for liquid Kr, in order to test the proposed method of the  $b_{ne}$  value obtaining. Moderate accuracy ( $\sim 5 \cdot 10^{-3}$ ) of these experimental  $S(q)$ , which was sufficient to obtain information about interatomic interaction potentials, nevertheless, allowed us to extract  $b_{ne}$  value with the accuracy  $\sim 10 - 20\%$ . To achieve better accuracy it is desirable to measure the scattered neutron intensity for noble gases with the relative accuracy  $3 \cdot 10^{-4} - 10^{-4}$ .

### 3.1. Gaseous Kr

In [14] we used experimental data  $S(q,n)$  measured for gaseous Kr and published in [11]. The structure factors were obtained for 17 gas densities  $n = (0.26\text{--}6.19)\cdot 10^{21} \text{ cm}^{-3}$  and 78 values of  $q$  up to  $4 \text{ \AA}^{-1}$ . To normalize the neutron scattering intensity the authors of [11] used vanadium, assuming that its scattering cross section is isotropic in the interval of  $q$  from 0 up to  $4 \text{ \AA}^{-1}$ , and the calculated  $S(q,n)$  value using the expression

$$\frac{dI(\mathcal{Q})}{d\Omega} = \frac{\sigma_s}{4\pi} [1 + B_0 f(q)] \cdot \{[S(q,n) - 1] \gamma + 1 + P_1(q)\}, \quad (5)$$

where  $B_0$  is the correction for n,e-scattering with  $b_{ne} = -1.34 \cdot 10^{-3} \text{ fm}$ ,  $P_1(q)$  is the well known Placzek correction, which is usually applied to describe thermal motion of atoms in solid state experiments. We used all  $S(q,n)$  from [11] and described them by fitting formula, which ensued after equating the right parts of equations (1) and (5) and finding a solution of combined equation relative to the experimental  $S(q,n)$  from (5). We kept the normalizing multiplier  $\alpha$  before the fitting formula to take into account inaccurate knowledge of krypton and vanadium cross sections. In our expression (1) term with  $n^2$  appeared in diffraction dependency on gas pressure due to linear in  $n$  function  $C(q) = C_0(q) - nC_1(q)$ . Thus, in the fitting formula for describing the experimental  $S(n,q)$  values for all  $n$  for each  $q$  there were three varied parameters:  $C_0$ ,  $C_1$  and  $B$ .

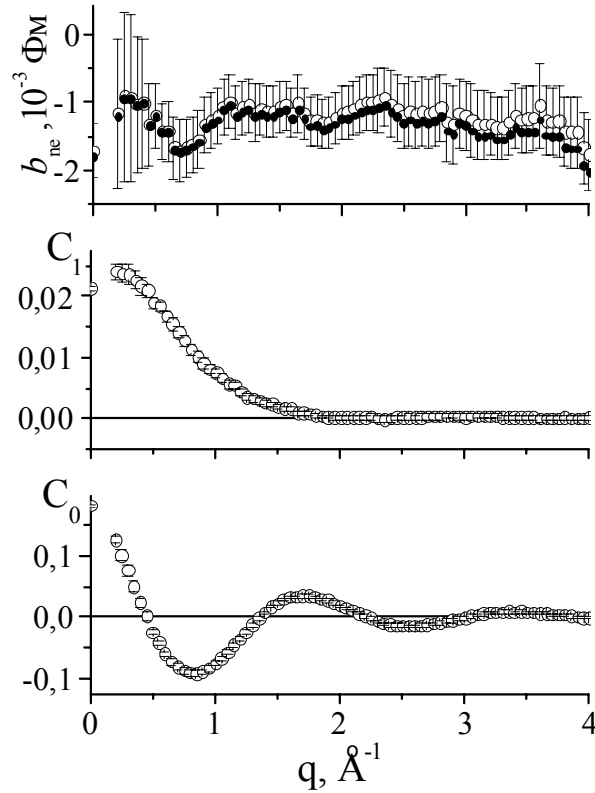


Fig.3. Fitted parameters  $b_{ne}$ ,  $C_0$  and  $C_1$  with  $F$ -corrections and  $\alpha = 0.975$  (light points) and with the Placzek corrections and  $\alpha = 1$  (black points).

The results of fits are shown in Fig.3. The upper picture shows a constancy of  $b_{ne}$  parameter within the error bars, which means good quality of the experimental data described with the accuracy  $3 \cdot 10^{-3}$ .

The performed fits with replacement of functions  $F_s$  by Placzek's  $P_1(q)$  showed that parameters  $C_0$  and  $C_1$  (see Fig.3) are practically indistinguishable, but  $b_{ne}$  systematically differ by  $\sim 0.1 \cdot 10^{-3}$  fm. This circumstance denotes once more the importance of correct calculation of atomic thermal motion influence on the extracted  $b_{ne}$  estimations.

Furthermore, the experimental data for all  $q$  and all  $n$  simultaneously were fitted by ten parameters:  $\alpha$ ,  $b_{ne}$  and eight parameters  $A_i$  for describing functions  $C_0$  and  $C_1$  by formula (4) (assuming that  $A_2=0$ ). Examples of experimental data describing for four chosen gas densities demonstrate the satisfactory quality of this fitting at the lower part of Fig.4. The result obtained with free parameter  $\alpha$  is placed in the first line of Table.

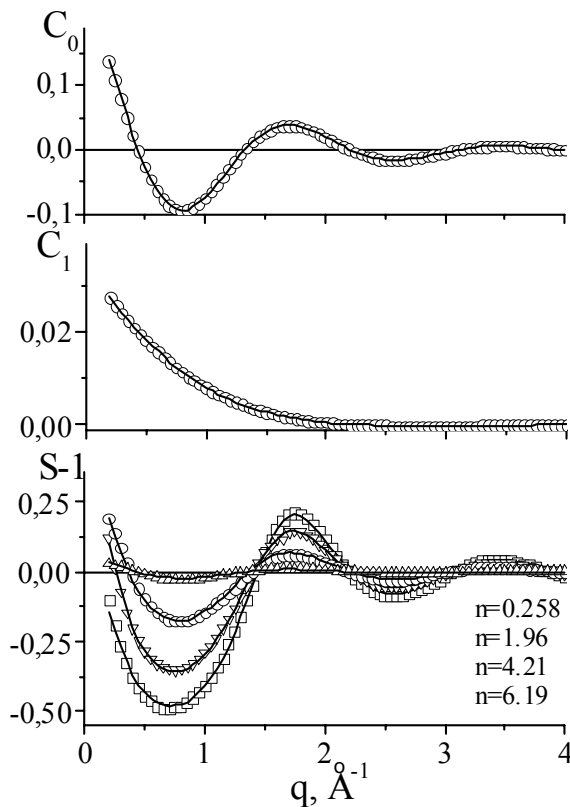


Fig.4. The result of simultaneous fitting to the data for all  $q$  and all  $n$ .

Thereby, in the proposed method the diffraction on neighboring atoms does not disturb obtaining the  $b_{ne}$  value, and that differentiates our method profitably from the researches with liquid metals [2], where correction for diffraction, which is more than  $n$ ,e-effect, is calculated analytically.

### 3.2. Gaseous isotope $^{36}\text{Ar}$

As  $^{36}\text{Ar}$  has an anomalously large scattering cross section  $\sigma_s \approx 78$  b, and  $n$ ,e-effect for it must be  $\sim 10$  times less than for natural Ar, so extracting  $b_{ne}$  value from the  $^{36}\text{Ar}$  diffraction data we made a check of our method sensitivity.

In [15] we used  $S(q)$  data obtained in the Institute Laue-Langevin in Grenoble [12] for  $q = (0.24 - 10.1) \text{ \AA}^{-1}$  at four densities of gaseous isotope  $^{36}\text{Ar}$  with the accuracy from 0.06% up to 0.2%.

Small number and narrow range of densities  $n$  did not allow us to get  $b_{ne}$  value for each given  $q$  separately (as in the case of gaseous Kr, see 3.1). We fitted these data for each density of  $^{36}\text{Ar}$  in the wide interval of  $q$  values using formulae (1) and (4). The authors of [12] normalized experimental  $S(q)$  values on the data at large  $q$  neglecting the diffraction there and not taking into account n,e-scattering. Their thermal motion corrections differed from  $F_s$ -corrections (2) by a constant multiplier close to 1 only, so their intensity we described by expression (1) with  $F_1 = F_2 = 1$  and with varied multiplier  $\alpha$  taking into account the difference of normalizations.

During data processing a strong correlation took place between  $b_{ne}$  value and  $\alpha$  ( $\Delta\alpha \sim 10^{-3}$  changed  $b_{ne}$  by 10%), and insufficient precision of normalization did not allow us to get  $b_{ne}$  value with the accuracy better than 10 %.

We could describe experimental data of  $S(q)$  satisfactorily at  $q \geq 3 \text{ \AA}^{-1}$  only. Moreover, all the data for the lowest density of argon were rejected because of large  $\chi^2$  criterion. The weighted average result for the rest three densities is shown in Table (line 2) with the statistical error. However, the systematic error of normalization evaluated over a wide interval  $q = (8 - 10) \text{ \AA}^{-1}$  turned out two times more than the statistical one.

### 3.3. Liquid Kr

Although  $b_{ne}$  value extracting from the neutron scattering on liquid is not so clear in comparison with the scattering on gases because of the problem of adequate consideration of thermal motion for atoms of liquid, the  $b_{ne}$  value was also obtained from the diffraction data measured in Grenoble [13] for seven close densities of liquid Kr in the wide range  $q \sim (0,4 - 17) \text{ \AA}^{-1}$ . We used these experimental data to verify different versions of  $b_{ne}$  value extracting. They were described in detail in [16,17].

Out of  $\sim 5000$  experimental data presented in [13] we used  $S(n,q)$  in the interval  $q \cong 4 - 16 \text{ \AA}^{-1}$ , because we could not get fits with  $\chi^2 \leq 1$  analyzing all the data (with  $q < 4 \text{ \AA}^{-1}$ ).

Simultaneous fitting of all seven densities with the same parameters  $A_i$  of function  $C(q)$  gave the result  $b_{ne} = -(1.39 \pm 0.04) \cdot 10^{-3} \text{ fm}$ . The result of fitting is shown in Fig.5. However, the correlation between  $b_{ne}$  value and normalizing constant  $\alpha$  led to  $b_{ne}$  values spread up to  $\pm 30\%$ .

Using individual diffraction parameters fitted for each of seven samples and fixing them afterwards in the following fitting with free  $b_{ne}$  value and with seven different normalizing parameters  $\alpha_i$  we obtained  $b_{ne} = -(1.63 \pm 0.02) \cdot 10^{-3} \text{ fm}$ . This error is 10–15 times less than for gaseous Kr and  $^{36}\text{Ar}$ , where it is caused by correlation between  $b_{ne}$  and  $\alpha$ . We succeeded in the break off correlation here due to wider region of  $q$  reached  $q > 16 \text{ \AA}^{-1}$ , where n,e-contribution is negligible. This example demonstrates future prospects of obtaining  $b_{ne}$  value with the accuracy  $\sim 2\%$  by means of performing similar measurements with gaseous samples.

Unfortunately, this result can not be accepted as significant one on account of essential change of the extracted  $b_{ne}$  value at varying the limits of the working  $q$ -interval. It can be evidently explained by insufficiently satisfactory description of neutron diffraction in liquid state of Kr.

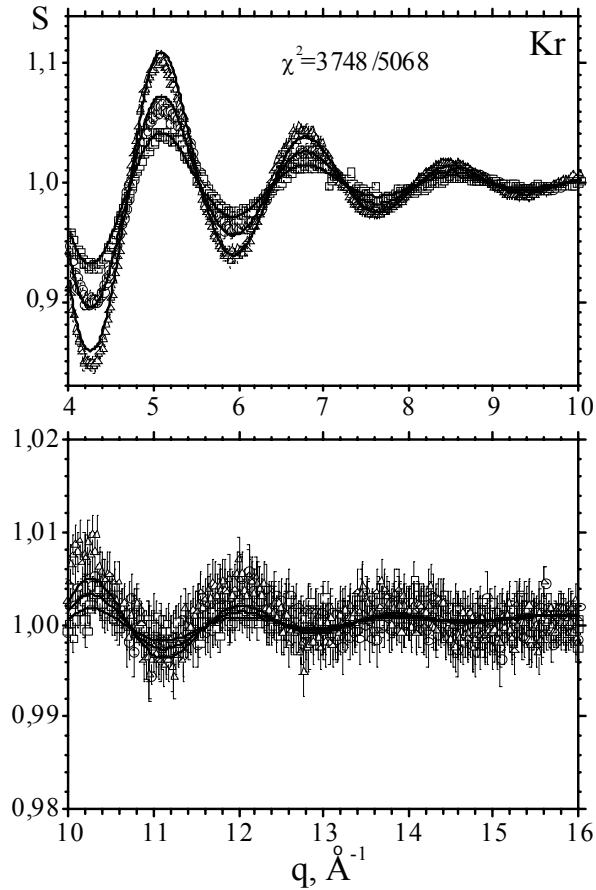


Fig.5. The simultaneous fitting for  $S(n, q)$  of liquid Kr for seven densities. The data for three densities  $n = 11.86, 14.57$  and  $17.01 \text{ nm}^{-3}$  are shown only. Points are experimental data, curves are fitting results.

Target	Fittings	Table $\langle b_{ne} \rangle \cdot 10^3, \text{ fm}$
Kr	for all $q$ and all $n$ simultaneously	$-1,53 \pm 0,24$
$^{36}\text{Ar}$	averaged value of simultaneous fits for each $n$	$-1,33 \pm 0,28 \pm 0,57$
liquid Kr	average value obtained by interval dividing	$-1,38 \pm 0,27$
	average value of fits for three samples with similar $n$	$-1,40 \pm 0,10$

To escape safely a correlation between  $\alpha$  and  $b_{ne}$  we separated n,e-part in our fitting function (details see in [16]):

$$p(q) = \alpha[1 + Bf'(q)] = S^{\text{exp}}(q) / \{1 + \gamma[S^{\text{fit}}(q) - 1]\},$$

where  $S^{\text{exp}}(q)$  are the experimental and  $S^{\text{fit}}(q)$  are the fitted structure factors, and after dividing the working  $q$  interval into six parts, which corresponded to six visible periods of



the diffraction, obtained three  $b_{ne}$  values from the sum ratios  $p_i / p_j$  for  $i / j = 1/4, 2/5$  and  $3/6$  (indexes  $i, j$  belong to different parts of the interval). Thus, we exclude  $\alpha$ . The average of three obtained  $b_{ne}$  values is placed in the third line of Table.

The averaged result of fittings to the experimental data for three groups of samples with similar densities, which were done in [17], is presented in the 4-th line of Table.

#### 4. Conclusion

Possibilities of the new method to extract the n,e-scattering length from the measured structure factors were entirely shown with the data of experiments [11–13]. The data analysis for gaseous Kr demonstrated two variants of the data processing for  $b_{ne}$  value extracting: with the use of  $n$ - and  $q$ -dependences of experimental structure factors.

Fundamental capability to solve the problem of  $b_{ne}$  obtaining by new method was also shown by the model experiment performed by the Monte Carlo procedure [18], where angle distributions of neutrons with the energy 0.0143 eV scattered by gaseous Kr were considered. Calculations allowed us to come to a conclusion that having the data for 20 or more angles at a few gas densities in the range from  $0.0269 \cdot 10^{21} \text{ cm}^{-3}$  to  $2.69 \cdot 10^{21} \text{ cm}^{-3}$  with the relative accuracy of experimental points  $\sim 3 \cdot 10^{-3}$ , we could extract the  $b_{ne}$  value with the accuracy no worse than 5%.

High sensitivity of the new method to the n,e-scattering length extracting was also shown in the work with  $^{36}\text{Ar}$ , where n,e-effect is 10 times less than for natural argon.

A problem of the extracted neutron-electron scattering length precision in the proposed method depends not only on the statistical accuracy of the measured angle distributions of neutrons scattered by gas but also on an extent of diffractometer isotropy – the constancy of the product of detector efficiency and the solid angle at all angles.

The exclusion of the dependency of neutron probability registration by the detectors on a scattering angle is fundamentally important task. In [11] this problem was solved by normalizing the angle distribution of neutrons scattered by gaseous krypton on such distribution of neutrons scattered by vanadium. However, the order of vanadium isotropy is not known with the accuracy, which would be sufficient for our purposes (see [19,20]).

To obtain  $b_{ne}$  value with the accuracy  $\sim 2\%$  the facility anisotropy must be less than  $\sim 3 \cdot 10^{-4}$ , that is practically impossible condition. The only possibility of this trouble avoidance is to realize relative measurements of two noble gases with strongly different n,e-contributions to scattering cross sections, for example Ar and  $^{36}\text{Ar}$ , which have n,e-contributions 1.7% and 0.2%, or Xe and Kr, whose ones are 2.1% and 1.2%, correspondingly.

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