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# NEUTRON-ELECTRON SCATTERING LENGTH EXTRACTED FROM NEUTRON DIFFRACTION ON LIQUID KRYPTON

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Магли Р. и др. Е3-2006-139

Длина рассеяния нейтрона на электроне, извлеченная из экспериментов по дифракции нейтронов на жидком криптоне

Из данных по структурным факторам $S(q)$ жидкого криптона, полученных в нейтронно-дифракционных экспериментах без учета нейтрон-электронного взаимодействия, была определена соответствующая ему длина рассеяния $b_{ne}$. Главная трудность — присутствие в данных неизвестной, близкой к единице константы — была преодолена разными способами, которые привели к практически одинаковым результатам, наиболее точный из которых $b_{ne} = (-1{,}38 \pm 0{,}04) \times 10^{-3}$ фм.

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Neutron-Electron Scattering Length Extracted from Neutron Diffraction on Liquid Krypton

Using data on the structure factors $S(q)$ for liquid krypton obtained in the neutron diffraction experiments without taking into account the neutron-electron interaction, the corresponding scattering length $b_{ne}$ has been extracted. The main difficulty, the presence in the data of an unknown constant close to unity, was overcome by different ways, which led to practically the same result, and the most accurate one is $b_{ne} = (-1.38 \pm 0.04) \cdot 10^{-3}$ fm.

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

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## INTRODUCTION

In the papers [1–4] the new method to extract the neutron-electron scattering length $b_{ne}$ was developed, which is characterized by the employment of dense targets of noble gases and by deriving the $b_{ne}$ value from the neutron diffraction occurring there. The method was tested using the data on the structure factor $S(q)$ of gaseous Kr from [5] (see [1, 3]) and gaseous isotope $^{36}$Ar from [6] (see [4]). It was shown that the method does work but the accuracy of the used data is insufficient for the satisfactory accuracy of the obtained $b_{ne}$ value. The present investigation is the next attempt to apply the method. This time, we use the $S(q)$ data for liquid Kr [7], which together with $S(q)$ for $^{36}$Ar were kindly given to us by the authors of [6, 7].

We have used already these data in our previous paper [8] and the present one is in fact its continuation. The point is that there are several different ways to extract the $b_{ne}$ value from 4000–5000 quantities of $S(q)$ for seven Kr samples of different densities $n$. Using the MINUIT fitting program two ways were applied in [8]: 1) joint processing of all data, 2) separate processing of data for three groups of samples with close densities, that gave the average result

$$b_{ne} = (-1.40 \pm 0.10) \cdot 10^{-3}\,\mathrm{fm}. \tag{1}$$

We report below the results on $b_{ne}$ obtained by four more ways.

## 1. DATA PROCESSING

Since the diffraction and $n, e$ interaction contributions to the neutron scattering have in principle different dependences on the transferred wave vector $q$, the $n, e$ contribution can be extracted by our method even at high densities of investigated samples. We had the structure factor $S(q)$ for dense liquid Kr at seven different thermodynamic states (densities from 11.28 nm$^{-3}$ to 17.01 nm$^{-3}$) in the wide range of $q$ up to $\sim 16$ Å$^{-1}$. The liquid phase of a scatterer excludes the possibility to make use of known dependence of $S(q) - 1$ value on the gas density $n$ (as in [1–4]). Therefore, the data for each Kr sample were processed independently and the first problem was to find adequate description of diffraction.

It turned out to be enough to use four free parameters $A_1 - A_4$ in the formula

$$C(q) = A_1 \exp\left(-A_2 q\right) \sin\left(\frac{2\pi q}{A_3} + A_4\right) \tag{2}$$

in order to describe the value

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

for a sample having density $n$ (in [8] there were six free parameters for $C(q)$).

Thus, taking the $S(q)$ values from [7] as the experimental points, we described them with taking the $n, e$ scattering into account as

$$S^{\exp}(q) = k\left\{1 + Bf'(q) + [\gamma + Bf'(q)] \cdot [S(q) - 1]\right\}. \tag{4}$$

Here $k$ is the unknown constant close to unity, which has arisen due to author's data normalization to $S(q_{\max})$, which has its own error. The value $B = 8\pi a b_{ne} Z/\sigma_s$ is the relative contribution of $n, e$ scattering to the total one, where $a$ is the length of nuclear coherent scattering of an atom, $Z$ is the number of atomic electrons, $\sigma_s$ is the cross section of nuclear scattering. The electron form factor is $f'(q) = f(q) - f(q_{\max})$, $f(q) = [1 + 3(q/q_0)^2]^{-1/2}$, for Kr $q_0 = 6.74$ Å$^{-1}$ according to [9] and $\gamma = 4\pi a^2/\sigma_s$. The searched $b_{ne}$ contained in $B$ can be found together with other five parameters ($k, A_1 - A_4$ from (2)) by fitting them to a set of $S^{\exp}(q)$ using description (4) with (2) and (3). It is worth noting that the difference $f(q) - f(q_{\max})$ appears in (4) as a result of obvious simplification of expression (3) in [8], which describes the ratio $S(q)/S(q_{\max})$. This simplification makes the work of the used fitting program FUMILI easier.

The pair of parameters $k$ and $b_{ne}$ deserve special attention because of a noticeable correlation between them, especially in the case of small change of the used $f(q)$. This was explicitly observed in the paper [3] where the neutron diffraction by gaseous Kr was analyzed. So we additionally apply the cancellation of constant $k$ by dividing two different domains of $S^{\exp}(q)$ one ofter another.

In order to make basis for the second processing way equation (4) has to be rewritten differently:

$$S^{\exp}(q) = k\,[1 + Bf'(q)] \cdot \left\{1 + \gamma\left[S^{\mathrm{fit}}(q) - 1\right]\right\}, \tag{5}$$

where some small terms are omitted and $S^{\mathrm{fit}}(q)$ already fitted by the first processing way stands instead of to be fitted $S(q)$ in (4). The second step was to divide the whole working interval of $q$ into several domains containing one diffraction period each and to sum up in each of them the experimental $S^{\exp}(q)$, the fitted $S^{\mathrm{fit}}(q)$ and the values $f'(q)$ as well. Then, performing simple mathematical operations with the obtained sums on the basis of (5) we came to

$$p_i = k\,[1 + B < f'(q) >_i] = \sum S^{\exp}(q) / \left\{N_i + \gamma \sum [S^{\mathrm{fit}}(q) - 1]\right\} \tag{6}$$

for the domain $i$ containing $N_i$ points of $S^{\exp}(q)$. Here $\langle f'(q)\rangle_i$ is the form factor averaged over domain $i$. At last the above-mentioned division of the value $p_i$

after (6) by the corresponding $p_j$ led to the final result for $b_{ne}$ without $k$:

$$b_{ne} = \left(\frac{p_i}{p_j} - 1\right) \frac{\sigma_s}{8\pi a Z \left[\langle f'(q)\rangle_i - \langle f'(q)\rangle_j\right]}. \qquad (7)$$

## 2. RESULTS

Unlike [8] we attribute here own normalizing constant $k$ to each sample separately. The interval $q = 4.74{-}15.21$ Å$^{-1}$ was chosen as the main working interval, which was used in all processing ways. It consists of six domain periods of diffraction numbered at $\sim 100$ points of $S^{\exp}(q)$ each. We did not use the $S^{\exp}(q)$ values at $q > 15.21$ Å$^{-1}$ where their obvious fall with increasing $q$ takes place. Really, at the diffraction amplitude $\sim (2{-}5) \cdot 10^{-4}$ the averages $\langle S^{\exp}(q) - 1\rangle$ over $q = (15.21{-}16.24)$ Å$^{-1}$ for five samples are by $\sim (8{-}19) \cdot 10^{-4}$ less than over $q = (13.49{-}14.52)$ Å$^{-1}$. As to the lower limit the use of $S^{\exp}(q)$ at $q < 4.74$ Å$^{-1}$ leads to an increase in $\chi^2$ value essentially.

The majority of obtained results are collected in the Table, where the samples are placed and numbered as in the paper [7]. The average $b_{ne}$ values in columns III, IV and VI are the mean arithmetical over 7 samples with the errors, which are the mean deviations from these averages.

**Table**

| I | II | III | IV | V | VI |
|---|---|---|---|---|---|
| Sample | $k$ | $b_{ne} \cdot 10^3$fm | $b_{ne} \cdot 10^3$fm | $k$ | $b_{ne} \cdot 10^3$fm |
| Kr-1 | 1.0014(1) | –1.25(9) | –1.30(9) | 1.0016(2) | –1.27(13) |
| Kr-2 | 1.0020(1) | –1.87(9) | –2.08(9) | 1.0020(3) | –1.85(18) |
| Kr-3 | 1.0005(1) | –1.07(9) | –1.08(9) | 1.0005(2) | –0.99(16) |
| Kr-4 | 1.0018(1) | –1.77(9) | –1.75(9) | 1.0018(2) | –1.73(17) |
| Kr-5 | 1.0014(1) | –1.05(9) | –0.96(9) | 1.0013(1) | –0.98(9) |
| Kr-6 | 1.0009(1) | –1.42(9) | –1.51(9) | 1.0010(2) | –1.37(12) |
| Kr-7 | 1.0010(1) | –0.87(9) | –0.95(9) | 1.0010(2) | –0.78(15) |
| Average | | –1.33(31) | –1.38(35) | | –1.28(32) |

**2.1. The First Way.** The results of the fitting of 6 parameters in formulas (2)–(4) over the whole working interval of $q$ at $q_{\max} = 16.24$ Å$^{-1}$ (to $N = 604$ points of $S^{\exp}(q)$) are presented in columns II and III of the Table. A description of the experimental points can be seen in Fig. 1, where the data for the least dense sample (Kr-5, $n = 11.28$ nm$^{-3}$) and the densest one (Kr-6, $n = 17.01$ nm$^{-3}$) are shown.

To our astonishment the $\chi^2$ values turned out to be approximately three times less than standard 598. So, assuming the errors of $S^{\exp}(q)$ had been

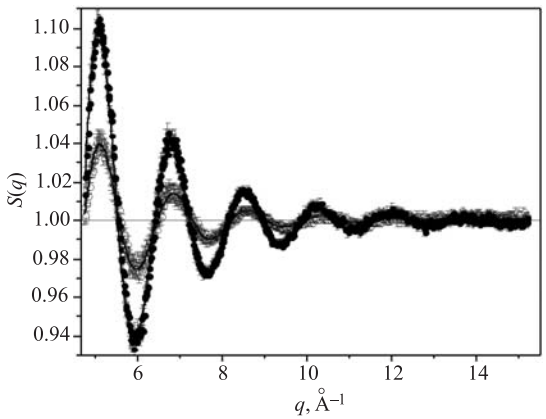


Fig. 1. Data on $S^{\exp}(q)$ and their description by function (4) for two samples: Kr-5 (open circles) and Kr-6 (full circles)

overestimated, we divided them by $\sqrt{3}$ and naturally obtained $\chi^2$ three times more and exactly the same all parameters with the errors $\sqrt{3}$ less. There was one exception: instead of $\sqrt{3}$ we had to use $\sqrt{1.5}$ only for Kr-4. All errors in the Table are given with taking these corrections into account. For justification of our «operation» on errors it is possible to say the following.

1) Neither initial nor decreased statistical errors of individual $b_{ne}$ values have no influence on the error of their average. This error is specified by the scatter of $b_{ne}$ values for different samples. It is 5.5 times more than the statistical error at the initial errors of $S^{\exp}(q)$ and 9.5 times more at the decreased ones.

2) It is said in the paper [7]: «the measuring time was chosen at each measured density in such a way that a statistical precision of $\sim 0.1\%$ on the counting could be achieved». This means that at $S^{\exp}(q) \cong 1$ its error is $\sim 0.001$, but we have it in the range of 0.002–0.004, i. e., essentially more.

3) We made a test for the statistical errors of $S^{\exp}(q)$ using the obtained values of the describing function (4) $S^{\mathrm{func}}(q)$ and the difference $x(q) = S^{\exp}(q) - S^{\mathrm{func}}(q)$ (see Fig. 2) and calculating the average $\bar{x} = \left(\sum x\right)/N$ and the dispersion $\sigma^2 = \left[\sum (x - \bar{x})^2\right]/N$ of $x(q)$ over an interval containing $N$ points of $q$. The averaged over samples values $\sigma \cong (2.7, 1.1, 1.3) \cdot 10^{-3}$ were obtained in the intervals $q$ = 5–7, 7.5–10, 10.5–12.5 Å$^{-1}$, respectively. Really, these $\sigma$ values are 1.5–2 times less than the errors of $S^{\exp}(q)$ in [7].

In order to show the quality of describing $S^{\exp}(q)$, we calculated $x(q)$ for all samples averaging it over 50 points. The result is presented in Fig. 3. As in Fig. 2, the curves of $S^{\mathrm{func}}(q)/10$ for Kr-1 ($n = 14.57$ nm$^{-3}$) and $Bf'(q)$ at

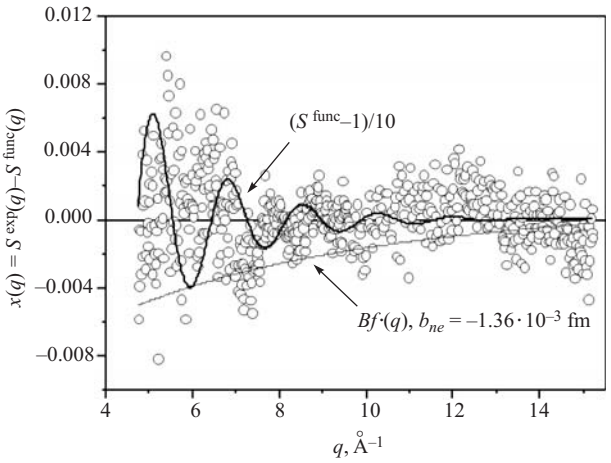


Fig. 2. Inaccuracy of the experimental data description for Kr-1 sample

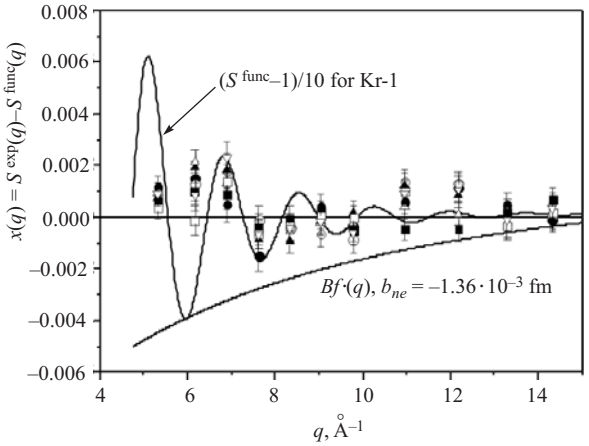


Fig. 3. The summed over 50 points inaccuracies in description of $S^{\exp}(q)$ for all krypton samples (Kr-1 – full circles, Kr-2 — open circles, Kr-3 — full triangles with the bottom down, Kr-4 — open triangles with the bottom down, Kr-5 — full squares, Kr-6 — open squares, Kr-7 — reverse open triangles)

$b_{ne} = -1.36\cdot10^{-3}$ fm are placed there for comparison. As compared with Fig. 2, the scatter of points in $q$ here is 3–4 times less, but some structure for all samples is obvious. Its reason can be incomplete description of the diffraction, erroneous measurements or (and) the data processing as well as some physics of liquid. The average $\bar{x}$ over all $q$ is $(0.9 \div 3.5)\cdot10^{-4}$ for different samples with the error $\sim 1.4\cdot10^{-4}$.

**2.2. The Second Way.** In this way using formula (6), six experimental values of $p_i$ for each sample were calculated. Then 3 values of $b_{ne}$ were obtained from the ratios $p_i/p_j$ according to (7) for $i/j = 1/4$, 2/5 and 3/6. Their weighted mean values for each sample are placed in the column IV of the Table.

The comparison of the results in columns III and IV shows that they are practically the same and undergo quite similar fluctuations from one sample to another. Consequently the problem of the constant $k$ in the first processing way can be considered as solved.

An additional decisive confirmation of this was obtained as follows. Fitting 5 parameters at different fixed constants $k$ in both processing ways, we found the derivatives $\Delta b_{ne}/\Delta k$, where numerator and denominator were the deviations of corresponding parameters from their values in columns III and II or IV and II of Table. The derivatives for all samples practically did not depend on the $\Delta k$ value in both ways, but their values turned out to be essentially different: –0.59 fm in the first way and –0.039 fm in the second way. It means that correlation between $k$ and $b_{ne}$ is suppressed in the second way by $\sim 15$ times and it acts only through the function $S^{\rm fit}(q)$ in (6).

At last, we were able to decrease a little the error of $b_{ne}$ using $S^{\rm fit}(q)$ obtained at the fixed $b_{ne} = -1.36 \cdot 10^{-3}$ fm, which is more real than the scattered quantities in column III of the Table. That decreased the scatter of the $b_{ne}$ values and gave the same average with the smaller error:

$$b_{ne} = (-1.38 \pm 0.27) \cdot 10^{-3}\,\text{fm}. \tag{8}$$

**2.3. The Third Way.** We have found one else possibility to confirm the results described above. In addition to six $p_i$ values obtained before for each sample, we received seven more on the broadened by two half-periods interval of $q = 3.92{-}16.13$ Å$^{-1}$. All $p_i$ being as a matter of fact the ratios of averaged over a domain period $S^{\rm exp}(q)$ and $S^{\rm fit}(q)$ are presented in Fig. 4 and demonstrate their rather smooth course with $q_i$, which is the middle point in the domain $i$.

The fitting of the parameters $k$ and $b_{ne}$ to them by the formula

$$p_i = k\,\{1 + B\,[f(q_i) - f(q_{\rm max})]\} \tag{9}$$

resulted in the quantities of columns V and VI. It is worth emphasizing almost ideal coincidence of the constants $k$ in columns II and V and noting the increased errors of $b_{ne}$ in column VI for individual samples due to a significant scatter of the $p_i$ points. It seems that all points $p_i$ lie approximately on two periods of a certain sinusoid, which is something like the structure in Fig. 3.

In calculations of all results placed in the Table the values $q_{\rm max} = 16.24$ Å$^{-1}$, $a = 7.81$ fm, $\sigma_s = 7.68$ b, $\gamma = 0.998$ were used. Three last items were taken from the compilation [10] and are consistent with the values used in [5, 11]. We also tested the influence on the results of unexpectedly precise quantity

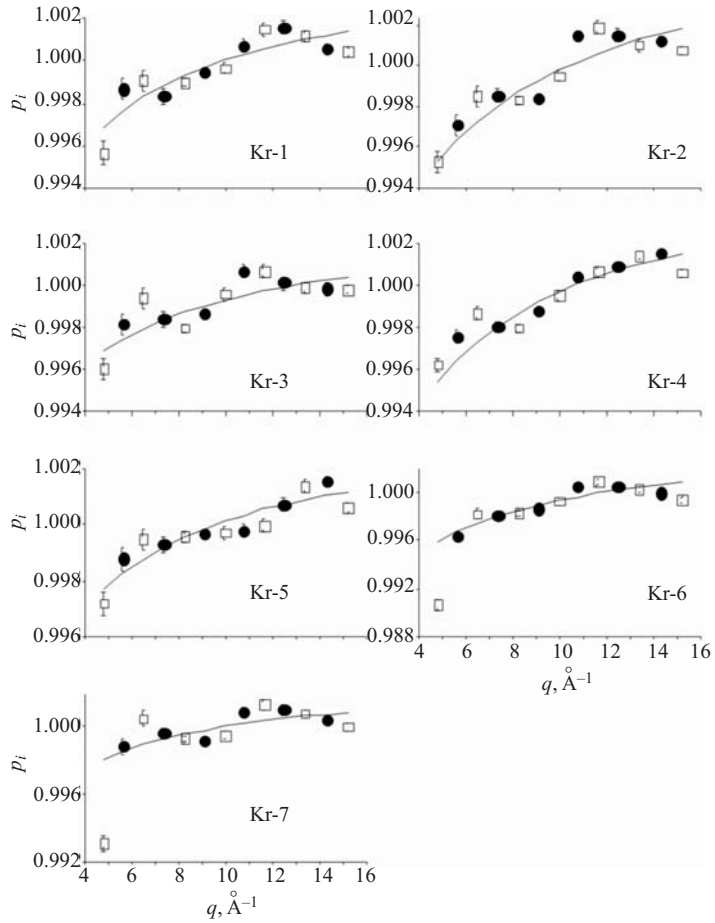


Fig. 4. The $p_i$ values determined by expression (6) for the main domains (full circles) and for the shifted ones by half-period (open squares)

$\gamma = 0.936 \pm 0.002$ obtained in [7] by the original method. The substitution of such $\gamma$ in (4)–(6): 1) at $a = 7.56$ fm in $B$ gives an increase of $|b_{ne}|$ by $\sim 0.06 \cdot 10^{-3}$ fm, 2) $\sigma_s = 8.19$ b in $B$ increases $|b_{ne}|$ by $\sim 0.10 \cdot 10^{-3}$ fm. This is a significant change although for the present in the error's limits.

**2.4. The Fourth Way.** Of course, observed in the Table large scatter of $b_{ne}$ over the different samples and originated from it large error of the mean $b_{ne}$ could not satisfy us. So, we tried to find the common $b_{ne}$ value for all samples, how it should be. For this aim we did the fit with one parameter $b_{ne}$ and seven parameters $k_1 \div k_7$ to all data $S_1^{\exp}(q) \div S_7^{\exp}(q)$, simultaneously, at the fixed

diffraction parameters $R_1 - R_4$ fitted before for each sample separately by the first way (Subsec. 3.1). This led to a very good result

$$b_{ne} = (-1.35 \pm 0.03) \cdot 10^{-3}\,\mathrm{fm} \tag{10}$$

with $\chi^2/4220 = 1.225$ that increased the error from 0.028 to 0.031.

But unfortunately, this result cannot be accepted as the final one. The talking point is that varying the limits of the working $q$ interval changes the extracted $b_{ne}$ value essentially, what is demonstrated in Fig. 5. We can see a smooth course of $b_{ne}$ (crosses) as a function of lower limit $q_l$ at the constant upper limit $q = 15.21$ Å$^{-1}$ (left panel of Fig. 5) and as a function of the upper limit $q_u$ at constant lower limit $q = 4.74$ Å$^{-1}$ (right panel of Fig. 5). If we look attentively at all crosses in Fig. 5, we will see that they lie just within the errors of (8). It means that we have obtained a result approximately equivalent to (8).

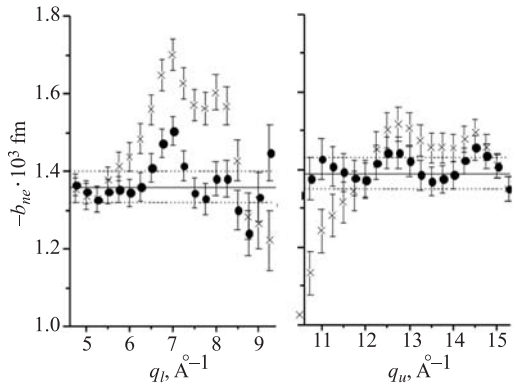


Fig. 5. The extracted $b_{ne}$ value as a function of lower $q_l$ and upper $q_u$ limits of the working interval: crosses — without removing the structure from $S^{\exp}(q)$ and points — with correction for the structure

Nevertheless, we tried to improve the situation with $b_{ne}$ error. Seemingly, such a behaviour of $b_{ne}$ is due to some structure that was discussed in connection with Figs. 3 and 4. Visible structure distorts the real functions $y = k(1 + Bf')$ leading to wrong $b_{ne}$ values. Really, if $y(q_l)$ becomes less, the fitted $-b_{ne}$ increases and vice versa (this takes place at $q_l = 6 \div 9$ Å$^{-1}$, see the left panel of Fig. 5). And if $y(q_u)$ becomes more, the fitted $-b_{ne}$ increases and vice versa (see the right panel of Fig. 5, at $q_u = 12 \div 15$ Å$^{-1}$). All this means that the most correct $b_{ne}$ value lies probably along a «pedestal» of two maxima of crosses in Fig. 5.

In order to find such a «pedestal» we described the points $x(q) = S^{\exp}(q) - S^{\mathrm{func}}(q)$ by the function (2) with four varied parameters. The fitted functions

$x^{\rm fit}(q)$ came out with good $\chi^2$ values, but with rather irregular sinusoid parameters for different samples: amplitudes $A_1 \sim 0.0004 \div 0.0022$, periods $A_3 \sim 4.3 \div 9.9\text{Å}^{-1}$, initial phases $A_4 \sim (0.001 \div 0.85) \cdot 2\pi$, four of fitted functions are diminishing sinusoids ($A_2 > 0$) and three are increasing ones ($A_2 < 0$, see examples in Fig. 6). Thus, considering $x^{\rm fit}(q)$ as a false structure and taking $S^{\rm exp}(q) - x^{\rm fit}(q)$ instead of $S^{\rm exp}(q)$ we obtained the black points in Fig. 5. This operation decreased the $b_{ne}$ scatter significantly and allowed us to get rather satisfactory results: for the left points in Fig. 5

$$b_{ne} = (-1.36 \pm 0.04) \cdot 10^{-3}\,\text{fm} \tag{11}$$

and

$$b_{ne} = (-1.39 \pm 0.04) \cdot 10^{-3}\,\text{fm} \tag{12}$$

for the right ones. They both are the mean arithmetical quantities over 19 values of $b_{ne}$ and of its deviation from the average. The errors in (11) and (12) are statistical mainly, because they are only a little larger than a statistical error in (10).

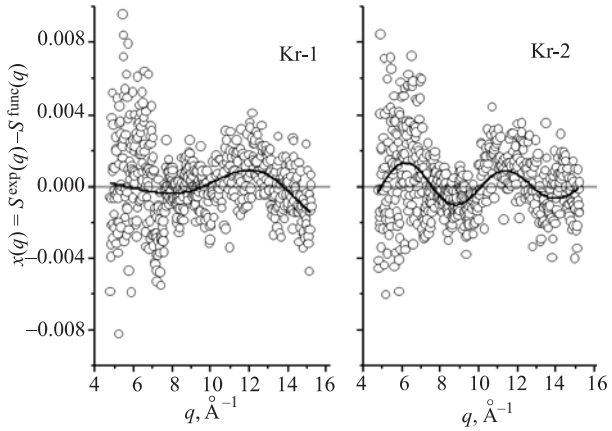


Fig. 6. Examples of differences of the experimental $S(q)$ and $S^{\rm fit}(q)$. Lines are the descriptions of these differences by function (2)

## CONCLUSION

Thus completing the data processing, we dispose of three results for $b_{ne}$ obtained by different ways. They are (1), (8) and implied consequence from (11) and (12)

$$b_{ne} = (-1.38 \pm 0.04) \cdot 10^{-3}\,\text{fm}. \tag{13}$$

At rather different errors, the values of $b_{ne}$ are practically the same and this fact allows us to consider (13) as the main result demonstrating a definite progress in perfecting the method as compared with two previous ones [3, 4]. The reached accuracy of $b_{ne}$ places this result among the best ones.

However certainly, this result is correct only in the case if the erroneous monotonous deviation of the $S^{\exp}(q)$ points from their true values (for example, due to wrong corrections) in the whole interval $q > 4$ Å$^{-1}$ does not exceed $\sim 0.0003$.

We must also emphasize that in future investigations it is necessary to have (in addition to improvement of statistics) a very precise ratio $a/\sigma_s$ (better than 1% of accuracy). According to [10] here it is $\sim$1.7%. It gives the systematical error of $b_{ne} \sim 0.02 \cdot 10^{-3}$ fm.

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