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New method to extract the neutron–electron scattering length

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Abstract. A novel 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 dividing the experimental data into two parts: the first, nearly proportional to n, corresponding to diffraction on neighboring atoms and the second one, a small contribution of n, e scattering independent on n. The proposed technique is demonstrated using the structure factor $S(q)$ for gaseous krypton.

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1 Introduction

Since the neutron has a complex electromagnetic structure, it has to interact with atomic electrons not only via its magnetic moment. The electric structure of the neutron can be characterized by a fundamental constant, the mean square charge radius of the neutron $\langle r_n^2 \rangle$, which is connected directly with the neutron–electron scattering length

$$b_{ne} = \frac{M_n e^2}{3\hbar^2} \langle r_n^2 \rangle \,,$$

where M_n is the neutron mass, and e is the charge of the electron.

Experiments with the aim to determine the b_{ne} value were initiated more than fifty years ago and continued up to now. Different methods were exploited to determine b_{ne} with errors $< 0.05 \cdot 10^{-3}$ fm (see Table 1). The values are concentrated in the $-1.6 \cdot 10^{-3}$ to $-1.3 \cdot 10^{-3}$ fm range but differ by several standard deviations. Of course, unaccounted systematic errors must be the reason of the large divergence of the data. In each of the methods of the b_{ne} determination there are specific problems connected with the necessity to introduce large corrections with magnitudes which are of the same order or even larger than the investigated effect.

It is important to note that the measured b_{ne} values are scattered around the value of the so-called Foldy scattering length $b_{\rm F} = \mu_n e^2/(2M_n c^2) = -1.468 \cdot 10^{-3}$ fm caused by the neutron anomalous magnetic moment μ_n interacting with the electron electrical field [10]. If $b_{ne} = b_{\rm F}$, it would signify that μ_n is connected with $\langle r_n^2 \rangle$ directly. Such a bond of magnetic and electrical constants for elementary particles is unexpected for present theories. It clearly justifies a re-analysis of the previous data and new measurements.

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Table 1. The best results on b_{ne}

Experiment	Target	b_{ne}, 10^{-3} fm	References
Transmission (time-of-light)	Bi	-1.56 ± 0.05	[1]
		-1.44 ± 0.07	[2]
	^{208}Pb	-1.31 ± 0.05	[3]
		-1.33 ± 0.04	[2]
Angle scattering	Ne, Ar,	-1.34 ± 0.03	[4]
	Kr, Xe	-1.30 ± 0.03	[5]
Single crystal scattering	^{186}W	-1.60 ± 0.05	[6]
Transmission, mirror reflection	Pb	-1.364 ± 0.025	[7]
	Bi	-1.393 ± 0.025	[7]
	Pb, Bi	-1.32 ± 0.04	[8]
	Isotopes Pb, Bi	-1.32 ± 0.03	[9]

The simplest experiment to obtain the b_{ne} value is to scatter neutrons in a noble gas. Since an amplitude of n, e scattering is a very small addition to the nuclear one, the experiments for extracting b_{ne} are based on a measurement of the interference between these two amplitudes. The scattering cross section for scattering a neutron off one atom at rest can thus be written as

$$\sigma_s^{\rm atom}(\theta) = \sigma_s + 8\pi a_{\rm coh} b_{ne} Z f(q) \,,$$

where σ_s is the nuclear part of the scattering cross section, $a_{\rm coh}$ is the nuclear coherent scattering length, Z is the number of electrons, $f(q)$ is the atomic form factor, $q = 4\pi \sin(\theta/2)/\lambda$, θ is the scattering angle, λ is the neutron wavelength. The second term, which is about one percent of the cross section, can be extracted due to the known atomic form factor $f(q)$.

In many experiments with the purpose to obtain b_{ne}, it is necessary to take into account neutron diffraction of the

neighboring atoms described by the structure factor $S(q)$. Even in the experiments with noble gases [4] a correction for the diffraction can be essential [11]. Unfortunately, nobody tried to separate experimentally the diffraction and n,e scattering contributions. Model calculations [2] cannot reach an accuracy of $\sim 10^{-4}$ of the nuclear cross section, which is necessary to obtain b_{ne} with the relative accuracy $\sim 10^{-2}$ (see, for example, one of the last and detailed papers [2] and the critique of it in [12]).

2 Method

In the method proposed here the diffraction at neighboring atoms is not a hindrance for n,e scattering research, and the n,e scattering effect can be extracted in an experimental situation where the structure factors of the noble gases are carefully investigated.

To pass from the intensities of neutron scattering $I(q)$ to the structure factors $S(q)$ a lot of corrections have to be introduced. A number of these corrections (for thermal motion of atoms, container influence, efficiency of neutron registration, etc.) also includes the correction for the n,e scattering contribution, which is supposed to be known. But the n,e effect $B = 8\pi a_{\rm coh} b_{ne} Z/\sigma_s$ can be determined together with the $S(q)$ due to the fact that the diffraction has a known dependence on the gas density n (almost linear at not very high n), while B does not depend on n. Therefore, in accordance with [13] the scattering intensity per unit of neutron flux and one atom of gas can be described as

$$I(\theta) = \sigma_s \Bigg\{ (1+Q_1) + f(q)B + \frac{nC(q)}{1-nC(q)} \left[\frac{\sigma_{\rm coh}}{\sigma_s} (1+Q_2) + f(q)B \right] \Bigg\} , \quad (1)$$

where Q_1 and Q_2 take into account the thermal motion of one atom and a pair of atoms, respectively [4, 12, 14] (in [14] $F = 1 + Q_1$), the function $C(q)$ is connected with the structure factor $S(q)$ directly [13, 15]:

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

and $\sigma_{\rm coh}$ and σ_s are the coherent and total nuclear scattering cross sections.

3 Test of the method

To confirm the principal possibility to obtain the b_{ne} value from the angle distributions of neutrons at different densities of the noble gas the model experiment was performed [16]. Its main aim was to find out the necessary statistics level and the number of scattering angles and gas densities for obtaining the result with sufficient accuracy. Neutrons with the energy $E_0 = 0.0143\,\text{eV}$ (as in [13]) were scattered by krypton in the angle interval 0–180° ($q = 0$–$5.2\,\text{Å}^{-1}$) at 15 gas densities $(0.0269 \div 5.58) \cdot 10^{21}\,\text{cm}^{-3}$. Using (1) the simulated data (99 points in the angle interval for each gas density) were generated and then statistically scattered with the average relative error $3 \cdot 10^{-3}$.

Two variants of the data analysis were carried out. (1) The data at the certain q for all gas densities are fitted consecutively. Two parameters b_{ne} and $C(q)$ are obtained for each q and then an average value of b_{ne} is evaluated. (2) All the data for all q and the chosen number of gas densities are fitted simultaneously and then the parameters b_{ne} and $C(q)$ are determined.

Both variants gave very close results; in particular b_{ne} values averaged over q coincided with b_{ne} in the second variant. Of course, the most accurate $b_{ne} = -(1.337 \pm 0.017) \cdot 10^{-3}$ fm (the original one is -1.340) was obtained using all 1485 "experimental" points, but for the accuracy on the present-day level ($\Delta b_{ne} = 0.03$–0.04) 220–300 points were enough. These very good results were obtained in idealized conditions, so, taking into account the background, the influence of the container for gas and different corrections remain the main difficulties of our method.

4 Examples of the method application

To make a realistic test of our method we chose a very detailed paper [13], where neutrons with the energy $E_0 = 0.0143\,\text{eV}$ were scattered at 200 angles $\theta \cong 6° \div 109°$ (with statistics of $3.5 \cdot 10^5$ counts per angle) by gaseous krypton at 17 different densities $n = (0.25 \div 6.19) \cdot 10^{21}\,\text{cm}^{-3}$. There are a table of $S(q)$ values for all gas densities and 78 different q up to $4.0\,\text{Å}^{-1}$ and almost full information about corrections in this paper. The authors of [13] wrote the neutron scattering intensity (after background and multiple scattering subtracting) as

$$I(\theta) = \sigma_s (1 + f(q) B_0) \{ [S(q,n) - 1]\,\gamma_0 + 1 + P_1(q) \} , \quad (2)$$

where B_0 is a correction for n,e scattering made in [13], which contains $b_{ne} = -1.34 \cdot 10^{-3}$ fm, $\gamma_0 = \sigma_{\rm coh}/\sigma_s = 0.976$ is the fraction of coherent scattering in the total one, and $P_1(q) = 0.01056 - 0.001727 q^2$ is the well-known Placzek correction for the thermal motion of the atoms.

We have made two attempts to obtain the b_{ne} value from the $S(q)$ data of [13]. In the first one [12] we tried to reconstruct the ratios of the initial scattering intensities of krypton and vanadium using the $S(q)$ values and information about the corrections from [13]. To describe scattering on krypton we used formula (1) with $\sigma_{\rm coh} = 6.96b$ and $\sigma_s = 7.51b$ and the free parameter B. We took not all the data for fitting but chose only those which satisfied the linearity of the dependence $S(n)$ for each q. From the fit we obtained for each q a new S value, which is very close to the original one from [13], and searched the parameter B. The stability of the value of the parameter B obtained in fitting for different q we consider as a success of the method. However, we obtained the quantity $b_{ne} = -1.34 \cdot 10^{-3}$ fm from the B values averaged over all q after introducing the factor 0.971 before σ_s in

(1). The close factor $[1 + P_1(0)] / [1 + Q_1(0)] = 0.975$ is necessary because of the difference in corrections for the thermal motion between [12] and [13] (this can be seen from a comparison of (1) and (2)).

Doubtless, the reason of such a vague result is the insufficient accuracy of numerous corrections and incomplete information on them given in [13]. For example, the authors report only the limits of the corrections changing and nothing about their accuracy. Meanwhile, in order to derive b_{ne} with an accuracy $\sim 5\%$ the changing with q of all real corrections (for background, absorption, self-screening, multiple scattering) has to be known with a relative accuracy not worse than 2–3%. The absolute value of the correction is not so important because it influences only the data normalization, which must be fitted (see below). Therefore, we realized another attempt to get b_{ne}. Believing in corrections for the absorption and multiple scattering made in [13], we used all the data on $S(q)$ from [13], including a term with n^2 in the expression for the scattering intensity:

$$I(\theta) = \sigma_s \left[(1 + Q_1)(1 + fB) + (1 + Q_2)(\gamma + fB)\, X_1 - (1 + Q_3)\,(\gamma + fB)\, X_2\right] . \quad (3)$$

Since $C(q)$ is a linear function in gas density, which can be written as $C(q) = C_0(q) - nC_1(q)$, according to [15], the terms $X_1 = nC_0/(1 - nC_0 + n^2C_1)$ and $X_2 = n^2C_1/(1 - nC_0 + n^2C_1)$ appeared in (3). The functions $Q_1 = 0.0360 - 0.00184q^2$, $Q_2 = 0.0172 - 0.000887q^2$ and $Q_3 = 0.0114 - 0.000584q^2$ take into account the thermal motion of one, two and three scattering atoms, respectively. Combining (2) and (3) we obtain the fitting formula

$$S - 1 = \frac{1}{\gamma_0}\left\{\frac{a}{(1 + fB_0)}\left[(1 + Q_1)(1 + fB) + (1 + Q_2)(\gamma + fB)X_1 - (1 + Q_3)(\gamma + fB)X_2\right] - (1 + P_1)\right\}. \quad (4)$$

As for σ_s, it canceled out, but we keep a normalizing constant a. Here the more correct value $\gamma = 0.927$ in the diffraction terms differs from the γ_0 used by authors of [13].

Fitting the experimental $S(q, n) - 1$ from [13] by formula (4) for all gas densities, we obtained three parameters: b_{ne}, C_0 and C_1 for each q. Besides that, for the comparison of taking into account the thermal motion by different methods, we have also done calculations with Placzek corrections. With this purpose the functions Q_1, Q_2, Q_3 in the fitting formula (4) were replaced by P_1, P_2 and P_3, where P_2 and P_3 correspond to the mass of two and three atoms and are found by division of P_1 by 2 and 3, respectively. Results of the fits are shown in Fig. 1. In both cases the parameters C_0 and C_1 are indistinguishable in the picture, and parameters b_{ne} systematically differ by $\sim 0.1 \cdot 10^{-3}$ fm. We cleared up also how the fitting results depend on γ value. When we took $\gamma = 0.976$ (equal to γ_0) instead of 0.927, the result of b_{ne} shifted to zero by $\sim 0.02 \cdot 10^{-3}$ fm only. The error bars in the upper part of Fig. 1, which are significantly more than the observed scatter of the b_{ne} points ($\chi^2 < 1$ for each q), are the errors of fitting with the data

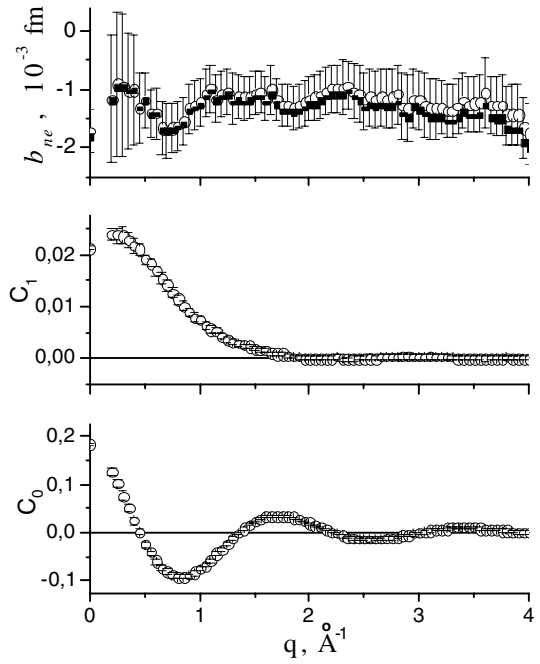

Fig. 1. Parameters b_{ne}, C_0 and C_1 fitted using (4) with Q corrections and $a = 0.975$ (light squares) and with Placzek corrections and $a = 1$ (black circles)

Table 2. b_{ne} values obtained by the new method

Fitting		a	$\langle b_{ne}\rangle \cdot 10^{-3}$, fm
for each q separately	using Q- correction	0.975	-1.23 ± 0.02
	using P correction	1	-1.34 ± 0.02
for all q simultaneously	Q, a was fixed	0.975	-1.27 ± 0.03
	Q, a was fitted	0.976 ± 0.002	-1.53 ± 0.24

error $\Delta S = 5 \cdot 10^{-3}$ taken by us rather arbitrarily, being founded on the authors' estimations (it is not given directly in [13]; in particular, because the authors employed the smoothing points of $S(n, q)$ by "eye"). Results of these fits, averaged over the q values $\langle b_{ne}\rangle$ and the mean square deviation from them (that is the real error), are presented at the two upper lines of Table 2.

Naturally, fitting for each q separately did not allow us to fit the normalization parameter a. So, additionally, we fitted $S(q, n) - 1$ for all q and all n simultaneously using ten parameters: the parameter b_{ne}, the normalization parameter a, the four parameters for describing C_0 and the four parameters for C_1, as C_0 and C_1 were described by suitable convergent oscillating functions. Figure 2 demonstrates the satisfactory quality of the fitting. In the lower picture there are examples of describing the experimental data $S - 1$ (points) by the fitting function (4) (lines) for some chosen gas densities. The lines and points for C_0 and C_1 are obtained at different fitting conditions with free and fixed parameter a respectively. In the lower part of Fig. 1, they

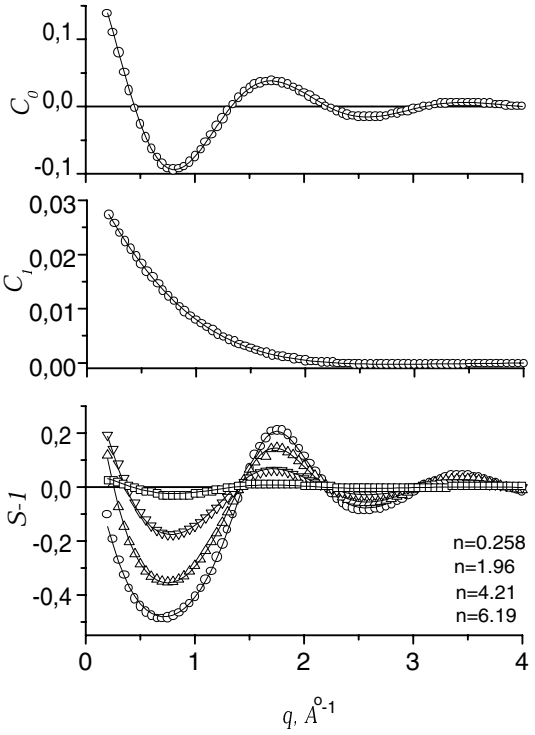

Fig. 2. The results of simultaneous fitting the data for all q and n

display a behavior with q typical for diffraction on gases (see [13,15] and references therein). The obtained b_{ne} values are placed in two lower lines of Table 2. In both cases, the χ^2 values were ~ 1.3 per point.

It is worth to explain the seeming contradictory between this good χ^2 value and the large error bars of b_{ne} in Fig. 1. The reason is that at the same errors $\Delta S = 0.005$ for all q and n, Fig. 1 is the result of describing of 78×17 points of S by 78×3 free parameters, while Fig. 2 and the lower line of Table 2 are the result of describing the same points by ten free parameters only. Therefore, the systematic errors existing in the data (and which can be noticed in Fig. 1) are described lightly in the first case and cannot be described in the second one.

5 Discussion

To discuss the obtained results, the following should be noted.

(1) The thermal motion taken into account through the P and Q functions gives different $\langle b_{ne} \rangle$ values, which differ by almost 9% although their errors are less than 2%. So, the question which correction is true remains open.

(2) It is shown that the diffraction on neighboring atoms can be eliminated as a hindrance for obtaining b_{ne}. This distinguishes the proposed method essentially from the research like [2], where the calculated model correction for diffraction reaches about 100% of the n, e effect.

(3) The form factor $f(q)$ (and the b_{ne} contribution fB) decreases only by 30% at increasing q from 0 to 4 Å^{-1}, and therefore the parameter B correlates with a rather strongly. As a result, changing of a by 0.001 changes b_{ne} by $\sim 8\%$. And although the statistical accuracy of each $S(q, n)$ value in [13] is close to 0.001, the accuracy of the normalizing constant a is significantly worse due to errors of the corrections and cross sections of Kr, V and Al (containers). This means that the normalization has to be a fitted parameter, and only such a fit is worthy of a serious consideration. Thus, the three upper lines of Table 2 are only a demonstration of our new method efficiency, and they display only prospects of the measurements like those in [13] for the b_{ne} derived. On the contrary, the lower line of Table 2 represents a new (even though modest in accuracy) result obtained by the proposed new method. Since some quantities in [13] are not precise enough, new experiments would be indispensable.

6 Conclusion

We have demonstrated the feasibility to extract the n, e scattering length with an accuracy better than 5% from a study of the angular distributions of mono-energetic thermal neutrons scattered off single-atom noble gases by investigating the structure factors of noble gases.

From the data of [13] the new result $b_{ne} = -(1.53 \pm 0.24) \cdot 10^{-3}$ fm has been obtained, which is not of high accuracy but free from model corrections.

For the future experiments with gases xenon, krypton or argon using the new method:
(1) it is necessary to have statistics not less than 10^6 counts for each bin in q; (2) it is necessary to have a reliable and exact normalization of both absolute and angular distributions (correctly accounting for background and other corrections); (3) it is desirable to have a wider range of q up to 10–20 Å^{-1} (for more changes in $f(q)$) in order to decrease the correlation between parameters b_{ne} and a and the error of b_{ne} .

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