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INTERATOMIC PAIR POTENTIAL AND $n{-}e$ AMPLITUDE FROM SLOW NEUTRON SCATTERING BY NOBLE GASES

Yu. N. Pokotilovski [1]

Joint Institute for Nuclear Research, Dubna

Recently proposed new precision experiments to increase accuracy of neutron–electron scattering amplitude consist in the energy-dependence measurement of the asymmetry of slow neutron scattering by noble gases. It is shown that additional diffraction effect, due to correlations in positions of atoms in gas, has significant value and depends on particular form of realistic interatomic pair potential.

Недавно были предложены новые прецизионные эксперименты по уточнению амплитуды нейтрон-электронного взаимодействия посредством измерения энергетической зависимости асимметрии рассеяния медленных нейтронов благородными газами. Показано, что дополнительный дифракционный эффект из-за корреляции в положении атомов газа имеет значительную величину и зависит от конкретной формы межатомного потенциала.

As is well known, experimental situation in the value of neutron–electron scattering amplitude looks rather controversial:

$$\begin{aligned} a_{n-e} &= -\,1.56 \pm 0.05 \ [1], \\ a_{n-e} &= -\,1.59 \pm 0.04 \ [2], \\ a_{n-e} &= -\,1.31 \pm 0.03 \ [3,\ 4], \\ a_{n-e} &= -\,1.44 \pm 0.033 \pm 0.06 \ [5], \\ a_{n-e} &= -\,1.33 \pm 0.027 \pm 0.03 \ [5]. \end{aligned} \tag{1}$$

It is seen that the progress in the precision was not significant during the last 40 years, and strong disagreement exists between different experiments. New experiments have been proposed recently to measure $n{-}e$ scattering amplitude by the method of Fermi–Marshall [6, 3] — angular asymmetry in slow neutron scattering, and by the transmission method — measuring the energy-dependence of total neutron cross-section by noble gases [7, 8]. It was also reminded that small effect of neutron diffraction has to be taken into account to infer $n{-}e$ amplitude from asymmetry data [9]. The model of hard-sphere interatomic potential was taken relying on the paper by Akhiezer and Pomeranchuk [10].

But rigorous calculations of the diffraction effect, based on the realistic interatomic potentials, demonstrate that diffraction effect has significant value especially in the cold-neutron energy range reaching dozens percent or even prevailing over the $n{-}e$ interaction effect.

[1] e-mail: pokot@nf.jinr.ru

Neutron–atom scattering amplitude

$$a(\theta) = a_N + a_{n-e} Z f(\theta) \tag{2}$$

in result of interference of the nuclear and electron scattering leads to scattering cross-section

$$\frac{d\sigma(\theta)}{d\Omega} = a_N^2 + 2a_N a_{n-e} Z f(\theta), \tag{3}$$

with the relative value of the anisotropic term

$$\delta\Big(\frac{d\sigma(\theta)}{d\Omega}\Big) = 2\frac{a_{n-e}}{a_N} Z f(\theta). \tag{4}$$

Atomic formfactor may be calculated with sufficient precision according to [11]

$$f(q) = \left[1 + 3\left(\frac{q}{q_0}\right)^2\right]^{-1/2}, \tag{5}$$

with

$$q_0 = \beta Z^{1/3} (\text{Å}^{-1}). \tag{6}$$

In these expressions a_N is the nuclear scattering amplitude; a_{n-e} is the amplitude of $n-e$ scattering; Z is the charge number. The value of β is taken from the tables [12].

Static-structure factor depends on interatomic interaction potential $U(r)$ and atomic density n:

$$S(q) = 1 + n\int_0^\infty \Big(\mathrm{e}^{-U(r)/kT} - 1\Big)\mathrm{e}^{i\mathbf{qr}} d^3\mathbf{r}. \tag{7}$$

For spherically symmetric potential $U(r)$ the structure factor is

$$S(q) = 1 + n\frac{4\pi}{q}\int_0^\infty \Big(\mathrm{e}^{-U(r)/kT} - 1\Big)\sin(qr) r dr. \tag{8}$$

The scattering asymmetry is introduced as the ratio of intensities of scattered neutrons to the angles θ_1 and θ_2 (usually, $\theta_1 + \theta_2 = \pi$)

$$\frac{S(\theta_1)}{S(\theta_2)}. \tag{9}$$

The figures show the results of calculation of asymmetry for the forward and backward angles, respectively, 45 and 135°. For every noble gas of interest (Ar, Kr, Xe) several best approximations for the potential of interatomic interaction were taken from the literature.

For all used potentials $r = r_m\bar{r}$, $U(r) = U^*(r)\epsilon$.

Lenard-Jones (L-J) potential for Ar [13]:

$$U^*(r) = (\bar{r}^{-12} - 2\bar{r}^{-6}),\ \epsilon/k = 119.8\ \text{K},\ r_m = 3.822\ \text{Å}. \tag{10}$$

Barker–Fisher–Watts (BFW) potential [14]:

$$U^*(r) = \exp\left[\alpha(1-\bar{r})\right]\sum_{i=0}^{n} A_i(\bar{r}-1)^i + \sum_{j=0}^{2} C^*_{2j+6}/(\delta + \bar{r}^{2j+6}). \tag{11}$$

Parameters of BFW potential for Ar:

$$\begin{array}{llll} \epsilon/k = 142.1\,\mathrm{K}, & r_m = 3.761\,\text{Å}, & \alpha = 12.5, & \delta = 0.01, \\ C_6 = -1.10727, & C_8 = -0.16971, & C_{10} = -0.01361, & \\ A_0 = 0.27783, & A_1 = -4.50431, & A_2 = -8.33122, & \\ A_3 = -25.2696, & A_4 = -102.0195, & A_5 = -113.25. & \end{array} \tag{12}$$

Barker–Bobetic–Maitland–Smith (BBMS) potential [15]:

$$U^*(r) = U^*(\mathrm{BFW}) + \alpha' \exp\left[-50(\bar{r}-1.33)^2\right]. \tag{13}$$

Parameters of BBMS potential for Ar:

$$\begin{array}{llll} \epsilon/k = 142.5\,\mathrm{K}, & r_m = 3.76\,\text{Å}, & \alpha = 12.5, & \delta = 0.01, \\ C_6 = -1.11976, & C_8 = 0.171551, & C_{10} = -0.01361, & \\ A_0 = 0.29214, & A_1 = -4.41458, & A_2 = -7.70182, & \\ A_3 = -31.9293, & A_4 = -136.026, & A_5 = -151. & \end{array} \tag{14}$$

Parson–Siska–Lee (Morse–Spline–Van der Waals, MSV III) potential [17]:

$$\begin{array}{ll} U^*(r) = \exp\left[-2\beta(\bar{r}-1)\right] - 2\exp\left[-\beta^{'}(\bar{r}-1)\right], & 0 \le \bar{r} \le x_1, \\ U^*(r) = b_1 + (\bar{r}-x_1)b_2 + (\bar{r}-x_2)[b_3 + (\bar{r}-x_1)]b_4, & x_1 \le \bar{r} \le x_2, \\ U^*(r) = C^*_6\bar{r}^{\,-6} + C^*_8\bar{r}^{\,-8} + C^*_{10}\bar{r}^{\,-10}, & x_2 \le \bar{r} \le \infty. \end{array} \tag{15}$$

Parameters of MSV III potential for Ar:

$$\begin{array}{llll} \epsilon/k = 140.7\,\mathrm{K}, & r_m = 3.76\,\text{Å}, & & \\ C_6 = -1.180, & C_8 = -0.6118, & C_{10} = 0, & \\ x_1 = 1.12636, & x_2 = 1.400, & \beta = \beta^{'} = 6.279, & \\ b_1 = -0.7, & b_2 = 1.8337, & b_3 = -4.5740, & b_4 = 4.3667. \end{array} \tag{16}$$

Aziz–Chen (Hartree–Fock, HFD–C) potential [16]:

$$U^*(r) = A\exp\left(-\alpha\bar{r}\right) + (C_6\bar{r}^{-6} + C_8\bar{r}^{-8} + C_{10}\bar{r}^{-10})F(\bar{r}),$$

where

$$\begin{array}{ll} F(\bar{r}) = \exp\Big[-\Big(\dfrac{D}{\bar{r}}\Big)^2\Big], & \bar{r} \le D, \\ F(\bar{r}) = 1, & \bar{r} \ge D. \end{array} \tag{17}$$

Parameters of HFD–C potential for Ar:

$$\begin{array}{lll} \epsilon/k = 143.224\,\mathrm{K}, & r_m = 3.759\,\text{Å}, & \alpha = 16.345655, \\ C_6 = -1.0914254, & C_8 = -0.6002595, & C_{10} = -0.3700113, \\ A = 0.9502720\cdot 10^7, & D = 1.4, & \gamma = 2.0. \end{array} \tag{18}$$

BWLSL potential for krypton [19] has the form of BFW potential with additional term:

$$\Delta U(\bar r) = \Big[P(\bar r - 1)^4 + Q(\bar r - 1)^5\Big] e^{\alpha(1-\bar r)}, \quad \bar r > 1, \\ \Delta U(\bar r) = 0, \qquad \bar r < 1. \tag{19}$$

Parameters of BWLSL potential for Kr:

$$\begin{array}{llll} \epsilon/k = 201.9\,\mathrm{K}, & r_m = 4.0067\,\text{Å}, & \alpha = 12.5, & \delta = 0.01, \\ C_6 = -1.0632, & C_8 = -0.1701, & C_{10} = -0.0143, & \\ A_0 = 0.23526, & A_1 = -4.78686, & A_2 = -9.2, & A_3 = -8.0, \\ A_4 = -30.0, & A_5 = -205.8, & P = -9.0, & Q = 68.67. \end{array} \tag{20}$$

BDVKS potential for krypton [20]:

$$\begin{array}{lll} U(r) = \epsilon f_m(\bar r, \beta), & 0 < r < r_1, & \\ U(r) = \sum_{k=0}^{3} a_k z_k, & r_1 < r < r_2, & z = (r - r_1)/(r_2 - r_1), \\ U(r) = -C_6 r^{-6} - C_8 r^{-8}, & r_2 < r < \infty, & \\ f_m = e^{2\beta(1-x)} - 2e^{\beta(1-x)}. & & \end{array} \tag{21}$$

Parameters of BDVKS potential for krypton have two slightly different variants (I and II):

$$\begin{array}{rl} \text{for variant I} & \epsilon/k = 200.0\,\mathrm{K},\ r_m = 4.03\,\text{Å},\ r_1 = 4.5,\ r_2 = 5.0, \\ & C_6 = -908000,\ C_8/C_6 = 10.9,\ \beta = 6.2, a_0 = -147.01, \\ & a_1 = 76.856,\ a_2 = -18.172,\ a_3 = 4.8747 \\ \text{and for variant II} & \beta = 6.3,\ a_0 = -145.84,\ a_1 = 78.034, \\ & a_2 = -24.022,\ a_3 = 8.3822 \end{array} \tag{22}$$

BWLSL potential for xenon [19] has the form of BFW potential. Parameters of BWLSL potential for xenon:

$$\begin{array}{llll} \epsilon/k = 293.8\,\mathrm{K}, & r_m = 4.355\,\text{Å}, & \alpha = 15.5, & \delta = 0.01, \\ C_6 = -1.0052, & C_8 = -0.1590, & C_{10} = -0.03105, & \\ A_0 = 0.18345, & A_1 = -4.2620, & A_2 = -27.0, & \\ A_3 = -58.0, & A_4 = 10.0, & A_5 = 10.0. & \end{array} \tag{23}$$

A more compromised form of the potential for xenon is specified by BWLSL potential with parameters

$$\begin{array}{llll} \epsilon/k = 281.0\,\mathrm{K}, & r_m = 4.3623\,\text{Å}, & \alpha = 12.5, & \delta = 0.01, \\ C_6 = -1.0544, & C_8 = -0.1660, & C_{10} = -0.0323, & \\ A_0 = 0.2402, & A_1 = -4.8169, & A_2 = -10.9, & A_3 = -25.0, \\ A_4 = -50.7, & A_5 = 200.0, & P = 59.0, & Q = 71.1. \end{array} \tag{24}$$

It is seen from Figs. 1–3 that additional diffraction effect, due to correlations in positions of atoms in gas, has significant value and depends on particular form of realistic interatomic pair potential. In the energy range below ~ 10 meV, diffraction contribution to the asymmetry

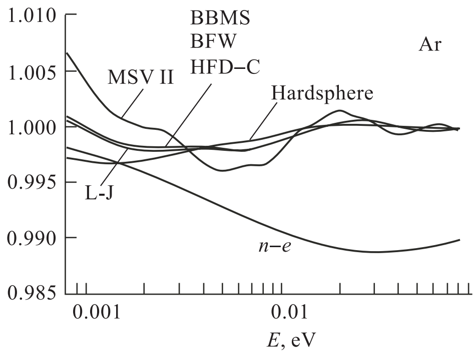

Fig. 1. The neutron energy-dependence of the scattering asymmetry ($\theta_1 = \pi/6$, $\theta_2 = 5\pi/6$) from 1 atm pressure Ar gas target in result of $n{-}e$ interaction and diffraction for different approximations of the interatomic Ar–Ar interaction: L-J — Lenard-Jones potential [13], BFW potential [14], BBMS approximation [15], HFD–C potential [16], MSV II potential [17]

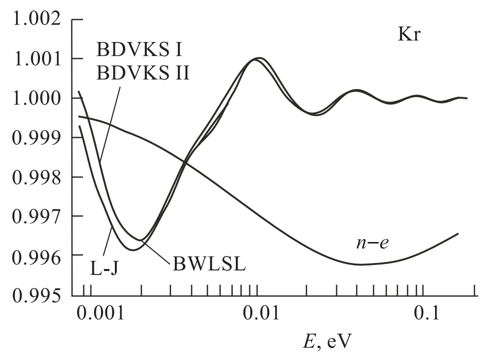

Fig. 2. The neutron energy-dependence of the scattering asymmetry ($\theta_1 = \pi/4$, $\theta_2 = 3\pi/4$) from 1 atm pressure Kr gas target in result of $n{-}e$ interaction and diffraction for different approximations of the interatomic Kr–Kr interaction: L-J — Lenard-Jones potential for Kr [18], BWLSL potential [19], BDVKS I and BDVKS II — two variants of approximation [20]

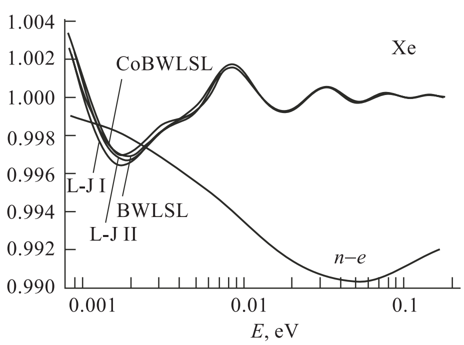

Fig. 3. The neutron energy-dependence of the scattering asymmetry ($\theta_1 = \pi/4$, $\theta_2 = 3\pi/4$) from 1 atm pressure Xe gas target in result of $n{-}e$ interaction and diffraction for different approximations of the interatomic Xe–Xe interaction: L-J I and L-J II — two approximations of Lenard-Jones potential for Xe [21,22], BWLSL [19], CoBWLSL-corrected approximation potential [19]

of slow neutron scattering by noble gases achieves dozens percent of the asymmetry due to $n{-}e$ interaction, and in the meV energy range even exceeds the $n{-}e$ asymmetry effect. To infer the value of $n{-}e$ scattering amplitude with percent precision from the neutron scattering asymmetry data, it is necessary to perform precise asymmetry measurements at the pressures significantly lower than 1 atm with subsequent extrapolation to zero pressure, or to take into account the diffraction effect using the particular approximation of the interatomic interaction potential as true one. In view of disagreement (significant in some cases) between different approximations of interatomic potential inferred from the large amount of experimental data on various physical quantities, the latter procedure does not seem reliable. It would be of value to perform the special high-precision measurements of neutron scattering asymmetry (or static structure factor) for noble gases, similar to the neutron-diffraction experiments on Ar [23–25] and to the experiments on Kr [26,27]. But in this case effect of $n{-}e$ interaction must be taken into account, which was not done in the cited experimental works. So the problem consists in the indeterminancy of both effects contributing to the asymmetry of slow neutron scattering by noble gases: $n-e$ interaction and diffraction. This complicates seriously the task of the measurement of the $n-e$ scattering amplitude with percent precision by this method.

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REFERENCES

1. *Melkonian E., Rustad B. M., Havens W. W.* // Phys. Rev. 1959. V. 114. P. 1571.
2. *Alexandrov Yu. A. et al.* // Yad. Fiz. 1974. V. 60. P. 1190; Sov. J. Nucl. Phys. 1975. V. 60. P. 623; *Alexandrov Yu. A.* // Z. Physik A. 1992. V. 344. P. 219.
3. *Krohn V. E., Ringo G.* // Phys. Rev. D. 1973. V. 8. P. 1305.
4. *Koester L., Washkovski W., Kluver A.* // Physica B. 1986. V. 137 P. 282.
5. *Kopecky S. et al.* // Phys. Rev. C. 1997. V. 56. P. 2229.
6. *Fermi E., Marshall L.* // Phys. Rev. 1947. V. 72. P. 1139.
7. *Bunatian G. G. et al.* JINR Preprint E3-96-79. Dubna, 1996; Z. Physik A. 1997. V. 359. P. 337.
8. *Enik T. L. et al.* Neutron Spectroscopy, Nuclear Structure, Related Topics // Proc. of the Intern. Seminar on Interaction of Neutrons with Nuclei, ISINN-9, Dubna, May 23–26, 2001. P. 70.
9. *Mitsyna L. V. et al.* JINR Preprint E3-2002-40. Dubna, 2002.
10. *Akhiezer A., Pomeranchuk I.* // ZhETF. 1949. V. 19. P. 558.
11. *Sears V. F.* // Phys. Rep. 1986. V. 141. P. 281.
12. International Tables for X-Ray Crystallography / Eds. Ibers J. A., Hamilton W. C. Birmingham: Kynoch Press, 1974. V. IV.
13. *Michels A., Wijker Hk., Wijker Hub.* // Physica. 1949. V. 15. P. 627.
14. *Barker J. A., Fisher R. A., Watts R. O.* // Mol. Phys. 1971. V. 21. P. 657.
15. *Barker J. A., Pompe A.* // Aust. J. Chem. 1968. V. 21. P. 1683; *Maitland G. C., Smith E. B.* // Mol. Phys. 1971. V. 22. P. 657.
16. *Aziz R. A., Chen H. H.* // J. Chem. Phys. 1977. V. 67. P. 5719.
17. *Parson J. M., Siska P. E., Lee J. T.* // J. Chem. Phys. 1972. V. 56. P. 1511.
18. *Hirshfelder J. O., Curtis C. F., Bird R. B.* Molecular Theory of Gases and Liquids. N. Y.: John Wiley, 1954.
19. *Barker J. A. et al.* // Chem. Phys. 1974. V. 61. P. 3081.
20. *Buck U. et al.* // Phys. Rev. A. 1973. V. 8. P. 2409.

21. *Van den Biesen J. J. H. et al.* // Physica A. 1980. V. 100. P. 375.

22. *Maitland G. C., Smith E. B.* // Seventh Symp. on Thermophysical Propreties. Am. Soc. Mech. Eng., 1977.

23. *Andriesse C. D., Legrand E.* // Physica. 1972. V. 57. P. 191.

24. *Fredrikze H., Andriesse C. D., Legrand E.* // Ibid. V. 62. P. 474.

25. *Fredrikze H. et al.* // Phys. Rev. Lett. 1989. V. 62. P. 2612.

26. *Teitsma A., Egelstaff P. A.* // Phys. Rev. A. 1980. V. 21. P. 367.

27. *Barocchi F., Zoppi M., Egelstaff P. A.* // Phys. Rev. A. 1985. V. 31. P. 2732.

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