L.A. BULAVIN, YU.F. ZABASHTA

Taras Shevchenko National University of Kyiv, Faculty of Physics
(64/13, Volodymyrs'ka Str., Kyiv 01601, Ukraine; e-mail: bulavin221@gmail.com)

PACS 28.20.Cz, 61.05.fg

ANOMALOUS ASYMPTOTIC OF SMALL-ANGLE NEUTRON SCATTERING INTENSITY

An anomalous asymptotic dependence of the small-angle neutron scattering intensity $I(\mathbf{Q})$, when $I(\mathbf{Q})$ increases infinitely as $\mathbf{Q} \to 0$, has been studied. This behavior is shown to be associated with the presence of the random field of a scattering density, whose typical linear size is much larger than the reciprocal magnitude of $\mathbf{Q}$. In the considered case, the sought asymptotic dependence is found to have the form $I(\mathbf{Q}) \sim Q^{-3}$.

Keywords: small-angle neutron scattering, classical asymptotics, anomalous asymptotics.

1. Introduction

According to the classical theory [1], the scattering intensity at $\mathbf{Q} \to 0$ has the following dependence:

$$I_{\text{clas}}(\mathbf{Q}) \sim 1 - Q^2 b^2, \tag{1}$$

where b is a characteristic linear dimension of the system, which coincides by its order of magnitude with the correlation length (the inhomogeneity size). We will refer to the behavior of the intensity described by formula (1) as the classical asymptotics.

In some experiments [2–5], deviations from the classical dependence (1) are observed (see Figure, where the dashed curve is determined by formula (1), and the solid one corresponds to the experimental dependence). The behavior of the intensity described in the figure by the solid curve will be referred to as the anomalous asymptotics of a small-angle neutron scattering. In this paper, a possible physical mechanism of its emergence is discussed.

2. Anomalous Asymptotics of Neutron Scattering Intensity

One of the known models used to describe the scattering of neutrons by a physical system [2] is the continuum one. In its framework, the system is considered as a statistically homogeneous field $\varphi(\mathbf{x})$ of a random variable φ, which is called the scattering density. This field, as any other random homogeneous field, is characterized by the correlation coefficient

$$\Gamma(\mathbf{r}) = \frac{\langle \varphi(\mathbf{x})\varphi(\mathbf{x}')\rangle}{\sigma^2}, \tag{2}$$

where $\mathbf{r} = \mathbf{x} - \mathbf{x}'$, $\mathbf{x}$ is the radius vector of the point in the space occupied by the system, $\langle ... \rangle$ the operator of averaging over the field, and σ^2 the dispersion of the random variable.

Another characteristic of the indicated field is the quantity $s(\mathbf{q})$ called the normalized spectral density or the normalized spectrum (below, the term "spectrum" will be used). This quantity is connected with the correlation coefficient by the Fourier transformation:

$$s(\mathbf{q}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Gamma(\mathbf{r}) \exp(-i\mathbf{r}\mathbf{q})\, d\mathbf{r}, \tag{3}$$

$$\Gamma(\mathbf{r}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} s(\mathbf{q}) \exp(i\mathbf{r}\mathbf{q})\, d\mathbf{q}. \tag{4}$$

According to the classical theory of scattering [1], the scattering intensity is proportional to the random field spectrum. This result is used to find the spectrum from experimental data. Namely, by measuring the scattering intensity $I(\mathbf{Q})$ for various scattering vectors $\mathbf{Q}$ and using the mentioned dependence, the experimental spectrum $s_{\exp}(\mathbf{Q})$ is calculated as

$$I(\mathbf{Q}) \sim s_{\exp}(\mathbf{Q}). \tag{5}$$

It is evident that

$$s_{\exp}(\mathbf{Q}) = s(\mathbf{q} = \mathbf{Q}). \tag{6}$$

We associate the emergence of the anomalous asymptotics in the small-angle neutron scattering intensity with the existence of a random field, for which the following condition is satisfied:

$$b \gg Q^{-1}. \tag{7}$$

Provided that condition (7) holds true, let us consider a passage to the limit defined by the dependences

$$Q^{-1} \to \infty, \tag{8}$$

$$b \to \infty. \tag{9}$$

Then, for the correlation coefficient, the relation

$$\Gamma(\mathbf{r}) \to 1 \tag{10}$$

takes place. Substituting it into equality (3), we obtain

$$s(\mathbf{q}) \to \delta(\mathbf{q}). \tag{11}$$

Dependence (8) can be rewritten in the form

$$\mathbf{Q} \to 0. \tag{12}$$

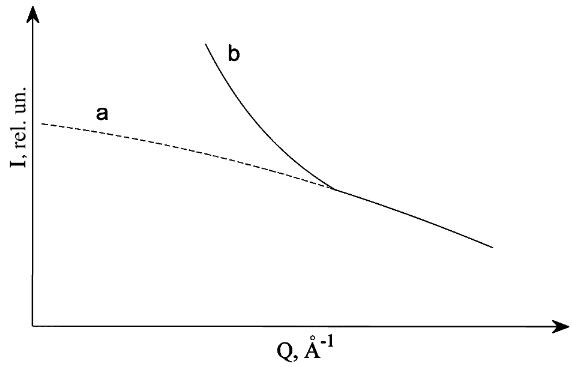
Here, some numerical sequence tending to zero is meant:

$$\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, ..., 0; \tag{13}$$

whereas, when writing down relation (11), the sequence of functions

$$s(\mathbf{q})_1, s(\mathbf{q})_2, s(\mathbf{q})_3, ..., \delta(\mathbf{q}) \tag{14}$$

converging to the delta-function in the space of generalized functions was assumed [6]. By comparing relations (13) and (14), one can see that every dispersion vector $\mathbf{Q}_J$ in sequence (13) has its "counterpart" term $s_J(\mathbf{q})$ in sequence (14). Such a sequence is called the



Classical (a) and anomalous (b) asymptotics of the neutron scattering intensity

delta-sequence [6]. It is supposed [6] that since the indicated sequence converges to the delta-function, any term in the sequence can be considered, in principle, as a delta-function approximation. For this purpose, it is necessary that the indicated term should have the properties of the delta-function. Proceeding from the last condition, let us determine the analytical form of the function $s_J(\mathbf{q})$, i.e. the J-th term in the delta-sequence.

In the physical literature [7], the delta-function is considered as a function with the following properties:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(\mathbf{q})\, d\mathbf{q} = 1, \tag{15}$$

$$\delta(\mathbf{q}) = 0 \ (\mathbf{q} \neq 0), \tag{16}$$

$$\delta(\mathbf{q}) = \infty \ (\mathbf{q} = 0). \tag{17}$$

The approximate delta-function (the term $s_J(\mathbf{q})$ in the delta-sequence) must have similar properties. Property (15) of the delta-function remains the same for the $s_J(\mathbf{q})$ term in the delta-sequence,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} s_J(\mathbf{q})\, d\mathbf{q} = 1. \tag{18}$$

But the formulations that give rise to properties (16) and (17) of the delta-function have to be corrected in the case of an approximate delta-function, i.e. the $s_J(\mathbf{q})$ term. As follows from formula (16), the values of delta-function are equal to zero for all scattering vectors, except for the vector $\mathbf{q} = 0$. It is clear that the zero value is unattainable for the scattering vector in the real experiment. We may say only that the magnitude of the vector $\mathbf{Q}_J$ given in the experiment is small enough for it to be considered as equal to zero. In this case, the magnitude of scattering vector $\mathbf{Q}_J$ plays the role of the determination error for the so-called "zero" in this experiment.

It was already mentioned that the term $s_J(\mathbf{q})$ in the delta-sequence corresponds to the magnitude of $\mathbf{Q}_J$. Therefore, if we intend to consider the term $s_J(\mathbf{q})$ in the delta-sequence as an approximate delta-function, we should approximately adopt that we deal with a "zero" that occupies the region $|\mathbf{q}| \leq |\mathbf{Q}_J|$. The obtained approximate delta-function $s_J(\mathbf{q})$ is "smeared" over a spherical region with the radius $|\mathbf{Q}_J|$. Beyond this region, the values of term $s_J(\mathbf{q})$ in the delta-sequence must be equal to zero as is inherent to the delta-function,.

It is evident that the indicated "smearing" does not allow property (16) of the delta-function to be attributed to the term $s_J(\mathbf{q})$ in the delta-sequence at full scale, because the approximate delta-function "smeared" over the indicated sphere $|\mathbf{q}| \leq |\mathbf{Q}_J|$ cannot be equal to infinity, since equality (16) becomes violated otherwise. At the same time in our case, it is important that the delta-function has a unique value at zero, and just this peculiarity of the delta-function has to be preserved for the terms of the delta-sequence. In other words, if we want to consider the term $s_J(\mathbf{q})$ in the delta-sequence as the delta-function, we have to accept that, at "zero" in the region $|\mathbf{q}| \leq |\mathbf{Q}_J|$, this term has a unique value, which will be denoted below as h_J.

Taking all the aforesaid into account, the function $s_J(\mathbf{q})$ is selected in the form

$$s_J(\mathbf{q}) = h_J\{H(|\mathbf{q}|) - H(|\mathbf{q}| - |\mathbf{Q}|)\}, \quad (19)$$

where $H(z)$ is the Heaviside step function. Substituting it into equality (18) and integrating, we obtain

$$h_J = \frac{3}{4\pi} Q_J^{-3}. \quad (20)$$

By definition, the experimentally observed spectrum at the given scattering vector $\mathbf{Q}_J$ equals

$$s_{\text{exp}}(\mathbf{Q}_J) = s_J(\mathbf{q} = \mathbf{Q}_J). \quad (21)$$

Substituting $s_J(\mathbf{q} = \mathbf{Q}_J)$ calculated with the use of formulas (19) and (20) into equality (21), we obtain

$$s_{\text{exp}}(\mathbf{Q}) = \frac{3}{4\pi} Q^{-3}. \quad (22)$$

In addition, according to formula (5), we have

$$I_{\text{anom}}(\mathbf{Q}) \sim Q^{-3} \quad (\mathbf{Q} \to 0) \quad (23)$$

for the anomalous asymptotics of the small-angle neutron scattering intensity.

As is seen from the figure, a specific feature of the anomalous asymptotics in comparison with its classical analog is a sharp growth of the intensity in the case where the scattering vector tends to zero. Relation (23) describes this feature. Therefore, we have all grounds to consider the mechanism of anomalous asymptotics at the small-angle neutron scattering considered above as a true one. It is clear that the condition of thermodynamic limit is not realized in a real experiment, and the neutron scattering intensity at the zero angle will not be infinite [8].

3. Conclusion

The speculations presented above bring us to a conclusion that inequality (7) is the unique reason for the anomalous asymptotics (23) to emerge. This means that we will always observe experimentally the described anomalous behavior of the small-angle neutron scattering intensity, if the examined system includes a large-scale random field of the scattering condensed medium density with characteristic linear dimensions considerably exceeding the inverse magnitudes of scattering vectors realized in this experiment. In addition, this also means that since no microscopic ideas were used while deriving formula (23), the latter remains valid for any field satisfying condition (7).

Which field is it? On the one hand, the presence of the indicated field can testify to the existence of a large-scale superstructure in the condensed medium. On the other hand, it is not excluded that when the scattering vector tends to zero, the small-angle scattering intensity starts to be affected by the spatial confinement of the examined system. Then the system size will play the role of a characteristic dimension b. The answer to this question should be obtained in further experiments planned by us.

1. P. Debye, *Selected Works* (Nauka, Moscow, 1987) (in Russian).
2. L.A. Feigin and D.I. Svergun, *Structure Analysis by Small-Angle X-Ray and Neutron Scattering* (Plenum Press, New York, 1987).

3. M.V. Avdeev and V.L. Aksenov, Usp. Fiz. Nauk **180**, 1109 (2010).
4. V.V. Runov and V.N. Skorobagatykh, Fiz. Tverd. Tela **56**, 68 (2014).
5. T.V. Khamova and O.A. Shilova, Fiz. Tverd. Tela **56**, 107 (2014).
6. W. Kecs and P.P. Teodorescu, *Applications of the Theory of Distributions in Mechanics* (Acad. RSR, Bucharest, 1970) (in Romanian).
7. L.D. Landau and E.M. Lifshitz, *Quantum Mechanics. Non-Relativistic Theory* (Pergamon Press, New York, 1977).
8. K.O. Chalyi, L.A. Bulavin, and O.V. Chalyi, Zh. Fiz. Dosl. **9**, 66 (2005).

Received 08.02.15
Translated from Ukrainian by O.I. Voitenko

Л.А. Булавін, Ю.Ф. Забашта

АНОМАЛЬНА МАЛОКУТОВА АСИМПТОТИКА ІНТЕНСИВНОСТІ РОЗСІЯННЯ НЕЙТРОНІВ

Р е з ю м е

Стаття присвячена розгляду асимптотичної залежності інтенсивності малокутового розсіяння нейтронів $I(\mathbf{Q})$ при $\mathbf{Q} \to 0$. Розглядається аномальна асимптотика інтенсивності розсіяння, коли $I(\mathbf{Q})$ різко зростає при $\mathbf{Q} \to 0$. Показано, що така поведінка інтенсивності зумовлена присутністю випадкового поля розсіюючої густини з характерним лінійним розміром, який значно перевищує обернене значення модуля $\mathbf{Q}$. Встановлено, що в розглянутому випадку шукана асимптотична залежність має вигляд $I(\mathbf{Q}) \sim Q^{-3}$.