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THEORY OF NEUTRON ELASTIC SCATTERING BY NEMATIC LIQUID CRYSTALS

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THEORY OF NEUTRON ELASTIC SCATTERING BY NEMATIC LIQUID CRYSTALS

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I. INTRODUCTION

Recently, Novaković and Shukla /1/ have presented a new approach to nematic liquid crystals by exploring the pseudo-spin formalism. Also several neutron experiments were carried out on these types of liquids /2-4/. Therefore, there is a need to develop a model-scattering theory which would be invoked to verify the consistency of the proposed pseudo-spin Hamiltonian with the existing observations by neutron techniques.

In this paper we present a method for an explicit evaluation of the angular cross section for the elastic neutron scattering by nematic liquids. To do this, it is necessary to quote briefly their physical nature in addition to the pseudo-spin model and its theoretical consequences /1/.

As it is well known /5,6/, in distinction from the smectic liquid crystals, in nematic and cholesteric ones the molecules are not confined in layers but are capable of random orientations which are more or less continuous throughout the liquid. Furthermore, nematic liquids possess certain invariance under reflections, while this is not the case with the cholesteric liquids.

II. THE PSEUDO-SPIN HAMILTONIAN

Assuming that 2S + 1 (S = b/2; b = 0,1,...) orientations of an effective electrical dipole, $\vec{d}_i = 2e\vec{R}_{0i}$ ($2|\vec{R}_0|$ being the distance between effective charges e) inside of each long elongated rod-like molecule, are described by deviations of the S_i^z pseudo-spin components (i,j= 1,...N label the molecular sites)*, the proposed Hamiltonian of the system is /1/

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* To effective dipoles $\vec{d}_i = 2e\vec{R}_{0i}$ one makes correspond the pseudo-spin $\vec{S}_i = \mathrm{ort}\vec{R}_{0i}$, such that $\vec{d}_i = d_0\vec{S}_i$ ($d_0 = 2eR_0$).

$$H = - \sum_{j} \sum_{b=1}^{2S} \Omega_j (S_{jx})^b - \sum_{jk} J_{jk} S_{jz} S_{kz} . \tag{1}$$

Here Ω_j are quantum parameters related to a transfer energy of dipoles, while $J_{jk} = J(|\vec{r}|)$, $\vec{r} = |\vec{r}_i - \vec{r}_j|$, are coupling parameters related to the intermolecular (namely interdipole) potential, as a continuously varying function for a fluid. The above Hamiltonian, being thus very general, was simplified a bit further assuming that all dipoles have only 3 possible orientations ($S = 1$). However, the treatment and the obtained results are essentially identical for general S.

The further procedure, which is used also hereafter, consisted in a rotation of the pseudo-spin system through an angle φ. Then the pseudo-spin raising (lowering) operators $S_j^{\pm} = S_j^x \pm iS_j^y$ were introduced, assuming their bosonic representation /7/. After this, going over to the Fourier transformed bosons, performing the standard Bogolubov's diagonalization and assuming the Lennard-Jones intermolecular potential, the collective excitation frequency was obtained. Such a frequency was analysed around the origin $\vec{q} = 0$ and in the neighbourhood of the second maximum in the Fourier transformed intermolecular potential $\vec{q}_o$, wherefrom a zero-sound velocity and a rotonic mass were estimated.

III. GENERAL EXPRESSION FOR ELASTIC NEUTRON SCATTERING

The elastic scattering of slow neutrons by nematic liquid crystals can be described with high accuracy by a pure nuclear interaction, while the other ones can be discarded as being the effects of a considerably less order of magnitude. Actually, for an asymmetric effective dipole (i.e. rotator, defined later on in Sec. IV) an interaction would exist between the neutron magnetic moment and a resulting magnetic moment generated by the rotation of a dipole proportional to

$$|\vec{\mu}_n||\vec{\mu}_{eff}| = |2\gamma \frac{e\hbar}{2m_p c} \vec{I}_n||\frac{1}{2c} (\frac{e_1}{m_1} + \frac{e_2}{m_2})\vec{L}|; \qquad (2)$$

m_p is the proton mass and $\vec{I}_n$ - the neutron spin; $\gamma = -1{,}93$ is the neutron magnetic moment in nuclear Bohr magnetons, and $\vec{L}=\hbar(\mathrm{ort}\vec{d} \times \mathrm{ort}\vec{p})$ is an effective orbital moment operator associated with a rotating dipole masses m_1 and m_2, $\vec{p}$ being a dipole momentum. Since masses $m_1 \approx m_2$ are probably relatively large, such a magnetic scattering would result in a negligible effect.

The elastic differential cross section per unit solid angle for unpolarized neutrons can be expressed in the concise form /8,9/

$$\frac{d\sigma}{d\Omega} = \frac{m_n^2}{(2\pi)^2\hbar^4} \sum_{ij} \sum_{rr'} \langle\langle \overline{a_{ir} a_{jr'}} \rangle\rangle \langle e^{-i\vec{q}\vec{R}_{ir}(o)} e^{i\vec{q}\vec{R}_{jr'}(\infty)} \rangle. \quad (3)$$

Here the bracket <<...>> stands for the average of the expectation value of the enclosed operator, as well as for the average over the nuclear spin and effective orbital moments (dipoles) orientations, and the line above denotes the average over the initial neutron spin orientations; m_n is the neutron mass, $\vec{q}=\vec{p}-\vec{p}'$ is the scattering momentum transfer and $\vec{p}$, $\vec{p}'$ are incoming and outgoing wave vectors of the neutron, respectively. The atoms along any rod-like molecule, as well as the two ends of each effective dipole, are labelled by the index r ($1 \leqslant r \leqslant n + 2$, n being the total number of atoms in the molecule), and their position vectors are denoted by $\vec{R}_{ir}$. The scattering amplitude of nuclei, i.e. scattering amplitudes associated with effective dipole nuclear masses, are $a_{ir} = A_{ir} + B_{ir}(\vec{I}_n \vec{I}_{ir})$ ($\vec{I}_{ir}$ is the spin operator of the ir-th target, and A_{ir} and B_{ir} are the corresponding nuclear constants).

Let us now perform decomposition of the ir-th position vector

$$\vec{R}_{ir}(t) = \vec{R}_i + \vec{R}_r(t); \tag{4}$$

$\vec{R}_i$ refers to the middle (gravity) point of the i-th rod-like molecule and $\vec{R}_r(t)$ is an instantaneous distance of the r-th atom, i.e., an instantaneous distance of one or the other dipole end, inside a molecule, with respect to its gravity point.

These position vectors have not any correlation at an infinite time-like distance, so the correlator in (3) can be written

$$\langle e^{-i\vec{q}\vec{R}_{ir}(o)} e^{i\vec{q}\vec{R}_{jr'}(\infty)}\rangle = e^{-i\vec{q}(\vec{R}_i-\vec{R}_j)} \langle e^{-i\vec{q}\vec{R}_r(o)}\rangle \langle e^{i\vec{q}\vec{R}_{r'}(\infty)}\rangle. \tag{5}$$

As we deal with neutron scattering by effective dipoles inside long rod-like molecules, we shall use the adiabatic approximation. The correlators

$$\langle e^{-i\vec{q}\vec{R}_{i\mu}(o)} e^{i\vec{q}\vec{R}_{j\nu}(\infty)} = e^{-i\vec{q}(\vec{R}_i-\vec{R}_j)} \langle e^{-i\vec{q}\vec{R}_\mu(o)}\rangle \langle e^{i\vec{q}\vec{R}_\nu(\infty)}\rangle F(T) \tag{6}$$

$$(\mu,\nu = 1,\ldots n),$$

will, as a good approximation, determine only Bragg-like peaks, depicting an ordinary elastic scattering in liquids, i.e. a "background" to which the scattering on the "basic (dipole-like) mode" would be superposed. The "pure" dipole correlators

$$\langle e^{-i\vec{q}\vec{R}_{i\gamma}(o)} e^{i\vec{q}\vec{R}_{j\beta}(\infty)}\rangle = e^{-i\vec{q}(\vec{R}_i-\vec{R}_j)} |\langle e^{-iqR_\gamma(o)}\rangle|^2 \tag{7}$$

$$(\gamma,\beta = n + 1, n + 2),$$

and the "mixed" correlators between atoms and effective dipoles

$$\langle e^{-i\vec{q}\vec{R}_{i\mu}(o)}\, e^{i\vec{q}\vec{R}_{j\gamma}(\infty)}\rangle = e^{-i\vec{q}(\vec{R}_i-\vec{R}_j)}\langle e^{-i\vec{q}\vec{R}_\mu(o)}\rangle\langle e^{i\vec{q}\vec{R}_\gamma(o)}\rangle F(T) \quad (8)$$

will describe a characteristic elastic scattering by effective dipoles themselves, as well as correlated with the atomic motion, respectively. In the above expressions $F(T)\sim 1$ is a thermal factor due to the internal degrees of freedom of the molecule.

Actually, these two last correlators are concerned with the neutron scattering by "basic elementary excitations", the latter reflecting once more the collective atomic effect in addition to that manifested in the formation of an effective dipole, as a consequence of a specific atomic cooperation.

Then from (3) one can write

$$\frac{d\sigma}{d\Omega} = \Big[\sigma_1^{coh}\Big|\sum_i e^{i\vec{q}\vec{R}_i}\Big|^2 + N\sigma_1^{inc}\Big]\Big|\langle e^{i\vec{q}\vec{R}(o)} + e^{-i\vec{q}\vec{R}(o)}\rangle\Big|^2 +$$

$$\Big[\sigma_2^{coh}\Big|\sum_i e^{i\vec{q}\vec{R}_i}\Big|^2 + N\sigma_2^{inc}\Big]S(\vec{q})\ \langle e^{i\vec{q}\vec{R}(o)} + e^{-i\vec{q}\vec{R}(o)}\rangle\ F(T) \quad (9)$$

($\vec{R}(o) = \vec{R}_\gamma(o)$ - the position vector of any dipole end, independent of γ)

where

$$\sigma_f^{coh} = \frac{m_n^2}{(2\pi\hbar^2)^2}\langle A_f\rangle^2,\quad \sigma_f^{inc} = \frac{m_n^2}{(2\pi\hbar^2)^2}\Big[\langle A_f^2\rangle - \langle A_f\rangle^2 + \frac{1}{4}\langle B_f\rangle I(I+1)\Big],$$

$$(f = 1,2)\ ; \quad (10)$$

$$S(\vec{q}) = \Big|\sum_{\mu=1}^{n} e^{i\vec{q}\vec{R}_\mu}\Big|^2 \simeq n\,\frac{\sin(\vec{l}\vec{q})}{(\vec{l}\vec{q})}\ . \quad (11)$$

$S(\vec{q})$-structural factor of the molecule, $2|\vec{L}|$ being the molecular length; $\langle A_f\rangle = (\sum_s A_s\, c_s)_f$, c_s being the concentration of atoms (isotopes), i.e., of effective dipoles, for which $A_{ir} = A_s$. The index "1" is referred to the "pure" scattering by dipoles, provided that a possible estimation of a corresponding scattering amplitudes will be outlined hereafter, when model description of dipoles will be closely adjusted; the index "2" is related to the "mixed" scattering events, when dipoles correlate with atoms.

IV. MODEL DESCRIPTION OF THE EFFECTIVE DIPOLE AND PSEUDO-SPIN FORMFACTORS

To explore the pseudo-spin formalism for the explicit evaluation of the angular elastic cross section (9), it is necessary to find an equivalent correlator between pseudo-spins /10-12/. Since the effective dipoles have 3 discrete orientations (restriction to the case of S=1), one assumes that their corresponding states can be desribed by a set of real trial wave functions for every dipole

$$|x\rangle = \frac{1}{R_o^2}\,\delta^{1/2}(R-R_o)\{-\frac{1}{\sqrt{2}}\,[Y_{11}(\theta,\phi) + Y_{1-1}(\theta,\phi)]\}$$

$$|y\rangle = \frac{1}{R_o^2}\,\delta^{1/2}(R-R_o)\{\frac{1}{\sqrt{2}}[Y_{11}(\theta,\phi) - Y_{1-1}(\theta,\phi)]\} \qquad (12)$$

$$|z\rangle = \frac{1}{R_o^2}\,\delta^{1/2}(R-R_o)Y_{10}\,(\theta,\phi).$$

The radial part of the above wave function is assumed according to Schwinger /11/ for a rigid rotator, while the spherical functions are

$$Y_{\ell m}(\theta,\phi) = \frac{(-1)^{\ell+m}}{2^{\ell}\,\ell!}\left[\frac{(2\ell+1)(\ell-m)}{4\pi\,(\ell+m)!}\right]^{1/2}(\sin\theta)^m\,\frac{d^{\ell+m}(\sin\theta)^{2\ell}}{(d\cos\theta)^{\ell+m}}\exp(im\phi) \tag{13}$$

In such a way we also associate to each effective dipole $\vec{d}_i = d_o\vec{s}_i$ a corresponding rotator with an effective orbital moment operator $\vec{L}_i = \hbar\vec{s}_i^{\,\prime}$ ($\vec{s}_i^{\,\prime} \sim \vec{s}_i$; $|\vec{s}^{\,\prime}| = |\vec{s}| = 1$), so that it holds

$$\frac{\vec{L}^2}{2I}\,|\alpha\rangle = \frac{\hbar^2\ell(\ell+1)}{2I}, \quad (\ell = 1;\ \alpha = x,y,z); \tag{14}$$

$\left(I = (m_1 + m_2)R_o^2\right.$ is the inertia-moment of the rotator$\left.\right)$. Restricting ourselves to the case of a symmetric rotator ($m_1=m_2=m$), it is obvious that the above equation (14) is equivalent to the equation for a free rotating dipole with 3 discrete orientations (free pseudo-spin or "dipolar-like" spin)

$$\vec{d}^2|\alpha\rangle = d_o^2\,\ell(\ell+1), \quad d_o = 2eR_o . \tag{15}$$

Hence, in the proposed model figure parameters of the effective dipole such as m, e and R_o, although for the final scattering cross section, as we shall see later, only the estimation of dipole magnitude, i.e. the estimation of its effective length, is needed along with the assumptions for the ratios e/m, m/M to be of the order $e_o/2m_p$, R_o/L , respectively, M being the molecular mass. Accordingly, for effective nuclear constants, associated with nuclear dipole mass, one can assume

$$A_d = \left(\sum_\mu A_\mu c_\mu\right)\frac{R_o}{L}\ ; \quad B = \left(\sum_\mu B_\mu c_\mu\right)\frac{R_o}{L} . \tag{16}$$

If one makes correspond the spin-wave functions (namely those of pseudo-spin) $|\chi_\alpha\rangle$ (for $S = 1$) to the wave functions $|\alpha\rangle$, then one can make correspond the pseudo-spin-like operator to the exponential one in (9). This comes from equality of the corresponding matrix elements of these two operators in their respective bases, so one postulates.

$$e^{i\vec{q}\vec{R}} \Leftrightarrow f(\vec{q},\vec{S}) = A_q I + B_q S_x + C_q S_y + D_q S_z + E_q S_x^2 + F_q S_z^2 + G_q S_x S_y + H_q S_x S_z + K_q S_y S_z;$$

$$\text{(I is the unit [3x3] matrix)}, \qquad (17)$$

where the above formfactors are determined from the conditions

$$\langle\alpha|e^{i\vec{q}\vec{R}}|\beta\rangle = \langle\chi_\alpha|f(\vec{q},\vec{S})|\chi_\beta\rangle = M_{\alpha\beta}(\vec{q}). \qquad (18)$$

Applying now the well known expansion

$$e^{i\vec{q}\vec{R}} = 4\pi \sum_{\ell m} i^\ell j_\ell(qR) Y^*_{\ell m}(\vec{q}_o) Y_{\ell m}(\vec{r}_o); \quad \vec{q}_o = \mathrm{ort}\vec{q},\ \vec{r}_o = \mathrm{ort}\vec{R}, \qquad (19)$$

and the formula for the product of two spherical functions

$$Y_{\ell_1 m_1}(\theta,\phi) Y_{\ell_2 m_2}(\theta,\phi) = \sum_{\ell m} \left[\frac{(2\ell_1+1)(2\ell_2+1)(2\ell+1)}{4\pi}\right]^{1/2} \cdot \qquad (20)$$

$$\cdot \begin{pmatrix} \ell_1 & \ell_2 & \ell \\ m_1 & m_2 & m \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell \\ o & o & o \end{pmatrix} Y_{\ell m}(\theta,\phi),$$

as well as the hermiticity and unitarity of the $\|M_{\alpha\beta}(\vec{q})\|$ matrix, one obtains

$$M_{xz}(\vec{q}) = \tfrac{3}{2}j_2(qR_o)\sin 2\theta_q \sin\phi_q \; ; \quad M_{yz}(\vec{q}) = -\tfrac{3}{2}j_2(qR_o)\sin 2\theta_q \cos\phi_q \; ;$$

$$M_{xy}(\vec{q}) = \tfrac{3}{2}j_2(qR_o)\sin^2\theta_q \sin 2\phi_q \quad M_{zz}(\vec{q}) = j_o(qR_o)+j_2(qR_o)(1-3\cos^2\theta_q);$$

$$M_{xx}(\vec{q}) = \tfrac{1}{2}j_2(qR_o)\left[3(\sin^2\theta_q\cos 2\phi_q + \cos^2\theta_q) - 1\right] \tag{21}$$

$$M_{yy}(\vec{q}) = -\tfrac{1}{2}j_2(qR_o)\left[3(\sin^2\theta_q\cos 2\phi_q - \cos^2\theta_q) + 1\right] - j_o(qR_o),$$

where θ_q and ϕ_q are the spherical angles of the wave vector $\vec{q}$ in an ordinary x,y,z space.

For the claiming formfactors then one finds

$$A_q = \left[M_{zz}(\vec{q}) - 2M_{xy}(\vec{q})\right] = j_o(qR_o) + j_2(qR_o)\left[1-3(\cos^2\theta_q+\sin^2\theta_q\sin 2\phi_q)\right],$$

$$B_q = \frac{1}{\sqrt{2}}\left[M_{yz}(\vec{q}) + M_{xz}(\vec{q})\right] = \frac{3}{2\sqrt{2}}j_2(qR_o)\sin 2\theta_q(\sin\phi_q-\cos\phi_q),$$

$$C_q = \frac{1}{i\sqrt{2}}\left[M_{yz}(\vec{q}) - M_{xz}(\vec{q})\right] = i\frac{3}{2\sqrt{2}}j_2(qR_o)\sin 2\theta_q(\sin\phi_q+\cos\phi_q),$$

$$D_q = \frac{1}{2}\left[M_{xx}(\vec{q}) - M_{yy}(\vec{q})\right] = \tfrac{3}{2}j_2(qR_o)\sin^2\theta_q\cos 2\phi_q \; , \tag{22}$$

$$E_q = 2M_{xy}(\vec{q}) = 3j_2(qR_o)\sin^2\theta_q\sin 2\phi_q \; ,$$

$$F_q = \frac{1}{2}\left[M_{xx}(\vec{q}) + M_{yy}(\vec{q})\right] - A_q - \tfrac{1}{2}E_q = \tfrac{3}{2}j_2(qR_o)\left[3(\cos^2\theta_q-2\sin^2\theta_q\sin 2\phi_q) - 1\right] - 2j_o(qR_o),$$

$$H_q = -iC_q, \qquad K_q = 0.$$

V. FINAL EXPRESSIONS

To test the pseudo-spin model for nematic liquids* ,it is of

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* In /1/, the numerical values are chosen for para-azoxyanisole, as a typical nematic liquid crystal.

interest to calculate the neutron elastic cross section in the zero-sound ($\vec{q} \sim 0$) and the rotonic ($\vec{q} \sim \vec{q}_o$) parts of the frequency spectrum /1/ both at temperature region $T \sim 0$ and at $T \sim T_c = \frac{S^2}{k_B} |J(\vec{q}_m)|$ ($\vec{q}_m$ is the first minimum in the Fourier transform of the intermolecular potential /1/).

Now, with the aid of (8), (17) and (22), the angular elastic cross sections around $T \sim 0$ and $T \sim T_c$ are as follows

$$\left(\frac{d\sigma}{d\Omega}\right)_{T\sim 0} = \left[\sigma_1^{coh}\frac{(2\pi)^3 N}{V_o}\sum_{\tau}\delta(\vec{q}-\vec{\tau}) + N\sigma_1^{inc}\right]\cdot$$
$$4\left(A_q + B_q\langle S_x\rangle + D_q\langle S_z\rangle + E_q\langle S_x\rangle^2 + F_q\langle S_z\rangle^2 + H_q\langle S_x\rangle\langle S_z\rangle\right)^2$$
$$+ \left[\sigma_2^{coh}\frac{(2\pi)^3 N}{V_o}\sum_{\tau}\delta(\vec{q}-\vec{\tau}) + N\sigma_2^{inc}\right]\cdot 4\pi\,\frac{\sin(\vec{l}\vec{q})}{(\vec{l}\vec{q})}\,F(T)\cdot \tag{23}$$
$$\left(A_q + B_q\langle S_x\rangle + D_q\langle S_z\rangle + E_q\langle S_x\rangle^2 + F_q\langle S_z\rangle^2 + H_q\langle S_x\rangle\langle S_z\rangle\right)\;;$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{T\sim T_c} = \left[\sigma_1^{coh}\frac{(2\pi)^3 N}{V_o}\sum_{\tau}\delta(\vec{q}-\vec{\tau}) + N\sigma_1^{inc}\right]\cdot$$
$$4\left[A_q^2 + 2A_qB_q\langle S_x\rangle + 2A_qD_q\langle S_z\rangle + (B_q^2 + 2A_qE_q)\langle S_x\rangle^2 + 2(A_qH_q + B_qD_q)\cdot\right.$$
$$\cdot\langle S_x\rangle\langle S_z\rangle + 2B_qE_q\langle S_x\rangle^3 + 2(B_qH_q + D_qE_q)\langle S_x\rangle^2\langle S_z\rangle + E_q^2\langle S_x\rangle^4$$
$$\left. + 2E_qH_q\langle S_x\rangle^3\langle S_z\rangle\right] \tag{24}$$
$$+ \left[\sigma_2^{coh}\frac{(2\pi)^3 N}{V_o}\sum_{\tau}\delta(\vec{q}-\vec{\tau}) + N\sigma_2^{inc}\right]\cdot 4\pi\frac{\sin(\vec{l}\vec{q})}{(\vec{l}\vec{q})}\,F(T)\cdot$$
$$\left(A_q + B_q\langle S_x\rangle + D_q\langle S_z\rangle + E_q\langle S_x\rangle^2 + H_q\langle S_x\rangle\langle S_z\rangle\right)\;,$$

($V_o = \frac{V}{N}$ is the volume of an effective unit cell).

In the above two expressions we have the coherent and incoherent parts. It is obvious that the former describes only the shapes of peculiar Bragg peaks at a given reciprocal lattice-like point $\vec{q} = \vec{\tau}$. But the incoherent part could give information about zero-sound and rotonic scattering in both temperature regions.* Thus, it remains to evaluate $\langle S_x\rangle$ and $\langle S_z\rangle$ around these temperatures. Using a standard procedure for zero temperatures /12,13/ and combining a selfconsistent field approximation with an expansion for the thermodynamical functions $\cos^2\varphi$ and H /1,14,15/ in powers of $(T-T_c)$ (a second-order phase transition is assumed)**, one finds:

a) At $T\sim 0$:

$$\langle S_z\rangle_T = \cos\varphi\ (S-\langle b_i^+b_i\rangle_T)\ ,$$
$$\langle S_x\rangle_T = \sin\varphi\ (S-\langle b_i^+b_i\rangle_T)\ , \qquad (25)$$

where $\sin\varphi = \Omega_1/2S(J-\Omega_2)$, coming from the condition for the system to achieve a ground state at T=0 /1/.

Assuming, as a good approximation, for small $\vec{q}$ the dispersion law in the form

$$\omega_q = \omega_o + \omega_1 q^2\ ,$$

$$\omega_o = S\cos\varphi\sqrt{J(J-\Omega_2)},\quad \omega_1 = \frac{1}{2}\ \frac{J\alpha_1}{(J-\Omega_2)\cos^2\varphi}\ , \qquad (26)$$

(α_1 being estimated in /1/),

* If the condition $2lq_o < 1$ is violated, one has to multiply the incoherent scattering intensity by the factor 1/2.
**At critical temperatures $\cos^2\varphi\sim 0$ /1/. As a consequence, it comes out, from the Hamiltonian (1), that, with a good accuracy, one can apply such a procedure.

one obtains

$$\langle b_i^+ b_i \rangle_T = \frac{V_o}{(2\pi)^2}\, \Gamma(3/2) \left(\frac{k_B T}{\omega_1}\right)^{3/2} Z_{3/2}\left(\frac{\omega_o}{k_B T}\right) ; \tag{27}$$

$\Gamma(3/2)$ is the gamma-function and

$$Z_h(x) = \sum_{\kappa=1}^{\infty} \kappa^{-h}\, e^{-\kappa x} .$$

Since the Fourier transformed Lennard-Jones potential $V(\vec{q}) = S^2 N_o J(\vec{q}$, $(N_o = 2\cdot 10^{32}\ cm^3)$ /1/ has the main contribution as being integrating over $\vec{q}$ from zero to approximatly $\vec{q}_o \sim \vec{q}_{Brill/2}$, the above obtained expressions should be applied for the elastic scattering around $\vec{q} \sim \vec{q}_o$, too.

b) At $T \sim T_c$:

By convenient definitions

$$H_x = \Omega_1 + 2\Omega_2 \langle S_x \rangle, \quad H_z = 2J\langle S_z \rangle ; \quad H = (H_x^2 + H_z^2)^{1/2} , \quad J = \sum_j J_{ij} , \tag{28}$$

and with the expansions /1,15/

$$\cos^2\varphi = \begin{cases} \lambda(T-T_c), & T>T_c \\ 2\lambda|T-T_c|, & T<T_c \end{cases} ; \tag{29}$$

$$H = \begin{cases} H_x\left[1+\lambda|T-T_c|+\dots\right], & T<T_c \\ H_x, & T>T_c \end{cases} , \tag{30}$$

on the basis of the selfconsistent equation

$$\langle S_\alpha \rangle = S\, \frac{H_\alpha}{H}\, th\left(\frac{H}{2k_B T}\right), \tag{31}$$

one obtains

$$\langle S_x \rangle = \begin{cases} K, & T<T_c \\ K-SQ\,\dfrac{T-T_c}{2k_BT_c{}^2}\,, & T>T_c \end{cases}, \tag{32}$$

$$\langle S_z \rangle = \begin{cases} Q\,\sqrt{2\lambda}\,|T-T_c|^{1/2}, & T<T_c \\ Q\,\sqrt{\lambda}\,(T-T_c)^{1/2}, & T>T_c \end{cases}; \quad K = \Omega_1/2(J-\Omega_2) \quad Q = \frac{\Omega_1}{2J}\Big[1 + \frac{\Omega_2}{\Omega_1}\,K\Big]. \tag{33}$$

The constant λ, which was only required earlier /1/ to have the dimension T^{-1}, can be determined by a slight adaptation from Ref. /14/, wherewith it follows

$$\lambda = \frac{1}{H_x}\,\frac{\partial H}{\partial T}\Big|_{T=T_c} = \frac{2SJ(1-z^2)}{T_c\big[2k_BT_c-2SJ(1-z^2)\big]}, \tag{34}$$

where $z = H_x/2k_BT_c$.

To conclude, a new approach to neutron scattering by liquid crystals, especially of nematic type, is presented. The obtained results provide the possibility to reproduce the shapes of the coherent and incoherent peaks in elastic neutron scattering spectra in the acoustic ($\vec{q} = 0$) and the rotonic ($\vec{q} = \vec{q}_o$) parts of the collective excitations, both at temperature regions $T \approx 0$ and at $T = T_c$. Since the cross sections are expressed in terms of parameters Ω_1, Ω_2, J, α_1, λ and q_o, the fitting to experiments could give the possibility to verify the validity of the pseudo-spin model and the theoretical estimations of the parameters in it. At the same time, one could obtain closer estimations of effective dipole parameters, which would be of basic interest. Nevertheless, one could expect much more information from inelastic neutron scattering spectra, which can be, in principle, described by the same pseudo-spin formalism and the here proposed method.

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