Relationship between molecule shape and hydrodynamics in a nematic substance

G. E. Volovik
L.D. Landau Institute of Theoretical Physics

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It is shown by the Poisson brackets method that the reactive coefficient in the hydrodynamics equations for a nematic substance must be close to $+1$ for rod-shaped molecules and -1 for disk-shaped molecules.

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An experimental study of nematic dynamics showed that the reactive coefficient λ in the hydrodynamic equations

$$\lambda = \frac{\alpha_2 + \alpha_3}{\alpha_2 - \alpha_3}, \tag{1}$$

where α_2 and α_3 are the Leslie coefficients, is close to unity (see Ref. 1). Using the Poisson brackets method to derive the hydrodynamic equations, we shall show that the closeness of λ to $+1$ is a consequence of the rod-shaped form of the molecules, and for the recently discovered nematic with disk-shaped molecules[2] the coefficient λ should be close to -1.

The Poisson brackets method for deriving the hydrodynamic equations in condensed media was developed in a paper by Dzyaloshinskiĭ and the author.[3] In contrast to Ref. 3, where an auxiliary variable—the angular momentum density, which was assumed to be zero in the final equations—was used, at the outset we shall use the hydrodynamic variables: ρ is the liquid density, $\mathbf{p}$ is the momentum density, and $\mathbf{n}$ is a unit vector—the director.

The Poisson brackets between these variables can be obtained by knowing the transformation of the hydrodynamic variables due to the action of a nonuniform displacement $\mathbf{r} \to \mathbf{r} + \mathbf{u}(\mathbf{r})$ generated by the momentum operator[3] (see also Ref. 4). Thus, it follows from the transformation of $\mathbf{p}$ and ρ than

$$\{ p_i(\mathbf{r}), p_k(\mathbf{r}') \} = p_k(\mathbf{r}) \nabla_i \delta(\mathbf{r} - \mathbf{r}') - p_i(\mathbf{r}') \nabla'_k \delta(\mathbf{r} - \mathbf{r}') \tag{2}$$

$$\{ p_i(\mathbf{r}), \rho(\mathbf{r}') \} = \rho(\mathbf{r}) \nabla_i \delta(\mathbf{r} - \mathbf{r}'). \tag{3}$$

The transformation properties of the director $\mathbf{n}$, which are strongly dependent on the molecule shape, must be determined. If the molecules are rod shaped, then in the ideal case of infinitely thin and straight rods the vector $\mathbf{n}$ coincides with the direction of the rod axis. Therefore, being frozen in the substance, the vector $\mathbf{n}$ is a contravariant vector for coordinate transformations. We recall that contravariant vectors are transformed in accordance with the law

$$A^k \to A^k(\mathbf{r} - \mathbf{u}) + A^l \nabla_l u^k, \tag{4}$$

and covariant vectors in accordance with the law

$$A_k \to A_k(\mathbf{r} - \mathbf{u}) - A_l \nabla_k u^l. \tag{5}$$

Using (4) and taking into account the uniqueness of the director, we obtain the following Poisson bracket for a nematic substance with rod-shaped molecules:

$$\{\mathbf{p}_i(\mathbf{r}), n_k(\mathbf{r}')\} = -(\nabla_i n_k)\delta(\mathbf{r} - \mathbf{r}') + (\delta_{ik} - n_i(\mathbf{r}')n_k(\mathbf{r}'))\mathbf{n}(\mathbf{r}')\overleftarrow{\nabla}\delta(\mathbf{r} - \mathbf{r}'). \tag{6}$$

If the molecules have a disk shape, then in the ideal case of infinitely thin disks the nematic substance is a system of surfaces frozen in the medium. The vector $\mathbf{n}$, normal to these surfaces, must behave like a covariant vector during a coordinate transformation. Therefore, again taking into account the uniqueness of the director, we have from (5):

$$\{\mathbf{p}_i(\mathbf{r}), n_k(\mathbf{r}')\} = -(\nabla_i n_k)\delta(\mathbf{r} - \mathbf{r}') + n_i(\mathbf{r}')(n_k(\mathbf{r}')n_l(\mathbf{r}') - \delta_{kl})\nabla'_l\delta(\mathbf{r} - \mathbf{r}'). \tag{7}$$

The hydrodynamic equations are the Liouville equations, which, taking into account the dissipation, have the following form:

$$\dot{\rho} + \{\rho, H\} = 0, \tag{8}$$

$$\dot{\mathbf{p}}_k + \{\mathbf{p}_k, H\} = -\frac{\delta R}{\delta v_k}, \tag{9}$$

$$\dot{n}_k + \{n_k, H\} = \frac{\delta R}{\delta h_k}. \tag{10}$$

Here H is the energy of the system

$$H = \int d^3r \left(\epsilon_0(\rho) + \epsilon(\mathbf{n}) + \frac{\mathbf{p}^2}{2\rho}\right), \tag{11}$$

and R is the dissipative function which is expressed in terms of the velocity

$$\mathbf{v} = \frac{\delta H}{\delta \mathbf{p}} = \frac{\mathbf{p}}{\rho}$$

and the molecular field

$$\mathbf{h} = -\frac{\delta H}{\delta \mathbf{n}} = -\frac{\partial \epsilon}{\partial \mathbf{n}} + \nabla_i \frac{\partial \epsilon}{\partial \nabla_i \mathbf{n}}.$$

According to Ref. 1, R has the following form in the incompressible liquid approximation ($\nabla \mathbf{v} = 0$):

$$R = \int d^3r \left[\frac{1}{2\gamma_1}(\mathbf{h}^2 - (\mathbf{n}\mathbf{h})^2) + 2(\nu_3 - \nu_2)(A_{ik}n_k)^2\right.$$

$$+ \nu_2 A_{ik} A_{ik} + (\nu_1 + \nu_2 - 2\nu_3)(n_i A_{ik} n_k)^2 \Big] . \qquad (12)$$

Here $A_{ik} = \frac{1}{2}(\nabla_i v_k + \nabla_k v_i)$. We have written (12) in terms of the positive dissipative coefficients ν_1, ν_2, ν_3, and γ_1, which were introduced by the so-called Harvard group.[5]

Expanding Eq. (10) with the aid of Eqs. (11) and (12) and the Poisson bracket (6) or (7), we obtain the known equation for the director (see Refs. 1, 5)

$$\frac{\partial \mathbf{n}}{\partial t} + (\mathbf{v}\nabla)\mathbf{n} - \frac{1}{2}[\operatorname{rot} \mathbf{v}, \mathbf{n}] - \lambda(\mathbf{n}\overleftrightarrow{A} - \mathbf{n}(\mathbf{n}\overleftrightarrow{A}\mathbf{n})) = \frac{1}{\gamma_1}(\mathbf{h} - \mathbf{n}(\mathbf{hn})) . \qquad (13)$$

Here λ is the reactive parameter, which is not defined in Ref. 5 and which must be determined from experiment. In the scheme presented here λ is completely defined. It is equal to $+1$ if the Poisson bracket (6) is used, i.e., if the molecules are rod shaped, and -1 if the Poisson bracket (7) is used, i.e., if the molecules are disk shaped.

In reality, if deviations from the ideal are taken into account, for example, the finite ratio of the rod length to thickness or the presence of a spread in the rod orientations relative to the average direction defining the director vector, then our statement reduces to the following. For nematics with rod-shaped molecules λ is close to $+1$, and for nematics with disk-shaped molecules λ is close to -1. The first statement is well verified; thus, for example, the value of λ for MBBA, given in Ref. 1, is 1.04 at 22 °C. It is still difficult to test the second statement in view of a lack of an adequate quantity of such nematic material.

Let us note that as one approaches the phase transition to an isotropic liquid, when the deviations of the molecule axes from the average direction increase, the difference between $|\lambda|$ and unity should increase. The situation is analogous as one approaches the smectic A, when the director becomes the normal to the smectic layers.

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