Correlation Functions in the Isotropic Phase of Nematics

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The orientational correlation functions in the isotropic phase of nematics are calculated starting from the expression of De Gennes for the free energy density of this phase.

1. Introduction

Short range order effects are quite pronounced in the isotropic phase of nematics as demonstrated e.g. by light scattering experiments [1]. The relevant short range order concerns the local state of orientational order in the isotropic phase. This orientational order is described by a symmetric traceless tensor of the second rank denoted by $Q_{\alpha\beta}(\boldsymbol{r})$. The Greek indices refer to the axes of a given cartesian co-ordinate system, e.g. the laboratory frame. The amount of short range order is expressed by correlation functions of the type $\langle Q_{\alpha\beta}(\boldsymbol{r})\, Q_{\gamma\delta}(\boldsymbol{r}')\rangle$, where $\alpha, \beta, \gamma, \delta = x, y, z$.

In order to describe the short range orientational effects De Gennes [2] proposed the following contribution of the orientational fluctuations to the free energy density of the isotropic phase

$$\begin{aligned} f(\boldsymbol{r}) &= \tfrac{1}{2} A(T)\, Q_{\alpha\beta}(\boldsymbol{r})\, Q_{\beta\alpha}(\boldsymbol{r}) \\ &\quad + \tfrac{1}{2} L_1 [\partial_\alpha Q_{\beta\gamma}(\boldsymbol{r})][\partial_\alpha Q_{\beta\gamma}(\boldsymbol{r})] \\ &\quad + \tfrac{1}{2} L_2 [\partial_\alpha Q_{\alpha\gamma}(\boldsymbol{r})][\partial_\beta Q_{\beta\gamma}(\boldsymbol{r})] , \end{aligned} \tag{1.1}$$

where $\partial_\alpha = \partial/\partial\alpha$ and repeated indices must be summed. Only second order terms in $\mathbf{Q}$ are taken into account because of the smallness of $\mathbf{Q}$, whereas the higher order derivatives of $\mathbf{Q}$ are neglected because of the assumption that $\mathbf{Q}(\boldsymbol{r})$ still varies slowly from point to point.

Here the physical meaning and validity of expression (1.1) are not questioned or discussed, but the stand is taken that this expression seems to be able to give a satisfactory phenomenological description of short range order effects. Strangely enough, however, the general expression for the correlation function $\langle Q_{\alpha\beta}(\boldsymbol{r})\, Q_{\gamma\delta}(\boldsymbol{r}')\rangle$ has never been correctly derived with the exception of the case $L_2 = 0$. The purpose of this paper is to make up for this deficiency.

The error arises directly after substituting the Fourier transformation

$$Q_{\alpha\beta}(\boldsymbol{r}) = \sum_{\boldsymbol{k}} Q_{\alpha\beta}(\boldsymbol{k}) \exp[i\, \boldsymbol{k} \cdot \boldsymbol{r}] \tag{1.2}$$

into the free energy density (1.1) and integrating the resulting expression over the volume V of the system. Then the following free energy F is obtained

$$\begin{aligned} F &= \tfrac{1}{2} \sum_{\boldsymbol{k}} [VA(T) + VL_1]\, Q^*_{\alpha\beta}(\boldsymbol{k})\, Q_{\alpha\beta}(\boldsymbol{k}) \\ &\quad + \tfrac{1}{2} VL_2 \sum_{\boldsymbol{k}} k_\alpha k_\beta\, Q^*_{\alpha\gamma}(\boldsymbol{k})\, Q_{\beta\gamma}(\boldsymbol{k}) , \end{aligned} \tag{1.3}$$

where

$$Q^*_{\alpha\beta}(\boldsymbol{k}) = Q_{\alpha\beta}(-\boldsymbol{k}) . \tag{1.4}$$

In order to calculate the short range order effects expectation values like $\langle Q^*_{\alpha\beta}(\boldsymbol{k})\, Q_{\gamma\delta}(\boldsymbol{k})\rangle$ must be calculated. Unfortunately former calculations (see e.g. [3]) have been based upon the incorrect view that $\boldsymbol{k}$ can be chosen along the z-axis without loss of generality. Such a procedure is correct indeed as long as only one wave vector $\boldsymbol{k}$ is considered. However, the procedure is incorrect in the underlying calculation because not all wave vectors $\boldsymbol{k}$ determine the same z-direction, i.e. the same cartesian system. This means a violation of the starting point that the tensor elements $Q_{\alpha\beta}(\boldsymbol{k})$ are defined with respect to the same co-ordinate system irrespective of the wave vectors $\boldsymbol{k}$.

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2. The Calculation of the Expectation Values

The calculation of the expectation values $\langle Q^*_{\alpha\beta}(\boldsymbol{k})\, Q_{\gamma\delta}(\boldsymbol{k})\rangle$ is based upon the assumption that the amplitudes $Q_{\alpha\beta}(\boldsymbol{k})$ may be conceived as random variables, i.e. the probability of a given set of amplitudes $\{Q_{\alpha\beta}(\boldsymbol{k})\}$ is given by

$$P(\{Q_{\alpha\beta}(\boldsymbol{k})\}) = \frac{1}{Z}\exp[-\beta F], \tag{2.1}$$

where Z is a normalization constant and $\beta=(k_B T)^{-1}$, with k_B denoting Boltzmann's constant and T the temperature. Next the complex amplitude is written as

$$Q_{\alpha\beta}(\boldsymbol{k}) = r_{\alpha\beta}(\boldsymbol{k}) + i\, s_{\alpha\beta}(\boldsymbol{k}), \tag{2.2}$$

where the real tensors $\mathbf{r}(\boldsymbol{k})$ and $\mathbf{s}(\boldsymbol{k})$ are symmetric and traceless and

$$r_{\alpha\beta}(\boldsymbol{k}) = r_{\alpha\beta}(-\boldsymbol{k}), \quad s_{\alpha\beta}(\boldsymbol{k}) = -s_{\alpha\beta}(-\boldsymbol{k}). \tag{2.3}$$

Consequently the free energy can be expressed like

$$F = \sum_{\boldsymbol{k}}{}' F(\boldsymbol{k}), \tag{2.4}$$

where

$$F(\boldsymbol{k}) = (VA(T) + VL_1 k^2)\,(r^2_{\alpha\beta}(\boldsymbol{k}) + s^2_{\alpha\beta}(\boldsymbol{k})) + VL_2\, k_\alpha k_\beta\,(r_{\alpha\gamma}(\boldsymbol{k})\, r_{\beta\gamma}(\boldsymbol{k}) + s_{\alpha\gamma}(\boldsymbol{k})\, s_{\beta\gamma}(\boldsymbol{k})) \tag{2.5}$$

and $\sum_{\boldsymbol{k}}{}'$ denotes the summation over all $\boldsymbol{k}$-vectors that label the independent random variables. The variables themselves, which appear in expression (2.5), are not all independent because of the constraint $r_{\alpha\alpha}(\boldsymbol{k}) = s_{\alpha\alpha}(\boldsymbol{k}) = 0$. In order to keep the full symmetry between the involved variables the constraint is incorporated into the probability distribution by means of the Dirac delta function

$$\delta(x) = \lim_{\varepsilon\to 0}\frac{1}{\sqrt{2\pi\varepsilon}}\exp\left[-\frac{x^2}{2\varepsilon^2}\right]. \tag{2.6}$$

Then the probability distribution reads

$$P(\{Q_{\alpha\beta}(\boldsymbol{k})\}) = \frac{1}{Z}\prod_{\boldsymbol{k}}{}'\exp[-\beta F(\boldsymbol{k})]\,\delta(r_{\alpha\alpha}(\boldsymbol{k}))\,\delta(s_{\gamma\gamma}(\boldsymbol{k}))\,. \tag{2.7}$$

Clearly this distribution is a product of Gaussian distributions of the form

$$P_{\boldsymbol{k}} = \frac{1}{Z_{\boldsymbol{k}}}\exp\left[-\frac{1}{2}\sum_{i=1}^{6}\sum_{j=1}^{6} A_{ij}(\boldsymbol{k})\,\sigma_i(\boldsymbol{k})\,\sigma_j(\boldsymbol{k})\right], \tag{2.8}$$

where $Z_{\boldsymbol{k}}$ is a normalization constant and $\sigma_i(\boldsymbol{k})$ denotes whether $r_{\alpha\beta}(\boldsymbol{k})$ or $s_{\alpha\beta}(\boldsymbol{k})$ with $i=1,2,3,4,5,6$ corresponding respectively with

$$\alpha\beta = xx,\ yy,\ zz,\ xy,\ xz,\ yz\,.$$

The matrix $A(\boldsymbol{k})$ is given by

$$A(\boldsymbol{k}) = \begin{pmatrix}
\alpha(\boldsymbol{k})+\gamma k_x^2+\frac{1}{\varepsilon} & \frac{1}{\varepsilon} & \frac{1}{\varepsilon} & \gamma k_x k_y & \gamma k_x k_z & 0 \\
\frac{1}{\varepsilon} & \alpha(\boldsymbol{k})+\gamma k_y^2+\frac{1}{\varepsilon} & \frac{1}{\varepsilon} & \gamma k_x k_y & 0 & \gamma k_y k_z \\
\frac{1}{\varepsilon} & \frac{1}{\varepsilon} & \alpha(\boldsymbol{k})+\gamma k_z^2+\frac{1}{\varepsilon} & 0 & \gamma k_x k_z & \gamma k_y k_z \\
\gamma k_x k_y & \gamma k_x k_y & 0 & 2\alpha(\boldsymbol{k})+\gamma(k_x^2+k_y^2) & \gamma k_y k_z & \gamma k_x k_z \\
\gamma k_x k_z & 0 & \gamma k_x k_z & \gamma k_y k_z & 2\alpha(\boldsymbol{k})+\gamma(k_x^2+k_z^2) & \gamma k_x k_y \\
0 & \gamma k_y k_z & \gamma k_y k_z & \gamma k_x k_z & \gamma k_x k_y & 2\alpha(\boldsymbol{k})+\gamma(k_y^2+k_z^2)
\end{pmatrix} \tag{2.9}$$

where

$$\alpha(\boldsymbol{k}) = 2\beta V(A(T) + L_1 k^2), \quad \gamma = 2\beta V L_2. \tag{2.10}$$

Then the required expectation value $\langle\sigma_i\,\sigma_j\rangle$ reads [4]

$$\langle\sigma_i\,\sigma_j\rangle = A^{-1}(\boldsymbol{k})_{ij}, \tag{2.11}$$

where $A^{-1}(\boldsymbol{k})_{ij}$ is an element of the matrix inverse to $A(\boldsymbol{k})$. Consequently the problem consists of determining the matrix inverse to $A(\boldsymbol{k})$. This problem is quite simple in the case $\boldsymbol{k}=0$. Then it holds

$$A^{-1}(0)=\begin{pmatrix} \frac{\alpha\varepsilon+2}{\alpha^2\varepsilon+3\alpha} & \frac{-1}{\alpha^2\varepsilon+3\alpha} & \frac{-1}{\alpha^2\varepsilon+3\alpha} & 0 & 0 & 0 \\ \frac{-1}{\alpha^2\varepsilon+3\alpha} & \frac{\alpha\varepsilon+2}{\alpha^2\varepsilon+3\alpha} & \frac{-1}{\alpha^2\varepsilon+3\alpha} & 0 & 0 & 0 \\ \frac{-1}{\alpha^2\varepsilon+3\alpha} & \frac{-1}{\alpha^2\varepsilon+3\alpha} & \frac{\alpha\varepsilon+2}{\alpha^2\varepsilon+3\alpha} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2\alpha} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2\alpha} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2\alpha} \end{pmatrix} \tag{2.12}$$

with $\alpha=\alpha(0)$. The required expectation values are obtained by taking the limit $\varepsilon\to 0$, i.e.

$$\begin{aligned} &\langle Q_{xx}^2(0)\rangle=\langle Q_{yy}^2(0)\rangle=\langle Q_{zz}^2(0)\rangle=\frac{2}{3\alpha}, \\ &\langle Q_{xy}^2(0)\rangle=\langle Q_{xz}^2(0)\rangle=\langle Q_{yz}^2(0)\rangle=\frac{1}{2\alpha}, \\ &\langle Q_{xx}(0)\,Q_{yy}(0)\rangle=\langle Q_{xx}(0)\,Q_{zz}(0)\rangle \\ &\qquad=\langle Q_{yy}(0)\,Q_{zz}(0)\rangle=\frac{-1}{3\alpha}, \end{aligned} \tag{2.13}$$

whereas the remaining thermal averages, e.g. $\langle Q_{xx}(0)\,Q_{xy}(0)\rangle$, are zero.

The general case, i.e. $\boldsymbol{k}$ is an arbitrary vector, has to be solved by means of a computer. According to the computer program REDUCE (Hearst 1974) the matrix elements $A^{-1}(\boldsymbol{k})_{ij}$ read in the limit $\varepsilon\to 0$,

$$\begin{aligned} A^{-1}(\boldsymbol{k})_{11}&=N(\boldsymbol{k})\,[2\alpha(\boldsymbol{k})+\gamma(k_y^2+k_z^2)]^2, \\ A^{-1}(\boldsymbol{k})_{12}&=A^{-1}(\boldsymbol{k})_{21}=-N(\boldsymbol{k})\,[(2\alpha(\boldsymbol{k})+\gamma k^2) \\ &\quad\cdot(\alpha(\boldsymbol{k})+\gamma k_z^2)-\gamma^2 k_x^2 k_y^2], \\ A^{-1}(\boldsymbol{k})_{13}&=A^{-1}(\boldsymbol{k})_{31}=-N(\boldsymbol{k})\,[(2\alpha(\boldsymbol{k})+\gamma k^2) \\ &\quad\cdot(\alpha(\boldsymbol{k})+\gamma k_y^2)-\gamma^2 k_x^2 k_z^2], \\ A^{-1}(\boldsymbol{k})_{14}&=A^{-1}(\boldsymbol{k})_{41} \\ &=-N(\boldsymbol{k})\,\gamma k_x k_y[\alpha(\boldsymbol{k})+\gamma(k_y^2+k_z^2)], \\ A^{-1}(\boldsymbol{k})_{15}&=A^{-1}(\boldsymbol{k})_{51} \\ &=-N(\boldsymbol{k})\,\gamma k_x k_z[\alpha(\boldsymbol{k})+\gamma(k_y^2+k_z^2)], \\ A^{-1}(\boldsymbol{k})_{16}&=A^{-1}(\boldsymbol{k})_{61} \\ &=N(\boldsymbol{k})\,\gamma k_y k_z[2\alpha(\boldsymbol{k})+\gamma(k^2+k_x^2)], \\ A^{-1}(\boldsymbol{k})_{22}&=N(\boldsymbol{k})\,[2\alpha(\boldsymbol{k})+\gamma(k_x^2+k_z^2)]^2, \\ A^{-1}(\boldsymbol{k})_{23}&=A^{-1}(\boldsymbol{k})_{32}=-N(\boldsymbol{k})\,[2\alpha(\boldsymbol{k})+\gamma k^2) \\ &\quad\cdot(\alpha(\boldsymbol{k})+\gamma k_x^2)-\gamma^2 k_y^2 k_z^2], \\ A^{-1}(\boldsymbol{k})_{24}&=A^{-1}(\boldsymbol{k})_{42} \\ &=-N(\boldsymbol{k})\,\gamma k_x k_y[\alpha(\boldsymbol{k})+\gamma(k_x^2+k_z^2)], \\ A^{-1}(\boldsymbol{k})_{25}&=A^{-1}(\boldsymbol{k})_{52} \\ &=N(\boldsymbol{k})\,\gamma k_x k_z[2\alpha(\boldsymbol{k})+\gamma(k^2+k_y^2)], \\ A^{-1}(\boldsymbol{k})_{26}&=A^{-1}(\boldsymbol{k})_{62} \\ &=-N(\boldsymbol{k})\,\gamma k_y k_z[\alpha(\boldsymbol{k})+\gamma(k_x^2+k_y^2)], \\ A^{-1}(\boldsymbol{k})_{33}&=N(\boldsymbol{k})\,[2\alpha(\boldsymbol{k})+\gamma(k_x^2+k_y^2)]^2, \\ A^{-1}(\boldsymbol{k})_{34}&=A^{-1}(\boldsymbol{k})_{43} \\ &=N(\boldsymbol{k})\,\gamma k_x k_y[\alpha(\boldsymbol{k})+\gamma(k^2+k_z^2)], \\ A^{-1}(\boldsymbol{k})_{35}&=A^{-1}(\boldsymbol{k})_{53} \\ &=-N(\boldsymbol{k})\,\gamma k_x k_z[\alpha(\boldsymbol{k})+\gamma(k_x^2+k_y^2)], \\ A^{-1}(\boldsymbol{k})_{36}&=A^{-1}(\boldsymbol{k})_{63} \\ &=-N(\boldsymbol{k})\,\gamma k_y k_z[\alpha(\boldsymbol{k})+\gamma(k_x^2+k_y^2)], \\ A^{-1}(\boldsymbol{k})_{44}&=\tfrac{1}{2}N(\boldsymbol{k})\,[(3\alpha(\boldsymbol{k})+2\gamma k^2) \\ &\quad\cdot(2\alpha(\boldsymbol{k})+\gamma k_z^2)+2\gamma^2 k_x^2 k_y^2], \\ A^{-1}(\boldsymbol{k})_{45}&=A^{-1}(\boldsymbol{k})_{54} \\ &=-N(\boldsymbol{k})\,\gamma k_y k_z[3\alpha(\boldsymbol{k})+2\gamma(k_y^2+k_z^2)], \\ A^{-1}(\boldsymbol{k})_{46}&=A^{-1}(\boldsymbol{k})_{64} \\ &=-N(\boldsymbol{k})\,\gamma k_x k_z[3\alpha(\boldsymbol{k})+2\gamma(k_x^2+k_z^2)], \\ A^{-1}(\boldsymbol{k})_{55}&=\tfrac{1}{2}N(\boldsymbol{k})\,[(3\alpha(\boldsymbol{k})+2\gamma k^2) \\ &\quad\cdot(2\alpha(\boldsymbol{k})+\gamma k_y^2)+2\gamma^2 k_x^2 k_z^2], \\ A^{-1}(\boldsymbol{k})_{56}&=A^{-1}(\boldsymbol{k})_{65} \\ &=-N(\boldsymbol{k})\,\gamma k_x k_y[3\alpha(\boldsymbol{k})+2\gamma(k_x^2+k_y^2)], \\ A^{-1}(\boldsymbol{k})_{66}&=\tfrac{1}{2}N(\boldsymbol{k})\,[(3\alpha(\boldsymbol{k})+2\gamma k^2) \\ &\quad\cdot(2\alpha(\boldsymbol{k})+\gamma k_x^2)+2\gamma^2 k_y^2 k_z^2], \end{aligned} \tag{2.14}$$

where (2.15)

$$N(\boldsymbol{k}) = \alpha^{-1}(\boldsymbol{k})\,[2\alpha(\boldsymbol{k}) + \gamma k^2]^{-1}[3\alpha(\boldsymbol{k}) + 2\gamma k^2]^{-1}.$$

It follows directly that the elements of the inverse matrix possess poles in the complex k-plane. According to (2.15) these poles are situated along the imaginary-axis at the positions

$$\xi_1 = \left[\frac{L_1}{A(T)}\right]^{1/2}, \quad \xi_2 = \left[\frac{L_1 + \frac{1}{2}L_2}{A(T)}\right]^{1/2},$$
$$\xi_3 = \left[\frac{L_1 + \frac{2}{3}L_2}{A(T)}\right]^{1/2}, \tag{2.16}$$

and they have the dimension of a length. These lengths govern the behaviour of the correlation function at long distances. Obviously only the largest length makes sense and is called the correlation length. This means that ξ_3 is the correlation length for positive values of L_2, whereas ξ_1 is the correlation length for negative values of L_2.

3. Correlation Functions

Using the Fourier transformation (1.2) and replacing the summation over $\boldsymbol{k}$ by an integration over $\boldsymbol{k}$, the correlation function $\langle Q_{\alpha\beta}(\boldsymbol{r})\, Q_{\gamma\delta}(\boldsymbol{r}')\rangle = \langle Q_{\alpha\beta}(0)\, Q_{\gamma\delta}(\boldsymbol{R})\rangle$, where $\boldsymbol{R} = \boldsymbol{r}' - \boldsymbol{r}$, is given by

$$\langle Q_{\alpha\beta}(0)\, Q_{\gamma\delta}(\boldsymbol{R})\rangle = \frac{V}{4\pi^3} \int_{k<k_D} d\boldsymbol{k}\, \langle r_{\alpha\beta}(\boldsymbol{k})\, r_{\gamma\delta}(\boldsymbol{k})\rangle \exp[i\,\boldsymbol{k}\cdot\boldsymbol{R}], \tag{3.1}$$

where the Debye wave number $k_D = \left(6\pi^2 \frac{N}{V}\right)^{1/3}$ appears as a cut-off, because the system consists of only N molecules, i.e. only N $\boldsymbol{k}$-values are independent.

As an example the correlation function $\langle Q_{xx}(0)\, Q_{xx}(\boldsymbol{R})\rangle$ is calculated, where the vector $\boldsymbol{R}$ is taken along the z-direction denoted by the unit vector $\hat{z}$, i.e. $\boldsymbol{R} = R\hat{z}$, whereas k_D is replaced by ∞ in order to perform the calculation analytically. Then the following expression is obtained

$$\langle Q_{xx}(0)\, Q_{xx}(\boldsymbol{R}\hat{z})\rangle = \frac{V}{4\pi^3}\int d\boldsymbol{k}\, \langle r_{xx}^2(\boldsymbol{k})\rangle \exp[i\,R\,\boldsymbol{k}\cdot\hat{z}]$$
$$= \frac{V}{4\pi^3}\int d\boldsymbol{k}\, A^{-1}(\boldsymbol{k})_{11} \exp[i\,R\,\boldsymbol{k}\cdot\hat{z}]$$
$$= \frac{V}{(2\pi)^3}\int d\boldsymbol{k}\left[\frac{1}{\alpha(\boldsymbol{k})} + \frac{1}{3\alpha(\boldsymbol{k}) + 2\gamma k^2} + \frac{2\gamma k_x^2}{(2\alpha(\boldsymbol{k}) + \gamma k^2)\,(3\alpha(\boldsymbol{k}) + 2\gamma k^2)} - \frac{2\gamma k_x^2}{\alpha(\boldsymbol{k})\,(2\alpha(\boldsymbol{k}) + \gamma k^2)} + \frac{2\gamma^2 k_x^4}{\alpha(\boldsymbol{k})\,(2\alpha(\boldsymbol{k}) + \gamma k^2)\,(3\alpha(\boldsymbol{k}) + 2\gamma k^2)}\right] \cdot \exp[i\,R\,\boldsymbol{k}\cdot\hat{z}]. \tag{3.2}$$

The easiest way to perform the integration is by making use of spherical co-ordinates for $\boldsymbol{k}$, which explains the choice of $\boldsymbol{R}$ along the z-axis. It appears that

$$\langle Q_{xx}(0)\, Q_{xx}(R\hat{z})\rangle = \frac{k_B T A_1}{4\pi L_1 R}\left[\frac{1}{2} + \frac{L_2 B_1}{(2L_1 + L_2)\, D_{12}} + \frac{3L_2^2 C_1}{(2L_1 + L_2)\,(3L_1 + 2L_2)\, D_{21} D_{31}}\right] + \frac{k_B T A_2}{4\pi (2L_1 + L_2) R}\left[\frac{L_2 B_2}{L_1 D_{21}} + \frac{L_2 B_2}{(3L_1 + 2L_2) D_{32}} + \frac{3L_2^2 C_2}{L_1 (3L_1 + 2L_2) D_{12} D_{32}}\right] + \frac{k_B T A_3}{4\pi (3L_1 + 2L_2) R}\left[\frac{1}{2} + \frac{L_2 B_3}{(2L_1 + L_2) D_{23}} + \frac{3L_2^2 C_3}{L_1 (2L_1 + L_2) D_{13} D_{23}}\right], \tag{3.3}$$

where

$$A_i = \exp\left[-\frac{R}{\xi_i}\right],$$
$$B_i = \left(\frac{R}{\xi_i} + 1\right),$$
$$C_i = \left(\frac{R^2}{\xi_i^2} + 3\frac{R}{\xi_i} + 3\right),$$
$$D_{ij} = \frac{R^2}{\xi_i^2} - \frac{R^2}{\xi_j^2},$$

with $i, j = 1, 2, 3$.

In order to obtain the correlation functions for an arbitrary direction of $\boldsymbol{R}$ the original coordinate system, described by the unit vectors $\hat{x}$, $\hat{y}$ and $\hat{z}$, is rotated in such a way that the direction of the z-axis of the new system, which is described by the

unit vectors $\hat{x}'$, $\hat{y}'$ and $\hat{z}'$ coincides with the direction of $\boldsymbol{R}$. An arbitrary $\boldsymbol{R}$ is given by

$$\boldsymbol{R} = R\sin\theta\cos\varphi\,\hat{x} + R\sin\theta\sin\varphi\,\hat{y} + R\cos\theta\,\hat{z} = R\,\hat{z}'\,. \tag{3.4}$$

The tensor $Q_{\alpha\beta}$ in the original system and the tensor $Q_{\alpha'\beta'}$ in the rotated system are related by

$$Q_{\alpha\beta} = R_{\alpha\gamma'} R_{\beta\delta'} Q_{\gamma'\delta'}\,,$$

where

$$R = \begin{pmatrix} R_{xx'} & R_{xy'} & R_{xz'} \\ R_{yx'} & R_{yy'} & R_{yz'} \\ R_{zx'} & R_{zy'} & R_{zz'} \end{pmatrix} = \begin{pmatrix} \cos\theta\cos\varphi & -\sin\varphi & \sin\theta\cos\varphi \\ \cos\theta\sin\varphi & \cos\varphi & \sin\theta\sin\varphi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}. \tag{3.5}$$

This means that the general expression for the correlation function $\langle Q_{\alpha\beta}(0)\, Q_{\gamma\delta}(\boldsymbol{R})\rangle$ reads

$$\langle Q_{\alpha\beta}(0)\, Q_{\gamma\delta}(\boldsymbol{R})\rangle = R_{\alpha\mu'} R_{\beta\nu'} R_{\gamma\varrho'} R_{\delta\sigma'} \langle Q_{\mu'\nu'}(0)\, Q_{\varrho'\sigma'}(R\,\hat{z}')\rangle\,. \tag{3.6}$$

Finally it should be mentioned that expression (3.3) clearly shows that only one correlation length is present, for the long distance behaviour of the correlation function is completely governed by the factor A_1 or A_3 according to the sign of L_2.

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