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THREE-DIMENSIONAL ROTATOR MODEL AND VORTEX PLASMA (*)

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Résumé. — On établit une relation triangulaire entre les modèles statistiques suivants : le modèle des excitations discrètes, le modèle des rotateurs généralisés et le plasma de tourbillons. On montre que la fonction de corrélation du modèle rotateur en dimension $D \geq 2$ décroît exponentiellement à haute température.

Abstract. — We establish a triangular relation between discrete excitation models, generalized rotator models and generalized vortex plasma models. The high temperature correlation function for the planar rotator models in dimensions $D \geq 2$ is shown to decrease exponentially.

In a recent letter Knops [1] gave an exact relation between solid-on-solid interfacial models and generalized planar rotator (GPR) models in two dimensions (2D). In particular he showed that the discrete Gaussian (DG) interfacial model [2] maps onto the Villain [3] rotator model and which corresponds to the 2D plasma model [3], as does the DG model [2]. Similar methods have been developed by José *et al.* [4]. Based on these ideas a similar triangular relation for the corresponding 3D models will be established.

We consider on a 3D simple cubic (sc) lattice with N lattice sites the Hamiltonian

$$\mathcal{H}_{\text{DE}} = J_{\text{DE}}/2 \sum_{\langle i,j,k,l \rangle} V(n_{\langle i,j,k,l \rangle}), \quad (1)$$

where $n_{\langle i,j,k,l \rangle} = 0, \pm 1, \dots$, and $V(x)$ is a positive function of x which will be specified later. Each elementary square of the sc lattice is labeled by $\langle i, j, k, l \rangle$, where i, j, k, l are taken consecutively counterclockwise around the square face. Each face carries only two labels $\langle i, j, k, l \rangle$ and $\langle l, k, j, i \rangle$ giving the face two orientations. Correspondingly we require

$$n_{\langle i,j,k,l \rangle} = -n_{\langle l,k,j,i \rangle}. \quad (2)$$

The set $\{n_{\langle i,j,k,l \rangle}\}$ is thus defined on a face centred cubic (fcc) lattice. Furthermore we require that

$$\sum_{\langle i,j,k,l \rangle} n'_{\langle i,j,k,l \rangle} = 0 \quad (3)$$

holds for each point i' on the dual lattice (dsc) to the sc lattice. Here $n'_{\langle i,j,k,l \rangle} = n_{\langle i,j,k,l \rangle}$ holds for the six neighbouring outward oriented faces to the point i' otherwise it vanishes. Accordingly the discrete excitation (DE) model defined by equations (1), (2) and (3) has $2N$ degrees of freedom. Using the integral representation for equation (3)

$$(2\pi)^{-1} \int_0^{2\pi} d\varphi_{i'} \exp \left\{ i\varphi_{i'} \sum_{\langle i,j,k,l \rangle} n'_{\langle i,j,k,l \rangle} \right\} = \delta_{\sum_{\langle i,j,k,l \rangle} n'_{\langle i,j,k,l \rangle}, 0} \quad (4)$$

the partition function of the problem can be written

$$Z_{\text{GPR}} = (2\pi)^{-N} \prod_{i'=1}^N \int_0^{2\pi} d\varphi_{i'} \times \exp \left\{ -\beta_{\text{DE}} \sum_{\langle i',j' \rangle} \tilde{V}(\varphi_{i'} - \varphi_{j'}) \right\}, \quad (5)$$

where $\langle i', j' \rangle$ indicates summation over nearest neighbours of the dsc lattice, and

$$\tilde{V}(\varphi) = -(2\beta_{\text{DE}})^{-1} \ln \left\{ \sum_{n=-\infty}^{\infty} e^{in\varphi - \beta_{\text{DE}} J_{\text{DE}} V(n)} \right\}. \quad (6)$$

This is a GPR model with nearest neighbour interaction and which, in the case of $V(n) = n^2$, corresponds to the Villain [3] model for the 3D rotator model.

A further representation of the DE model similar to the one obtained in [2] for the DG model will now be derived. Because equation (3) implies that the set $\{n_{\langle i,j,k,l \rangle}\}$ forms a divergenceless field, it may

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be obtained *via* a rot-operation [4] from a vector field $\{\mathbf{m}_i\}$ defined on the sc lattice. Using the following representation

$$\begin{aligned} n_{\langle 1234 \rangle} &= m_2^z - m_1^z + m_3^z - m_4^z - (m_4^y - m_1^y + m_3^y - m_2^y), \\ n_{\langle 6721 \rangle} &= m_6^y - m_1^y + m_7^y - m_2^y - (m_2^x - m_1^x + m_7^x - m_6^x), \end{aligned} \quad (7)$$

$$n_{\langle 4561 \rangle} = m_4^x - m_1^x + m_5^x - m_6^x - (m_5^z - m_4^z + m_6^z - m_1^z)$$

for the three faces illustrated in figure 1 and the rules stated earlier one confirms that equation (7) satisfies equation (3). Using in addition the condition

$$\begin{aligned} \text{Div}_i \{\mathbf{m}_i\} &\equiv \\ &\equiv \sum_{\mathbf{K}=\mathbf{x},\mathbf{y},\mathbf{z}} \delta_{\mathbf{K}} \cdot (\mathbf{m}_{i+\delta_{\mathbf{K}}} - \mathbf{m}_{i-\delta_{\mathbf{K}}}) = 0, \quad i = 1, \dots, N, \end{aligned} \quad (8)$$

FIG. 1. — Relation between subindices used in equation (7) and square face orientations. Arrows point inside first quadrant.

where $\delta_{\mathbf{K}}$ is a nearest neighbour vector, one confirms that to the $2N$ independent variables of the set $\{n_{\langle ijkl \rangle}\}$ correspond $2N$ independent variables of the set $\{\mathbf{m}_i\}$. A unique mapping between these two sets of variables is therefore provided if the transformation matrix A constructed from equation (7)

$$\mathbf{x}_n = A \mathbf{y}_m \quad (9)$$

has rank $2N$. Here $\mathbf{x}_n$ and $\mathbf{y}_m$ are $3N$ vectors and A is a $3N, 3N$ matrix. Using Fourier transforms and for sake of simplicity a long wave length approximation one gets

$$\mathbf{x}_n^+ \cdot \mathbf{x}_n = \mathbf{y}_m^+ A^+ A \mathbf{y}_m \approx 2 \sum_{\mathbf{q}} q^2 (Y_{\mathbf{q}}^1 Y_{-\mathbf{q}}^1 + Y_{\mathbf{q}}^2 Y_{-\mathbf{q}}^2), \quad (10)$$

where $(Y_{\mathbf{q}}^1, Y_{\mathbf{q}}^2, Y_{\mathbf{q}}^3)$ are normal coordinates referred to the orthogonal trihedron with $\mathbf{e}_{\mathbf{q}}^3 = \mathbf{q}/|\mathbf{q}|$, and $\mathbf{q}$ assumes N values in the first Brillouin zone of the sc lattice. It follows from equation (10) that rank

FIG. 2. — Planar part of some loop conformation. C_1 and C_2 are closed loops. The loop parts C_3 and C_4 enter the plane at circular drawn points and coalesce to C_5 . Construction satisfies equation (8). Vortex strengths are $\sigma_1 = \sigma_2 = \sigma_4 = 1/2$, $\sigma_3 = 1$, $\sigma_5 = 3/2$. Dashed drawn circuits indicate sense of integration in equation (12).

$[A] = 2N$. All sets $\{\mathbf{m}_i\} \subset \{\mathbf{y}_i\}$ satisfying equation (8) can now be constructed as an oriented and interconnected loop system (Fig. 2) obeying Kirchhoff's law in the form of equation (8) and corresponding uniquely *via* equation (9) to a set $\{n_{\langle ijkl \rangle}\}$ with integer valued entries as required for the derivation of equation (5). The question if all sets $\{n_{\langle ijkl \rangle}\}$ which satisfy equation (3) and which can be constructed in an obvious fashion are obtained in this way is of different nature and will not be considered further. Let me point out that Villain [5] has already studied the relation between Hamiltonians expressed in terms of sets of variables $\{q_{\rho}\}$ and $\{v_{ij}\}$, which are essentially equivalent to the sets $\{n_{\langle ijkl \rangle}\}$ and $\{\mathbf{m}_i\}$ respectively although he does not introduce the DE model explicitly. The difference in the two procedures to construct the set $\{n_{\langle ijkl \rangle}\}$ from the set $\{\mathbf{m}_i\}$ and the analogous construction in [5] has two reasons. First the v_{ij} are bond variables whereas the $\mathbf{m}_i$ are variables on the sc lattice and second in the present method both sets of variables used are confined from the outset to $2N$ degrees of freedom.

The constructions of sets of $\{\mathbf{m}_i\}$ satisfying equation (8) and which involves the oriented loops presented in figure 2 allows to associate with each part C_i of the loop system a vortex strength σ_i defined by

$$\sigma_i \equiv j_{\langle ij \rangle}(C_i) = (\mathbf{m}_i + \mathbf{m}_j) \cdot \delta_{\langle ij \rangle} / 2,$$

which can be interpreted as a current $j_{\langle ij \rangle}$ associated with the bond $\langle i, j \rangle$.

Now we can express the partition function in the form

$$Z_{\text{GVL}} = \sum_{\substack{\{\mathbf{m}_i\} = -\infty \\ \text{Div}_i\{\mathbf{m}_i\} = 0}}^{\infty} \prod_{i=1}^N \prod_{\alpha=x,y,z} \int_{-\infty}^{\infty} dh_i^{\alpha} \exp \left\{ 2 \pi i \sum_i \mathbf{h}_i \cdot \mathbf{m}_i \right\} \times \\ \times \exp \left\{ - \beta_{\text{DE}} J_{\text{DE}} / 2 \sum_{\langle i,j,k,l \rangle} V(n_{\langle i,jkl \rangle}(\{\mathbf{h}_i\})) \right\}. \quad (11)$$

From the generalized vortex loop (GVL) models defined by equation (11) only the one obtained from $V(n) = n^2$ leads to a Coulomb vortex loop (CVL) model. One obtains after standard manipulations taking into account that $\sum_i \mathbf{m}_i = 0$ holds for each closed loop

$$Z_{\text{CVL}} = \sum_{\substack{\{\mathbf{m}_i\} = -\infty \\ \text{Div}_i\{\mathbf{m}_i\} = 0}}^{\infty} \left(\frac{\pi}{4 \beta_{\text{DE}} J_{\text{DE}}} \right)^{2N} \exp \left\{ \frac{\pi^2}{\beta_{\text{DE}} J_{\text{DE}}} \sum_{i,j} \sigma_i \sigma_j \times \frac{1}{N} \sum_{\mathbf{q}} \int_{C_i} \int_{C_j} d\mathbf{r}_i \cdot d\mathbf{r}_j (1 - \cos \mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)) / q^2 \right\}, \quad (12)$$

where $\sigma_i = (0, \pm 1, \pm 2, \dots)/2$, and integration is performed along the conformations of the loop system extending along the edges of the sc lattice, and at each vertex Kirchhoff's law in the form of equation (8) has to be satisfied. In equation (12) the discrete summation over the $\mathbf{m}_i$ has been approximated by a continuous integration which involves the σ_i as defined above. Because these quantities are defined with respect to bonds they can assume half integer values. The interaction in equation (12) is the Coulomb interaction known from the interaction of Amperian currents but is of apposite sign. Equation (12) represents the grand canonical ensemble partition function of a vortex plasma with coupling constant

$$\beta_{\text{CVL}} e_{\text{CVL}}^2 = \pi/2 \beta_{\text{DE}} J_{\text{DE}} \quad (13)$$

and chemical potential

$$\beta_{\text{CVL}} \mu_{\text{CVL}} = 2 \pi^2/3 \beta_{\text{DE}} J_{\text{DE}} \quad (14)$$

for the loop bordering a square face on the sc lattice.

Further relations can be established by expanding equation (5) for $\beta_{\text{DE}} J_{\text{DE}} \gg 1$ and using $n = 0, \pm 1$ only. This leads to the planar rotator PR model

$$\mathcal{H}_{\text{PR}} = - J_{\text{PR}} \sum_{\langle i', j' \rangle} \cos(\varphi_{i'} - \varphi_{j'}) \quad (15)$$

with

$$\beta_{\text{PR}} J_{\text{PR}} = e^{-\beta_{\text{DE}} J_{\text{DE}}}. \quad (16)$$

It follows from equations (15) and (16) that the high temperature CVL- and PR-model can be mapped onto each other for $\beta_{\text{PR}} J_{\text{PR}} \ll 1$ leading to

$$e_{\text{CVL}}^2 = 2 \pi J_{\text{PR}} (1 + g(1/\beta_{\text{PR}} J_{\text{PR}})), \\ \mu_{\text{CVL}} = \frac{8 \pi^2}{3} J_{\text{PR}} \left(1 + g \left(\frac{1}{\beta_{\text{PR}} J_{\text{PR}}} \right) \right) \quad (17)$$

and

$$1 + g(1/\beta_{\text{PR}} J_{\text{PR}}) = 1/4 \beta_{\text{PR}} J_{\text{PR}} \ln(1/\beta_{\text{PR}} J_{\text{PR}}). \quad (18)$$

For low and intermediate temperatures one uses Berezinskii's [6] representation of equation (15) to derive the following Hamiltonian

$$\mathcal{H} = J_{\text{PR}} \sum_{\mathbf{q}} q^2 \psi_{\mathbf{q}} \psi_{-\mathbf{q}} - \frac{4 \pi^2 J_{\text{PR}}}{N} \times \\ \times \sum_{i,j} \sigma_i \sigma_j \sum_{\mathbf{q}} \int_{C_i} \int_{C_j} \frac{d\mathbf{r}_i \cdot d\mathbf{r}_j (1 - \cos \mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j))}{q^2} \\ + \text{anharm. terms}. \quad (19)$$

Here the first term represents spin wave excitations, the second term represents the vortex plasma on the sc lattice with $\sigma_i = 0, \pm 1, \dots$ and the anharmonic terms couple spin waves and vortices such that

$$|\psi_i - \psi_{i+\delta_K}| \leq 2 \pi$$

is satisfied for all dsc lattice sites. For $\beta_{\text{PR}} J_{\text{PR}} \gg 1$, equation (19) is characterized by the coupling constant and chemical potential given in equation (17) with $g(1/\beta_{\text{PR}} J_{\text{PR}}) \rightarrow 0$. For increasing temperature the third term in equation (19) can be taken into account by means of a wave function renormalization of the spin propagator [7]

$$1/q^2 \rightarrow 1/(1 + g(1/\beta_{\text{PR}} J_{\text{PR}})) q^2 \quad (20)$$

yielding the renormalized expressions given in equation (17). It apparently follows from this and the exact high temperature limit equation (18) that the PR model equation (15) can be studied over the whole temperature range by means of equation (19) where the last term is taken into account over equation (20) and $g(1/\beta_{\text{PR}} J_{\text{PR}})$ can be calculated *via* a perturbative procedure. Apparently therefore no

dimensional change of the spin propagator in the disordered phase takes place. It should, however, be pointed out that the plasma model defined by equation (19) allows integer valued vortex strengths, whereas the plasma model defined by equation (12) allows also half integer vortex strengths. The topological conformations of the vortex loops in the latter model are, however, severely constrained due to Kirchhoff's law in the form of equation (8), whereas the usual Kirchhoff's law as applied to equation (19) allows more configurations. For instance the elementary vortex loop of the CVL-model equation (12) borders four square faces implying a chemical potential four times the value given in equation (14) whereas the elementary loop to equation (19) borders one square face. Accordingly there is still a certain difference between the two models.

The most interesting case, however, arises for $V(n) = n^2$, $n = 0, \pm 1$, which allows only $n_{\langle ijkl \rangle} = 0, \pm 1$ excitations. Equation (1) and its constraints define this time a vortex loop problem on the sc lattice with an excluded volume effect as interaction and vortex strengths $\sigma = \pm 1$. It is obvious that this holds for all hypercubic lattices with $D \geq 2$ when the $n_{\langle ij \dots \rangle}$ are defined with respect to the $(D-1)$ dimensional elementary hypercube faces. Equation (5) gives in that case

$$\tilde{V}_{\infty}(\varphi) = -(2\beta_{DE})^{-1} \ln(1 + 2 \cos \varphi e^{-\beta_{DE} J_{DE}}). \quad (21)$$

The PR model equation (15) can now be studied for the range

$$\beta_{DE} J_{DE} \gg \ln 2 \quad (22)$$

as follows from equation (21). A lower bound for the PT in the DE model follows from the Peierls type argument [8] namely that below a certain temperature calculated within a random walk approximation no infinitely extended loop can be present,

$$\beta_{DE} J_{DE} \leq \ln(2D-1)^{1/2}. \quad (23)$$

Comparison of equations (22) and (23) shows that the PT in the PR model for $D = 2$ cannot be studied via the present DE model, but only its high temperature properties. For $D \geq 3$ this is, perhaps, possible and has recently been done by Helfrich [9] who derived the present representation of the PR model by means of a different procedure. The correlation functions for the PR model are easily derived by substituting the right hand side of equation (3) for $i' = 0, \mathbf{r}$ by $+1$, and -1 respectively. This leads to

$$\begin{aligned} \langle \cos(\varphi_0 - \varphi_{\mathbf{r}}) \rangle &= \\ &= \sum_{\{C_S\}, \{C_L\}} \exp \left[-\beta_{DE} J_{DE} \left(\int_0^{\mathbf{r}} dS_S + \oint dS_L \right) \right] / \\ &\quad \sum_{\{C_L\}} \exp \left(-\beta_{DE} J_{DE} \oint dS_L \right), \end{aligned} \quad (24)$$

where all string conformations attached to $i' = 0, \mathbf{r}$ and all loop conformations are summed over. Equation (24) holds for $\beta_{PR} J_{PR}$ given by equation (16) under the restriction equation (22) and for $D \geq 2$. It can be studied by the methods of polymer physics and leads for $\beta_{DE} J_{DE} \gg 1$ to exponential decay of correlations.

Finally we would like to point out with respect to the GVL model that due to the constraints imposed by the requirements of the DE model, to permit $n = 0, \pm 1$ excitations only, onto the set $\{\mathbf{m}_i\}$ via equation (9) vortex strengths and loop conformations of the GVL model are severely constrained. This may invalidate the conclusions reached below equation (20) because the PR model is obtained from the GPR model with $n = 0, \pm 1$ excitations only.

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