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H.Chamati*, N.S.Tonchev

LONG-RANGE ORDER IN A QUANTUM MODEL OF STRUCTURAL PHASE TRANSITION

*Georgy Nadjakov Institute of Solid State Physics,
Bulgarian Academy of Sciences,
Tzarigradsko Chaussée 72, 1784 Sofia, Bulgaria

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Шамати Х., Тончев Н.С. E17-92-565

Дальний порядок в одной квантовой модели структурного фазового перехода

Вычислены параметр порядка m и среднеквадратичный параметр порядка m_0 в точно решаемой модели структурного фазового перехода. В этой модели учтены как классические, так и квантовые критические флуктуации, зависящие от температуры и размерности пространства d. Для величины $r(d, T) = m/m_0$ получено $r(d, T) = \sqrt{3}$. Этот результат не зависит от флуктуаций в системе.

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Long-Range Order in a Quantum Model of Structural Phase Transition

We calculate the order parameter m and the root mean square order parameter m_0 of an exactly soluble model of structural phase transition. In this model classical and quantum critical fluctuations depending on the temperature T and the dimension of the space are present. For the ratio $r(d, T) = m/m_0$ we obtain $r(d, T) = \sqrt{3}$. This result does not depend on the quantum and\or classical fluctuations.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. Introduction

The discussion about $r = m / m_0$, the relation between the two measures of the long-range order (LRO) m and m_0: the usual magnetization m and the root mean square magnetization m_0, is one of the most interesting questions in the theory of phase transitions [1-8]. Though the "folk-lore" statement is that in the thermodynamic limit both quantities coincide (see, e.g., the review [1]), the problem of equivalence of the different definitions of the LRO is a rather sophisticated one [2] and has a long history (see also refs. [3,4]). Recently the interest in this subject has been renewed by Kaplan et al. [5,6] in connection with the theory of some quantum spin systems (see also refs. [1,7,8]).

By definition

$$m = \lim_{h\to 0^+} \lim_{N\to\infty} \langle L_z \rangle_{H(h)} , \tag{1}$$

$$m_0 = \lim_{N\to\infty} \sqrt{\langle (L_z)^2 \rangle_H} , \tag{2}$$

where

$$\langle L_z \rangle_{H(h)} = \mathrm{Tr} \left\{ L_z \exp[-\beta H(h)] \right\} . \left\{ \mathrm{Tr} \exp[-\beta H(h)] \right\}^{-1}$$

$$H(h) = H - hNL_z \quad , \quad \beta = 1/T ,$$

H is the Hamiltonian of the system under consideration. L_z is the z-component of the operator of the magnetization (staggered magnetization) for ferromagnets (antiferromagnets) and N is the number of spins. Let us note that the physical quantity m is obtained by introducing an infinitesimal symmetry breaking field h, while m_0 does not require such a field, the expectation values in (1) and (2) are calculated over symmetry-broken and symmetry-unbroken states, respectively. This lies at the basis of the difference between the two measures m and m_0.

In ferromagnet where $[L_z,H]=0$, the result $r\geq1$ is found at any temperature [3] . When $[L_z,H]=0$ and H is invariant under the uniform spin rotation, we have $r \geq\sqrt{3}$ [4]. In ref. [5] the estimate $r\geq1$ is obtained in the more complicated case of antiferromagnet, where $[L_z,H]\neq0$. The exact value $r =\sqrt{3}$ is obtained in the framework of the Lieb-Mattis model in the ground state (T=0) [6] and at arbitrary temperatures T and an arbitrary value of the spin [7].

All the results cited above have been attached to the localized spin models of a Heisenberg type. Recently the problem of the LRO in an itinerant magnetic system (the simple Vonsovskii-Zener model of antiferromagnetism with imperfect nesting conditions [8]) was examined and the result $r =\sqrt{3}$ found. For this model it has been shown that the ratio r is independent of the band filling, which is a measure of the nesting.

All efforts in this area have been attached to magnetic system, however this problem is not of a smaller interest in the other physical systems exhibiting a phase transition.

In this paper we shall examine the ratio r in a 3-component model, exhibiting a structural phase transition of a ferrodistortion type, with cubic symmetry (the model is a generalization of the two-component one, see refs.[9]). The Hamiltonian of this system is

$$H= \sum_{l\alpha} \left(\frac{P^2_{l\alpha}}{2M} - \frac{A}{2} Q^2_{l\alpha}\right) + \frac{1}{4} \sum_{ll'\alpha} A_{ll'} \left(Q_{l\alpha}-Q_{l'\alpha}\right)^2 + \frac{B_1}{4N} \left(\sum_{l\alpha} Q^2_{l\alpha} \right)^2 + \frac{B_2}{4N} \sum_{ll'\alpha} Q^2_{l\alpha} Q^2_{l'\alpha} , \qquad (3)$$

$\alpha=x,y,z$; $P_{l\alpha}$ and $Q_{l\alpha}$ are canonically conjugated momenta and coordinates, respectively, of the lth atom with the α component of the displacement, N denotes the number of atoms. $A>0$, B_1, B_2 are model constants. $\Phi_{ll'}$ is non-zero only for the nearest neighbors.

The thermodynamic behavior of the system can be studied exactly with the aid of the approximating Hamiltonian method (AHM) [10,11], in the sense that instead of (3) we can use a simplified approximating Hamiltonian (see eq.(4) below), which generates the same thermodynamic behavior under a proper choice of its free variational parameters (for details see refs.[9]). The approximating Hamiltonian for the model (3) in normal coordinate representation is

$$T_0= \frac{1}{2}\sum_{q\alpha} \left|P_{q\alpha}\right|^2 +\nu_0^2\Omega^2_{q\alpha} \left|Q_{q\alpha}\right|^2 - \frac{N}{9} E_0 C , \qquad (4)$$

where we use the notations

$$\nu_0^2 = \frac{A}{M} \quad , \quad E_0 = \frac{A^2}{4(B_1+B_2)} \quad ,$$

$$\Omega_{q\alpha} = \Delta_\alpha + \frac{1}{A}(A_0 - A_q) = \Delta_\alpha + s^2q^2 \; ,$$

$$C = \frac{1}{b_1}(\Delta_x+\Delta_y+\Delta_z+3)^2 + \frac{1}{b_2}(2\Delta_x-\Delta_y-\Delta_z)^2 + \frac{3}{2b_2}(\Delta_y-\Delta_z)^2 \; ,$$

$$b_1 = \frac{1}{2}\,\frac{3B_1 + B_2}{B_1 + B_2} \; , \qquad b_2 = \frac{2}{3}\,\frac{B_2}{B_1 + B_2} \; ; \tag{5}$$

and Δ_α are variational parameters. They obey the equations

$$9\, y_{xN} = \frac{1}{b_1}(\Delta_x+\Delta_y+\Delta_z+3) + \frac{2}{b_2}((2\Delta_x - \Delta_y - \Delta_z) \; , \tag{6.1}$$

$$9\, y_{yN} = \frac{1}{b_1}(\Delta_x+\Delta_y+\Delta_z+3) + \frac{2}{b_2}((2\Delta_y - \Delta_z - \Delta_x) \; , \tag{6.2}$$

$$9\, y_{zN} = \frac{1}{b_1}(\Delta_x+\Delta_y+\Delta_z+3) + \frac{2}{b_2}((2\Delta_z - \Delta_x - \Delta_y) \; , \tag{6.3}$$

where

$$y_{\alpha N} = \frac{1}{N}\sum_q \frac{\lambda}{2\Omega_{q\alpha}} \coth\frac{\lambda\Omega_{q\alpha}}{2t} \; , \tag{7}$$

$$\lambda = \frac{\hbar\nu_0}{4E_0} \quad , \quad t = \frac{T}{4E_0} \; .$$

We note that the Hamiltonian (3) is exactly soluble only in the region (see refs.[9] for the two-component case)

$$3B_1 + B_2 > 0 \quad \text{and} \quad B_2 > 0 \; . \tag{8}$$

Equations (6) have a simple solution

$$\Delta_x = \Delta_y = \Delta_z = \Delta \; , \tag{9}$$

and the investigation of the system (3) is similar to

that of the one-component version [12-14] proposed by T.Schneider et al. [15].

2. The parameters m and m_0

In calculating m from (1) we use the Hamiltonian $H(h) = H - hNL_z$, where $L_z = (M^{1/2}/N)\sum_l Q_{lz}$. In this case we have the approximating Hamiltonian $H_0(h) = H_0 - hNL_z$ and the free energy (normalized to $4E_0$) is

$$f(h) = \lim_{N\to\infty} f[H(h)] = \lim_{N\to\infty} -(t/N)\ln\mathrm{Tr}\{\exp-[H(h)]/T)\} =$$

$$= \frac{S_d}{\kappa^d}\, t\sum_\alpha \int_0^{x_D} \ln[2\mathrm{sh}\frac{\lambda\sqrt{x^2+\Delta_\alpha}}{2t}] - \frac{C}{36} - \frac{h^2}{8E_0\nu_0^2\,\Delta_z} \; . \tag{10}$$

In eq.(10) $\alpha = x,y,z$; $S_d = 2(\pi)^{d/2}/\Gamma(d/2)$ is the surface of the unit d-dimensional sphere, $x_D = \kappa(d/S_d)^{1/d}$, $\kappa = 2\pi s/a$ (a is the lattice constant) and $\Delta_x, \Delta_y, \Delta_z$ are the solutions of the equations

$$9y_x = \frac{1}{b_1}(\Delta_x+\Delta_y+\Delta_z+3) + \frac{2}{b_2}((2\Delta_x - \Delta_y - \Delta_z) \; , \tag{11.1}$$

$$9y_y = \frac{1}{b_1}(\Delta_x+\Delta_y+\Delta_z+3) + \frac{2}{b_2}((2\Delta_y - \Delta_z - \Delta_x) \; , \tag{11.2}$$

$$9y_z = \frac{1}{b_1}(\Delta_x+\Delta_y+\Delta_z+3) + \frac{2}{b_2}((2\Delta_z - \Delta_x - \Delta_y) - \frac{9h^2}{4E_0\nu_0^2\Delta_z^2} \; , \tag{11.3}$$

where

$$y_\alpha = \lim_{N\to\infty} y_{N\alpha} =$$

$$= \frac{\lambda}{2}\,\frac{S_d}{\kappa^d}\, x_D^{d-1} \int_0^1 \frac{z^{d-1}\,dz}{\sqrt{\Delta_\alpha x_D^{-2} + z^2}} \coth\frac{\lambda x_D}{2t}\sqrt{\Delta_\alpha x_D^{-2} + z^2} \; . \tag{12}$$

Adding the equations (11), we have

$$\frac{h^2}{4E_0\nu_0^2\ \Delta_z^2} = \frac{1}{3b_1}(\Delta_x+\Delta_y+\Delta_z+ 3) - y_x - y_y - y_z \ . \qquad (13)$$

The functions $f_N(h)$ are differentiable and convex at any h. The limit function $f(h)$ is convex and differentiable at $h\neq 0$. Then applying the Griffiths-Fisher lemma [16], we have

$$\limsup_{N\to\infty} \langle L_z\rangle \le \lim_{h\to 0^-} \partial f(h)/\partial h \ ,$$

$$\liminf_{N\to\infty} \langle L_z\rangle \ge \lim_{h\to 0^+} \partial f(h)/\partial h \ .$$

However we can choose a sequence of points $h_n^+ > 0$, $h_n^+\to 0$ at which the derivatives

$$\left.\frac{\partial f(h)}{\partial h}\right|_{h=h_n^+} = \lim_{N\to\infty} \langle L_z\rangle_{H(h_n^+)}$$

exist. Now from the right continuity of $\partial f(h)/\partial h$ at $h = 0$ and from eqs.(10) and (13) it follows that

$$m = \frac{2}{\nu_0}\left[\frac{E_0}{3b_1}\right]^{1/2}\left\{\Delta_x+\Delta_y+\Delta_z+ 3 - 3b_1(y_x+ y_y+ y_z)\right\}^{1/2} . \qquad (14.1)$$

Similarly it can be shown that there exists a sequence for $h_n^- > 0$, $h_n^-\to 0$, and we get

$$m = -\frac{2}{\nu_0}\left[\frac{E_0}{3b_1}\right]^{1/2}\left\{\Delta_x+\Delta_y+\Delta_z+ 3 - 3b_1(y_x+ y_y+ y_z)\right\}^{1/2} . \qquad (14.2)$$

In zero field $(h=0)$, equations (11) reduce to equations (6) in the thermodynamical limit . Then taking into account (9), we can write (14) (as $y_x=y_y=y_z=y$)

$$m = \operatorname{sign}h\,\frac{2}{\nu_0}\left[\frac{E_0}{b_1}\right]^{1/2}\left\{\Delta + 1 - 3b_1 y\right\}^{1/2} . \qquad (15)$$

The source term $-hNL_z$ breaks the symmetry of H. The function $f(h)$ is not differentiable at $h=0$ and $m \neq \langle L_z\rangle_H = 0$. This is an example of Bogolubov's "quasi-averages" [17].

The calculation of m_0 from (2) requires the use of a source term which does not break the symmetry of H [7]. Let us consider the Hamiltonian $H(\rho) = H - \rho N\vec{L}^2$, which has the same basic symmetry properties as H. In this case we have the approximating Hamiltonian $H_0(\rho) = H_0 - \rho N\vec{L}^2$ and the free energy is

$$f(\rho) = \lim_{N\to\infty} f_N[H_0(\rho)] \ ,$$

where

$$f_N[H_0(\rho)] = 3\frac{t}{N}\sum_q \ln[2\operatorname{sh}\frac{\lambda\Omega_q(\rho)}{2t}] - \frac{1}{4}\ \frac{(1 + \Delta)^2}{b_1}, \qquad (16)$$

$$\Omega_q^2(\rho) = \Omega_q^2 - (2\rho/\nu_0^2)\delta_{q0} \ ,$$

δ_{q0} is the Kronecker symbol and Δ is the solution of the equation

$$\Delta + 1 = 3b_1 y_N . \qquad (17)$$

The functions $f_N[H_0(\rho)]$ are differentiable at $\rho=0$. Then from the Griffiths-Fisher lemma [16], the continuity of the derivatives $\partial f_N[H_0(\rho)]/\partial\rho$ (which permits one to inverse the order of the operation $\lim_{\rho\to 0} \lim_{N\to\infty}$) at $\rho=0$ and equation (16), we obtain

$$\lim_{N\to\infty} < \vec{L}^2 >_H = -\lim_{N\to\infty} \frac{\partial f_N[H_0(\rho)]}{\partial \rho}\bigg|_{\rho=0} . \qquad (18)$$

Now using the unitary transformation $U_{\alpha\beta} = \exp\{-i(\pi/2\hbar)\sum_l (P_{l\alpha}Q_{l\beta} - Q_{l\alpha}P_{l\beta})\}$, which transforms L_α into L_β , L_β into $-L_\alpha$ and keeps invariant the other axes, one can easily show that

$$< L_x^2 >_H = < L_y^2 >_H = < L_z^2 >_H . \qquad (19)$$

Let us note that $U_{\alpha\beta}$ conserves the commutation relations $[P_{l\alpha}, Q_{l'\beta}] = i\hbar\delta_{ll'}\delta_{\alpha\beta}$.

Finally from (2),(17),(18) and (19) we obtain

$$m_0^2 = \frac{4E_0}{3b_1\nu_0^2}\left\{ 1 + \Delta - 3b_1 y \right\} , \qquad (20)$$

and (*cf.* eq.(15))

$$r(d,T) = m / m_0 = \sqrt{3} . \qquad (21)$$

3. Discussion

In this paper we have investigated the relation $r(d,T)$ between the two different measures of the LRO in the symmetry breaking state and in the state with unbroken symmetry. The most interesting physical consequences in this area have been provoked by the fact that in the quantum models the order parameter operator does not commute with the Hamiltonian (see refs.[1-8,18]). The quantum model studied here is exactly soluble in the thermodynamical limit. The peculiarity of this model comes from the presence of quantum and classical critical fluctuations, depending on the temperature T and the space dimensionality d [13]. In the classical limit, the one-component version of the model (3) belongs to the class of universality of spherical models. It has been also shown that there is a classical to quantum dimensional crossover in the zero temperature limit [13]. The obtained result $r(d,T) = \sqrt{3}$ shows that the critical fluctuations (quantum and/or classical) do not violate the equality $m = m_0\sqrt{3}$ found earlier for some exactly soluble mean-field models in the theory of magnetism [6-8]. At last, let us note that the generalized model obtained for an arbitrary number of the components n of $\vec{L}$ gives the result $r(d,T) = \sqrt{n}$.

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