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INFINITE SUSCEPTIBILITY WITHOUT LONG-RANGE ORDER: THE TWO-DIMENSIONAL HARMONIC "SOLID"

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It is pointed out that the classical two-dimensional harmonic "solid" exhibits an infinite generalized susceptibility at low temperature, although there is no long-range order and no phase transition.

It has been rigorously proven that there is no ferromagnetism in the two-dimensional isotropic Heisenberg model.[1] There are, however, strong indications that the magnetic susceptibility becomes infinite below some critical temperature.[2] It has therefore been speculated that, below this critical temperature, the curve of the magnetization versus the field might have a vertical tangent at zero field, without having a finite discontinuity.

In the present note, it is proven that a very simple soluble model, the classical two-dimensional harmonic "solid," does exhibit this very behavior. Let $\vec{K}$ be a vector of the reciprocal lattice. The analog of the spontaneous magnetization per particle is N^{-1} times the average value $\langle\rho_{\vec{K}}\rangle_0$ of the Fourier component of the density $\rho_{\vec{K}}$ in the limit of no external field. The analog of the susceptibility is the linear response $\chi_{\vec{K}}$ of $(1/N)\langle\rho_{\vec{K}}\rangle$ to the static external potential $V\exp(i\vec{K}\cdot\vec{r})$. It is well known that a harmonic system undergoes no phase transition, in any number of dimensions, and also that $(1/N)\langle\rho_{\vec{K}}\rangle_0$ is zero in one and two dimensions. We shall prove, however, that in two dimensions, $\chi_{\vec{K}}$, finite above a critical temperature T_c, becomes infinite at and below that temperature.

We consider a two-dimensional square lattice of N particles of mass m which interact through harmonic forces; periodic boundary conditions are assumed. Let $\vec{R}_i$ be the equilibrium positions of the particles and $\vec{u}_i$ the deviations of these positions from their equilibrium values. The $\vec{u}_i$ are linear combinations of the phonon coordinates[3] $\vec{v}_{\vec{k}}$:

$$\vec{u}_i = N^{-1/2}\sum_{\vec{k}} \exp(i\vec{k}\cdot\vec{R}_i)\vec{v}_{\vec{k}}. \tag{1}$$

The potential energy of the system is $\sum_{\vec{k}} \frac{1}{2}m\omega_{\vec{k}}^2 \times |\vec{v}_{\vec{k}}|^2$, where $\omega_{\vec{k}}$ is the angular frequency associated with the wave number $\vec{k}$; and the sums on $\vec{k}$ always run over the first Brillouin zone. A component $v_{\vec{k}\lambda}$ of $\vec{v}_{\vec{k}}$ has a Gaussian distribution with a width given by the energy equipartition at temperature T:

$$\tfrac{1}{2}m\omega_{\vec{k}}^2\langle|v_{\vec{k}\lambda}|^2\rangle = \tfrac{1}{2}k_B T. \tag{2}$$

The total internal energy (including the kinetic energy) is $2Nk_BT$. Since this is a regular function of T, there is no phase transition in the the thermodynamic sense.

The Fourier component of the density $\rho_{\vec{K}}$ is

defined as

$$\rho_{\vec{K}} = \sum_i \exp[-\vec{K}\cdot(\vec{R}_i + \vec{u}_i)] = \sum_i \exp(-i\vec{K}\cdot\vec{u}_i), \quad (3)$$

and, since $\vec{u}_i$ is a linear combination of Gaussianly distributed variables,

$$(1/N)\langle\rho_{\vec{K}}\rangle_0 = \exp[-(\tfrac{1}{2})\langle(\vec{K}\cdot\vec{u}_i)^2\rangle]. \quad (4)$$

From (1) and (2), one gets the following in the limit of an infinite system:

$$\langle(\vec{K}\cdot\vec{u}_i)^2\rangle = \frac{k_B T K^2}{4\pi^2 m}\int\frac{d^2\vec{k}}{\omega_{\vec{k}}^2} \quad (5)$$

(we take the equilibrium distance between nearest neighbors as the unit of length). Since $\omega_{\vec{k}}$ behaves like ck (c is the sound velocity) for small k values, the integral in (5) diverges; $\vec{u}_i$ has infinite fluctuations, and $(1/N)\langle\rho_{\vec{K}}\rangle_0$ is washed out to zero. The system has no long-range order and is not a solid in the usual sense.

The generalized susceptibility is defined by applying an external potential $V\exp(i\vec{K}\cdot\vec{r})$ and looking at the response of $(1/N)\langle\rho_{\vec{K}}\rangle$:

$$\chi_{\vec{K}} = (1/N)(\partial\langle\rho_{\vec{K}}\rangle/\partial V)_{V=0} = -(1/Nk_B T)\langle|\rho_{\vec{K}}|^2\rangle_0, \quad (6)$$

where the last equality follows from the relation[4] between the linear response and the fluctuations at zero field. Therefore,

$$\chi_{\vec{K}} = -(1/Nk_B T)\sum_{ij}\langle\exp[i\vec{K}\cdot(\vec{u}_i - \vec{u}_j)]\rangle = -(1/k_B T)\sum_j \exp\{-(\tfrac{1}{2})\langle[\vec{K}\cdot(\vec{u}_1 - \vec{u}_j)]^2\rangle\}. \quad (7)$$

From (1) and (2), one gets

$$\langle[\vec{K}\cdot(\vec{u}_1 - \vec{u}_j)]^2\rangle = \frac{2k_B T K^2}{mN}\sum_{\vec{k}\neq 0}\frac{1-\cos[\vec{k}\cdot(\vec{R}_1 - \vec{R}_j)]}{\omega_{\vec{k}}^2}. \quad (8)$$

For a given value of $\vec{R}_1 - \vec{R}_j$, (8) remains finite as $N\to\infty$: Although $\vec{u}_1$ and $\vec{u}_j$ each have infinite fluctuations, they are correlated in such a way that their difference has only finite fluctuations. Incidentally, this shows that the usual assumption of harmonic forces between neighboring particles remains a consistent one, since the local deformations of the lattice are finite. When, however, $R_{1j} = |\vec{R}_1 - \vec{R}_j|$ increases, (8) behaves like a constant times $\ln R_{1j}$.

A crude argument for this result is the following: The $\vec{k}$ sum in (8) may be split into two regions. For $k < 1/R_{1j}$, $1-\cos(\vec{k}\cdot\vec{R}_{1j})$ is small, and this region does not contribute much to the sum; for $k > 1/R_{1j}$, $\cos(\vec{k}\cdot\vec{R}_{1j})/\omega_{\vec{k}}^2$ is an oscillating function, the sum of which is also small. The main contribution therefore is

$$\frac{1}{N}\sum_{k>1/R_{1j}}\frac{1}{\omega_{\vec{k}}^2} \sim \frac{1}{4\pi^2 c^2}\int_{1/R_{1j}} 2\pi k\frac{dk}{k^2} \sim \left(\frac{1}{2\pi c^2}\right)\ln R_{1j}. \quad (9)$$

The argument can be made rigorous through the introduction of upper and lower bounds for the functions which are involved, and then leads to the inequality, valid for all $\vec{R}_{1j}\neq 0$,

$$|\langle[\vec{K}\cdot(\vec{u}_1 - \vec{u}_j)]^2\rangle - (k_B T K^2/\pi m c^2)\ln R_{1j}| < AT, \quad (10)$$

where A is a constant, independent of $\vec{R}_{1j}$, N, and T. R_{1j} however must be understood as the shortest distance between the lattice points 1 and j when the periodic boundary conditions are taken into account, i.e., the shortest path on the torus on which the lattice may be wrapped.

Going back to the susceptibility (7), one sees that

$$\chi_{\vec{K}} = \frac{1}{k_B T}\left[1 + B\sum_{j\neq 1}\left(\frac{1}{R_{1j}}\right)^{2T/T_c}\right], \quad (11)$$

where $\exp(-\frac{1}{2}AT) < B < \exp\frac{1}{2}AT$ and

$$k_B T_c = 4\pi m c^2/K^2. \quad (12)$$

In the limit of an infinite system,[5] the j sum in (11), which runs over the two-dimentional lattice, will converge at infinity if $T > T_c$, but will diverge as soon as $T \leq T_c$.[6]

For temperatures just above T_c, the susceptibility behaves like

$$\chi_{\vec{K}} \sim -(B/k_B T)\int_1^\infty 2\pi R dR\, R^{-2T/T_c} \sim C(T - T_c)^{-1}, \quad (13)$$

where C is some constant.

The same dependence R_{1j}^{-2T/T_c} that we find for our

$$\exp\{-\tfrac{1}{2}\langle[\vec{K}\cdot(\vec{u}_1 - \vec{u}_j)]^2\rangle\}$$

has been suggested[7] for the correlation function $\langle\vec{\sigma}_1\cdot\vec{\sigma}_j\rangle$ in the Heisenberg model. Our susceptibility, however, diverges with a $(T-T_c)^{-1}$ law which differs from the nonentire power law proposed[2] for the Heisenberg model.

It may be worth emphasizing again that, in the present model, T_c is not a thermodynamical singularity; moreover, T_c depends on that wave number $\vec{K}$ which has been considered.

It is possible that the above considerations might serve as a guide for obtaining further results on the two-dimensional Heisenberg model, and perhaps on the hard-disc system.[8]

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ABSOLUTE MEASUREMENT OF STRUCTURE FACTORS WITH HIGH PRECISION

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Recently, Hattori et al. have measured the structure factors of Si single crystals on the absolute scale with an accuracy of about 1%.[1,2] The method is entirely different from the conventional one based on x-ray intensity measurements. The new method is based on the spacing measurement of the Pendellösung fringes[3] due to the interference of doubly refracted x rays under the condition of the Bragg reflection. The results are free from extinction effects and less ambiguous in applying the theoretical formula connecting the structure factor $|F_g|$ with the observable quantities.

The spacing $\Lambda_g{}^c$ of the Pendellösung fringes along the net plane is given by[1,2,4]

$$\Lambda_g{}^c=\frac{\pi v}{\lambda\cos\theta_B}\left(\frac{mc^2}{e^2}\right)|F_g|^{-1}, \tag{1}$$

including the effect of x-ray polarization, where λ is the wavelength, θ_B is the Bragg angle, v is the volume of unit cell, and e, m, and c are the physical constants having usual meanings. The observable spacing Λ_g is connected with this spacing $\Lambda_g{}^c$ through a geometrical factor Φ_g:

$$\Lambda_g=\Lambda_g{}^c\Phi_g. \tag{2}$$

If a perfect wedge crystal of wedge angle φ is used and either the entrance surface or the exit surface of the crystal is perpendicular to the plane determined by the incident beam and the Bragg-reflected beam, the factor Φ_g turns out to be $\cot\varphi$.

We confirmed through internal check that Λ_g itself could be determined with an accuracy of about 0.1% under suitable experimental conditions, particularly in low-order reflections. A difficulty, however, for obtaining $|F_g|$ accurately arises in determining the wedge angle φ with sufficient accuracy. Moreover, it is rather difficult to prepare an ideally perfect wedge of the crystal. For this reason, in the previous work, the accuracy of the structure factor was not better than about 1%.

Here, it is shown that the geometrical factor Φ_g can be eliminated by combining the experiment of Pendellösung fringes with that of thickness fringes in x-ray interferometry which has been recently demonstrated by Bonse and Hart.[5] The principle of the present interferometer is illustrated in Fig. 1. The incident beam satisfies the Bragg condition simultaneously at the interferometer crystals S, M, and A. Contrary to that of Bonse and Hart, an extremely narrow beam (20~100 μ) was used