

A transition from a commensurate phase to an incommensurate phase in a continuous medium with dislocations

T. Bor, V. L. Pokrovskii, and A. L. Talapov

L. D. Landau Institute of Theoretical Physics

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A transition from a commensurate phase to an incommensurate phase is studied in an anisotropic system with a commensurability order $p = 2$. A term which describes the formation of dislocations is added to the sine-Gordon theory. The phase transition acquires an Ising nature if the dislocations are taken into account.

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Theoretical and experimental studies of the phase transition from a commensurate phase to an incommensurate phase are continuing.^{1–3} In regard to systems which are incommensurate with the substrate in one direction, it has recently been pointed out^{4–6} that the dislocations in the soliton structure must be taken into account. It was shown that the regular soliton lattice is unstable to the formation of dislocations. The nature of the corresponding phase transition and the structure of a new “molten” phase, however, have not been studied. According to Refs. 5 and 6, an instability appears only if the commensurability order p is sufficiently low, i.e., at $p^2 < 8$.

In this letter we shall consider a phase transition when $p = 2$. This phase transition has been studied experimentally by Jaubert and his co-workers.⁷ Using the methods developed by Luther and Peschel⁸ and Mandel'stam,⁹ we show that an exact solution can be obtained in this case at a certain temperature. The experiment is described by a field theory similar to the sine-Gordon theory. The Hamiltonian appearing in the transition-matrix of this system can be written by using the boson field φ and its momentum $P = (1/i)(\delta/\delta\varphi)$

$$H = \int_0^L dx \left\{ \frac{P^2}{2} + \frac{1}{2} \left(\frac{\partial \varphi}{\partial x} \right)^2 - \mu' \left(\frac{\partial \varphi}{\partial x} \right) + m' \cos \beta \varphi + \lambda' \cos \left(\frac{2\pi p}{\beta} \int_{-\infty}^x P dx \right) \right\}, \quad (1)$$

where L is the length of the system in the x direction. The first two terms correspond to the harmonic elastic interaction between the adsorbed atoms. The third term describes the initial incommensurability with the substrate. The term containing $\cos \beta \varphi$ is a periodic potential of the interaction of atoms with the substrate. The last term describes the dislocation effect.¹⁰ The constant λ' is proportional to the probability of formation of a dislocation and β is proportional to the square root of the temperature.

We introduce the fermionic variables ψ_1 and ψ_2 . According to Refs. 8 and 9, Eq. (1) can be rewritten as a Hamiltonian of the generalized massive Thirring model

$$H = \int \left\{ \frac{c}{i} (\psi_1^\dagger \partial_x \psi_1 - \psi_2^\dagger \partial_x \psi_2) - \mu (\psi_1^\dagger \psi_1 + \psi_2^\dagger \psi_2) + g \psi_1^\dagger \psi_1 \psi_2^\dagger \psi_2 + m (\psi_1^\dagger \psi_2 + \psi_2^\dagger \psi_1) + \lambda (\psi_1^\dagger \psi_2^\dagger + \psi_2 \psi_1) \right\} dx, \quad (2)$$

where

$$c = \frac{1}{2} \left(\frac{\beta^2}{4\pi} + \frac{4\pi}{\beta^2} \right), g = \pi \left(\frac{4\pi}{\beta^2} - \frac{\beta^2}{4\pi} \right), m = m' \pi a, \lambda = \lambda' \pi a, \mu = \mu' \frac{2\pi}{\beta}. \quad (3)$$

Here a is the lattice constant.

For $\beta^2 = 4\pi$ we have $g=0$, and we find a quadratic Hamiltonian with $c=1$. Diagonalizing it by using the Bogolyubov transformation, we find the spectrum

$$\epsilon(k) = \pm (k^2 + m^2 + \mu^2 + \lambda^2 + 2\sqrt{\mu^2 k^2 + \mu^2 m^2 + \lambda^2 m^2})^{1/2}. \quad (4)$$

The free energy density F is equal to the ground-state energy of the Hamiltonian H divided by L . Only those states in Eq. (4) whose energy is negative are occupied. In contrast to the case $\lambda=m=0$, the free energy varies in the following way:

$$\Delta F = -\frac{1}{L} \sum_{k>0} \left\{ \sqrt{2} (k^2 + m^2 + \mu^2 + \lambda^2 + \sqrt{(k^2 + m^2 - \mu^2 - \lambda^2)^2 + 4k^2 \lambda^2})^{1/2} - 2k \right\}. \quad (5)$$

The phase transition occurs when

$$\mu_c^2 = m^2 - \lambda^2, \quad (6)$$

as $\partial^2 F / \partial \mu^2$ tends to infinity logarithmically.

The difference in the densities of the solitons and antisolitons is $n = -\partial \Delta F / \partial \mu$. For $|\mu - \mu_c| \ll m$ and $\lambda \ll m$ we find

$$n = \frac{\lambda}{\pi} E \left(\frac{\sqrt{m^2 - \mu^2}}{\lambda} \right), \quad (7)$$

where E is a complete elliptic integral.

According to Eq. (4), the fundamental-excitation spectrum at $\lambda \neq 0$ has no gap only at $\mu = \mu_c(m, \lambda)$. The correlation length is therefore finite at any $\mu \neq \mu_c$. Consequently, in contrast to the case $\lambda=0$, the system is not a two-dimensional incommensurate crystal with power-law correlations at $\mu > \mu_c$. The soliton density (7), nonetheless, obeys the law $n \sim \sqrt{\mu - \mu_c}$, on condition that $\mu - \mu_c \gg \lambda$, consistent with the results of Refs. 1 and 7. The correlation length is proportional to λ^{-1} in this region, and the system behaves as an ordinary incommensurate crystal at a distance less than λ^{-1} .

In the limit $\mu \rightarrow \mu_c$ the energy gap Δ_0 vanishes in a manner $\Delta_0 \sim \mu - \mu_c$. The correlation length ξ_0 therefore diverges according to the law $\xi_0 \sim (\mu - \mu_c)^{-1}$. Since

$\mu - \mu_c$ plays the role of the reduced temperature, the critical index ν has an Ising value $\nu = 1$. The behavior of the free energy and of the correlation length shows that this phase transition resembles very closely the transition in a two-dimensional Ising model. Such behavior has been predicted elsewhere¹¹ and in the private communication of Schulz, in which the discrete models were studied. If, in fact, the Hamiltonian in (2) ($cg = 0$) is converted to the variables in which it is diagonal at $\lambda = 0$ and the spectrum branches, whose energy is of the order of m at $k = 0$ are ignored, then we would have a Hamiltonian at small k , which is the same as that in Ref. 11.

Until now, we have considered a special case in which $\beta^2 = 4\pi$. We expect that the results obtained by us will hold for other values of β if m and λ are replaced by their renormalized values m_R and λ_R .

The equations for renormalization of m and λ were obtained by Wiegmann¹⁰ and Jose *et al.*¹² The presence of a term with μ in Eq. (1) does not change them, since the momenta $k \gg m$ contribute to the renormalization. Therefore,

$$m_R(\xi) \sim m \exp\left(1 - \frac{\beta^2}{4\pi}\right) \xi, \quad \lambda_R(\xi) \sim \lambda \exp\left(1 - \frac{4\pi}{\beta^2}\right) \xi, \quad (8)$$

where ξ is a logarithm of the characteristic length. The renormalization stops at $\xi = -1/2 \ln \times (m_R^2 + \lambda_R^2)$, and for $\lambda \ll m$ we have

$$m_R \sim m \frac{1}{(2 - \beta^2/4\pi)}, \quad \lambda_R \sim \lambda m \left(\frac{4\pi}{\beta^2} - 1 \right) / \left(2 - \frac{\beta^2}{4\pi} \right). \quad (9)$$

According to Eq. (6), the transition occurs only on condition that $m \geq \lambda$. The critical point on the phase diagram is therefore determined by the equation $m_R = \lambda_R$. We determine from (9) the critical value of β

$$\frac{\beta_c^2}{4\pi} = 1 - q + \sqrt{1 - q + q^2}, \quad q = \frac{\ln m}{\ln \lambda}. \quad (10)$$

In the limit $\lambda \rightarrow 0$ we obtain the known result $\beta_c^2 = 8\pi$.

At $p = 2$ the commensurate state is doubly degenerate, corresponding to the arrangement of atoms in two different sublattices. The solitons form a boundary between these two states. At $|\mu| \ll \mu_c$ virtually the entire plane is occupied by one of these states and at $\mu = \mu_c$ both states are in the domains of infinite size. This is completely analogous to the behavior of the Ising model. We expect that the order parameter $\langle \exp(i\beta\phi/2) \rangle$, i.e., the Debye-Waller factor, decreases in the commensurate phase as $(\mu_c - \mu)^{1/8}$, as in the Ising model. Such a pretransition effect is missing at $\lambda = 0$. The logarithmic increase of the specific heat and of the two-dimensional compressibility is also regarded as the pretransition effect.

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