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COMMENT

Pseudo-first-order phase transitions in one dimension

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Abstract. A study is made of the one-dimensional Ginzburg–Landau system with a cubic term, a model of the first-order phase transition. Fluctuations are taken into account by means of the WKB method. It is pointed out that the transition is of continuous type for any value of the coefficient of the cubic term. This results from the excitation of domain walls between two coexisting phases.

The simple Landau theory (Landau 1965) predicts a first-order transition whenever a cubic term is allowed in the expansion of the free energy with respect to the order parameter. Alexander and Amit (1975) criticised this theory and concluded that the above prediction is not always valid, but that the transition can be of continuous type for a certain range of the parameter involved.

In this Comment we treat a one-dimensional system with a cubic term, in which the effect of fluctuations is expected to be especially important, and study what kind of transition this system shows. A one-dimensional system is simple, so that many of its properties can be obtained in explicit form. This may give a better understanding of a general theory of the first-order phase transition.

Let us consider a generalised Ginzburg–Landau system whose free energy functional is given by

$$H(\phi(x))/k_{\mathrm{B}}T = \int \mathrm{d}x[\tfrac{1}{2}(\mathrm{d}\phi/\mathrm{d}x)^2 + \tfrac{1}{2}u_2\phi^2 - u_3\phi^3 + u_4\phi^4], \tag{1}$$

where the parameter u_2 is an increasing function of the temperature and u_3 and u_4 are assumed to be positive constants. We take $\phi(x)$ to be a real field satisfying periodic boundary conditions $\phi(L) = \phi(0)$, where L is the length of the system.

The partition function for this system is obtained by calculating a functional integral of $\exp[-H(\phi(x))/k_{\mathrm{B}}T]$ over all field configurations. For a one-dimensional field, the transfer operator technique (Scalapino *et al* 1972) reduces the calculation of this integral to the problem of solving the Schrödinger equation

$$[-\tfrac{1}{2}(\mathrm{d}^2/\mathrm{d}\phi^2) + V(\phi)]\Psi_\lambda(\phi) = E_\lambda\Psi_\lambda(\phi), \tag{2}$$

where

$$V(\phi) = \tfrac{1}{2}u_2\phi^2 - u_3\phi^3 + u_4\phi^4. \tag{3}$$

In the thermodynamic limit the free energy per unit length is given, by using the lowest eigenvalue E_0 of equation (2), as

$$F/L = S_0 + E_0, \tag{4}$$

where S_0 is a constant independent of the temperature originating from a certain integral.

Before proceeding further, let us refer to the results by the usual mean-field theory. In this theory, the system we consider shows a first-order transition when

$$u_2 = \tfrac{1}{2}u_3^2/u_4 \equiv u_{2c} \tag{5}$$

is satisfied. For u_2 just above u_{2c}, the system is disordered with $\phi = 0$, while for u_2 just below u_{2c}, the system is ordered with $\phi = \tfrac{1}{2}u_3/u_4$. Through this transition the entropy of the system undergoes a finite jump.

The correct theory will be obtained by solving the Schrödinger equation (2). We solve this equation by means of the WKB method. In the vicinity of the transition point, i.e. $u_2 = u_{2c}$, the potential $V(\phi)$ has two minima. Confining ourselves to the low-lying eigenvalues near the potential minima, we divide the ϕ axis into five regions: (I) $\phi < \alpha$; (II) $\alpha < \phi < \beta$; (III) $\beta < \phi < \gamma$; (IV) $\gamma < \phi < \delta$; (V) $\delta < \phi$. Here α, β, γ and δ are the turning points at which the classical momentum

$$p(\phi) = [2(E - V(\phi))]^{1/2} \tag{6}$$

vanishes. Regions (II) and (IV) form two potential wells separated from each other by the barrier in region (III).

Next we take in region (I) the exponentially growing WKB wavefunction which vanishes for $\phi \to -\infty$ and, applying the connecting formula at the turning points, obtain the wavefunctions in the other regions successively. From the requirement that the wavefunction in region (V) should vanish for $\phi \to \infty$, we finally obtain the quantisation condition

$$\cot\left(\int_\alpha^\beta p \, \mathrm{d}\phi\right) \cot\left(\int_\gamma^\delta p \, \mathrm{d}\phi\right) = \tfrac{1}{4} \exp\left(-2 \int_\beta^\gamma |p| \, \mathrm{d}\phi\right). \tag{7}$$

It is difficult to determine the energy levels from this complicated condition as it stands. However, observing that the transparency through the potential barrier is very small, we can approximate (7) by a simpler form

$$\left(\int_\alpha^\beta p \, \mathrm{d}\phi - \pi(n + \tfrac{1}{2})\right)\left(\int_\gamma^\delta p \, \mathrm{d}\phi - \pi(n + \tfrac{1}{2})\right)$$

$$= \tfrac{1}{4} \exp\left(-2 \int_\beta^\gamma |p| \, \mathrm{d}\phi\right) \qquad (n = 0, 1, 2, \ldots). \tag{8}$$

We solve this equation by expanding the potential involved in p in a power series of ϕ about each of the minima and retaining it up to second order. The low-lying eigenvalues are found as

$$E_n = \frac{1}{4}\left(\frac{u_2}{2u_4}\right)^{1/2}(u_2 - u_{2c}) + (n + \tfrac{1}{2})\sqrt{u_2} \pm \left(t_n^2 + \frac{1}{32}\frac{u_2}{u_4}(u_2 - u_{2c})^2\right)^{1/2}, \tag{9}$$

where

$$t_n = \frac{\sqrt{u_2}}{2} \exp\left(-\int_\beta^\gamma |p| \, \mathrm{d}\phi\right) \simeq \frac{\sqrt{u_2}}{2\pi}\left(\frac{2eu_2\sqrt{u_2}}{(2n+1)u_4}\right)^{(2n+1)/2} \exp\left(-\frac{u_2\sqrt{u_2}}{12u_4}\right). \tag{10}$$

In evaluating the tunnel integral, we have retained only the lowest order in $u_4/u_2\sqrt{u_2}$ because of the small transparency through the potential barrier which is assumed. Clearly this assumption is consistent with confining ourselves to the low-lying states.

Substituting (9) into (4), we obtain the free energy near the transition point as

$$\frac{F}{L}=S_0+\frac{\sqrt{u_2}}{2}+\frac{1}{4}\sqrt{\frac{u_2}{2u_4}}(u_2-u_{2c})-\left(t_0^2+\frac{u_2}{32u_4}(u_2-u_{2c})^2\right)^{1/2}. \tag{11}$$

If we fix u_3 and u_4 as certain constants and vary u_2, which measures the temperature, then we can observe the thermodynamic behaviour of the system. If the tunnelling term t_0 were missing, a first-order transition would take place at $u_2=u_{2c}$. This is the mean-field result. However, the presence of t_0, i.e. the tunnelling between the two nearly degenerate minima, prevents a clear-cut first-order transition, so that the transition is of continuous type. This fact holds for any value of u_3. Following the work of Krumhansl and Schrieffer (1975) on the one-dimensional ϕ^4 model, we note that the tunnelling between the two minima is caused by domain walls, i.e. boundaries between coexisting disordered and ordered phases. Our argument thus provides an intuitive picture of the pseudo-first-order transition; that is, the formation of domain walls near the transition. This picture has been overlooked in mean-field theory. Also in higher dimensions, the concept of domain walls plays a crucial role in a better understanding of the first-order transition (Toulouse and Kléman 1976).

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