ANALOGY BETWEEN LANDAU THEORY OF PHASE TRANSITIONS AND LAGRANGIAN MECHANICS

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It is shown that the definition of a stable point in Landau theory is different from that used in mechanics. The implications for numerical work on phase transitions for systems that have a Lifshitz invariant are discussed.

Our intention in this note is to give a geometric view of the theory of phase transitions with inclusion of a Lifshitz invariant. We consider a system with a two-component order parameter (ξ_1, ξ_2) in which the free energy density has the form

$$F = K + W + L\,, \tag{1}$$

where

$$K = \tfrac{1}{2}\kappa\,[(\mathrm{d}\xi_1/\mathrm{d}z)^2 + (\mathrm{d}\xi_2/\mathrm{d}z)^2]\,, \tag{2}$$

and L is a Lifshitz invariant

$$L = \Lambda(\xi_1\,\mathrm{d}\xi_2/\mathrm{d}z - \xi_2\,\mathrm{d}\xi_1/\mathrm{d}z)\,. \tag{3}$$

The form of W depends on the system under discussion. We use two specific examples for illustration. For an incommensurate–commensurate transition in a crystal W may take the form [1]

$$W = \tfrac{1}{2}a(\xi_1^2 + \xi_2^2) + \tfrac{1}{4}\beta(\xi_1^4 + \xi_2^4) + \tfrac{1}{2}\gamma\xi_1^2\xi_2^2\,. \tag{4}$$

It is assumed as usual that $a = a_0(T - T_0)$ while the other parameters are independent of temperature. In the high temperature (prototype) phase $\xi_1 = \xi_2 = 0$. At temperature $T_c = T_0 + \Lambda^2/a_0\kappa$ there is a transition to the incommensurate phase in which both ξ_1 and ξ_2 are non-zero and z dependent. At a lower temperature T_{LI} there is a "lock-in" transition to the commensurate phase in which ξ_1 and ξ_2 are independent of z. In the minimization of F, L favours the precession of the incommensurate phase, while W favours the uniformity of the commensurate phase. Writing $\xi_1 = |\xi|\cos\phi$, $\xi_2 = |\xi|\sin\phi$ one sees easily from the fourth order terms of W that for $\gamma > \beta$ the commensurate phase has $\phi = 0$ or $\pi/2$, while for $\gamma < \beta$ $\phi = \pm\pi/4$.

Eq. (1) also applies to the "unwinding" of the smectic C* phase of liquid crystals in an external magnetic field H [2]. In this case (ξ_1, ξ_2) is the molecular director $\boldsymbol{n}$, and

$$W = \tfrac{1}{2}(a - \chi H^2)\xi_1^2 + \tfrac{1}{2}a\xi_2^2 + \tfrac{1}{4}b(\xi_1^2 + \xi_2^2)^2\,. \tag{5}$$

The prototyne phase $\xi_1 = \xi_2 = 0$ is now smectic A, and the analogue of the incommensurate phase is smectic C* in which $\boldsymbol{n}(z)$ precesses round the $\hat{\boldsymbol{z}}$ direction as z varies. As H is increased at constant temperature, the C* helix elongates until eventually there is a transition to the C phase. Here $\xi_2 = 0$, and $\xi_1 \neq 0$ is independent of z. Thus the C phase is the analogue of the commensurate phase of the crystal. Again, the presence of L favours the C* phase, while minimization of W alone gives the C phase.

To begin with, we consider the simpler free energy density $F_0 = K + W$. The Euler–Lagrange equations for a minimum value of $\int F_0\,\mathrm{d}z$ are

$$\kappa\,\mathrm{d}^2\xi_1/\mathrm{d}z^2 - \partial W/\partial\xi_1 = 0\,, \tag{6}$$

$$\kappa\,\mathrm{d}^2\xi_2/\mathrm{d}z^2 - \partial W/\partial\xi_2 = 0\,. \tag{7}$$

The minimum obviously corresponds to a uniform

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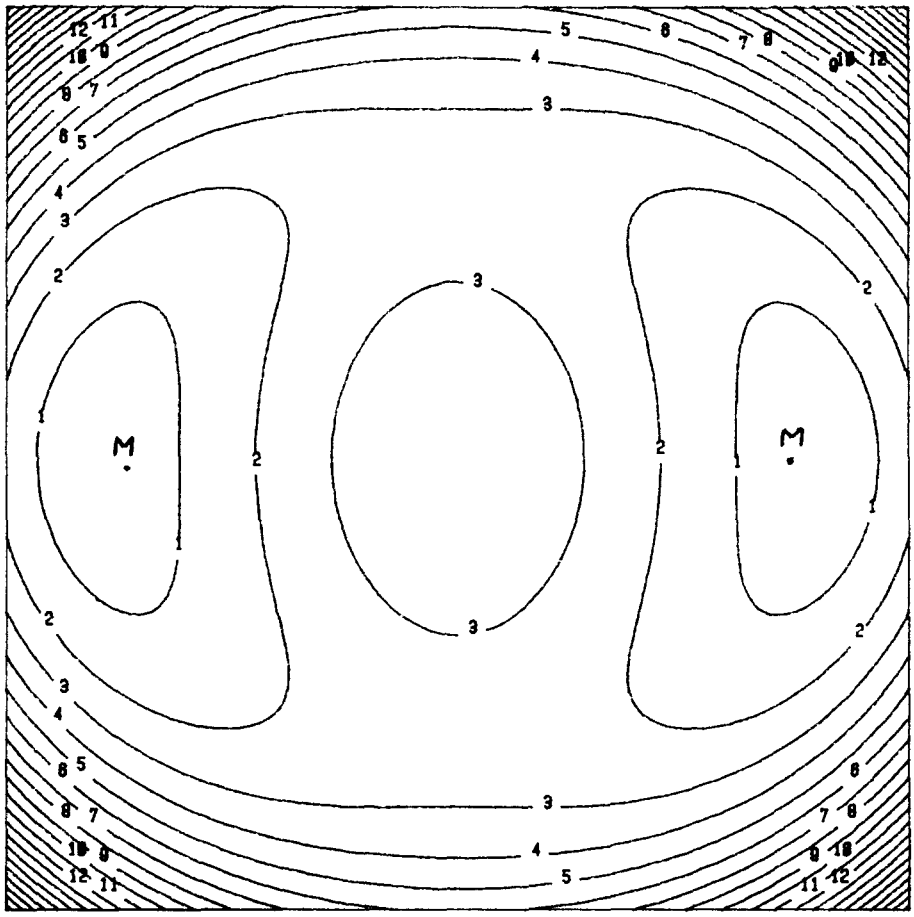

Fig. 1. Contour lines of potential function W of (5) for $a = -1.5$, $\chi H^2 = 1.0$, $b = 1.0$. The contour lines are drawn at intervals of 0.478, line 1 corresponding to the value -1.323.

solution, $d\xi_1/dz = d\xi_2/dz = 0$ and minimum W. Typical contour lines of W as given in (5) are shown in fig. 1; minimum W is at the points M on the x axis. If (ξ_1, ξ_2) departs at some point from its equilibrium value (ξ_1^0, ξ_2^0), say $(\xi_1, \xi_2) = (\xi_1^0 + \delta\xi_1, \xi_2^0 + \delta\xi_2)$, then it is seen from (6) and (7) that the z dependence of the fluctuations is

$$\delta\xi_1 \sim \exp(-\alpha_x |z|), \quad \delta\xi_2 \sim \exp(-\alpha_y |z|), \tag{8}$$

where α_x and α_y are real because (ξ_1^0, ξ_2^0) is a minimum of W. Positive signs of α_x, α_y are taken to ensure boundedness of $(\delta\xi_1, \delta\xi_2)$. Specifically, for (5)

$$\alpha_x^2 = -2(a - \chi H^2)/\kappa, \tag{9}$$

$$\alpha_y^2 = \chi H^2/\kappa. \tag{10}$$

We now define an analogy with the mechanics of a particle moving in two dimensions by putting $z \equiv t$, the time, and $(\xi_1, \xi_2) \equiv (x, y)$, the particle position. Clearly K becomes the kinetic energy. However, in order to write F_0 as a langrangian $L_0 = K - V$, we must put $W = -V$. Now in mechanics the stable equilibria are points of minimum V, and if the system is perturbed from equilibrium the ensuing motion is an oscillation:

$$\delta x \sim \exp(-i\omega_x t), \quad \delta y \sim \exp(-i\omega_y t). \tag{11}$$

Thus the analogy is not straightforward. Points that are "Landau-stable", minima of W, are maxima of V, and therefore "mechanically unstable". The different definitions of stability are reflected in the different

ways in which fluctuations behave, (8) and (11).

We now return to the full free energy density F including the Lifshitz invariant. The Euler–Lagrange equations are

$$\kappa(\mathrm{d}^2\boldsymbol{\xi}/\mathrm{d}z^2 + 2\boldsymbol{\Omega}\times \mathrm{d}\boldsymbol{\xi}/\mathrm{d}z) - \mathrm{grad}\ W = 0\,, \tag{12}$$

where

$$\boldsymbol{\Omega} = (0, 0, \Lambda/\kappa)\,, \tag{13}$$

The term in $\boldsymbol{\Omega}$ has the form of a Coriolis force, although it will be noticed that there is no centrifugal term. This is simply included by rewriting (12):

$$\kappa[\mathrm{d}^2\boldsymbol{\xi}/\mathrm{d}z^2 + 2\boldsymbol{\Omega}\times \mathrm{d}\boldsymbol{\xi}/\mathrm{d}z + \boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{\xi})] - \mathrm{grad}\ W_1 = 0\,, \tag{14}$$

where

$$W_1 = W + \tfrac{1}{2}\Omega^2\xi^2\,. \tag{15}$$

The energy integral derived from (11) is

$$\tfrac{1}{2}\kappa[(\mathrm{d}\xi_1/\mathrm{d}z)^2 + (\mathrm{d}\xi_2/\mathrm{d}z)^2] - W = E\,. \tag{16}$$

It is seen from (14) that the mechanical analogy is the motion of a particle in the x–y plane in which the potential $V_1 = -W_1$ is rotated with angular velocity Ω about the z axis. However, the particle trajectory must be such as to minimise F rather than a mechanical lagrangian. We conjecture that a "Landau-stable" trajectory is one in which perturbations relax as in (8), whereas a "mechanically-stable" trajectory is one in which perturbations oscillate as in (11). This has important implications for attempts at numerical integration of the Euler–Lagrange equations. A mechanically stable trajectory is also numerically stable, since a small error in an integration step leads to small oscillations about the true solution. However, a Landau-stable trajectory is not numerically stable. A small error may result in pick up of a diverging solution, $\exp(+\alpha_x|z|)$ rather than the $\exp(-\alpha_x|z|)$ of (8), with the result that the trajectory veers right away from the required solution. In other words, the Euler–Lagrange equations are very stiff along a Landau trajectory. This has been found to be the case in practice [3], and our point in that the stiffness is intrinsic to the problem.

It is helpful to consider the commensurate–incommensurate or the C–C* transition as induced by an increase in Ω. For $\Omega = 0$ $\boldsymbol{\xi}$ is at one of the points M of fig. 1, which as we pointed out is a minimum of W but a maximum of the mechanical potential V. For non-zero Ω, the potential is rotating about the z axis. For sufficiently small Ω the point representing the system travels round at M with the potential: the C phase persists. For larger Ω the system point moves round the potential surface, this being the C* phase. Since M is a maximum of V, the mechanical and therefore numerical instability of the trajectory is evident from this description.

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