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HAMILTONIAN DYNAMICS OF THE LANDAU MODEL OF FERROELECTRIC LIQUID CRYSTALS - I

by

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- Abstract

We present a Hamiltonian treatment of the Landau theory of phase transitions. In this formulation we are based on the analogy between the order parameter space and the ordinary coordinate space of a particle moving in two dimensions. As an application, we consider the ferroelectric smectic liquid crystals.

Key-words: Ginzburg-Landau theory; Ferroelectric liquid crystals; Hamiltonian Dynamics; Poincaré section.

1) Alternative Formulation

Recently some authors [1,2] have discussed analogies between the Landau theory of Phase Transitions and Lagrangian mechanics. We aim at to developing those ideas using a Hamiltonian formulation in this work. At first, we construct an alternative dynamical theory which allows to study the "time" evolution of the order parameter components in the Landau theory. For this we correlate, at the beginning, the usual configuration space $(q_1,q_2,...,q_m)$, with the one of the order parameter components $(n_1,n_2,...,n_m)$. We can write the Hamiltonian density $\mathcal{H}$ in terms of the free energy density F as

$$\mathcal{H} = \dot{n}_i\, p_i - F \quad . \tag{1}$$

Where p_i is the canonical momentum conjugated to n_i. We have employed in (1) and hereafter the summation convention in the repeated indices and p_i are the canonical momenta.

The Hamilton's equations for the order parameters take the form

$$\dot{n}_i = \frac{\partial \mathcal{H}}{\partial p_i} \quad ; \quad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial n_i} \tag{2}$$

Sections 2 and 3 present the basic procedures for the analysis of a Hamiltonian system in the Ginzburg-Landau theory.

2) Application of the Poincaré Section in the Ginzburg-Landau Theory

We will study in this work the evolution of order parameter components and the corresponding commensurate and incommensurate frequency regime of the dynamical system, analysing the Poincaré section [3] of the two-dimensional torus embedded in the phase space (n_i, p_i).

As we have already stressed before (see eq.1) the evolution of our dynamical system is described in terms of the free energy density F, considering now the degeneracy parameter N = 2 [2,4]. This thermodynamical potential has been used for the particular case of ferroelectric smectic liquid crystals in the presence of an external magnetic field (H) [5], such that

$$F = C_1 n_x^2 + C_2 n_y^2 + C_3(n_x^2 + n_y^2)^2 + \frac{1}{2}\left[\left(\frac{dn_x}{dz}\right)^2 + \left(\frac{dn_y}{dz}\right)^2\right] \qquad (3)$$

where we define in this case:

$$C_1 = \frac{1}{2}(A - \chi_a H^2) \quad , \quad C_2 = \frac{1}{2}A \quad \text{and} \quad C_3 = \frac{1}{4} \qquad (4)$$

being χ_a the diamagnetic anisotropy; the Landau parameter A is dependent linearly upon temperature; and $n = (n_x, n_y)$ is the molecular director of the pitch and the last part is the elastic term.

This expression (eq.3) can be applied to the three smectic liquid crystal phases A (prototype), C^* and C . These systems have been intensively studied and it is very established that in a smectic C liquid crystal rod-like molecules are arranged in parallel layers, within which they have the character of a two-dimensional liquid. There is a tilt angle θ between the molecular director and the layer normal, being the same within all layers. In the case of chiral molecules (non centro symmetrical), in addition to the smectic C phase there is the chiral smectic C^* phase, whose basic property is that it is modulated in the layer normal direction in the form of a helix [6,7]. This last characteristic arises from the presence of the Lifshitz invariant term (3). So a characteristic potential (Fig. 1) of the system and the Hamiltonian density (1) are

$$W = C_1 n_x^2 + C_2 n_y^2 + C_3 (n_x^2 + n_y^2)^2 \tag{5}$$

$$\mathcal{H} = \frac{1}{2} (p_x^2 + p_y^2) - W \tag{6}$$

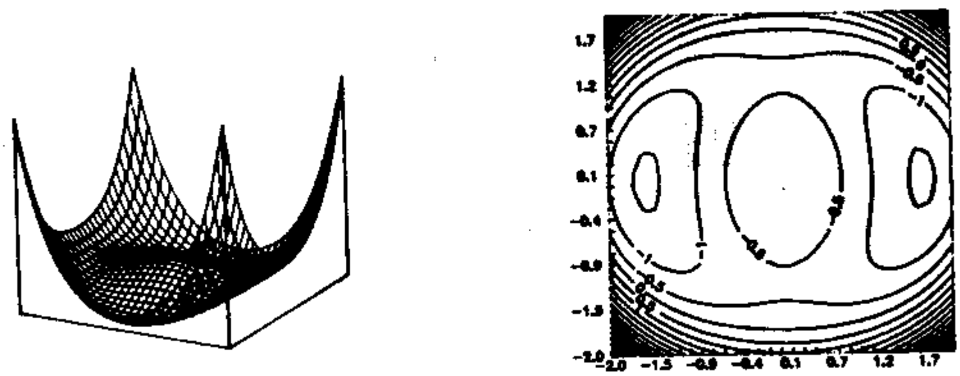

Fig.1 a) A tree dimensional view of the W potencial and b) is a top view of the same potential.

We assume no Lifshitz invariant term in eq.3 in this note. The most general problem which contains this invariant will be studied in the near future. In the present case the equations of motion are:

$$\dot{n}_x = \frac{\partial \mathcal{H}}{\partial p_x} = p_x \qquad (7a)$$

$$\dot{n}_y = \frac{\partial \mathcal{H}}{\partial p_y} = p_y \qquad (7b)$$

$$\dot{p}_x = -\frac{\partial \mathcal{H}}{\partial n_x} = 2C_1\, n_x + 4C_3\, (n_x^2 + n_y^2)\, n_x \qquad (7c)$$

$$\dot{p}_y = -\frac{\partial \mathcal{H}}{\partial n_y} = 2C_2\, n_y + 4C_3\, (n_x^2 + n_y^2)\, n_y \qquad (7d)$$

In this case, despite the phase space be a four-dimensional one, meanwhile it reduces to three dimensions because our system is not dissipative (constant energy). The existence of second conserved quantity implicates in the reduction of the phase space to two-dimensional torus. The determination of the invariant torus has been done from Poincaré section analysis. This section is defined by the intersection points of orbits with the ($n_y = 0$,$p_y >$ 0) -plane.

We have used a numerical algorithm based on the Runge-Kutta method in order to integrate the Hamilton's equation and to construct the Poincaré sections. The analysis of the Poincaré section results enable us in clearly discussing the commensurate frequencies regime from the incommensurate one. In the former case the orbits along the torus are closed such that the Poincaré section presents a finite number of points. In the incommensurate case this section is established by a dense set of points meaning that the orbits are quasiperiodic (see Fig. 2 and 3 of the Poincaré section and Fourier analysis). We have used the KAOS package [8] in order to obtain the figures 2 to 4.

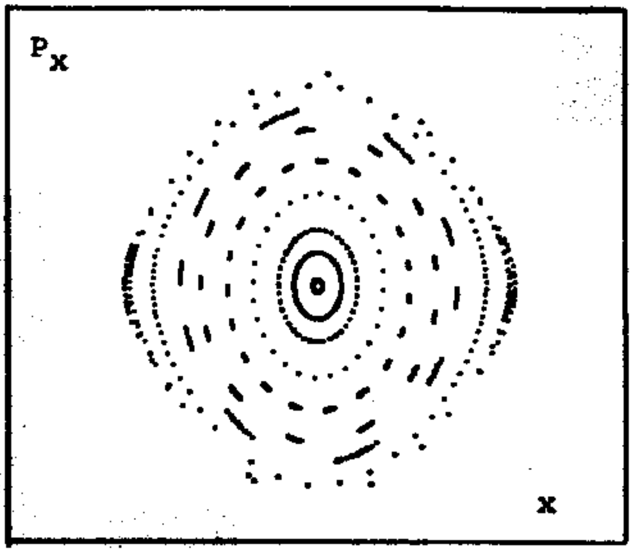

Fig.2 Poincare' section. The used parameters: $C_1 = -1.125$, $C_2 = 0.625$, $C_3 = 0.25$, Energy = 1.333, $X_i = -3.15$, $P_{xi} = 0.18$, $y_i = 0.0$, $P_{yi} = 0.0$

The periodic and quasiperiodic motions will give rise more complex motions (chaotic) when there is not a second constant of integration. The Poincaré section is showed in this case as a set of points that cannot be orderly connected with the evolution of parameter z. A more accurate analysis of these cases will be done in the next note.

The numerical analysis of this problem (see Fig. 2) shows that the order parameter components n_x , n_y and their canonical momenta p_x , p_y are quasi-periodic and the order parameter space frequencies are incommensurable ones (see Fig. 3). This incommensurability arises from the disturbance (one-directional) due to the magnetic field H (see eq.3).

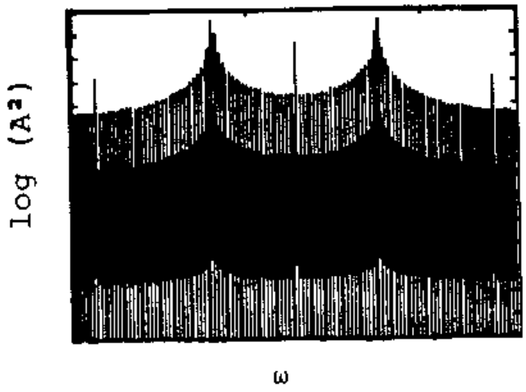

Fig. 3 Power spectral by a Fast Fourier Transform (FFT) with period two. The vertical axis represents logaritm of the sum of the squared Fourier amplitudes (A) of that frequency and the horizontal axis is the frequency ω.

From Landau point of view the prototype phase $n_x = n_y = 0$ corresponds to the smectic A phase. In the second part of this work we can also think in terms of the soliton-like picture. There, we will study the behaviour of the angle $\phi(z)$ between the position vector of the particle and horizontal axis, considering the presence of the Lifshitz term's parameter. In the present case we have the situation where there is no variation of that parameter and in the Ginzburg-Landau theory this situation corresponds to the smectic C phase, where the angle $\phi(z)$ is more-or-less constant for a determined range z.

3) The Trajectory Analysis in the Order Parameter Phase Space

Another important feature of this alternative formulation is that it allows to describe the stability of the system from a simple and general manner within a linear approximation.

The stability notion arises when a system, in the equilibrium position, is softly disturbed. When we look for the formal concept of stability of an orbit, in general we say that the motion is stable if we can understand the time evolution from an interval $[(0,t_o)$ to $(0,\infty)]$. We must to remember that the orbit denoted here are defined within a 2m-dimensional phase space (m = 2). Then a trajectory is stable if for each $\epsilon > 0$ (arbitrarily small) there is $\delta(\epsilon) > 0$ such that

$$| x_o - a | < \delta(\epsilon) \tag{8}$$

and

$$| X(x_o,t_o;t) - X(a,t_o;t) | < \epsilon \quad , \quad \text{for all } \ t \geq t_o$$

The stability analysis of a dynamical system can be treated within a linear approximation, by equation

$$\dot{X} \cong A\, X \tag{9}$$

which in the case of our potential W has the explicit form

$$\begin{pmatrix} \dot{n}_x \\ \dot{n}_y \\ \dot{p}_x \\ \dot{p}_y \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 2C_1 & 0 & 0 & 0 \\ 0 & 2C_2 & 0 & 0 \end{pmatrix} \begin{pmatrix} n_x \\ n_y \\ p_x \\ p_y \end{pmatrix} = \begin{pmatrix} p_x \\ p_y \\ 2C_1 n_x \\ 2C_2 n_y \end{pmatrix} \tag{10}$$

We must find the eigenvalues of the following characteristic equation in this linear approximation

$$\det(\lambda I - A) = \lambda^4 - 2(C_1 + C_2)\lambda^2 + 4C_1C_2 = 0 \qquad (11)$$

Making the change of variable $\bar{\lambda} = \lambda^2$ we have

$$\bar{\lambda}^2 - 2(C_1 + C_2)\bar{\lambda} + 4C_1C_2 = 0 \qquad (12)$$

and the solution is

$$\lambda_1 = + \sqrt{(A-\chi_a H)} = - \lambda_2 \qquad (13)$$

$$\lambda_3 = + \sqrt{A} = - \lambda_4 \qquad (14)$$

In order do make clear this theoretical background we present below some phase space trajectories (see Fig. 4).

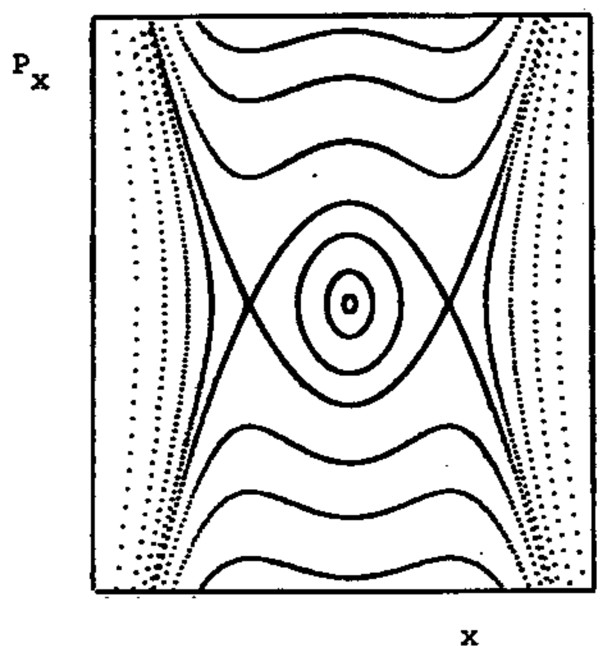

Fig. 4 Represents some trajectories in phase space. We have used the same parameters as in Fig. 2.

In the numerical analysis we have used standard parameters values [2] A = -1.25 and $\chi_a H^2 = 1$. In this case the eigenvalues are pure imaginary numbers and the singularity is called vortex point or centre, because the A - matrix is real.

4) Conclusion

We have developed the first part of the Hamiltonian formalism of the Ginzburg- Landau theory of phase transitions in the case of ferroelectric liquid crystals, considering no contribution of the Lifshitz invariant. In this case the minimum value of the free energy corresponds to a uniform solution, $\frac{dn_x}{dz} = \frac{dn_y}{dz} = 0$ and minimum W. For $A - \chi_a H^2 < 0$ (eqs.4 and 5) W has a relative maximum at the origin, and if we consider n_x-axis, the equilibrium configuration is one of minimum W. Similarly if we consider n_y-axis, we get a saddle point, as sketched in Fig. 1 a,b. Typical contour lines of W are showed in Fig. 1b . In this analogy with the mechanics of a particle moving in two dimensions we have put z ≡ t (time) and $(n_x, n_y) \equiv (x,y)$ is the particle position such that the elastic term in (3) becomes the kinetic energy. However, in order to write the free energy density as a Lagrangian we must put W = -V [1].

From mechanical point of view the stability analogies of this system shows that when the eigenvalues are pure imaginary numbers the singularity is called vortex point or centre . The trajectories in the (n_x, n_y)-plane are ellipses or circles and all orbits are periodic around the λ_1 point (see Fig. 4).

We will present the complete Hamiltonian treatment of the Ginzburg-Landau theory of phase transitions in the next part of this work . In this system we will consider the contribution of the Lifshitz invariant term which favors the smectic C^* phase, as well as the arising of solitons.

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