# Different states of incommensurate phase with solitons of one and two types

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We obtain and investigate two-soliton as well as one-soliton states of a noncommensurate phase the transition to which is described by a two-dimensional irreducible representation that admits of the Lifshitz gauge invariant. The boundaries between the different phases are drawn on the phase diagram. We show that the boundary between the one- and two-soliton states of the incommensurate phase is not a phase-transition line.

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The incommensurate phase observed in crystals, for example in certain ferroelectrics (see Ref. 1), spans as a rule an intermediate temperature region between the usual crystalline phases having high symmetry (initial) and low symmetry (commensurate). The closer the temperature to the point of the transition between the incommensurate and commensurate phases, the more similar the incommensurate and commensurate phases become in structure if the latter contains regular domains.[2,3] In other words, the regions of almost uniform distribution of the order parameter are separated in the incommensurate phase by comparatively narrow transition regions, which will be called here solitons. It is well known, however, that several different commensurate phases can correspond to one multidimensional irreducible representation of the symmetry group of the initial phase of the crystal. Consequently, an incommensurate phase that is adjacent on the phase diagram to different commensurate phases will likewise have near these boundaries different structures close to those of the corresponding commensurate phases. Thus, for example, if the commensurate phase has two types of domain wall, the incommensurate phase can also be expected to have solitons of two types. In this paper, using a two-component order parameter as the example, we investigate the states of an incommensurate phase with solitons of one and two types, and assess the possibility of a phase transition between these states.

We represent the thermodynamic potential in the form

$$\Phi=\int \Phi(x)\,dx\Big/\int dx,$$

$$\Phi(x)=\alpha\rho^2+\beta\rho^4+\alpha'\rho^4\cos 4\varphi+\beta'\rho^8\cos^2 4\varphi-\sigma\rho^2\varphi_x+\delta(\rho_x^2+\rho^2\varphi_x^2), \qquad (1)$$

where $\rho(x)$, $\varphi(x)$ are the polar coordinates of the two-component order parameter $\eta=\rho\cos\varphi$, $\xi=\rho\sin\varphi$, which transforms in accord with the two-dimensional irreducible representation of the symmetry group of the initial phase of the crystal. Account is taken in (1) of two degrees of the isotropic invariant $\rho^2$ and of two degrees of the spatially isotropic components of the order parameter of the invariant $\rho^n\cos n\varphi$ (we consider for the sake of argument the case $n=4$), as well as the Lifshitz gauge invariant[4] $\rho^2\varphi_x$ (the subscript $x$ denotes a derivative with respect to $x$: $\varphi_x=\partial\varphi/\partial x$) and a gauge invariant of higher order. It is assumed that the coefficients $\beta>0$, $\delta>0$.

The phase diagram corresponding to the thermodynamic potential (1) on the $(\alpha,\alpha')$ plane is shown schematically in Fig. 1 for small values of $\alpha'$: $|\alpha'|\ll\beta$ at $\beta'>0$. The numbers 1, 2, and 3 denote the regions where different commensurate phases exist, and 0 denotes the region of the initial phase. The solution for $\rho$ and $\varphi$ in phase 1 is

$$\cos 4\varphi=-1,\quad \rho^2=\frac{-\alpha}{2\beta}(1+\varepsilon-\tau);$$
$$\Phi=-\frac{\alpha^2}{4\beta}\left[1+\varepsilon-\frac{\tau}{2}+(\varepsilon-\tau)^2\right], \qquad (2)$$

where we have introduced for brevity the dimensionless parameters

$$\varepsilon=\alpha'/\beta,\quad \tau=\beta'\alpha^2/2\beta^3. \qquad (3)$$

We used in (2) an expansion in the parameters (3), which are assumed to be small: $\varepsilon\ll 1$, $\tau\ll 1$ (weak-anisotropy approximation). The solution in phase 2 differs from Eq. (2) in that the signs of $\alpha'$ and $\cos 4\varphi$ are reversed. The solution for $\rho$ and $\varphi$ in phase 3 is

$$\cos 4\varphi=-\varepsilon/\tau,\quad \rho^2=-\alpha/2\beta;$$
$$\Phi=-\frac{\alpha^2}{4\beta}\left(1+\frac{\varepsilon^2}{2\tau}\right). \qquad (4)$$

The boundary between phases 1 and 3 is a second-order phase transition line (see Ref. 5 for details)

$$\varepsilon=\tau \qquad (5)$$

(the boundary between phases 2 and 3 is the line $\varepsilon=-\tau$). Phase 3 is stable if $\beta'>0$. The case $\beta'<0$ will be considered below.

The solutions for $\rho$ and $\varphi$ in the incommensurate phase will be sought in the approximation with constant amplitude $\rho_x=0$ (Ref. 2). Varying the thermodynamic

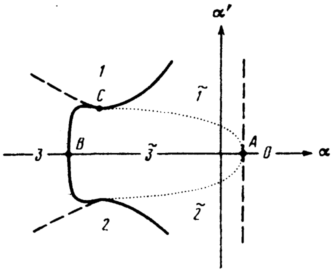

FIG. 1. Phase diagram on the $(\alpha,\alpha')$ plane, corresponding to the thermodynamic potential (1) at $\beta'>1$. Dashed lines—second-order phase transition lines.

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potential (1) with respect to $\varphi$ we obtain

$$\delta\varphi_{xx}+2\alpha'\rho^2\sin 4\varphi+2\beta'\rho^8\sin 8\varphi=0. \tag{6}$$

Multiplication by $\varphi_x$ and integration reduce this equation to a first-order equation that can be solved by separating the variables. The result is an elliptic integral

$$x=\frac{\sqrt{\delta}}{4}\int\frac{du}{[(1-u^2)(c_1+\alpha'\rho^2u+\beta'\rho^8u^2)]^{1/2}}+c_2, \tag{7}$$

where $u=\cos 4\varphi$, and $c_1$ and $c_2$ are integration constants. We consider those solutions (7) for which $\varphi$ increases (or decreases) monotonically with increasing $x$, as near the point of the transition between the initial and incommensurate phases. This excludes from consideration "oscillatory" solutions for $\varphi$. There exist three solutions of this type, which we designate $\tilde{1}$, $\tilde{2}$, and $\tilde{3}$.

The function $u(x)$ can be obtained from (7) by reducing in standard fashion the elliptic integral (7) to normal form and using Jacobi elliptic functions. Replacing $c_1$ by a new constant $l$ and choosing the value of $c_2$, which depends on the choice of the null point of $x$, we can represent solution $\tilde{1}$ in the form

$$\cos 4\varphi=\frac{\operatorname{cn}(z,k)-l\operatorname{dn}(z,k)}{\operatorname{dn}(z,k)-l\operatorname{cn}(z,k)},$$
$$z=4qx,\quad q^2=\frac{\alpha'\rho^2}{2\delta l}(1-l\gamma),\quad k^2=l\frac{l-\gamma}{1-l\gamma}, \tag{8}$$

where $k$ is the modulus of the Jacobi elliptic functions. Here and elsewhere we use the notation

$$\gamma=\frac{2\beta'\rho^6}{\alpha'},\quad \alpha_0=\frac{\sigma^2}{4\delta},\quad \varepsilon_0=\frac{2}{\beta}(\beta'\alpha_0^2)^{1/3}. \tag{9}$$

The solution (8) exists if $\alpha'>0$ and $\gamma\leqslant l\leqslant 1$. The solution $\tilde{2}$ differs from (8) in that the signs of $\alpha'$ and $\cos 4\varphi$ are reversed.

The solution $\tilde{3}$ is given by

$$\cos 4\varphi=\frac{\operatorname{cn}(z,k)-l}{1-l\operatorname{cn}(z,k)},\quad z=4qx,\quad q^2=\frac{\alpha'\rho^2}{2\delta l}(1-l^2),\quad k^2=l\frac{\gamma-l}{1-l^2}. \tag{10}$$

It exists in the interval $|l|\leqslant\min(|\gamma|,\ 1/|\gamma|)$, and the sign of $l$ must be the same as the sign of $\alpha'$.

The solutions obtained contain the arbitrary parameter $l$ (or the uniquely related quantity $k$), as well as the quantity $\rho$, which by virtue of the employed approximation $\rho_x=0$ can also be regarded as a parameter. It is natural to determine these parameters[6] from the minimum condition for the thermodynamic potential (1), in which the solution for $\varphi$, (8) or (10), is substituted and integration is carried out with respect to $x$. The results of this calculation are relegated to the Appendix. We present here only the main consequences concerning the phase diagram (see Fig. 1). The boundary between solutions 1 and 3, i.e., (8) and (10), is defined by the equation

$$\frac{\alpha}{\alpha_0}=\left[1-\left(\frac{\varepsilon}{\varepsilon_0}\right)^6\right]^{1/2}-\frac{4}{\varepsilon_0}\left(\frac{\varepsilon}{\varepsilon_0}\right)^2 \tag{11}$$

(shown dotted in Fig. 1). On this boundary $k=0$, hence

$$\cos 4\varphi=\frac{\cos z-l}{1-l\cos z},\quad q^2=\frac{\alpha_0}{\delta}(1-l^2),\quad l=\gamma=\left(\frac{\varepsilon}{\varepsilon_0}\right)^3. \tag{12}$$

The parameter $l$ runs through values from $l=0$ at the point $A$ to $l=1$ at the point $C$. The coordinates of these points are $\alpha=\alpha_0$, $\alpha'=0$ for $A$ and $\alpha=-4\alpha_0/\varepsilon_0$, $\alpha'=\beta\varepsilon_0$ for $C$.

The equations for the boundaries of the existence of the incommensurate phase are determined from the condition $k=1$. For the solution $\tilde{1}$ [Eq. (8)] the boundary takes the parametric form

$$\frac{\alpha}{\alpha_0}=-\frac{4}{\varepsilon_0}\left(\frac{\pi\sin^2\theta}{2\theta+\sin 2\theta}\right)^{2/3}+\left(\frac{\pi\sin 2\theta}{2\theta+\sin 2\theta}\right)^2,$$
$$\frac{\varepsilon}{\varepsilon_0}=\left(\frac{\pi\sin^{1/2}\theta}{2\theta+\sin 2\theta}\right)^{4/3}, \tag{13}$$

where $\theta$ ranges from 0 to $\pi/2$ at the point $C$. For solution $\tilde{3}$ [Eq. (10) we have correspondingly

$$\frac{\alpha}{\alpha_0}=-\frac{4}{\varepsilon_0}\left(\frac{\pi/2}{\cos\theta+\theta\sin\theta}\right)^{2/3},$$
$$\frac{\varepsilon}{\varepsilon_0}=\sin\theta\left(\frac{\pi/2}{\cos\theta+\theta\sin\theta}\right)^{4/3} \tag{14}$$

with $\theta$ ranging from $\pi/2$ at point $C$ to 0 at point $B$ (see Fig. 1).

We note that Eqs. (A.1) to (A.5) describe the transitions $\tilde{1}$–1 and $\tilde{3}$–3 as first-order phase transitions. Actually, the values $k'=(1-k^2)^{1/2}$ corresponding to the condition for the loss of stability ($\Phi_{\rho\rho}\Phi_{ll}-\Phi_{\rho l}^2=0$) of the incommensurate solution (8) or (10) and to the condition that the thermodynamic potential be equal for solutions (8) and (2) or for (10) and (4) differ from the value $k'=0$ corresponding to the condition that the incommensurate solution vanish (the character of the dependence of $\Phi$ on $\alpha$ or $\alpha'$ in the vicinity of the transitions $\tilde{1}$–1 and $\tilde{3}$–3 is similar to that considered in Ref. 6). However, these differences of the values of $k'$ are exponentially small relative to $\varepsilon$ and $\varepsilon_0$ (3) and are therefore outside the scope of the employed constant-amplitude approximation $\rho_x=0$. This approximation is valid when the anisotropy in the space of the components of the order parameter is small: $\varepsilon\ll 1$, $\varepsilon_0\ll 1$. The solutions for $\rho$ and $\varphi$ are then valid only accurate to the first term of the expansion in powers of $\varepsilon$ and $\varepsilon_0$ (for details see Ref. 7). Therefore Fig. 1 does not show details that exceed the inaccuracies of the employed approximation. Thus, for example, the lines defined by Eqs. (11) and (13) likewise intersect at a point whose coordinates differ from those of $C$ by terms of higher order in $\varepsilon_0$.

The boundary between the initial and incommensurate phases is given by

$$\alpha=\alpha_0 \tag{15}$$

and is a second-order phase-transition line. On this boundary $k=l=0$.

Let us explain the differences between the incommensurate-phase structures corresponding to the solution $\tilde{1}$ (8) and the solution $\tilde{3}$ (10). Figure 2 shows schematically the function $\cos 4\varphi(x)$ for these solutions near the $\tilde{1}$–1 and $\tilde{3}$–3 phase-transition lines, when $k$ is close to unity. In this case the period $K/q$ of the function $\cos 4\varphi$ is large and the structure of the incommensurate phase is similar to that of the corresponding commensurate phase if the latter contains regular domains. For the solution (8) we have $\cos 4\varphi=-1$ [cf. Eq. (2)], and the transition regions (at $qx/K=0$, ±1, ±2, ...) are solitons

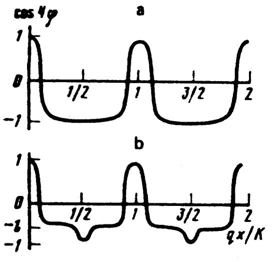

FIG. 2. Plots of $\cos 4\varphi$ vs $x$ near the boundaries $\tilde{1}-1$ (a) for the solution (8) and $\tilde{3}-3$ (b) for the solution (10).

of one type, i.e., the state $\tilde{1}$ (as well as $\tilde{2}$) of the incommensurate phase is one soliton. For the solution (10) we have inside the domains $\cos 4\varphi = -l = -\varepsilon/\tau$ [cf. (4)], and transition regions exist—solitons of two types (at $qx/K = \pm 1, \pm 2, \ldots$ and at $qx/K = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$), i.e., the state 3 of the incommensurate phase is two-soliton. The difference between states $\tilde{1}$ and $\tilde{3}$ of the incommensurate phase corresponds to the difference between the domain structures of the commensurate phases 1 (four domains of the same type) and 3 (eight domains of two different types).

The boundary between the two states of the incommensurate phase is the line (11), which is shown by analysis not to be a phase boundary. Indeed, any derivative of the thermodynamic potential with respect to $\alpha$ or $\alpha'$ is continuous on this boundary. The point is that the value $k^2 = 0$, which determines the boundary between the solutions $\tilde{1}$ and $\tilde{3}$, is not singular for elliptic functions and integrals, which remain real also at $k^2 < 0$, i.e., at pure imaginary $k$ (we note that all the equations contain $k^2$ and not $k$). The transformation $k^2 \to -k^2$ (i.e., $k \to ik$) permits a change from Eqs. (8), (A.1), and (A.3) to Eqs. (10), (A.4) and (A.5) and conversely, i.e., the functions contained in them are in essence different representations of the same analytic functions of $k^2$.

The transition from the one-soliton to the two-soliton state is thus continuous, similar to the transcritical gas-to-liquid transition. The anomalies of the heat capacity and of other quantities, which exist on the line (5) that determines the 1–3 phase boundary, become smoothed out on going through the point $C$ (see Fig. 1). We emphasize also that the solutions $\tilde{1}$ and $\tilde{3}$, as is seen in particular from Fig. 2 [see also Eq. (12)] have equal periods, i.e., with respect to the translational and hence also the total symmetry the solutions $\tilde{1}$ and $\tilde{3}$ correspond to the same phase.

We consider now briefly the case $\beta' < 0$. Strictly speaking, for the thermodynamic potential to be bounded as $\rho \to \infty$ it is necessary to add $\Phi(x)$ (1), for example, a term $\beta'' \rho^8$, assuming $\beta' + \beta'' > 0$, but this term is of no significance for the results that follow. If $\beta' < 0$, the solution 3 is unstable. The phase transition 1–2 is of first order and takes place on the line $\alpha' = 0$, while the line (5) is the stability boundary of phase 2.

The commensurate phase has no solution $\tilde{3}$, only the solutions $\tilde{1}$ [which is of the same form as (8)] and $\tilde{2}$. Equations (A.1)–(A.3) remain valid. Now, however, $k^2 > l^2$, and this leads to a different behavior of the elliptic integral $\pi$ of the third kind (A.1), especially as $k \to 1$. The equation for the $\tilde{1}-1$ boundary therefore does not coincide with (13), but takes the form

$$\frac{\alpha}{\alpha_0} = -\frac{4}{\varepsilon_0}\left(\frac{\pi\,\mathrm{sh}^2 z}{2z+\mathrm{sh}\,2z}\right)^{4/3} + \left(\frac{\pi\,\mathrm{sh}\,2z}{2z+\mathrm{sh}\,2z}\right)^2,$$
$$\frac{\varepsilon}{\varepsilon_0} = \left(\frac{\pi\,\mathrm{sh}^{1/2} z}{2z+\mathrm{sh}\,2z}\right)^{4/3}, \tag{16}$$

where $z$ runs through values from 0 to $\infty$ at a triple point with coordinates

$$\alpha = -(4\alpha_0/\varepsilon_0)\pi^{2/3} + \pi^2, \quad \alpha' = 0.$$

The boundary $\alpha' = 0$ between the two incommensurate solutions $\tilde{1}$ and $\tilde{2}$ is shown by investigation not to be a phase-transition line. With increasing $\alpha$, on going through the triple point, the hysteresis vanishes and all the anomalies become smoothed out. We note that the absence of a phase-transition line between the incommensurate states $\tilde{1}$ and $\tilde{2}$ agrees with the Gibbs phase rule, since three phase-transition lines converge already at the triple point.

## APPENDIX

After substituting (8) in (1) and integrating with respect to $x$ we obtain for the solution $\tilde{1}$

$$\Phi = \alpha\rho^2 + \beta\rho^4 - \frac{l}{2}\alpha'\rho^4 - \frac{1-l\gamma}{2lK}\alpha'\rho^4[(3-2k^2)K - 2E$$
$$-2(1-k^2)\Pi] - \frac{\pi}{K}\left[\frac{1-l\gamma}{2l}\alpha_0\alpha'\rho^6\right]^{1/2}, \tag{A.1}$$
$$\Pi = \Pi(-l^2),$$

where $K$, $E$, and $\pi$ are complete elliptic integrals of first, second, and third kind, respectively, with modulus $k$, and

$$\Pi(n) = \int_0^{\pi/2} \frac{d\theta}{(1+n\sin^2\theta)(1-k^2\sin^2\theta)^{1/2}}. \tag{A.2}$$

From the conditions $\partial\Phi/\partial\rho = 0$, $\partial\Phi/\partial l = 0$ for $\Phi$ (A.1) we obtain

$$\alpha + 2\beta\rho^2 - \frac{\alpha'\rho^2}{2lK}[(3-4l\gamma+l^2)K - 3(1-l\gamma)E + (1-l^2)\Pi] = 0, \tag{A.3}$$
$$E + (1-k^2)(\Pi - K) - \pi\left[\frac{l(1-k^2)}{2(1-l^2)}\frac{\alpha_0}{\alpha'\rho^2}\right]^{1/2} = 0, \quad \Pi = \Pi(-l^2).$$

These equations determine $\rho$ and $l$ for given values of the constants of the thermodynamic potential (1).

For the solution $\tilde{3}$ we obtain similarly

$$\Phi = \alpha\rho^2 + \beta\rho^4 - \frac{\alpha'\rho^4}{2lK}[(3+l\gamma-l^2)K + 2(1-l^2)E$$
$$-2\Pi] - \frac{\pi}{K}\left[\frac{1-l^2}{2l}\alpha_0\alpha'\rho^6\right]^{1/2}, \quad \Pi = \Pi\left(\frac{l^2}{1-l^2}\right) \tag{A.4}$$

and from the conditions $\partial\Phi/\partial\rho = 0$, $\partial\Phi/\partial l = 0$ we get

$$\alpha + 2\beta\rho^2 - \frac{\alpha'\rho^2}{2lK}[(3-4l\gamma+l^2)K - 3(1-l^2)E + \Pi] = 0,$$
$$\Pi + (1-l^2)(E-K) - \pi\left[\frac{l(1-l^2)}{2}\frac{\alpha_0}{\alpha'\rho^2}\right]^{1/2} = 0, \quad \Pi = \Pi\left(\frac{l^2}{1-l^2}\right). \tag{A.5}$$

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