An exact solution to the equations of the phenomenological theory of the incommensurate phase

V. A. Golovko

Moscow Metallurgical Evening Institute

(Submitted 31 January 1984)
Zh. Eksp. Teor. Fiz. **87**, 1092–1101 (September 1984)

An exact solution to the differential equations for the components of the order parameter describing the incommensurate phase is obtained. This solution corresponds to the equilibrium state of the incommensurate phase on a certain curve lying in the plane of the thermodynamic parameters between the critical point of the transition from the initial phase and the critical point of the transition into the commensurate phase, the latter transition in the case under consideration being a second-order transition. It is shown that the specific heat of the incommensurate phase diverges as this phase transition is approached. The solution found is valid for those values of the coefficients of the thermodynamic potential for which the approximate methods normally used to solve the equations are unsuitable. In a special case this solution allows the investigation of the incommensurate phase in the vicinity of the triple point, where the incommensurate, commensurate, and initial phases coexist. At this point the incommensurate phase is degenerate.

The phenomenological theory of the incommensurate phase, based on the Landau theory of phase transitions (see, for example, Refs. 1 and 2) leads to a system of nonlinear differential equations for the components of the order parameter. Because of the complexity of this system, its solution requires the use of approximate methods. The greatest difficulties are encountered in the investigation of the incommensurate phase in the vicinity of the critical temperature $T = T_c$ of the phase transition into the commensurate (low-temperature) phase (*a* transition which possesses a number of distinctive features), and here the "constant amplitude" approximation or its modification is often used, but the various methods of finding this amplitude give different answers to the question of the order of the phase transition in question.[1,3,4] Furthermore, the indicated approximation is valid only in the case of weak anisotropy in the space of the order-parameter components,[5] i.e., in the case when the coefficient β_2 is small (see below). If, on the other hand, this anisotropy is not weak, then we do not have any analytic methods for solving the indicated equations. The analysis can be carried out[6,7] only in the vicinity of the triple point, where the incommensurate, commensurate, and initial (symmetric) phases adjoin in the phase diagram,[1)] and where, according to Sannikov[6] and Jacobs and Walker,[7] the incommensurate-commensurate phase transition is a first-order transition, although a number of authors[9–12] hold a different opinion about the order of the transition. Notice that in many papers the conclusions are drawn on the basis of numerical computations, whereas in the region of the incommensurate-commensurate phase transition the use of numerical methods to solve the equations requires the exercise of care.[13] It can be seen from the foregoing that it is of interest, having rejected the approximate methods, to try to obtain exact solutions to the equations in question, even if for particular cases, to which the present paper is devoted.

Let us consider the case of a two-component order parameter with components η and ξ that transform according to that two-dimensional irreducible representation of the symmetry group of the initial phase which admits of the Lifshitz gradient invariant. Let us denote the axis along which the incommensurability arises by x, and assume that the linear thermodynamic-potential density along x has the form

$$\bar{\Phi}(x)=\frac{\alpha}{2}(\eta^2+\xi^2)+\frac{\beta_1'}{4}(\eta^2+\xi^2)^2+\frac{\beta_2}{2}(\eta^2-\xi^2)^2$$
$$+\frac{\gamma}{6}(\eta^2+\xi^2)^3+\sigma\left(\frac{d\eta}{dx}\xi-\eta\frac{d\xi}{dx}\right)+\frac{\delta}{2}\left[\left(\frac{d\eta}{dx}\right)^2+\left(\frac{d\xi}{dx}\right)^2\right].$$

Here, besides the second-order invariant, we have taken into account two fourth-order invariants, a sixth-order invariant, as well as the Lifshitz invariant, with coefficient σ, and an invariant quadratic in the derivatives. Such a thermodynamic-potential density, with its fairly general form, is widely used in theoretical papers on incommensurate phases.[2,4,6,9] It is used, in particular, to describe the phase transitions in ferroelectric crystals: ammonium fluoroberyllate,[2] ammonium Rochelle salt and rubidium trihydroselenite,[14] in which the incommensurate phase has been experimentally observed.[15–18]

Let us write down the thermodynamic potential per unit length:

$$\Phi=\frac{1}{d}\int_0^d\bar{\Phi}\,dx, \tag{1}$$

where d is the period of the density $\bar{\Phi}(x)$. Going over to the polar coordinates ρ and φ in the space of the order-parameter components ($\eta=\rho\cos\varphi$, $\xi=\rho\sin\varphi$), we obtain for the thermodynamic-potential density the expression

0038-5646/84/090624-06$04.00

$$\Phi=\frac{\alpha}{2}\rho^2+\frac{\beta_1}{4}\rho^4+\frac{\gamma}{6}\rho^6+\frac{\beta_2}{4}\rho^4\cos 4\varphi-\sigma\rho^2\frac{d\varphi}{dx}+\frac{\delta}{2}\left[\left(\frac{d\rho}{dx}\right)^2+\rho^2\left(\frac{d\varphi}{dx}\right)^2\right],\tag{2}$$

where $\beta_1=\beta'_1+\beta_2$. For Φ to be bounded from below, we must assume that $\gamma>0$ and $\delta>0$; furthermore, we assume, for simplicity, that $\beta_2>0$, since the sign in front of the coefficient β_2 can be changed with the aid of the substitution $\varphi\to\varphi+\pi/4$. The minimization of Φ with respect to ρ and φ yields the system of equations discussed in the introductory part of the present paper:

$$\delta\frac{d^2\rho}{dx^2}-\delta\rho\left(\frac{d\varphi}{dx}\right)^2+2\sigma\rho\frac{d\varphi}{dx}-\alpha\rho-\beta_1\rho^3-\gamma\rho^5-\beta_2\rho^3\cos 4\varphi=0,\tag{3}$$

$$\delta\rho\frac{d^2\varphi}{dx^2}+2\delta\frac{d\rho}{dx}\frac{d\varphi}{dx}-2\sigma\frac{d\rho}{dx}+\beta_2\rho^3\sin 4\varphi=0.\tag{4}$$

Arguments adduced in the Appendix show that this system possesses the solution

$$\begin{gathered}\rho^2=8\alpha_0k^2c(\beta_1+\beta_2c)\{(\beta_1-3\beta_2c)^2(2-k^2+k^2c)^{1/2}\\ \times[(2-k^2+k^2c)^{1/2}+\sqrt{2}\operatorname{dn}2q(x-x_0)]\}^{-1},\\ \varphi=\frac{1}{2}\operatorname{am}[2q(x-x_0)],\qquad q=\frac{q_0(\beta_1+\beta_2c)}{3\beta_2c-\beta_1}\left(\frac{2}{2-k^2+k^2c}\right)^{1/2},\end{gathered}\tag{5}$$

where $\alpha_0=\sigma^2/\delta$, $q_0=\sigma/\delta$, and $\operatorname{dn}z$ and $\operatorname{am}z$ are the Jacobi elliptic functions with modulus k, and the quantities c and k are found from the equations

$$3(1-c^2)(\beta_1-3\beta_2c)^2=64\alpha_0\gamma c^2,\tag{6}$$

$$\begin{aligned}k^2=2[&\alpha(\beta_1-3\beta_2c)^2+\alpha_0(\beta_1+\beta_2c)(3\beta_1-5\beta_2c)]\\ &\times\{\alpha(1-c)(\beta_1-3\beta_2c)^2\\ &+\alpha_0(\beta_1+\beta_2c)[\beta_1(3-5c)-\beta_2c(5-3c)]\}^{-1}.\end{aligned}\tag{7}$$

The signs in front of the radicals in (5) have been chosen such that the functions $\rho(x)$ and $\varphi(x)$ are real and bounded at any x; for $\rho(x)$ and $\varphi(x)$ to have these properties the following inequalities should also be satisfied:

$$-1\leqslant c\leqslant 1,\quad k^2\leqslant 1,\quad (\beta_1+\beta_2c)ck^2\geqslant 0.\tag{8}$$

The period of the function $\rho(x)$ is equal to $d=K(k)/q$, where $K(k)$ is the complete elliptic integral of the first kind with modulus k.

Naturally, the expressions (5) are not the general solution to the system of equations (3) and (4), since they do not contain arbitrary constants besides the trivial constant x_0. These expressions guarantee the minimality of Φ, (1), only with respect to functions with a definite period d, and functions with other d values can give smaller values of Φ [of the various solutions to the system (3) and (4) we consider here only those for which $\rho(x)$ and $d\varphi/dx$ are periodic]. Let us find the condition under which Φ attains its minimum value when we substitute into (1) solutions [to the system (3) and (4)] with different d. Computing the d derivative of (1) with the aid of the well-known formulas of variational calculus,[2)] and equating it to zero, we obtain the sought condition

$$\frac{\delta}{2}\left[\left(\frac{d\rho}{dx}\right)^2+\rho^2\left(\frac{d\varphi}{dx}\right)^2\right]-\frac{\alpha}{2}\rho^2-\frac{\beta_1}{4}\rho^4-\frac{\gamma}{6}\rho^6-\frac{\beta_2}{4}\rho^4\cos 4\varphi=-\Phi.\tag{9}$$

Notice that the left-hand side here does not depend on x, since it is in fact the "energy" integral.[19] If the expressions (5) satisfy the equation (9), then they give the equilibrium values of ρ and φ (provided, of course, that it is the absolute minimum of Φ that is realized, and not a maximum or a relative minimum).

If we substitute the expressions (5) into the left-hand side of (9), and take (6) and (7) into account, then we can reduce the relation (9) to the form

$$\Phi=-\frac{8\alpha_0{}^2k^2c(\beta_1-\beta_2c)(\beta_1+\beta_2c)^2}{(2-k^2+k^2c)(\beta_1-3\beta_2c)^4}.\tag{10}$$

Let us now compute Φ in accordance with (1) and (2). It is convenient to first integrate the $\delta(d\rho/dx)^2/2$ term in (2) by parts and, using Eq. (3), eliminate the derivatives:

$$\Phi=-\frac{1}{d}\int_0^d\left(\frac{\beta_1}{4}\rho^4+\frac{\gamma}{3}\rho^6+\frac{\beta_2}{4}\rho^4\cos 4\varphi\right)dx.\tag{11}$$

The substitution of the expressions (5) into (11) gives rise to elliptic integrals. Let us omit the intermediate, rather tedious calculations and give the final result, obtained after the substitution of the computer Φ value into (10):

$$\begin{aligned}\beta_2/\beta_1=[&(4-2k^2+3k^2c-k^2c^3)\Pi-2(2-c)(1+c)K+2c(1-c)E]\\ &\times\{c[(4-2k^2+k^2c-8c^2+4k^2c^2-3k^2c^3)\Pi-2(2-3c)\\ &\times(1+c)K-2c(1-c)E]\}^{-1},\\ \Pi=\Pi&[{}^1/{}_2k^2(c-1),k],\end{aligned}\tag{12}$$

where $E(k)$ and $\Pi(n,k)$ are respectively the complete elliptic integrals of the second and third kinds, $\Pi(n,k)$ being defined here as in Ref. 20 (one must, when using the formulas of Ref. 21, take account of the fact that $n=-\alpha^2$).

The expressions (6), (7), and (12) are three equations for the two unknowns c and k, and can be satisfied only when a certain relation exists between the coefficients of the thermodynamic potential (2). Therefore, the solution (5) corresponds to the equilibrium state of the incommensurate phase at points located on a certain curve in the phase diagram.

Let us also find the derivative $\partial\Phi/\partial\alpha$, which we shall subsequently need. From (1) and (2) we obtain

$$\frac{\partial\Phi}{\partial\alpha}=\frac{1}{2d}\int_0^d\rho^2\,dx,\tag{13}$$

it being not necessary to take the α dependence of d, ρ, and φ into account when performing the differentiation, since Φ has been minimized with respect to these quantities. Substituting ρ from (5) into (13), and evaluating the integral, we obtain

$$\frac{\partial\Phi}{\partial\alpha}=\frac{4\alpha_0c(\beta_1+\beta_2c)}{(1-c)(\beta_1-3\beta_2c)^2}\left(\frac{\Pi}{K}-1\right),\quad \Pi=\Pi\left[\frac{k^2}{2}(c-1),k\right].\tag{14}$$

Let us proceed to investigate the expressions (6), (7), and

(12), which it is convenient to do by giving different values to the parameters c and k^2 and finding the corresponding values of the dimensionless quantities β_2/β_1, $\alpha_0\gamma/\beta_1^2$, and α/α_0; we can then compute Φ from the expression (10). Let us first give some general results. All the quantities remain real when we go over to a purely imaginary modulus k, i.e., when $k^2<0$. But, we can, by using the transformation formulas for the elliptic functions and integrals,[20,21] show that the case $k^2<0$ reduces to the $k^2>0$ case if we change everywhere the sign in front of β_2. Since we assume that $\beta_2>0$, we can assume that $k^2\geqslant 0$. On account of (12), the last inequality in (8) is fulfilled automatically, and does not impose any limitations. At equilibrium we must have $\Phi\leqslant 0$; therefore, it makes sense to consider only this case. The use of the expressions (10) and (12) allows us to show that $\Phi<0$ only when $c\geqslant 0$, and then $\beta_1\geqslant 0$. Thus, it is sufficient to limit ourselves to the parameter-value ranges $0\leqslant c\leqslant 1$ and $0\leqslant k^2\leqslant 1$, assuming that $\beta_1\geqslant 0$.

All the expressions become significantly simpler if, as is often done when thermodynamic potentials of the type (1), (2) are used, we assume that $\gamma=0$. In this case it follows from (6) that $c=\pm 1$ [the quantity $\beta_1-3\beta_2 c$ cannot be equal to zero, a fact which can be seen, for example, from (5)]. Since only the case of positive c is of interest to us here, let us go over to the limit $c\to 1$ in (7) and (12) [the right-hand side of the expression (12) for $c=1$ has the form 0/0, since $\Pi(0,k)=K(k)$]:

$$k^2=-\frac{\alpha(\beta_1-3\beta_2)^2+\alpha_0(\beta_1+\beta_2)(3\beta_1-5\beta_2)}{\alpha_0(\beta_1+\beta_2)^2},$$

$$\frac{\beta_2}{\beta_1}=\frac{4(1-k^2)K-(4+k^2)E}{8(1-k^2)K-(8-k^2)E}. \tag{15}$$

When $\gamma=0$, these relations determine that connection between the coefficients of the thermodynamic potential for which the solution in question is an equilibrium solution. Figure 1 shows the corresponding curve in the (α,β_2) plane.

Let us consider the case $k\to 0$ for arbitrary γ. Using the formulas of Ref. 21, we expand the right-hand side of the expression (12) in powers of k^2; in the first approximations

$$\frac{\beta_2}{\beta_1}=\frac{1}{c}\left(1-\frac{k^2c}{4}\right). \tag{16}$$

Solving this equation for c, and substituting it into (6) and (7), we find

$$\beta_2^2=\beta_1^2+\frac{16}{3}\alpha_0\gamma-\frac{k^2\beta_1(3\beta_1^2-8\alpha_0\gamma)}{6(\beta_1^2+16\alpha_0\gamma/3)^{1/2}},\quad k^2=\frac{\beta_2}{\alpha_0\beta_1}(\alpha_0-\alpha). \tag{17}$$

From (5) and (10) we obtain in this case the expressions

$$\rho^2=\frac{\alpha_0-\alpha}{\beta_1},\quad \varphi=q_0(x-x_0),\quad \Phi=-\frac{(\alpha_0-\alpha)^2}{4\beta_1}. \tag{18}$$

The expressions (18), which are valid in the vicinity of the critical point ($\alpha=\alpha_0$) of the transition from the initial (symmetric) phase into the incommensurate phase, are well-known expressions.[2]

Let us now proceed to consider the case $k^2\to 1$. From the expression (12) we find, after making allowance for the pertinent expansions,[21] that

$$\begin{aligned}\beta_2/\beta_1=\{&(1+c)(2-c)\operatorname{arth}((1-c)/2)^{1/2}\\&-c[2(1-c)]^{1/2}\}\\\times\{&c[(1+c)(2-3c)\operatorname{arth}((1-c)/2)^{1/2}\\&+c(2(1-c))^{1/2}]\}^{-1}.\end{aligned} \tag{19}$$

Denoting the value of α for $k=1$ by α_f, we find from (7) that

$$\alpha_f=-\alpha_0\frac{(\beta_1+\beta_2c)[(3+5c)\beta_1-\beta_2c(5+3c)]}{(1+c)(\beta_1-3\beta_2c)^2}. \tag{20}$$

Thus, the curve along which the solution in question is at equilibrium lies in the (α,β_2) plane between the point given by (17) for $k=0$ and the point determined by the expressions (19) and (20), as well as (6). As γ increases, the ends of this curve move along the dashed lines shown in Fig. 1. Let us note that the solution obtained exists when the space of the order-parameter components is markedly anisotropic (i.e., when β_2 is not small). It can also be seen that the constant-amplitude approximation (i.e., the approximation in which we set $\rho=\text{const}$) is clearly inapplicable in the present case, since, for example, when $k=1$ the square of the ratio of the maximum value of $\rho(x)$ to the minimum value is, according to (5), equal to $1+[2/(1+c)]^{1/2}$, i.e., for $0\leqslant c\leqslant 1$ it lies within the range from $1+\sqrt{2}$ to 2.

As $k\to 1$, the period $d\propto|\ln(1-k^2)|\to\infty$, and the incommensurate phase acquires the well-known domain-like structure. In this case, from (10) we can, by discarding the terms of higher order in smallness, obtain

$$\Phi=\Phi_c-\frac{16\alpha_0^2c(\beta_1+\beta_2c)^2(2\beta_2c^2+\beta_2c-\beta_1)}{(1+c)^3(\beta_1-3\beta_2c)^4}(1-k^2), \tag{21}$$

where Φ_c is the thermodynamic potential of the commensurate phase:

$$\Phi_c=\frac{1}{24\gamma^2}\{(\beta_1-\beta_2)^3-6\alpha\gamma(\beta_1-\beta_2)-[(\beta_1-\beta_2)^2-4\alpha\gamma]^{3/2}\}. \tag{22}$$

Using (19), we can show that $2\beta_2c^2+\beta_2c-\beta_1>0$; therefore, $\Phi\leqslant\Phi_c$, with $\Phi=\Phi_c$ when $k=1$, i.e., when $\alpha=\alpha_f$.

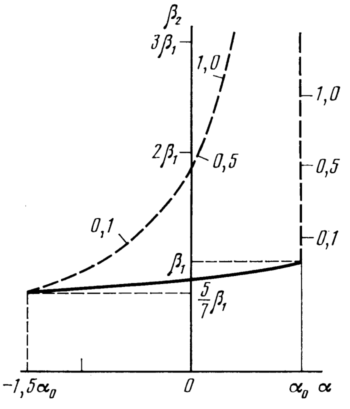

FIG. 1. The curve in the (α,β_2) plane on which the solution in question corresponds to the equilibrium state of the incommensurate phase for $\gamma=0$. As γ increases, the ends of the curve move along the dashed lines, on which the corresponding values of the quantity $\alpha_0\gamma/\beta_1^2$ are indicated.

Similarly, from (14) we obtain in the case $k \to 1$ the expression

$$\frac{\partial\Phi}{\partial\alpha}=\frac{\partial\Phi_c}{\partial\alpha}+\frac{8\sqrt{2}\,\alpha_0 c(\beta_1+\beta_2 c)\,\mathrm{arth}((1-c)/2)^{1/2}}{(1+c)(1-c)^{1/2}(\beta_1-3\beta_2 c)^2\ln(1-k^2)}. \tag{23}$$

From this it can be seen that $\partial\Phi/\partial\alpha = \partial\Phi_c/\partial\alpha$ when $k = 1$. Thus, the phase transition, occurring at $\alpha = \alpha_f$, into the commensurate phase is a second-order transition. Naturally, the present proof is correct only in the case of those parameter values for which the solution (5) can be used.

It is of interest to investigate the specific heat of the incommensurate phase for $\alpha \to \alpha_f$. From (6), (7), and (12) we can obtain in the $k \to 1$ case the expression

$$\alpha=\alpha_f+\bar{\alpha}(1-k^2)\ln(1-k^2),$$

where $\bar{\alpha}$ is some k-independent constant. From this we obtain the approximate expression

$$1-k^2=(\alpha-\alpha_f)\{\bar{\alpha}\ln[(\alpha-\alpha_f)/\bar{\alpha}]\}^{-1}. \tag{24}$$

Substituting (24) into (23), we obtain the dependence of $\partial\Phi/\partial\alpha$ on α, a dependence, which, having been found for the points where the solution (5) is an equilibrium solution, is, on account of its continuity, also valid in some neighborhood of these points. Differentiating $\partial\Phi/\partial\alpha$ with respect to α, and taking into consideration the fact that the derivative $\partial^2\Phi_c/\partial\alpha^2$ is finite, we find that for $\alpha \to \alpha_f$

$$\frac{\partial^2\Phi}{\partial\alpha^2}=-\frac{8\sqrt{2}\,\alpha_0 c(\beta_1+\beta_2 c)\,\mathrm{arth}((1-c)/2)^{1/2}}{(1+c)(1-c)^{1/2}(\beta_1-3\beta_2 c)^2(\alpha-\alpha_f)[\ln(\alpha-\alpha_f)]^2}, \tag{25}$$

where in accordance with (6) c is a fixed quantity. Notice that we can arrive at this relation in a different way, namely, by eliminating $1 - k^2$ from (21) and (23), obtaining a differential equation for $\Phi - \Phi_c$, and solving it.

If, as is usually done in the Landau theory, we consider the coefficient α to be a linear function of the temperature, then $\partial^2\Phi/\partial\alpha^2 \propto \partial^2\Phi/\partial T^2$ Therefore, as $\alpha \to \alpha_f$, the specific heat C diverges according to the law

$$C=-T\frac{\partial^2\Phi}{\partial T^2}\propto\frac{1}{(\alpha-\alpha_f)[\ln(\alpha-\alpha_f)]^2}. \tag{26}$$

Notice that a similar result can be obtained in the constant-amplitude approximation.[22]

The above-obtained solution (5) also allows us to investigate the incommensurate phase in the neighborhood of the triple point, where the initial, incommensurate, and commensurate phases adjoin in the phase diagram. For $\alpha \geqslant \alpha_0$ there exists an initial-commensurate phase boundary, determined by the equation $\Phi_c = 0$. Using (22), we find the equation of this boundary:

$$\alpha=(3/16\gamma)(\beta_2-\beta_1)^2,$$

ρ being real at this boundary when $\beta_2 > \beta_1$. Setting $\alpha = \alpha_0$ here, we find that at the triple point

$$\beta_2=\beta_1+4(\alpha_0\gamma/3)^{1/2}, \quad \alpha=\alpha_0. \tag{27}$$

Let us consider the above-obtained expressions in the case $c \to 0$. The relation (12) for $c \to 0$ has the form

$$\frac{\beta_2}{\beta_1}=\frac{1}{c}-g(k), \quad g(k)=\frac{2E-2K+k^2\Pi_0}{2K-(2-k^2)\Pi_0},$$
$$\Pi_0=\Pi\left(-\frac{k^2}{2},k\right), \tag{28}$$

where $g(0) = 0$, $g(k) > 0$ for $k \neq 0$, and $g(k) \neq \infty$. It can be seen from (28) that, for finite β_2, the case $c \to 0$ is possible only when $\beta_1 \to 0$. Solving (28) for c, and substituting it into (6) and (7), we obtain to within terms of the order of β_1^2:

$$\beta_2=4\left(\frac{\alpha_0\gamma}{3}\right)^{1/2}+\frac{1}{2}\beta_1 g(k), \quad \alpha=\alpha_0-\frac{\beta_1 k^2}{2(2-k^2)}\left(\frac{3\alpha_0}{\gamma}\right)^{1/2}. \tag{29}$$

These relations constitute the parametric equation of the curve on which the solution (5) is an equilibrium solution for small β_1. When $\beta_1 = 0$ the curve in question becomes a point, which, as can be seen from a comparison with (27), coincides with the triple point. The expression (10) leads, in the first approximation in β_1, to

$$\Phi=-3\alpha_0\beta_1 k^2 g(k)/8\gamma(2-k^2). \tag{30}$$

Hence we have $\Phi = 0$ at the triple point (in the present case, when $\beta_1 = 0$), but there are no single-valued expressions for $\rho(x)$ and $\varphi(x)$ corresponding to this value of Φ, since from (5) we obtain for $\beta_1 \to 0$ and $c \to 0$ the expressions

$$\rho^2=4\alpha_0 k^2\{\beta_2(2-k^2)^{1/2}[(2-k^2)^{1/2}+\sqrt{2}\,\mathrm{dn}\,2q(x-x_0)]\}^{-1},$$
$$\varphi=\frac{1}{2}\mathrm{am}[2q(x-x_0)], \quad q=q_0\left(\frac{2}{2-k^2}\right)^{1/2}, \tag{31}$$

where $0 \leqslant k \leqslant 1$. To remove any doubt that may arise about the admissibility of the passage to the limit, we can verify through direct substitution that the expressions (31) satisfy Eqs. (3) and (4), when $\beta_1 = 0$ and (27) is satisfied, regardless of the value of k, and that (11) yields $\Phi = 0$ for any k.

Thus, the incommensurate phase is degenerate at the triple point, a fact also noted in Refs. 7, 10, and 11. At the same time this result contradicts the assertion made in Ref. 23 that in the case of a thermodynamic potential with a $\rho^n\cos n\varphi$ term [in the expression (2) $n = 4$] there is no degeneracy point for the incommensurate phase when $n > 3$. Let us add that we have degeneracy at the triple point despite the presence in (2) of a term $\propto\rho^6$, even though, according to Refs. 11 and 23, such a term removes the degeneracy in the $n = 3$ case. It should be emphasized again that all the results for the triple point were obtained by us under the condition that $\beta_1 = 0$.

Notice that the expressions (18) become meaningless when $\beta_1 = 0$. Let us find out what they are replaced by in the general case. When $\alpha \approx \alpha_0$, the system (3) and (4) can be solved by the method of successive approximations, since $\rho \to 0$ as $\alpha \to \alpha_0$ (Ref. 2). Setting $\beta_1 = 0$ in (3) and (4), we obtain in place of (18) the expressions

$$\rho^4=\frac{16\alpha_0(\alpha_0-\alpha)}{16\alpha_0\gamma-3\beta_2^2}, \quad \varphi=q_0(x-x_0),$$
$$\Phi=-\frac{\rho^6}{48\alpha_0}(16\alpha_0\gamma-3\beta_2^2). \tag{32}$$

It can be seen from this that, in the present case, the triple point is a singular point on the initial—incommensurate phase transition line $\alpha = \alpha_0$ as well, since the denominator in the expression for ρ^4 vanishes at this point [the expression (27) yields the equation $3\beta_2^2 - 16\alpha_0\gamma = 0$ when $\beta_1 = 0$]. When $3\beta_2^2 > 16\alpha_0\gamma$, the quantity ρ is real only when $\alpha \geqslant \alpha_0$, and then, according to (32), $\Phi \geqslant 0$, which cannot correspond to a stable state. Let us note that a similar anomaly exists at the triple point in the case ($n = 3$) considered in Ref. 7.

Let us, in the light of the results obtained, discuss the nature of the transition along the entire boundary between the incommensurate and commensurate phases. The above-adduced arguments showing that the incommensurate-commensurate phase transition is of second order are valid for any values of the parameters entering into (5), including those pertaining to the vicinity of the triple point. Sannikov[6] and Jacobs and Walker[7] obtain a different result, according to which this transition is of first order in the vicinity of the triple point. The discrepancy between our results and the results obtained by Jacobs and Walker[7] is probably due to the fact that the thermodynamic potential used by these authors is different from (1), (2): it contains the term $\rho^3 \cos 3\varphi$ in place of $\rho^4 \cos 4\varphi$. As for Sannikov,[6] he does not analyze the special case $\beta_1 \rightarrow 0$, i.e., the case when the results of the present paper are valid in the vicinity of the triple point. Therefore, if the transition in question is of first order in the vicinity of the triple point, then it can be asserted that there exists in the interval between the β_2 value given by (19) and the β_2 value (27) at the triple point a critical point where the order of the transition changes, this critical point merging with the triple point and, thus, disappearing when $\beta_1 \rightarrow 0$. If there are no other critical points at the incommensurate-commensurate phase boundary (in the literature known to us there are no indications of the existence of several critical points at this boundary), then the incommensurate-commensurate phase transition is of second order in the range of β_2 values from zero to at least the value given by (19).

In conclusion, I thank D. G. Sannikov for a discussion of the results of the paper.

APPENDIX

Let us transform the system of equations (3) and (4) by introducing the function $f = d\varphi/dx$ and taking φ, and not x, as the independent variable. Then Eq. (4) assumes the form

$$\delta\rho f \frac{df}{d\varphi} + 2\delta f^2 \frac{d\rho}{d\varphi} - 2\sigma f \frac{d\rho}{d\varphi} + \beta_2\rho^3 \sin 4\varphi = 0. \qquad (A.1)$$

Instead of Eq. (3), let us take the energy integral, which constitutes the left-hand side of the relation (9). Denoting the energy by ε, and making the same substitutions carried out above, we obtain

$$\frac{\delta}{2} f^2 \left[\left(\frac{d\rho}{d\varphi}\right)^2 + \rho^2\right] - \frac{\alpha}{2}\rho^2 - \frac{\beta_1}{4}\rho^4 - \frac{\gamma}{6}\rho^6 - \frac{\beta_2}{4}\rho^4 \cos 4\varphi = \varepsilon. \qquad (A.2)$$

Thus, the two second-order equations have been transformed into two first-order equations. Let us introduce the variable $u = \cos 4\varphi$ in place of φ and the function $v = \rho^2(f - q_0)$ in place of f, and let us set $w = -4f d\rho/du$. Then from Eq. (A.1) and the definition of w we have

$$\delta w \frac{dv}{d\rho} + \beta_2\rho^4 = 0, \qquad w \frac{du}{d\rho} + \frac{4v}{\rho^2} + 4q_0 = 0, \qquad (A.3)$$

and Eq. (A.2) gives the relation

$$\frac{\delta}{2}(1-u^2)w^2 + \frac{\delta v^2}{2\rho^2} + \sigma v + \frac{1}{2}(\alpha_0 - \alpha)\rho^2 - \frac{\beta_1}{4}\rho^4 - \frac{\gamma}{6}\rho^6 - \frac{\beta_2}{4}\rho^4 u - \varepsilon = 0. \qquad (A.4)$$

Let us try to find the solution to this system, assuming that the function v has the simplest form:

$$v = a + b\rho^2, \quad a = \text{const}, \quad b = \text{const}. \qquad (A.5)$$

From the first equation in (A.3) we find w; from the second, u, the integration giving rise to another constant c. Let us substitute all this into (A.4), and, by equating the coefficients of the various powers of ρ to zero, obtain four algebraic equations for the quantities a, b, c, and ε, the fact that the coefficient of ρ^{-2} vanishes identically being of help. The constants a, b, and ε can be expressed in terms of c, and for c we obtain Eq. (6). The expression for ε coincides with (10) if we set $\varepsilon = -\Phi$.

Knowing the dependence of u and v on ρ, we can find the relation between $d\varphi/dx = f$ and $\cos 4\varphi = u$. The resulting differential equation can be solved with the aid of the elliptic functions with modulus k, (7), which, as a result, yields the expressions (5).

Let us note that we could not find any other exact solutions to the system (A.3) and (A.4) besides (A.5).

The above-considered method can be used in the case of a thermodynamic potential in which, instead of $\rho^4 \cos 4\varphi$, as in (2), we have a term of the more general form $\rho^n \cos n\varphi$. But when $n \neq 4$ the substitution of (A.5) yields five equations for the four parameters a, b, c, and ε. These equations can be satisfied only when the coefficients of the thermodynamic potential are connected by some relation; the additional relation is given by a condition of the type (9) for equilibrium. Therefore, the solution found will be an equilibrium solution only at one or several points of the phase diagram, or else it will not be an equilibrium solution at all. Such cases are of little interest. The indicated system of five equations admits of a special solution, when certain coefficients of the thermodynamic potential are equal to zero. For example, when $n \geqslant 5$, the coefficients of ρ^4 and ρ^6 should be equal to zero, but the coefficient of ρ^{2n-2} should be nonzero, which is not very realistic. If $n = 3$, the requisite coefficients should be equal to zero on the basis of symmetry arguments, and in this case $2n - 2 = 4$. But analysis shows that in this case the solution obtained does not guarantee an absolute minimum of the thermodynamic potential, except the solution for the triple point, which solution coincides with the one found in Ref. 7.

---

1) This point is sometimes called the Lifshitz point,[6] but in a number of papers this designation is reserved for a triple point occurring in a special case.[8]

2) The derivative of the functional

$$I = \int_{x_1}^{x_2} F(y_1, y_1', \ldots, y_n, y_n')\, dx$$

with respect to the upper limit of the integration is equal to

$$\frac{\partial I}{\partial x_2}=F-\sum_{i=1}^{n} y_i'\frac{\partial F}{\partial y_i'},$$

if the functions $y_i(x)$ satisfy the Euler equations. In our case we impose the conditions $\rho(d)-\rho(0)=0$ and $\varphi(d)-\varphi(0)=\pi/2$ on the functions.

[1] I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. **46**, 1420 (1964); **47**, 336, 992 (1964) [Sov. Phys. JETP **19**, 960 (1964); **20**, 223, 665 (1965)].

[2] A. P. Levanyuk and D. G. Sannikov, Fiz. Tverd. Tela (Leningrad) **18**, 423 (1976) [Sov. Phys. Solid State **18**, 245 (1976)].

[3] A. D. Bruce, R. A. Cowley, and A. F. Murray, J. Phys. C **11**, 3591 (1978).

[4] V. A. Golovko, Fiz. Tverd. Tela (Leningrad) **22**, 2960 (1980) [Sov. Phys. Solid State **22**, 1729 (1980)].

[5] D. G. Sannikov, Fiz. Tverd. Tela (Leningrad) **23**, 953 (1981) [Sov. Phys. Solid State **23**, 553 (1981)].

[6] D. G. Sannikov, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 173 (1979) [JETP Lett. **30**, 158 (1979)].

[7] A. E. Jacobs and M. B. Walker, Phys. Rev. B **21**, 4132 (1980).

[8] R. M. Nakanishi, M. Luban, and S. Shtrikman, Phys. Rev. Lett. **35**, 1678 (1975).

[9] H. Shiba and Y. Ishibashi, J. Phys. Soc. Jpn. **44**, 1592 (1978).

[10] K. Nakanishi and H. Shiba, J. Phys. Soc. Jpn. **45**, 1147 (1978).

[11] S. A. Jackson, P. A. Lee, and T. M. Rice, Phys. Rev. B **17**, 3611 (1978).

[12] H. Yamamoto, I. Nakayama, and T. Ohmi, Prog. Theor. Phys. **59**, 351 (1978).

[13] R. A. Cowley, Adv. Phys. **29**, 1 (1980).

[14] D. G. Sannikov and A. P. Levanyuk, Fiz. Tverd. Tela (Leningrad) **19**, 118 (1977) [Sov. Phys. Solid State **19**, 67 (1977)].

[15] M. Iizumi and K. Gesi, Solid State Commun. **22**, 37 (1977).

[16] M. Iizumi and K. Gesi, J. Phys. Soc. Jpn. **45**, 711 (1978).

[17] V. V. Gladkiĭ, S. N. Kallaev, V. A. Kirikov, and L. A. Shuvalov, Fiz. Tverd. Tela (Leningrad) **21**, 3732 (1979) [Sov. Phys. Solid State **21**, 2155 (1979)].

[18] K. Gesi and M. Iizumi, J. Phys. Soc. Jpn. **48**, 697 (1980).

[19] V. A. Golovko, Fiz. Tverd. Tela (Leningrad) **23**, 1643 (1981) [Sov. Phys. Solid State **23**, 958 (1981)].

[20] I. S. Gradshteĭn and I. M. Ryzhik, Tablitsy integralov, summ, ryadov i proizvedeniĭ (Tables of Integrals, Series, and Products), Fizmatgiz, Moscow, 1962 (Eng. Transl., Academic Press, New York, 1965).

[21] P. F. Byrd and M. D. Friedman, Handbook of Elliptic Integrals for Engineers and Physicists, Springer, Berlin, 1954.

[22] D. G. Sannikov, J. Phys. Soc. Jpn. **49**, Suppl. B, 75 (1980).

[23] A. E. Jacobs, D. Mukamel, and M. B. Walker, Phys. Rev. B **24**, 5195 (1981).

Translated by A. K. Agyei