One-dimensional crystal in the field of two potentials with incommensurate periods

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We study the phase diagram of a one dimensional crystal in the field of two potentials with incommensurate periods. We show that in the case of sufficiently weak potentials, the dependence of the period on the chemical potential has the form of a "devil's staircase."

1. Incommensurate structures are widespread experimental systems. They are found in three-dimensional (ferroelectrics, magnetic materials), two-dimensional (adsorbed films, reconstructed surfaces) and quasi-one-dimensional systems. The simplest model of incommensurate sturcture is the Frenkel-Kontorova model. In this model one studies a one-dimensional chain of atoms with period c in a potential with period b. The ground state has been extensively studied.[1] A natural extension of this model is the case of two potentials with incommensurate periods. If the periods of these two potentials were commensurate, the problem could be reduced to a model analogous to that of Frenkel and Kontorova.[1] For incommensurate periods, this is not the case. Before formulating a more concrete model let us look at a possible experimental realization.

The Frenkel-Kontorova model allows the description of the ground state of many experimental systems with uniaxial symmetry, in particular those known as uniaxial incommensurate two-dimensional crystals in adsorbed films. In these systems the surface of the substrate crystal is strongly anisotropic (the atomic surface is a system of furrows.) The presence of a preferred axis (which we call X) means that we consider displacements of atoms of the two-dimensional structure only in the direction X (along the furrows). In this case the period c is the period of the lattice of adatoms along X, while the period b of the potential is that of the substrate crystal in the same direction. In such systems we can realize experimentally also the situation with two incommensurate potentials. If the interaction between the adatoms is large compared with the potential variation of the substrate, the adatom lattice will be weakly deformed even for small differences between b and c. Examples are alkali adsorbates (potassium, cesium)[2] on furrowed (112) surfaces of tungsten and molybdenum. One can suppose that such an adsorbed system is a potential contour with preferred axis X for a lattice of adatoms of another kind, weakly interacting with each other. As a second adsorbate one could use noble gases. If the periods b and c are incommensurate, the description of the ground state of such a system (which depends only on the coordinate X) encounters the problem of a one-dimensional crystal in the field of two potentials with incommensurate periods.

2. Let us examine such a one-dimensional crystal with period a in the field of two potentials with incommensurate periods b and c ($c > b$). We will assume that all three periods are close together. For simplicity, we choose the functional form of both potentials to be the same. We will study the problem in the continuum approximation and write the potential energy of the crystal in the form:

$$H=\int dx\left\{\frac{\lambda}{2}\left(\frac{du}{dx}\right)^2+v_1 f\left[2\pi\left(\frac{u}{b}+\left(\frac{1}{b}-\frac{1}{a}\right)x\right)\right]+v_2 f\left[2\pi\left(\frac{u}{c}+\left(\frac{1}{c}-\frac{1}{a}\right)x\right)\right]\right\}, \tag{1}$$

$$f(x+2\pi)=f(x), \quad -1\leqslant f(x)\leqslant 1, \quad \overline{f(x)}=0.$$

Here u is the displacement of the atoms of the crystal at the point X. It is convenient to convert to the variables

$$\varphi=2\pi\left[\frac{u}{b}+\left(\frac{1}{b}-\frac{1}{a}\right)x\right],$$

$$t=2\pi\frac{c-b}{ab}x, \quad \gamma_{1,2}=\frac{v_{1,2}}{\lambda}\frac{a^2}{(c-b)^2}. \tag{2}$$

We shall use below both the original variables and the variables (2). The expression (1) for the energy takes the form

$$H=\frac{b(c-b)}{2\pi a}\lambda\int dt\left\{\frac{1}{2}\left(\frac{d\varphi}{dt}-\delta\right)^2+\gamma_1 f(\varphi)+\gamma_2 f[k(\varphi-t)]\right\}, \tag{3}$$

where $k=b/c$ and $\delta=(a-b)/(c-b)$. The equilibrium equation takes the form

$$d^2\varphi/dt^2=\gamma_1 f'(\varphi)+k\gamma_2 f'(k(\varphi-t)). \tag{4}$$

For $v_2=0$ Eqs. (3) and (4) describe the Frenkel-Kontorova model. Let us recall some of its properties. We note that the condition for the applicability of the continuum approximation is the smallness of the potential relief $v_{1,2}\ll\lambda$. For $v_2=0$, Eq. (4) is integrable. There are two types of solution corresponding to the commensurate ($\varphi=0$) and incommensurate ($\varphi=2\pi x/e+\varphi_1(x)$, $\varphi_1(x+l)=\varphi_1(x)$) structures. Near the transition between them, the latter is a lattice of solitons, of width $l_0\sim b(\lambda/v_1)^{1/2}$, separating domains of the commensurate phase. The soliton corresponds to a change of the phase φ by a period of the function $f(\varphi)$. The period l of the soliton lattice changes continuously with change of a. For large l/l_0, this dependence has the form $l/l_0\propto 1/\ln(|a-a_c|/a_c)$, where a_c corresponds to the transition point. For a_c we have $a_c-b\sim b(v_1/\lambda)^{1/2}\sim b^2/l_0$. For $l\sim l_0$ the incommensurate phase will be weakly modulated by the substrate potential.

If $v_2\neq 0$, Eq. (3) is not integrable. An equation analogous to (3) with $f(\varphi)=-\cos\varphi$ arises in the problem of the motion of a classical particle in the field of two waves. This problem was studied by Escande and Deveil.[3] A description of the results can also be found in the book of Lichtenberg and Liberman.[4] Although problems of the motion of

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a particle and of the ground state of a one-dimensional crystal are described by the same equation (4), they have some differences. The first is that the Hamiltonian of the mechanics problem corresponds to the Lagrangian of the crystal. More significant, however, is the requirement that the crystal energy (1) be a minimum. This leads to the fact that the ground state of the crystal is described by only a small subset of the solutions of Eq. (4). Unfortunately, because of the nonintegrability of (3), it is impossible to obtain a full description of all the possible phases of the problem at hand. Nevertheless, it is possible to obtain information about the phase diagram for some limiting cases. The transition to global stochasticity in (4) was studied by Escande and Deveil.[3,4] For $\gamma_1 \sim \gamma_2$ the critical value is $\gamma_s \lesssim 1$. Thus we will consider only the limiting case when γ_1 and γ_2 are small (weak potential).

3. It is convenient to study the weak-potential problem for $\gamma_1 \approx \gamma_2$. The smallness of the potential means that $c-b \gg b^2/l_0$. For simplicity we will assume that $f(\varphi) = -\cos\varphi$. For a close to b, two regimes can be distinguished: $\delta \ll \gamma_1^{1/2}$ $(a-b \ll b^2/l_0)$—region I and $\gamma_1^{1/2} \lesssim \delta \ll 1$ $(b^2/l_0 \lesssim a-b \ll c-b)$—region II. Since the threshold for the formation of solitons at $\gamma_2 = 0$ is $\delta_i = 4\gamma_1^{1/2}/\pi(a_c - b = (4/\pi)b(v_1/\lambda^{1/2}))$, in region I we can assume that φ is small. Keeping only the linear term in the expansion of the first term on the right of Eq. (4), we obtain

$$d^2\varphi/dt^2 = \gamma_1\varphi + F(\varphi,t),$$
$$F(\varphi,t) = k\gamma_2(\cos k\varphi \sin kt + \sin k\varphi \cos kt). \quad (5)$$

We use an approach analogous to that used for the analysis of the oscillation of a mathematical pendulum under the action of a rapid driving force.[5] The expression for φ now takes the form

$$\varphi = -(\gamma_2/k)\sin kt. \quad (6)$$

The period of (6) (in the usual units) is $ca/(c-b)$ and it varies continuously with a. It is not difficult to verify that the solution (6) does not have a continuous translation group. It is also easy to compute the energy of the solution (6) by using the results of the pendulum problem. We obtain

$$E = \gamma_2^2 + \delta^2/2. \quad (7)$$

We now consider the region II, where $\delta \gtrsim \gamma_1^{1/2}(a-b \gtrsim b^2/l_0)$. In this case solitons can be generated. Let us estimate the effect of a rapidly oscillating force on the energy of formation of a soliton and the structure of the soliton lattice. For the estimate of the energy we insert the one-soliton solution

$$\operatorname{tg}(\varphi/4) = \exp[\gamma_1^{1/2}(t-t_0)] \quad (8)$$

in expression (3) for the energy. The first two terms give a constant independent of the position t_0 of the center of the soliton. The third term in (3) gives an oscillatory contribution

$$-\frac{b(c-b)}{2\pi a}\lambda\gamma_2\int dt\cos k(\varphi - t)$$
$$\approx \frac{2b(c-b)}{a}\lambda\frac{\gamma_2}{\gamma_1}\frac{\exp(\pi/2\gamma_1^{1/2})}{\operatorname{sh}(\pi/\gamma_1^{1/2})}\cos kt_0$$
$$\approx \frac{2b(c-b)}{a}\lambda\frac{v_2}{v_1}\exp\left(-\frac{\pi}{2\gamma_1^{1/2}}\right)\cos kt_0 = v_p\cos kt_0. \quad (9)$$

Thus, with power-law accuracy, the energy of a soliton is not changed relative to its value in the Frenkel-Kontorova model, but now it does depend periodically on the position of the soliton. This pinning potential is analogous to the Peierls relief of a dislocation. Its period is equal to $2\pi/k$ (in usual units $ca/(c-b)$). We recall that the Peierls relief arises also in the Frenkel-Kontorova model but only when account is taken of the discreteness of the lattice. In this case its period is equal to that of the substrate. Near the soliton creation threshold, when the distance between the solitons is large, the pinning potential v_p will predominate over the repulsion of the solitons. There arises the problem of a one-dimensional lattice gas with repulsion. It was investigated by Burkov and Sinaĭ[6] and by Bak and Bruijnsma.[7] For the discrete Frenkel-Kontorova model, an analogous problem was investigated by Pokrovsky.[8] For large distances between solitons an infinite sequence of phases is produced with periods commensurate with the pinning potential. Such a sequence was named a "devil's staircase." If the ratio ϑ of the number of solitons to the number of minima of the pinning potential is $\vartheta = p/q$ (with integer p and q), the range of $\Delta\delta$ in which this structure is stable is[7]

$$\Delta\delta \propto p\frac{d^2J}{dx^2}\left[\frac{qac}{p(c-b)}\right], \quad (10)$$

where $J(x)$ is the interaction potential between solitons. With decreasing distance between solitons, this interaction increases. Let us estimate the characteristic distance t_1, at which this interaction becomes of the order of the amplitude of the Peierls relief. If the interaction falls off exponentially with distance, then

$$\gamma_1^{1/2}\exp(-\gamma_1^{1/2}t_1) \sim (\gamma_2/\gamma_1)\exp(-\pi/2\gamma_1^{1/2}), \quad (11)$$
$$t_1 \sim 1/\gamma_1. \quad (12)$$

Since the soliton size is about $\gamma_1^{-1/2}$, there is a range of values $\gamma_1^{-1/2} < t < \gamma_1^{-1}$ in which, on the one hand, the solitons can be considered point-like, while on the other the Peierls relief is weak compared with their interaction. Thus we have come again to the problem of a chain with a weak potential relief. For some $t_p \sim t_1$ the states of a lattice with incommensurate periods become energetically favorable. Such lattices have a continuous translation group.[1,8]

Let us return to Eq. (4), assuming as before that γ_1 and γ_2 are small, and regarding the term with γ_2 as a perturbation. Let the period of the unperturbed soliton (for $\gamma_2 = 0$) be τ. The perturbation is also a periodic function. The Poincare-Birkhoff and Kolmogorov-Arnold-Moser theorems then guarantee the existence of solutions of Eq. 4 for $\gamma_2 = 0$, which are stable with respect to such a perturbation,[1,4] both when $(k\tau/2\pi)$ is rational and when it is irrational. For an irrational ratio of the periods, an arbitrary translation does not change the total energy of the chain, i.e., the translation group is continuous.

In the investigation of the ground state for $a-b \ll (c-b)$, we have considered the term with γ_2 as a perturbation. For values a such that $c-a \ll c-b$, we should consider the term with γ_1 as a perturbation. Obviously, the picture of the ground state will be analogous to that previously considered.

Thus, for $\gamma_1, \gamma_2 \ll 1$, near $a = b$ and $a = c$ there are single phase regions of width $\sim b^2/l_0$, in which the displacements

of the atoms from the minima of the potentials with periods b and c respectively are small and are determined by Eq. (6). Next comes a transition to regimes in which there are infinite sequences of phases with periods commensurate with the periods of the modulation of the potential ($ca/(c-b)$ and $ba/(c-b)$). All these lattices have discrete translation groups. Finally, at large deviations of a from b (or from c), besides the solutions with discrete translation groups there appear solutions with continuous translation groups, whose period is incommensurate with the period of the modulation of the potential.

Now we turn to the phase diagram for $T \neq 0$. If the form of the ground state does not depend on the dimensionality of the system, the phase diagrams at $T \neq 0$ are different for systems of different dimensionality. We will discuss only two-dimensional systems. In the case of uniaxial systems (e.g., adsorbed films) the solitons are linear objects extending in the Y direction.[1] At finite temperatures, fluctuations lead to depinning of the structures with discrete translational symmetry[9,10] and to restoration of the continuous translation group. The transition temperature is determined by the kink energy E_k in the Peierls relief v_p, $E_k \sim [(\lambda v_1)^{1/2} v_p]^{1/2} ca/(c-b)$, and by the interaction between the solitons. For the simplest lattice with period $l = nca/(c-b)$ (n is an integer), the depinning temperature is determined by the expression

$$T_p \sim E_k / \ln[E_k / J(l)], \tag{13}$$

where $J(l)$ is the interaction energy between two solitons.[9,10] A more detailed description of the phase diagram of lattices of solitons in the presence of pinning can be found in Ref. (10).

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