Point defects and order in a two-dimensional soliton lattice

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It is shown that randomly distributed point defects disrupt the order in a two-dimensional soliton lattice. The size of the ordered state is found as a function of the defect density, temperature, and lattice parameters.

1. Solitons or domain walls are linear regions of disturbed commenurability (of characteristic length l_0), which appear in an adatom structure that is not commensurate with the substrate and compensate for the difference between the lattice and substrate periods (for details see the reviews[1,2]). The simplest soliton lattice is a set of parallel stripes with period l. When the elastic properties of such a lattice are examined, one can consider only its displacements in a direction perpendicular to the soliton line. Such lattices can occur in a tremendous number of incommensurate structures, e.g., when a commensurate structure is compressed along one of the crystallographic directions of the substrate (for a description of such systems see Ref. 3). Observation of an ordered striped soliton structure in diffraction experiments calls for very high precision. It was nevertheless observed experimentally in a freon-graphite system.[4] The properties of such a soliton lattice were investigated in detail in the case of an ideal substrate (see the reviews[1,2]) both theoretically and experimentally. On a real substrate there is always a finite density of defects, and as the point of transition into the commensurate phase is approached (i.e., with increasing period of the soliton lattice), the role of these defects, say in the loss of the order, should increase. Greatest interest attaches to the influence of nonequilibrium "frozen" substrate defects on the order in a soliton lattice. With respect to symmetry, the Hamiltonian of a striped soliton lattice is isomorphous[3] to the Hamiltonian of the XY model. It is known[5] that a random magnetic field destroys the order in a two-dimensional XY model. On the other hand, in a random-anisotropy field of order p with $p \geqslant 3$ ther exists a temperature region in which the thermal fluctuations restore the order.[6,7] However, the random field of substrate point defects in a soliton lattice differs noticeably from the random fields in magnets, and calls for an investigaiton of its own. The problem of loss of order, which is in itself of interest, is important also for the understanding of the diffusion dynamics of a soliton lattice,[8] where the point defects are shown by experiment to play a decisive role.

2. The concrete nature of the lattice point defects can vary. The defects can be impurity atoms, vacancies, and excess substrate atoms. The mobility of these defects can be extremely small at the experimental temperatures,[9] i.e., they are "frozen." The density c of such defects, even if the substrate is thoroughly cleaned, remains on the order of $c \sim 10^{-3}$ (Ref. 9). Such defects alter the potential relief of the substrate. The adatoms can be attracted to or repelled from such defects. This can cause the defects to attract or repel the solitons, which are in fact density waves. A defect will interact with a soliton only if it is in the vicinity of the latter. We consider by way of example the model of the so-called anisotropic two-dimensional crystal. In this model, which describes a large number of experimental systems, the anisotropy of the potential relief of the substrate permits the atoms to be displaced in only one direction (say, along the x axis).[3] The Hamiltonian of the model is

$$H=\int d^2r\left\{\frac{1}{2}K(\nabla u)^2 + v\left[1-\cos\left(\left(\frac{2\pi}{b}-\frac{2\pi}{a}\right)x+\frac{2\pi}{b}u\right)\right]\right\}. \quad (1)$$

Here u is the adatom displacement, K the elastic modulus, v the amplitude of the substrate potential relief, and a and b the periods of the film and of the substrate along the x axis. The single-soliton solution is of the form

$$u(x)=\frac{2b}{\pi}\operatorname{arctg}\left(\exp\left(\frac{2\pi x}{b(K/v)^{1/2}}\right)\right). \quad (2)$$

The simplest model of a point defect at a point x_0 in such a system is a potential in the form

$$V_0\left(1-\cos\frac{2\pi}{b}u(x_0)\right). \quad (3)$$

Substituting (2) in (3) we obtain the form of the potential barrier for the soliton:

$$V(x)=2V_0/\mathrm{ch}^2\frac{2\pi(x-x_0)}{b(K/v)^{1/2}}. \quad (4)$$

Thus, the field of a point defect acting on a soliton is localized in a region of the order of the soliton width $l_0 \sim b(K/v)^{1/2}$. Let us consider the approximate picture of the influence of randomly disposed defects on a substrate in a soliton lattice at $T=0$. The inhomogeneities of the defect arrangement cause certain regions to attract (or repel) the soliton lattice. The number N of defects interacting with the lattice in a region of size $r\times r$ is $N\sim c\Delta_0 r^2$, where $\Delta_0 = l_0/l$, and l is the period of the soliton lattice (we put henceforth $l=1$). The average fluctuation of the number of defects is $\sim N^{1/2}$, so that the energy associated with these inhomogeneities is $W\sim V_0 N^{12}$ and has the meaning of a pinning energy. As a result we get the estimate

$$W\sim V_0 N^{1/2}\sim V_0(c\Delta_0)^{1/2}r. \quad (5)$$

We see that the pinning energy W increases linearly with the dimension of the region r. At the same time, the energy of the elastic deformaiton of the lattice by an amount of the order

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of unity in a region of size $r\times r$ is $K(1/r)^2r^2\sim K$ and does not depend on r. Therefore with increasing r the pinning energy $W(r)$ reaches the value of the maximum deformation energy at

$$r\sim r_c\approx K/V_0(c\Delta_0)^{1/2}, \qquad (6)$$

meaning loss of the long-range order in regions of size $r\gtrsim r_c$. It should be noted that the actual form of the potential (4) is of no importance whatever for the foregoing estimates.

3. We have so far not taken into account the thermal fluctuations of the soliton lattice. We shall show now that they do not change the qualitative picture of the loss of order, but can lead to a substantial renormalization (more accurately, increase) of r_c. Since r_c is determined by comparing the pinning energy $W(r)$ with the elastic energy K, we must calculate $W(r)$ and K with account taken of the thermal fluctuations. It will be shown below that in the case of strong thermal fluctuations the renormalized potential of the interaction with the defects always becomes Gaussian; in the case of weak fluctuations, however, we return to Eqs. (5) and (6), which do not depend on the form of the potential. In the study of the thermal renormalizations it is therefore convenient to choose this potential right away in Gaussian form. As a result we have a Hamiltonian in the form

$$H=\int d^2r\left\{\frac{1}{2}K(\nabla u)^2+\sum_k\delta(\mathbf{r}-\mathbf{r}_k)V_0\sum_n\exp\left(-\frac{1}{2}\left(\frac{2\pi}{\Delta_0}\right)^2(u-x+n)^2\right)\right\}. \qquad (7)$$

Here $\Delta_0=l_0/l$, and the soliton-lattice periods are set equal to 1. The potential of the defects in (7) is a set of barriers randomly placed at the points r_k. The potential barrier in (7) can be represented in the form

$$V_0\Delta_0\frac{1}{\sqrt{2\pi}}\sum_m\exp\left(-\frac{m^2\Delta_0^2}{2}\right)\exp(2\pi im(u-x)). \qquad (8)$$

In contrast to the random field previously considered in the XY model,[6,7] all the harmonics p to $m\sim 1/\Delta_0$ are contained in (8). The expansion (8) always contains the first harmonic (the "magnetic field") which decreases more slowly upon renormalization than the higher harmonics.[10] The presence of the random magnetic field upsets the order in the lattice. Clearly, this is due not to the concrete shape of the barrier but to its localization in the region $\sim l_0$.

We average over the defects, just as in Refs. 6 and 7, by the replica method.[11] Expanding the partition function in powers of $V_0\Delta_0/T$ and averaging of the defects we can obtain the effective pinning potential. A contribution different from a constant appears in the second order and is of the form

$$\frac{V_0^2}{T}\Delta_0c\sum_{\alpha\neq\beta}\sum_m\exp\left(-\frac{1}{4}\left(\frac{2\pi}{\Delta_0}\right)^2(u_\alpha-u_\beta+m)^2\right). \qquad (9)$$

Here α and β are the replica indices. Expression (9) contains only terms that are linear in the defect density c. The higher-order corrections are small if $\Delta_0c\ll 1$, i.e., if the probability of the appearance of two defects in a region of size l_0 is low. This condition is not critical for our present results, but simplifies the analysis. After averaging over the impurities we can follow the standard renormalization-group transformation procedure.[10] Assuming next the number of replicas to be zero,[11] we obtain equations for the effective pinning potential W and for Δ:

$$d\Delta^2/d\xi=T/2\pi K,\quad \Delta(0)=\Delta_0, \qquad (10)$$

$$dW/d\xi=W(1-T/8\pi\Delta^2K),\quad W(0)=V_0(\Delta_0c)^{1/2}. \qquad (11)$$

Here $\xi=\ln r$, where r is the renormalized cutoff parameter. Equation (10 for the barrier width is obtained directly after integrating over the short-wave part u. The first term in (11) is connected with the change of scale, and the second can be obtained by stipulating conservation of form of the potential barrier. No renormalization of K takes place in this problem, in analogy with the situation in Ref. 7. The cause is the character of the defects, which are analogous to the phase fluctuations in the XY model. It follows from (10) and (11) that

$$W=V_0(c\Delta_0)^{1/2}(\Delta_0/\Delta)^{1/2}r, \qquad (12)$$

$$\Delta^2=\Delta_0^2+\frac{T}{2\pi K}\ln r. \qquad (13)$$

We see that the effective potential W of pinning by defects increases almost linearly with increasing size of the region. Thus, the thermal fluctuations of the soliton lattice lead to an increase of the effective thickness of the soliton ($\Delta>\Delta_0$) and to a decrease of the characteristic pinning energy $W(r)$ (the potential relief is partly smoothed out by the fluctuations). It can be seen from (12) and (13) that the thermal effects become substantial at $T\gtrsim T^*$, where $T^*\approx 2\pi K\Delta_0^2/\ln(K/V_0(c\Delta_0)^{1/2})$. At $T^*\ll T\ll T_{\text{melt}}\sim K$ the correlation radius $r_c(T)$ is determined with the aid of (12) (in analogy with the derivation of (6) for r_c) and is equal to

$$r_c(T)\approx\frac{K}{V_0(c\Delta_0)^{1/2}}\left(\frac{T}{2\pi K\Delta_0^2}\ln r_c\right)^{1/4}\simeq r_c(T/T^*)^{-1/4}, \qquad (14)$$

where r_c is defined in (6). Thus, at $T^*\ll T\ll K$ the soliton-lattice correlation radius is substantially larger than at $T\lesssim T^*$ (satisfaction of the condition $T^*\ll K$ is ensured by the smallness of $\Delta_0\ll 1$).

It must be noted that real soliton lattices are anisotropic,[3] but the anisotropy of the elastic properties and the difference between the periods of these lattices in different directions leads only to anisotropy of r_c and does not change its dependence (14) on c, V_0 and Δ_0.

In the derivation of the expression for $W(r)$ we used a power expansion in $V_0\Delta_0/T$. The qualitative estimate (5), however, hsows that this does not bound "from below" the temperature interval in which the results are applicable. On the other hand, no account was taken here of dislocations, meaning that the estimate (14) will be valid at $T\ll K$. Allowance for dislocations leads to a decrease of r_c at $T\lesssim K$.

We not also that the procedure used in this paper permits investigation of fluctuations of a $2D$ domain wall on account of pinning by defects on going from commensurate to an incommensurate phase.[12]

In the experiment, the subdivision of the crystal into regions will lead to an increase of the diffraction relfections.

According to (14), this width will increase like $c^{1/2}$. This result can be checked by experiment.

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