Lattice on Lattice in Two Dimensions

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Abstract

We study a harmonic triangular lattice, which relaxes in the presence of a weak, short-wavelength periodic potential. Monte Carlo simulations reveal that the elastic lattice has only short-ranged positional correlations, despite the absence of defects in either lattice. Long-range orientational order, however, persists in the presence of the background. Our results provide an alternative explanation for the hexatic glass phase observed in high-temperature superconductors, magnetic bubble lattices, and charge density waves in semiconductors.

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Vortex lattices in superconductors [1, 2], magnetic bubble lattices in ferromagnetic films [3], charge density waves [4] and Wigner crystals in semiconductors [5], are examples of elastic lattices which exist in a periodic potential having a much smaller period, and a different symmetry. In these systems, it is reasonable to treat the atomic lattice as static, since its elastic moduli are much larger than those of the large-scale lattice. It is widely believed that when the interaction between the two lattices is weak, crystalline order in the elastic lattice may be destroyed as a result of defects in either of the two lattices. The main purpose of this letter is to show that, rather surprisingly, no disorder in the atomic lattice is required to destroy translational long-range order in a defect-free elastic lattice. We perform Monte Carlo simulations of a two dimensional harmonic “lattice on lattice” system, in which the background lattice is static and defect-free, in order to learn the effect such a background has on translational and orientational order. We find that after the elastic lattice is cooled slowly to temperature zero, translational correlations are short-ranged, but that long-range orientational order persists. It follows that results of recent experiments [1, 3, 4] on elastic lattices subject to a background can be understood without appealing to defects in these quenched disorder in the underlying atomic lattice.

A fundamental observation of Halperin and Nelson [6] is that in disordered two dimensional lattices, orientational order is more robust than translational order. Consequently, there is a hexatic phase with short range translational order, but extended correlations in the orientation of local crystallographic axes. Two kinds of hexatic phase have been studied to date. The first appears in the theory of two-dimensional melting. As is known [7, 8], in two dimensions, true long-range translational order exists only at zero temperature. At low temperatures translational correlations exhibit power-law decay, while orientational order is long-range. Above the Kosterlitz-Thouless temperature [9], dislocation pairs dissociate into free dislocations [9, 10], and the solid melts into a hexatic phase [6] in which translational correlations decay exponentially with distance, while orientational correlations decay as a power law. Above the Halperin-Nelson temperature, dislocations (which are equivalent to pairs of disclinations) dissociate into free disclinations, which transforms the hexatic...
phase into a true liquid, with both translational and orientational correlations decaying exponentially.

A different kind of hexatic phase appears in the presence of quenched disorder at zero temperature, as in random pinning of such structures as vortex lattices, magnetic bubble lattices, and charge density waves, by defects in the underlying atomic lattice. Larkin [11, 2] demonstrated that quenched disorder, no matter how weak, destroys long-range translational order. The Imry-Ma theorem [12] generalizes this observation to assert that any long-range order described by a continuous-symmetry order parameter is destroyed by arbitrarily weak static random forces, below five dimensions. It was noticed later, however, that orientational order is more stable with respect to quenched randomness than is translational order [13]. At low temperatures it decays as a power law, leading to a solid phase called a hexatic glass [14]. The existence of this phase has been firmly established in vortex lattices of high-temperature superconductors [1], in magnetic bubble lattices [3], and in charge density lattices in semiconductors [4]. There is also reason to believe that at low temperatures, rare gas monolayers on solid substrates [15, 16], and two-dimensional Wigner crystals in semiconducting heterojunctions [5], also exist in the hexatic glass phase.

There is a vast literature on computer simulations of two-dimensional lattices in the presence of thermal disorder [17]. Simulations of the effect of quenched randomness have been less systematic and are limited to magnetic systems [18, 19, 20]. In this letter we report a numerical study of translational and orientational correlations in a triangular lattice of $10^4$ sites, subject to a weak periodic potential representing a quadratic lattice of much higher spatial frequency.

We consider a two dimensional triangular net of “particles” coupled by a harmonic, nearest-neighbour interaction. Let $a_1, \ldots, a_6$ be the basis vectors for the lattice, i.e., $a_1 = (a, 0), a_2 = (a/2, \sqrt{3}a/2)$, etc. The position of each particle in the ideal lattice is denoted by $r_i$, with $i = 1, 2, \ldots, N$; ($N$ is the total number of sites). The position of the i-th particle in the deformed lattice is $Y_i = Y(r_i)$, and the corresponding displacement is
\[ u_i = u(\mathbf{r}_i) = \Upsilon(\mathbf{r}_i) - \mathbf{r}_i. \] The potential energy of the lattice is purely harmonic:

\[
U_{\text{latt}} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{6} \{ a_j \cdot [ u(\mathbf{r}_i + \mathbf{a}_j) - u(\mathbf{r}_i)] \}^2.
\] (1)

(All quantities are dimensionless in our formulation; \( a = 1 \) in simulations.) The particles are subject to a periodic potential having the symmetry of a square lattice,

\[
V(x, y) = S \cos(kx) \cos(ky),
\] (2)

where \( 2\pi/k << a \). The interaction energy then becomes

\[
U_{\text{int}} = S \sum_{i=1}^{N} \cos\{ k[x_i + u_x(\mathbf{r}_i)] \} \cos\{ k[y_i + u_y(\mathbf{r}_i)] \}.
\] (3)

The translational correlation function is \[^3\]

\[
g_G(R) = \langle e^{iG \cdot [u(\mathbf{r}_i + R) - u(\mathbf{r}_i)]} \rangle = \langle \cos\{ G \cdot [u(\mathbf{r}_i + R) - u(\mathbf{r}_i)] \} \rangle,
\] (4)

where \( G \) is a reciprocal lattice vector and the average is taken over all sites. The angle brackets denote an equilibrium average, in the case of finite-temperature systems. For the lattice on lattice problem at zero temperature, they denote an average over initial configurations (at a certain temperature) as well as an average over noise during the ensuing cooling process. (Thus we are not particularly interested in the ground state of the system, but rather in typical configurations into which the lattice becomes frozen.) The orientational correlation function is defined as \[^3\]

\[
g_6(r) = \langle e^{i6[\theta(\mathbf{r}_i) - \theta(\mathbf{r}_j)]} \rangle = \langle \cos\{ 6[\theta(\mathbf{r}_i) - \theta(\mathbf{r}_j)] \} \rangle,
\] (5)

where \( r = |\mathbf{r}_i - \mathbf{r}_j| \) and \( \theta_i \) is the angle between \( \Upsilon(\mathbf{r}_i + \mathbf{a}_1) - \Upsilon(\mathbf{r}_i) \) and the x-axis.

We briefly review some exact results of elastic theory for the continuum limit of our discrete model, Eq. (1), in the absence of any background. In the continuum limit, the triangular lattice is described by an isotropic elastic tensor involving two constants \[^{21}\]

\[
U_{\text{latt}} = \frac{1}{2} \int d^2 r \left( 2\mu u_{\alpha\beta} u_{\alpha\beta} + \lambda u_{\gamma\gamma}^2 \right),
\] (6)
where
\[ u_{\alpha\beta} = \frac{1}{2} \left[ \frac{\partial u_{\alpha}}{\partial r_{\beta}} + \frac{\partial u_{\beta}}{\partial r_{\alpha}} \right] \quad (7) \]
is the strain tensor, \( \alpha, \beta = \{x, y\} \). (In Eq (6) repeated indices are summed over.) Comparison with the long-wavelength expansion of Eq (4) reveals that \( \mu = \lambda = \frac{\sqrt{3}}{2} a^2 \). Analysis of the continuum version of our model along the lines of Ref.[6] yields for the translational correlation function at the first Bragg point, \( G = 4\pi/a\sqrt{3} \),
\[ g_T^G = 1/R^n \quad (8) \]
with
\[ \eta = \frac{32\pi}{9\sqrt{3}} T \quad (9) \]
A similar analysis of the orientational correlation function yields \[ g_6 = \exp \left( -\frac{9\Lambda^2}{8\pi\mu T} \right) \quad (10) \]
where \( \Lambda \) is the ultraviolet cutoff. For \( \Lambda \sim 2\pi/a \) this gives
\[ \ln(g_6) \sim -3\sqrt{3}\pi T \quad (11) \]
These results will be used to test our numerical method.

Our main goal is to compute translational and orientational correlation functions in the presence of the underlying incommensurate, rapidly oscillating, periodic potential, Eq(2). This potential represents a highly non-linear contribution to the energy, and is not readily amenable to analytical treatment. One might suppose that it mimics some of the effects of a random background, in that the potentials affecting sites separated by more than a few lattice spacings are essentially uncorrelated. It may be useful, therefore, to compare our results with the predictions of a model with quenched randomness, i.e., an interaction of the form
\[ U_{\text{int}} = \sum_i f(\mathbf{r}_i) \cdot \mathbf{u}(\mathbf{r}_i) \quad (12) \]
where $f_\alpha(r_i)$ is a Gaussian random force with standard deviation $\sigma$. Continuum elastic theory [14] predicts that translational correlations are approximately Gaussian in form, $g^f_G(R) \approx \exp[-(R/\xi)^2]$, with

$$\xi \approx \sqrt{27/14\pi\sigma^{-1}} \tag{13}$$

at the first Bragg point. Orientational correlations are predicted to decay as a power law, $g^f_6(R) = 1/R^{\eta_6}$, with $\eta_6 = 3\pi\sigma^{-2}$. It is of course not clear that static disorder can be used to model the effects of the incommensurate periodic background. In any case one might suppose that a random potential would be more pertinent than the simple (but solvable) random force model. Although there is no reason to expect a Gaussian form for the translational correlation function in the presence of a random potential, the scaling of the correlation length, $\xi \propto 1/\sigma$ can be derived on the basis of a more general Imry-Ma type argument.

In our simulations we considered lattices with both periodic and open boundaries. The former systems were rhomboid in form, with $M \leq 100$ lattice sites to a side; the latter were hexagonal, with $M \leq 60$. In the open-boundary systems we compute correlation functions over the interior only, i.e., for sites at least $M/2$ distant from the edge. We computed the translational correlation function, Eq. (4), for two reciprocal lattice vectors, both of magnitude $4\pi/\sqrt{3}$, making angles of $30^\circ$ and $90^\circ$, respectively, with $R$, which lies along a principal lattice axis. In what follows we report on $g_G$ only for the former orientation; the results for the other orientation are very similar.

The model is simulated via the usual Metropolis procedure for a system in equilibrium at temperature $T$. At each step, a particle is selected at random and subjected to a trial displacement, in a random direction, and with a random magnitude, uniform on [0,$D$]. (We take $D = \max[2T, 0.05]$.) The move is accepted if the total change in energy $\Delta E \leq 0$. If $\Delta E$ is positive the new position is accepted only with probability $e^{-\Delta E/T}$. In studies of lattices subject to a background potential, the simulations begin at a temperature $T \approx S$, the strength of the background. Then the temperature is gradually reduced, typically over a series of ten steps, each consisting of about $10^3$ lattice updates, before the system is permitted to relax at temperature zero for several thousand lattice updates. (A “lattice
update” represents one trial displacement, on average, per particle.) For background potential strength \( S = 0.2 \), for example, we used the temperature sequence: \( T = 0.2, 0.13, 0.09, 0.06, 0.04, 0.25, 0.17, 0.12, 0.008, 0.005 \), each for 1400 lattice updates, followed by 3500 lattice updates at \( T = 0 \). The number of lattice updates per temperature step was sufficient that by the end of that step, the energy had reached an essentially constant value. We have also performed some preliminary studies using a continuously decreasing temperature. Correlation functions are computed in the final state.

As a check on our simulation method, we first consider the well-understood case of a harmonic lattice at finite temperature, in the absence of any background potential. Periodic systems with \( M = 100 \) (\( 10^4 \) sites), and open systems with \( M = 60 \), (\( N = 10621 \) sites), were studied in five independent realizations at temperatures ranging from 0.02 to 0.2. The results were independent of the boundary conditions. The mean elastic energy \( \langle U_{\text{latt}} \rangle = NT \) as required by equipartition. Fig. 1 shows correlation functions for temperatures 0.05 and 0.2.; the initial decay in the translational correlation function is well-described by a power law, \( g_G \approx Ar^{-\eta} \), as predicted by elastic theory, Eq(8). Power law decay of the positional correlations is observed at all of the temperatures studied, with \( \eta/T = 6.6 \pm 0.1 \), while theory gives 6.45 for this ratio. The orientational correlation \( g_6 \), also shown in Fig. 1, attains an essentially constant value \( \overline{g_6} \) after a few lattice spacings. \( \overline{g_6} \) is an exponentially decreasing function of temperature, as predicted by elastic theory, with \( -\ln \overline{g_6}/T = 17.3 \). Eq(11) yields 16.3 for this ratio, but this prediction depends on the value one takes for the cutoff \( \Lambda \), which is not precisely known. Thus the agreement between theory and simulation for the thermal case is quite satisfactory.

We studied systems subject to the potential \( V(x, y) \), with the coupling \( S \) ranging from 0.02 to 0.5, averaging in each case over 10 independent realizations. A snapshot of a typical zero-temperature configuration (Fig. 2), shows that while local positions are clearly disordered, the crystallographic directions are well-defined and globally correlated. Examples of correlation functions obtained for systems with open boundaries are shown in Fig. 3. The correlations decay fastest at small \( r \), which is incompatible with the Gaussian form
predicted for the random force model. In fact, the positional correlations are reasonably well-described by a simple exponential. The associated correlation length does not appear to follow any simple scaling with $S$, but if we identify $S$ with $\sigma$ in the random force model, then Eq (13) yields the correct order of magnitude: $\xi_{\text{rf}} = 39.2$, $\xi_{\text{sim}} = 24.7$, for $S = 0.02$; $\xi_{\text{rf}} = 7.8$, $\xi_{\text{sim}} = 10.7$, for $S = 0.1$. As in the thermal case, $g_6$ attains a steady value after a few lattice spacings. While the random force model predicts power-law decay of orientational correlations, we note that, the decay is very slow, i.e., $\eta_6 \approx 3S^2/2\pi \approx 0.1$ for $S = 0.5$, the largest value considered. Comparison of the correlation lengths and of $\overline{g_6}$ for the two wave numbers studied ($k = 39.984$, and $k = 20.0$), reveals no significant dependence upon $k$. We note that for the larger wavenumber, the potential energy per particle is $-S$, even for the smallest $S$-values studied, while for $k = 20$ saturation does not occur until $S \geq 0.1$. This indicates that for the larger wavenumber there is a potential minimum sufficiently near a particle’s equilibrium position that all particles can reach such a minimum.

We also studied harmonic lattices with periodic boundaries, subject to a background potential, as above, in systems of length $M = 100$, with $k = 39.984$. Positional correlations (Fig. 4) now decay more slowly than an exponential, but faster than a power law; for $r$ not too large they are well-represented by a “stretched exponential,” form, $g(r) = \exp[-ar^\beta]$. The decay rate $a$ is proportional to the potential strength $S$, while the exponent $\beta$ decreases with $S$ (for $S = 0.05$, $\beta = 0.71$; for $S = 0.2$, $\beta = 0.55$). Repeating the $S = 0.1$ study on a larger system ($M = 160$) yielded essentially identical results. As in the obc simulations, orientational correlations are essentially independent of $r$ beyond a few lattice spacings; $\overline{g_6}$ is in fact independent of the boundary conditions. We have also found stretched exponential decay of translational correlations in systems with open boundaries, when the temperature is decreased continuously. The correlation length is comparable to that obtained for step-wise cooling, and long-range orientational correlations persist. (A systematic investigation of cooling rate effects will be published elsewhere [22].) We stress that while the precise form of the translational correlation function depends on the cooling schedule and boundary
conditions, the appearance of hexatic order is independent of such details.

We propose the following scenario for the loss of translational order. As it is cooled in the periodic background potential, certain regions of the elastic lattice become frozen. Since the background is incommensurate with the elastic lattice, local order is reduced in the frozen regions. Moreover, these regions are well-separated, so that particle positions are not correlated between them. This does not preclude the presence of long-range orientational order. Thus we find that disorder typical of a hexatic glass may emerge in an elastic lattice, cooled in the presence of an underlying atomic lattice, even in the absence of quenched disorder. This provides an alternative explanation for recent experiments on such elastic lattices, and suggests that the hexatic phase is the generic low temperature state of such systems.

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References

[1] C.A.Murray et al., Phys. Rev. Lett. 64, 2312 (1990); C.A.Bolle et al., Phys. Rev. Lett. 66, 112 (1991); D.G.Grier et al., Phys. Rev. Lett. 66, 2270 (1990).

[2] For a recent review on vortex lattices see G.Blatter, M.V.Feigel’man, V.B.Geshkenbein, A.I.Larkin, and V.M.Vinokur, Rev. Mod. Phys., to appear.

[3] R.Seshardi and R.M.Westervelt, Phys. Rev. Lett. 66, 2774 (1991); Phys. Rev. B46, 5142 (1992).

[4] H.Dai, H.Chen, and C.M.Lieber, Phys. Rev. Lett. 66, 3183 (1991); H.Dai and C.M.Lieber, Phys. Rev. Lett. 69, 1576 (1992).

[5] E.Y.Andrei et al., Phys. Rev. Lett. 60, 2765 (1988).

[6] B.I.Halperin and D.R.Nelson, Phys. Rev. Lett. 41, 121 (1978); D.R.Nelson and B.I.Halperin, Phys.Rev. B19, 2457 (1979).

[7] L.D.Landau and E.M.Lifshitz, Statistical Physics, Part I, (Pergamon,1986), p. 432.

[8] N.D.Mermin, Phys. Rev. 176, 250 (1968).

[9] J.M.Kosterlitz and D.J.Thouless, J. Phys. C6, 1181 (1973); Prog. Low Temp. Phys. 7B, 371 (1978).

[10] V.L.Berezinskii, Zh. Eksp. Teor. Fiz. 59, 907 (1970) [Sov. Phys.-JETP 32, 493 (1971); 61, 1144 (1971) [34, 610 (1971)].

[11] A.I.Larkin, Zh. Eksp. Teor. Fiz. 58, 1466 (1970) [Sov. Phys.-JETP, 31, 784 (1970)]; A.I.Larkin and Yu.N.Ovchinnikov, J. Low Temp. Phys. 34, 409 (1979).

[12] Y.Imry and S.Ma, Phys. Rev. Lett. 35, 1399 (1975).

[13] E.M.Chudnovsky, Phys. Rev. B33, 245 (1986).
[14] E.M. Chudnovsky, Phys. Rev. B40, 11355 (1989); 43, 7831 (1991).

[15] S.E. Nagler et al., Phys. Rev. B32, 7373 (1985).

[16] N. Greiser et al., Phys. Rev. Lett. 59, 1706 (1987).

[17] For a review, see K.J. Strandburg, Rev. Mod. Phys. 60, 161 (1988).

[18] R.A. Serota and P.A. Lee, Phys. Rev. 34, 1806 (1986); J. Appl. Phys. 61, 3965 (1987).

[19] B. Dieny and B. Barbara, Phys. Rev. B41, 11549 (1990).

[20] R. Dickman and E.M. Chudnovsky, Phys. Rev. B44, 4397 (1991).

[21] L.D. Landau and E.M. Lifshitz, Theory of Elasticity (Pergamon, New York, 1970).

[22] E.M. Chudnovsky and R. Dickman, in preparation.
Figure Captions

Fig. 1 Translational (□) and orientational (+) correlations in harmonic lattices with open boundaries, at finite temperature. Upper set: \( T = 0.05 \); lower: \( T = 0.2 \). The straight lines represent power-law fits to the translational correlation functions.

Fig. 2. Snapshot of a frozen configuration in a background potential of strength \( S = 0.1 \), open boundaries.

Fig. 3. Translational (□) and orientational (+) correlations in a harmonic lattice in the presence of a background potential, \( T = 0 \), open boundaries. Upper set: \( S = 0.05 \); lower: \( S = 0.5 \). The straight lines represent exponential fits to the translational correlation functions.

Fig. 4. Translational (□) and orientational (+) correlations in a harmonic lattice in the presence of a background potential, \( T = 0 \), periodic boundaries. Upper set: \( S = 0.05 \); lower: \( S = 0.2 \). Solid lines represent stretched exponential fits to the translational correlation functions.