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Mobility of a driven elastic lattice in an incommensurate background

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Abstract. Using Monte Carlo simulations, we study the mobility of a harmonic triangular lattice subjected to an incommensurate short-wavelength potential and a steady driving force. At zero temperature ($T = 0$) the mobility jumps from zero to a finite value at a critical force F_c. For $T > 0$ the mobility shows Arrhenius behaviour, and grows exponentially with driving force before saturating at the free-particle limit for $F > F_c$. We find no evidence of a sharp depinning transition at finite temperature. This suggests that observations of depinning of charge-density waves, and the irreversibility line in high-temperature superconductors, may simply represent the onset of detectable motion on laboratory timescales, rather than an underlying phase transition.

1. Introduction

Wigner crystals [1], charge-density waves [2], atomic monolayers on crystal surfaces [3], magnetic bubble lattices [4], and vortex lattices in superconductors [5] are all examples of elastic lattices weakly coupled to an incommensurate background. It is of interest to study the mobility of an elastic lattice subjected to a background potential, under a steady driving force, since this model captures some of the key features of these systems, in particular the depinning of charge-density waves, and the irreversibility line in high-temperature superconductors. As one crosses the irreversibility line in the temperature–magnetic field plane, the response of a superconductor changes from hysteretic to reversible, due to a drastic increase in vortex mobility. In the presence of a current, the Lorentz force drags the vortices through the dissipative background, causing Ohmic resistance.

At low temperatures, and in the absence of pinning or a driving force, vortices form a triangular lattice. Random pinning destroys long-range translational order [6], leading to a vortex glass [7], in which translational correlations are expected to decay algebraically [8], while (hexatic) orientational order persists on a larger scale [9, 10]. In this immobile, low-temperature phase, the vortex is fixed to the pinning background. At higher temperatures, (i.e., above the irreversibility line, T_{IR}), there is a mobile phase that may be liquid-like. Topological defects, however, are largely absent in well-annealed systems at moderate to high magnetic fields [5].

Two scenarios have been suggested for the irreversibility line [11]. In one the vortex lattice melts at T_{IR}; above this temperature the shear modulus is zero, and vortices are mobile, since the random background does not pin individual vortices. Alternatively, it is possible that the lattice is preserved on a large scale even above the irreversibility line, and

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that it simply depins and becomes mobile when $T > T_{IR}$. Some experiments point to a first-order transition at the irreversibility line, which has been interpreted as the melting of an ordered flux-line lattice [12]. Other observations suggest that the irreversibility line and melting are distinct phenomena [13]. Recent molecular dynamics simulations in two dimensions [14] allow a role for both scenarios: they show melting [15–17] at the irreversibility line in the limit of zero pinning, and a crossover to thermally activated depinning of individual vortices, rather than a phase transition, for strong pinning. Simple arguments based on an 'effective shaking temperature', and simulations of the Langevin equation, indicate that when the driving force exceeds a critical value (well above the depinning threshold), long-range translational order is restored to the vortex lattice [18]. This view has been challenged by Giamarchi and Le Doussal, who argue that a moving glass state, free of topological defects, characterizes driven lattices in the presence of disorder [19]. The plastic flow regime has recently been studied in the absence of pinning by Braun *et al*, who solve the time-dependent Ginzburg–Landau equations numerically [20].

In addition to simulations of the relatively realistic models mentioned above, interest in the depinning transition has also prompted study of simpler models. An example is a driven elastic string in a random potential. Simulations at zero temperature demonstrated the existence of a threshold driving force below which the string is pinned, and above which it is mobile [21]. In this work we employ Monte Carlo simulations to study a minimal model of a defect-free, driven elastic lattice in a static, incommensurate background potential. (Because each particle is connected to its nearest neighbours—and only to its nearest neighbours—by a harmonic spring, it is not possible for defects such as dislocations to form.) In addition to its simplicity, our choice of a defect-free lattice is motivated by experimental decoration pictures showing remarkably large regions free of dislocations. Since the background potential is incommensurate with the unstrained lattice, well-separated regions of the latter experience essentially uncorrelated potentials, and it seems reasonable to expect that our model captures the main effects of a truly random potential. We address the question of whether a transition between low- and high-mobility phases is suppressed in the absence of defects. At zero temperature we find a sharp depinning transition at a critical force $F_c(0)$. For finite temperatures, by contrast, the mobility grows exponentially with the driving force before saturating when $F > F_c(0)$, and shows Arrhenius temperature dependence. There is no evidence of a sharp transition for $T > 0$. Because of the very rapid increase in mobility with driving force F, and with temperature, our results permit one to define an effective depinning line, $F_c(T)$, below which the mobility appears to be zero on the timescale of the simulations.

It should be stressed that our model can afford only a qualitative description of pinned vortex lattices, as it employs a harmonic lattice rather than a logarithmic interaction between vortices, and a short-wavelength periodic background, rather than a random pinning potential. We believe that the observed phenomenology is quite robust, however, and will persist for a wide variety of interactions. Indeed the effective depinning line, $F_c(T)$, obtained from our simulations is qualitatively similar to that observed in experiment and in molecular dynamics simulations [18]. In section 2 we introduce the model and simulation method. Our results are presented in section 3.

2. Model

We consider a two-dimensional triangular lattice of particles coupled by a harmonic, nearest-neighbour interaction, and subjected to a periodic potential and a uniform external force. In an earlier study of the model (without the driving force) [10], we found short-

range translational correlations and long-range orientational correlations, as predicted [9] and observed [5] for pinned flux-line lattices of high-temperature superconductors. Let $\boldsymbol{x}_i = (x_i, y_i)$ denote the position of particle i. For systems with open boundaries, the potential energy is

$$E = \frac{\kappa}{2}\sum_{\langle i,j\rangle}(r_{i,j}-a)^2 + \sum_{\langle i,j\rangle} u_{HC}(r_{i,j}) + S\sum_i \cos k_x x_i \cos k_y y_i - F\sum_i x_i \tag{1}$$

where the first two sums run over all nearest-neighbour pairs in the triangular lattice, $r_{i,j} = |\boldsymbol{x}_i - \boldsymbol{x}_j|$, and $u_{HC}(r)$ is a hard-core potential, infinite for $r < 1/2$, and zero otherwise. All quantities are dimensionless in our formulation. The simulations employ $\kappa = 2$, $a = 1$, and $k_x = k_y = 40$. (The hard-core contribution is included to prevent severe distortions of the lattice under a large driving force.) The third term in equation (1) represents a static periodic potential having the symmetry of a square lattice, and hence incommensurate with the triangular lattice. (The wavelength, $2\pi/k_x \simeq 0.157$, of the background potential is small compared to the elastic lattice spacing.) Our choice of parameters corresponds to the weak-pinning regime in which the translational (Larkin–Ovchinnikov) correlation length is large compared to the lattice constant, as we have demonstrated previously [10].

We simulated lattices of M particles to a side; both periodic and open lattices were studied. The former were rhomboid in form, the latter hexagonal. It is important to note that in the periodic case, the background potential (the third term in equation (1)) is unaltered: we simply provide particles at an edge of the central cell with their full complement of neighbours. (A particle on the rightmost edge, for example, interacts with the periodic images of two particles on the leftmost edge.) In periodic systems the driving force $F\hat{\boldsymbol{x}}$ is nonconservative, and cannot be represented as in equation (1), by the gradient of a potential. (This situation is familiar from studies of driven systems [22].) Study of periodic systems is motivated by a desire to rule out edge sites as special promoters of movement. In fact we find minimal difference between the mobilities for the two kinds of boundary.

In each step of the simulation, a particle is selected at random and subjected to a trial displacement uniform on a square of side D, symmetric about the origin. The move is accepted if the total change in energy $\Delta E \leqslant 0$; if ΔE is positive the new position is accepted with probability $\mathrm{e}^{-\Delta E/T}$. Our time unit comprises one attempted move per particle. While the Metropolis algorithm employed here is well suited to sampling an equilibrium ensemble, its application to dynamics requires some comment. Clearly all inertial effects are absent, as is appropriate to the strong-damping limit, in which velocity $\boldsymbol{v} = \boldsymbol{F}_{net}/\eta$, where η is the friction coefficient. Monte Carlo simulations are widely employed for studying polymer dynamics [23], and are equally valid for studying the motion of the vortex lattice, which is also strongly damped.

A related issue is the choice of D, which controls the step size, but has no obvious physical analogue. On general grounds, one would prefer to keep D fixed during a particular series of studies, and in any case small compared to the lattice spacing $a = 1$. Very small values of D will lead, on the other hand, to a slow, inefficient simulation. Another aspect bearing on the choice of D arises from consideration of single-particle motion in the tilted sinusoidal potential, $U(x) = S\cos kx - Fx$, at temperature zero. A classical particle is trapped in a well for $F < F_0 = kS$. But in a Monte Carlo simulation with finite displacements, the motion becomes unbounded at a force somewhat smaller than F_0, because acceptance of a displacement depends only on the energy difference between the initial and final positions. Thus it is possible for the particle to hop over a barrier of width less than D. To minimize this effect, we must limit the magnitude of D. For $D = 0.02$ and $k = 40$, the values used in our studies, the actual force, F^* required for escape is only

1% smaller than F_0. Since the step size is small compared to the lattice constant, it is also considerably smaller than the Larkin–Ovchinnikov correlation length.

Since D is fixed, the velocity saturates, and the mobility is $\propto 1/F$ for large F. To eliminate this artifact of the simulation method, we report *normalized* mobilities:

$$\mu = V_{CM}/F\mu_0 \tag{2}$$

where V_{CM} is the mean centre-of-mass (CM) velocity along the direction of the driving force, and μ_0 is the *free-particle* mobility in our algorithm:

$$\mu_0 = \frac{1}{F}\left\{\frac{D}{8} - \frac{T}{DF}\left[\frac{T}{F} - \left(\frac{T}{F} + \frac{D}{2}\right)\mathrm{e}^{-DF/2T}\right]\right\}. \tag{3}$$

This expression is derived by considering a single particle moving in the potential $-Fx$, and undergoing random displacements with an x-component uniform on $[-D/2, D/2]$. Displacements with $\Delta x > 0$ are always accepted. At $T = 0$ all displacements with $\Delta x < 0$ are rejected, so the mean displacement is $\langle \Delta x \rangle = D/8$. For $T > 0$, displacements with $\Delta x < 0$ are accepted with probability $\exp[F\,\Delta x/T]$. Dividing the mean displacement per move by the driving force F yields equation (3).

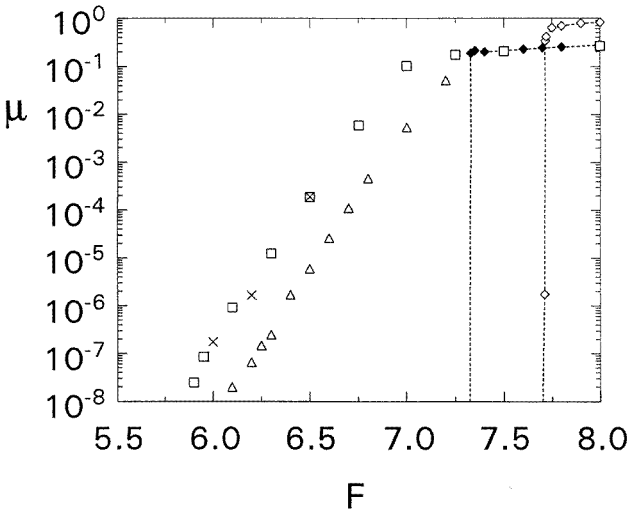

Figure 1. The mobility against the driving force; $S = 0.2$. Open diamonds: single particles, $T = 0$; filled diamonds: lattice ($M = 10$, periodic boundaries), $T = 0$; △: single particles, $T = 0.001$; □: lattice, $T = 0.001$, $M = 10$; ×: the same, except that $M = 20$.

3. Simulation results

We studied the CM motion of the driven harmonic lattice for background strengths S = 0.05, 0.1, and 0.2. Most of our results are for periodic systems of $M^2 = 100$ particles. Since we found good agreement between mobilities obtained with different system sizes ($M = 20$, 60—see figure 1), and with different boundary conditions, we used $M = 10$ (with periodic boundaries), since this permits longer simulations for a given cpu time. In order to eliminate transient effects, each study at given S, T, and F extended to a time $\geqslant 3 \times 10^6$, and in some cases (for very small mobilities), up to 5×10^7. We monitored

the mobility, and the elastic and potential energies, allowing us to identify and discard data reflecting the initial, nonsteady phase of the motion.

Our main results are for the steady-state normalized mobility μ. We begin by contrasting the mobility of an isolated particle with that of the lattice (see figure 1). At temperature zero, the mobility jumps from zero to a finite value as the force is increased beyond a critical value. For a single particle, the effective barrier to motion disappears at force F^*, as discussed above. The zero-temperature *lattice* mobility also exhibits a jump, but at a significantly smaller force, $F_c(0) = 1.70$, 3.525, and 7.31, for $S = 0.05$, 0.1, and 0.2, respectively. (Thus $F_c(0)/S \approx$ constant.) The incommensurate background potential is less effective in pinning the lattice, since, due to elastic forces, not all particles sit at local potential minima, even at $T = 0$. The lattice, that is to say, 'floats' over the incommensurate background, and at any moment certain particles are able to move in response to a driving force $F > F_c(0)$. Their displacement can then induce their neighbours to move. At larger values of the force (i.e., for $\mu \geqslant 0.1$), the single-particle mobility exceeds that of the lattice, as elastic forces begin to impede the motion. At finite temperature both the single-particle and lattice mobilities show an exponential dependence upon force, $\mu \propto \exp(-\Delta V/T)$, as expected for thermally activated transitions over a barrier $\Delta V \propto F_c(0) - F$. Again the lattice shows a substantially greater mobility than single particles, because the background is incommensurate with the unstrained lattice.

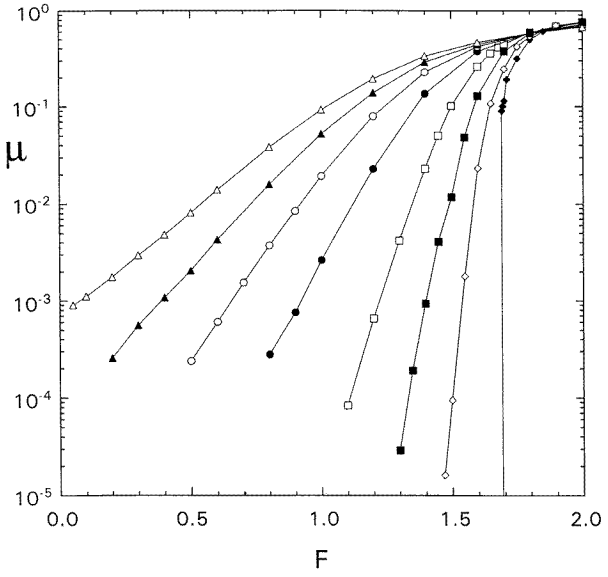

Figure 2. The mobility against the driving force for the background strength $S = 0.05$, and open boundaries. The temperatures, from right to left, are: 0, 2×10^{-4}, 5×10^{-4}, 0.001, 0.002, 0.003, 0.004, 0.005.

The dependence of the mobility on the driving force for a series of temperatures is illustrated in figure 2, which is for $S = 0.05$. (We obtained qualitatively similar results for $S = 0.1$ and 0.2.) At finite temperatures there is a regime in which the mobility depends exponentially on the force, $\mu \propto \exp(cF/T)$. As F is increased beyond $F_c(0)$, there is a smooth approach to the limiting free-particle mobility, $\mu = 1$. The dependence of the mobility on the temperature at fixed F is shown in figure 3, which confirms the Arrhenius

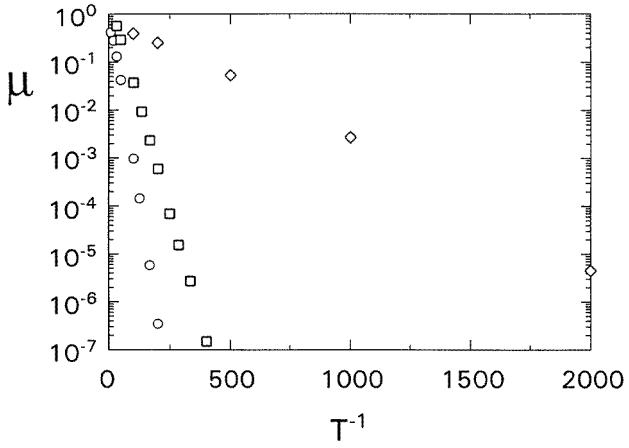

Figure 3. The mobility against the reciprocal temperature for $S = 0.1$ and fixed driving force. ○: $F = 0.5$; □: $F = 1.5$; ◇: $F = 3.0$.

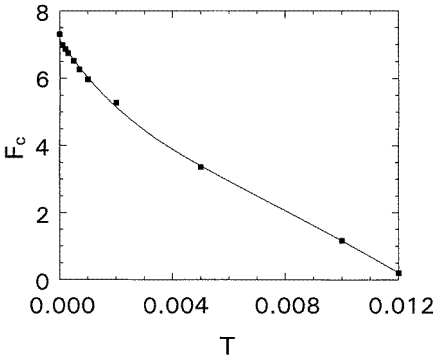

Figure 4. The critical force against the temperature for $S = 0.2$, and periodic boundaries.

behaviour noted above.

An outstanding question in the study of flux lattices is the existence of a sharp transition in mobility at nonzero temperatures. In the present study we only observe a sharp transition from a strictly immobile lattice to nonzero mobility at zero temperature. The exponential dependence of μ upon F (at finite temperatures) does however imply that over a narrow range of driving force there will be a change from a small (but nonzero) mobility to an absence of any apparent displacement of the centre of mass on simulation timescales. If we define a 'temperature-dependent critical force' $F_c(T)$ such that for $F < F_c(T)$, the lattice is motionless over an interval of 5×10^6 steps (comparable to the duration of our simulations); the resulting critical force approaches the zero-temperature value smoothly as $T \to 0$. (Observations extending over considerably longer intervals reveal that the mobility is not strictly zero, but rather is extremely small. Not surprisingly, for F well below $F_c(T)$ our longest runs show no displacement. But we have no evidence of a departure from the exponential dependence of mobility on force.) The critical force $F_c(T)$ decreases rapidly with increasing temperature, as shown in figure 4. The qualitative dependence of the critical force on temperature is quite similar to that observed in experiments on flux

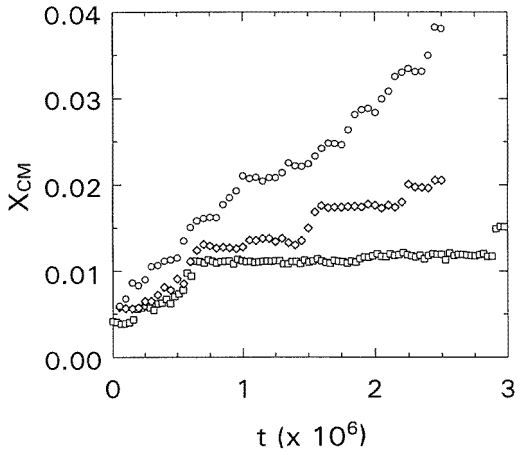

Figure 5. The centre-of-mass motion for $S = 0.2$, $T = 5 \times 10^{-4}$, and (bottom to top) $F = 6.60$, 6.61, and 6.65.

lattices in superconductors. When F is well above the critical force, we observe steady motion of the lattice. But for $F \gtrsim F_c(T)$, the motion is erratic, consisting of a series of jumps by individual particles or small groups, separated by periods during which the lattice is immobile (see figure 5). Our results pertain to low temperatures, as may be seen by noting that if our energy unit (the elastic coupling times the square of the lattice constant) is taken as of the order of the Fermi energy e_F, then $k_B T \leqslant 0.005 e_F$. In any event, $k_B T$ represents the smallest energy scale in our model.

In summary, we have studied the dynamics of a pinned elastic lattice subject to a steady driving force. There is a sharp depinning transition at zero temperature, while at finite temperatures we observe thermally activated collective motion. Due to the sensitive dependence of mobility on driving force, one may define an effective critical force $F_c(T)$ for motion on observational timescales. Our results indicate that a depinning line similar to that observed in high-temperature superconductors can be found in a model free of defects. This supports the assertion that depinning need not correspond to a phase transition.

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