Depinning phase transitions in 2D lattice Coulomb solids.

Søren Hattel and Joseph Wheatley*
Interdisciplinary Research Centre in Superconductivity, University of Cambridge, Madingley Road Cambridge, CB3 OHE, United Kingdom.
(Received 26 July 1994)

Collective depinning transitions in Coulomb solid-on-a-lattice systems are investigated in the low charge density limit. It is argued that depinning occurs at an inverted, continuous, dislocation unbinding transition of the Halperin-Nelson type. The depinning transition temperature is shown to be linear in the charge density, with a slope which is in good agreement with recent Monte Carlo simulations.

In this paper we discuss the thermodynamics of depinning phase transitions in 2D Coulomb solids where the charges are constrained to move on a regular background lattice. This problem arises in Josephson junction arrays in a magnetic field, for example. Josephson junction arrays where capacitance and screening effects are negligible can be modelled using a frustrated XY model.[1] The vortex degrees of freedom in this model interact at long distances via a 2D Coulomb interaction $V(r) = -e^2 \log r$ and the model maps, approximately, onto a lattice Coulomb gas. At sufficiently low temperatures and weak frustration (small vortex or charge density ρ_0), vortices on a square grid form a nearly hexagonal vortex solid, closely related to the Abrikosov lattice of continuum Ginzburg-Landau theory.

Teitel and co-workers[2] have recently discussed the 2D lattice Coulomb gas in the small ρ_0 limit, and associated the behavior of this model with the London limit of Ginzburg-Landau theory. In the dilute limit the low energy excitations of this system are expected to approach those of a 2D continuum Coulomb solid. These consist of a gapless transverse (shear) mode, with a plasma gap for longitudinal excitations. The gapless transverse mode is sufficient to guarantee that the Mermin-Wagner theorem[3] applies. Accordingly, true translational long range order (LRTO) is not possible, although algebraic translational order, corresponding to power law singularities in the structure function about Bragg vectors, and long range orientational order, do exist. These persist up to a 2D melting transition at $T = T_m$. The 2D melting transition may be first order or of the Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) dislocation mediated type[4,5]. In the latter case, an additional "hexatic" phase with power law orientational order was predicted by Halperin and Nelson[5].

This picture must be modified at finite values of ρ_0 because a finite energy barrier exists for moving a vortex through one lattice constant due to interaction with it's neighbours. Halperin and Nelson[5] also discussed 2D solids on a periodic substrate. They pointed out that a periodic substrate changes the universality class of the model and leads to a phase with true long range translational order at low temperature. For sufficiently weak periodic potentials, a phase transition from "epitaxial" or "floating" solid phases exists, the former characterized by LRTO, the latter by algebraic translational order. A 2D melting transition occurs at a second critical temperature. For strong substrate potentials the "floating solid" phase with algebraic order is absent, and $T_p = T_m$.

Franz and Teitel[2] observed that this picture describes their simulations of the 2D lattice Coulomb gas at low charge density. For $\rho_0 \lesssim \frac{1}{25}$ they found a phase transition to a floating phase at $T_p \propto e^2\rho_0$ while the melting temperature (vanishing orientational order) remains density independent[6] at $T_m = 0.0066e^2$. The upper transition (T_m) was found to be weakly first order. Distinct melting and depinning transitions has also been observed in the 2D frustrated XY model[7]. The situation is summarised in Fig. 1.

The purpose of this paper is to give an explicit derivation of the depinning or floating phase transition for a dilute lattice Coulomb gas. We argue that the transition is of the KTHNY type, not first order, at least in the limit of small ρ_0. We verify that the T_p is linear in ρ_0 in the dilute limit, and estimate its' slope.

At zero temperature the Coulomb solid forms an approximately hexagonal net[8] with solid lattice sites $\{\mathbf{R}\}$

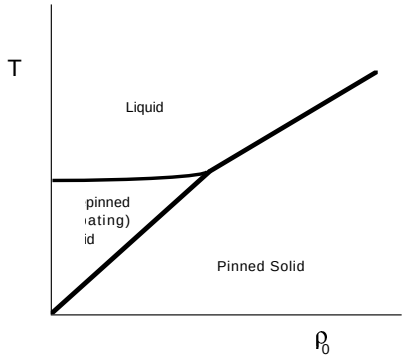

FIG. 1. Schematic phase diagram showing melting and depinning lines in the charge-density-temperature plane.

and lattice constant a_0 ($\rho_0 = \sqrt{\frac{4}{3}}a_0^{-2}$). Thermally excited displacements $\mathbf{R} \to \mathbf{R} + \mathbf{x_R}$ are constrained to belong to a square background grid, with lattice constant equal unity, i.e. $x^\alpha_{\mathbf{R}} =$ integer where α labels the x and y components. The partition sum is:

$$Z = \sum_{\{\mathbf{m_R}\}=-\infty}^{\infty} \int \prod_{\mathbf{R}} d\mathbf{x_R} e^{-S},$$

where the "action" S is,

$$S = -\frac{1}{T}\frac{e^2}{2}\sum_{\mathbf{R}\neq\mathbf{R}'} \log \mid \mathbf{x_R} + \mathbf{R} - \mathbf{x_{R'}} - \mathbf{R}' \mid + \frac{1}{T} e \sum_{\mathbf{R}} \phi \mid \mathbf{R} + \mathbf{x_R} \mid + 2\pi i \sum_{\mathbf{R}} \mathbf{m_R} \cdot \mathbf{x_R}. \quad (1)$$

The sums over integers $m^\alpha_{\mathbf{R}}$ impose the integer constraints on the $x^\alpha_{\mathbf{R}}$. $\phi(r)$ is the potential of a uniform neutralising background charge density; $\nabla^2\phi(r) = 2\pi e\rho_0$.

In common with the continuum case, the lattice Coulomb gas Eq. 1 has a finite 2D melting temperature T_m. Well below T_m it is usual to assume that the free energy density can be expanded keeping fluctuations up to quadratic order only. It will be verified later that this assumption is valid below T_p in the dilute limit. Fourier transforming the $\mathbf{x_R}$, and in terms of the Coulomb lattice dynamical matrix D, ($\sum_k$ denotes the hexagonal zone integral $\frac{1}{(2\pi)^2}\int d^2k$) we have,

$$Z = \sum_{\{\mathbf{m_R}\}=-\infty}^{\infty} \int \prod_{\mathbf{k}} d\mathbf{x_k} \exp\left\{ -\frac{1}{2}\sum_{\mathbf{k}} x^\alpha_{\mathbf{k}} D^{\alpha\beta}(\mathbf{k}) x^\beta_{\mathbf{k}} + 2\pi i \sum_{\mathbf{R},\mathbf{k}} m^\alpha_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}} x^\alpha_{\mathbf{k}} \right\} \quad (2)$$

The Coulomb solid dynamical matrix D is

$$D^{\alpha\beta}(\mathbf{k}) = -\sum_{\mathbf{R}\neq 0} \cos \mathbf{k}\cdot\mathbf{R} \left(\frac{\delta^{\alpha\beta}}{\mid \mathbf{R} \mid^2} - 2\frac{R^\alpha R^\beta}{\mid \mathbf{R} \mid^4} \right) - \pi\rho_0\delta^{\alpha\beta} \quad (3)$$

This model does not have a melting transition, which does not occur when only quadratic fluctuations about equilibrium are retained. However we show below that the non-linearity implied by the constraint in Eq. 2 does give rise to a depinning phase transition from a low temperature phase with LRTO to a high temperature phase with algebraic translational order only, in 2D.

The Gaussian integration over displacement modes $\mathbf{x_k}$ can be carried out to obtain an effective action for integer variables $\{\mathbf{m}\}$. After doing this, the partition sum takes the form $Z = Z_0(T)\sum_{\{\mathbf{m}\}} \exp -S[\{\mathbf{m}\}]$ where $Z_0(T)$ is the contribution of harmonic fluctuations. $Z_0(T)$ is non-singular and contributes a constant specific heat. The effective action is,

$$S[\{\mathbf{m}\}] = 2\pi^2 T \sum_{\mathbf{R},\mathbf{R}'} m^\alpha_{\mathbf{R}} \psi^{\alpha\beta}(|\mathbf{R} - \mathbf{R}'|) m^\beta_{\mathbf{R}} \quad (4)$$

where the interaction,

$$\psi^{\alpha\beta}(\mathbf{R} - \mathbf{R}') = \sum_{\mathbf{k}} (e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} - 1) \times \left[\omega_T^{-2}(\mathbf{k}) P_T^{\alpha\beta}(\mathbf{k}) + \omega_L^{-2}(\mathbf{k}) P_L^{\alpha\beta}(\mathbf{k}) \right] \quad (5)$$

In writing Eq. 5 we have imposed the charge neutrality conditions $\sum_R m^\alpha_R = 0$. $P_T^{\alpha\beta}(\mathbf{k})$ and $P_L^{\alpha\beta}(\mathbf{k})$ are the transverse and longitudinal mode projectors respectively for the hexagonal Coulomb solid. The corresponding eigenvalues are $\omega_T^2(\mathbf{k})$ and $\omega_L^2(\mathbf{k})$. The square roots of the eigenvalues are shown in Fig. 2.

We approximate these quantities by their short-wavevector forms up to the wavevector cutoff $\mid \mathbf{k} \mid < k_0 = \sqrt{4\pi\rho_0}$ corresponding to the Coulomb lattice zone area. Thus $P_T^{\alpha\beta}(\mathbf{k}) = \delta^{\alpha\beta} - \frac{k^\alpha k^\beta}{k^2}$, $P_L(\mathbf{k}) = \frac{k^\alpha k^\beta}{k^2}$, the shear mode is $\omega_T^2(\mathbf{k}) = \frac{1}{8}e^2 a_0^{-2} k^2$ and the plasma mode is $\omega_L^2(\mathbf{k}) = 2\pi e^2\rho_0$. Substituting these approximate forms into Eq. 5 we obtain,

$$S[\{m\}] \simeq 4\pi T \frac{a_0^2}{e^2} \sum_{R\neq R'} m^\alpha_R m^\beta_{R'} [-\log(|R - R'|)\delta^{\alpha\beta} + \frac{(R-R')^\alpha (R-R')^\beta}{|R-R'|^2} + \epsilon_c \delta_{R,R'}\delta^{\alpha\beta}] \quad (6)$$

This is the action of a 2D vector plasma, identical in form to that of a dislocation plasma in a 2D solid. This model is known to show a dislocation unbinding phase transition[5]. However, the temperature in Eq. 6 is inverted relative to the dislocation problem. Thus the "locations" $\{\mathbf{m}\}$ proliferate at low temperature, in a phase where the background lattice structure is important, and are confined at high temperature, when the lattice structure is expected to become unimportant. In this sense locations have the opposite effect to dislocations; they serve to order rather than disorder the lattice. The core energy term in Eq. 6 is,

$$\epsilon_c \simeq \log k_0^{-1} + 1 \quad (7)$$

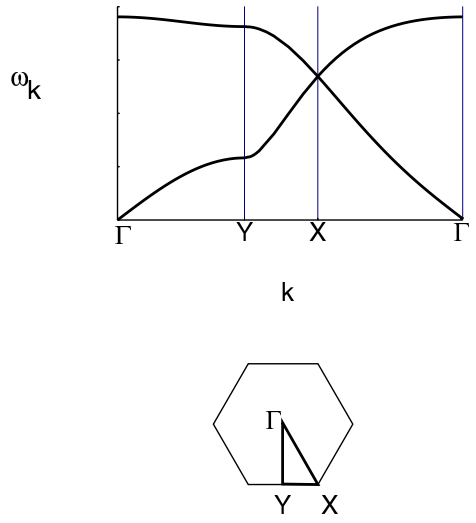

FIG. 2. Normal modes of a two dimensional hexagonal Coulomb lattice along symmetry directions.

The first term in the core energy Eq. 7 derives from the transverse fluctuations and becomes large in the low density limit. The density independent contribution to ϵ_c derives from the longitudinal (plasma) mode, and is unimportant in the low density limit.

The location binding transition corresponds to the transition between long range and algebraic order of the Coulomb solid. To show this we need to know the relation between the displacement and the location correlators. It follows from Eq. 2 that the transverse component (denoted $\langle \ldots \rangle_t$) of the displacement correlator is,

$$\langle x_k x_{-k} \rangle_t = \frac{1}{\tilde{\beta} k^2} - (2\pi)^2 \frac{\langle m_k m_{-k} \rangle_t}{(\tilde{\beta} k^2)^2} \tag{8}$$

where $\tilde{\beta} = \frac{1}{8} e^2/(T a_0^2)$. The small wave-vector behavior of the correlator $\langle m_k^\alpha m_{-k}^\beta \rangle$ can be obtained by applying Debye-Huckel theory to the vector plasma, which closely parallels the discussion for the scalar case[9]. The result is,

$$\langle m_k m_{-k} \rangle_t = \frac{1}{(2\pi)^2} \tilde{\beta} k^2 \frac{y}{\tilde{\beta} k^2 + y} + O(k^4) \tag{9}$$

which shows the expected suppression of long wavelength fluctuations. Here y is the fugacity of the location plasma. Combining Eqs. 8 and 9 we find,

$$\langle x_k x_{-k} \rangle_t = \frac{1}{\tilde{\beta} k^2 + y} \tag{10}$$

The binding transition leads to a phase with zero fugacity[4]. In the present case, the transition is inverted relative to the dislocation problem. The low temperature phase has $y > 0$ while the high temperature phase has vanishing fugacity. Thus the transverse displacement fluctuation Eq. 10 is *screened* below T_p. Screening cuts off the logarithmic growth of correlations i.e. for large r, $\langle (x_r - x_0)^2 \rangle \approx C e^{-\sqrt{\frac{y}{\beta}} r}$. Thus the structure function is

$$\frac{1}{N} \langle \rho_{Q+q} \rho_{-Q-q} \rangle \sim \sum_R \exp \left\{ i \mathbf{q} \cdot \mathbf{R} - \frac{1}{2} Q^2 C e^{-\sqrt{\frac{y}{\beta}} R} \right\}$$
$$\sim N \delta_{q,0}$$

in the vicinity of a Bragg peak Q. In other words true LRTO is present below T_p. It is worth emphasizing that there are no further phase transitions above T_p within the harmonic approximation of Eq. 2.

In a 3D version of the model Eq. 2, locations proliferate at all temperatures and there is no zero fugacity phase. The absence of a phase transition in this case corresponds to the fact that a 3D harmonic solid shows LRTO at any temperature, even in the absence of pinning. Thus a 3D lattice Coulomb gas has a melting, but no depinning phase transition. Conversely, in 1D the locations are always bound by a linear Coulomb potential. In 1D pinning is ineffective in restoring LRTO and the solid has short range correlations at all finite temperatures.

Chui[10] argued that 2D vector dislocation systems show a continuous KTHNY unbinding transition only when the core energy is above a critical value. This picture was confirmed by Saito[11] who studied Eq. 6 using Monte Carlo simulation and found a first order transition only for small core energies $\epsilon_c \lesssim 1$. On this basis, the depinning transition is expected to be continuous in the low density limit, where the core energy becomes large according to Eq. 7. The large core energy results thus lead to the following numerical estimate for the depinning phase transition temperature,

$$T_p \simeq \frac{\sqrt{3}}{8\pi t} e^2 \rho_0 \approx 0.31 e^2 \rho_0 \tag{11}$$

using Saito's value $t = 0.22$.[11] This compares well with Franz and Teitel's simulation result[2] for the Coulomb gas on a triangular grid, especially for smaller values of ρ_0.

The good agreement between simulation and theory suggests that the *harmonic* solid-on-a-lattice model Eq. 2 quantitatively describes the depinning transition for the dilute Coulomb solid. Indeed the screened displacement fluctuation Eq. 10 leads to a small local mean square displacement at T_p i.e. $\langle x_R^2 \rangle \sim \frac{1}{4\pi \mathrm{e}} a_0^2 T_p \log \frac{k_0^2}{T_p y}$. Thus $\langle x_R^2 \rangle \ll a_0^2$ in the small ρ_0 limit, we are far from the Lindemann melting criterion and the harmonic approximation is justified.

Clearly the harmonic approximation fails as the depinning and melting lines approach one another as shown schematically in Fig. 1. Since the numerical evidence[2] favors a first order transition at T_m, it is natural to ask whether the depinning line becomes first order at or before the critical point $T_p = T_m$. We cannot properly address this question using the present theory. However, the density independent longitudinal mode contribution to the core energy of Eq. 7 appears to guarantee that $\epsilon_c \gtrsim 1$ up to the point critical point $T_m = T_p$ at $\rho_0 \sim \frac{1}{25}$. Thus the possibility of a continuous depinning transition up to the melting line is not ruled out by estimates based on Eq. 2.

S.A.H is supported by Carlsbergfondet. The authors wish to thank M. A. Moore and S. Teitel for helpful discussions and remarks.

---

* Also at: Cavendish Laboratory, University of Cambridge, United Kingdom.

[1] W. Shih and D. Stroud, Phys. Rev. B **28**, 6575 (1983); S. Teitel and C. Jayaprakash, Phys. Rev. B **27**, 598 (1983).
[2] M. Franz and S. Teitel, Phys. Rev. Lett. **73**, 480 (1994).
[3] N. D. Mermin, Phys. Rev. **176**, 250 (1968).
[4] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[5] David R. Nelson and B. I. Halperin, Phys. Rev. B **19**, 2457 (1979).
[6] D. S. Fisher, Phys. Rev. B **22**, 1190 (1980).
[7] S. A. Hattel and J. M. Wheatley, to be published.
[8] The hexagonal symmetry is lifted on a square background grid, but this effect is small in the low density limit and plays no role in what follows. Note that a square Coulomb lattice has a shear mode instability (negative shear modulus).

[9] See for example A. M. Polyakov, *Gauge Fields and Strings*, Harwood Academic Publishers, 1987, p. 65-68.
[10] S. T. Chui, Phys. Rev. Lett. **48**, 931 (1979).
[11] Yukio Saito, Phys. Rev. B **26**, 6239 (1982).