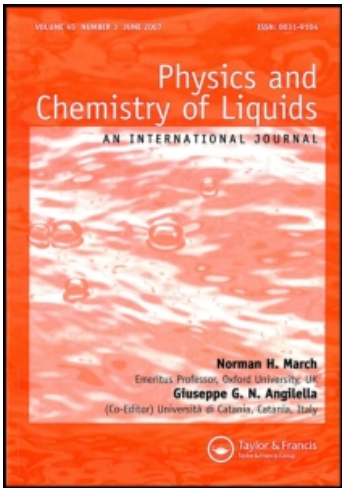

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F. Siringo[a]; M. J. Lea[b]; N. H. March[a]
[a] Theoretical Chemistry Department, University of Oxford, Oxford, England [b] Department of Physics, Royal Holloway and Bedford New College, University of London, Surrey, England

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LETTER

Self-consistent Force Constant Calculation for a Two-dimensional Wigner Electron Crystal in High Magnetic Fields, and Limitations of Lindemann's Law of Melting

F. SIRINGO*, M. J. LEA† and N. H. MARCH*

**Theoretical Chemistry Department, University of Oxford, 5 South Parks Road, Oxford 0X1 3UB, England.*

and

†Department of Physics, Royal Holloway and Bedford New College, University of London, Egham Hill, Egham, Surrey TW20 0EX, England.

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The Einstein oscillator model of the Wigner electron crystal takes a specified force constant, which is an explicit function of the electronic separation r_s. Here a method is devised for its self-consistent calculation. For the gaussian density of the Wigner oscillator, with width λ in terms of r_s, experimental data on the melting temperature T_m versus Landau filling factor ν is employed to plot the critical overlap parameter, λ_c say, versus T_m. This shows that λ_c increases as T_m decreases, which is in contrast to Lindemann's Law.

KEY WORDS: Landau filling factor, two-dimensional electron crystal, melting.

A body of work now exists on the melting of the Wigner electron crystal in zero magnetic field[1–4]. Unfortunately, no experiment is presently known in which the quantal regime of the melting curve can be explored in the laboratory. Therefore, attention has been focussing on magnetic field assisted Wigner crystallization[5]; the motivation being the recent experimental work of Andrei *et al.*[6] and Glattli *et al.*[7]. This was carried out on a GaAs–GaAlAs heterojunction in a magnetic field; the appearance of a new low frequency propagating mode is taken as a fingerprint of an electron solid. The conductivity in this new phase has the hallmarks of pinned Wigner crystallites: Bragg reflection studies have not proved feasible to date, but will eventually be required to confirm long-range order.

Because of the above motivation, we have been studying models of the melting curves of Wigner crystals in magnetic fields in 2 and 3 dimensions[8,9]. The present work focusses on the two-dimensional case. The new aspect of the investigation is to refine the harmonic oscillator model[10] and in particular to devise a method to make it self consistent, in a sense to be set out below. This treatment is then applied

to an analysis of the results of Glattli *et al.*[7], whose experiment gives data on the melting temperature T_m of the two-dimensional electron solid as a function of the Landau filling factor $\nu = nh/eB$, with B the magnetic field strength and n the density of electrons per unit area.

Turning immediately to the self-consistent approach to the Einstein model, we note first that such self-consistency is lacking in the normal procedure. This is because the spring constant $m\Omega^2$ in the harmonic potential $\frac{1}{2}m\Omega^2 r^2$ is usually written, with units of length the appropriate Bohr radius $a_b = h^2\varepsilon\varepsilon_0/\pi e^2 m$ (see below for numerical values):

$$m\Omega^2 = g/r_s^2(e^2/4\pi\varepsilon\varepsilon_0), \qquad n = (\pi r_s^2)^{-1} \tag{1}$$

where g has previously been taken as a constant which characterizes a given model. In fact Eq. (1) is valid only in the extreme low density limit, r_s tends to infinity. In general the scaling of Eq. (1) with r_s is correct but g is a somewhat complicated function of r_s and T, in addition to the magnetic field B if this is used, as here, to assist the Wigner transition.

Below, the question is raised, and answered in the affirmative, as to whether one can proceed self-consistently to a calculation of the oscillator force constant in such an Einstein description of the Wigner crystal. As already mentioned, the results are then combined with experimental data[7] on the melting temperature T_m vs. Landau filling factor ν to plot the overlap parameter λ_c (cf Eq. (13) below) corresponding to the melting transition, versus T_m.

The complete Hamiltonian for the single oscillator in 2 dimensions is

$$H = \frac{(\mathbf{p} - e\mathbf{A}/c)^2}{2m} + \tfrac{1}{2}m\Omega^2(x^2 + y^2) \tag{2}$$

Here the vector potential $\mathbf{A}$ is taken in terms of the magnitude of the field B in the z direction as $\mathbf{A} = (-By/2, Bx/2, Bx, 0)$ and we define $\omega = eB/2m$. Below we shall regard Ω^2 as a mean-field parameter which depends on the behaviour of the oscillators surrounding the one under discussion. Knowledge of Ω^2 allows the true potential felt by each oscillator to be evaluated in the harmonic approximation. The theory of March and Tosi[11] can be used in order to get the density matrix from the Hamiltonian (2). The electron density can then be evaluated, and in atomic units this can be written as

$$\rho(r, \beta) = \frac{1}{\pi\sigma^2}\exp(-r^2/\sigma^2) \tag{3}$$

where

$$\sigma^2 = \tilde{\omega}^{-1}\frac{\sinh(\beta\tilde{\omega})}{\cosh(\beta\tilde{\omega}) - \cosh(\beta\omega)}. \tag{4}$$

Here $\tilde{\omega} = [\omega^2 + \Omega^2]^{1/2}$ while $\beta = (k_B T)^{-1}$. Assuming a given geometrical structure for the crystal, and summing up over all the oscillator sites $i \neq j$ we find the density

surrounding the site j as

$$\rho_j(\mathbf{r}, \beta) = \sum_{i \neq j} \rho(\mathbf{r} - \mathbf{R}_i, \beta) \tag{5}$$

where $\mathbf{R}_i$ denote the lattice vectors.

The Coulomb repulsion energy for an electron on site j is then

$$\phi_j(\mathbf{r}) = \int d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \sum_{i \neq j} \rho(\mathbf{r} - \mathbf{R}_i, \beta). \tag{6}$$

From the rotational invariance symmetry of the crystal and in particular if the crystal is invariant under rotations through an angle $\Theta \neq 0, \pi$, then in general

$$\left.\begin{aligned} \left(\frac{\partial \phi_j}{\partial x}\right)_0 &= \left(\frac{\partial \phi_j}{\partial y}\right)_0 = 0 \\ \left(\frac{\partial^2 \phi_j}{\partial x\, \partial y}\right)_0 &= 0 \\ \left(\frac{\partial^2 \phi_j}{\partial x^2}\right)_0 &= \left(\frac{\partial^2 \phi_j}{\partial y^2}\right)_0 = \tfrac{1}{2}(\nabla^2 \phi_j)_0 \end{aligned}\right\} \tag{7}$$

Then the harmonic expansion of Eq. (6) reads

$$\phi_j(\mathbf{r}) \simeq \phi_j(0) + \tfrac{1}{4}(\nabla^2 \phi)_0 (x^2 + y^2). \tag{8}$$

This is the point now at which the model can be made self-consistent by imposing

$$\Omega^2 = \tfrac{1}{2}(\nabla^2 \phi_j)_0 = \int d\mathbf{r}' \frac{\mathbf{1}}{|\mathbf{r} - \mathbf{r}'|^3} \sum_{i \neq j} \rho(\mathbf{r} - \mathbf{R}_i, \beta). \tag{9}$$

Since for a uniformly charged 2-D layer $(\nabla^2 \phi) = 0$, we can invoke the superposition principle and we can add any constant uniform charge density to ρ:

$$\Omega^2 = \int d\mathbf{r}' \frac{\mathbf{1}}{|\mathbf{r} - \mathbf{r}'|^3} \sum_{i \neq j} \{\rho(\mathbf{r} - \mathbf{R}_i, \beta) - \rho_0\} \tag{10}$$

where ρ_0 is an arbitrary constant. In particular, the choice $\rho_0 = \sum_{i \neq j} \rho(-\mathbf{R}_i, \beta)$ removes divergence difficulties from the integration. Eq. (10) then becomes, after using Eqs. (3) and (4):

$$\Omega^2 = \sigma^{-3} \sum_i F\left(\left|\frac{\mathbf{R}_i}{\sigma}\right|\right) \tag{11}$$

where the function $F(x)$ is defined as

$$F(x) = \exp(-x^2) \int_0^\infty \frac{dr}{r^2} [\exp(-r^2) I_0(2rx) - 1]. \tag{12}$$

Here $I_0(y) = J_0(iy)$ is the Bessel function of imaginary argument.

Equations (11) and (4) provide a self-consistent way of calculating the spring

constant Ω^2 and the density $\rho(r, \beta)$ for the single oscillator. From Eq. (4) it is to be noted that the mean square displacement $\langle r^2 \rangle = \sigma^2$, and it is convenient to introduce the overlap parameter

$$\lambda = \sigma / r_s. \tag{13}$$

In Eq. (11), the quantity $\sum_i F(|\mathbf{R}_i| r_s/\lambda)$ is a function of λ only if the geometry of the crystal is fixed. If we define

$$g(\lambda) = \lambda^{-3} \sum_i F\left(\frac{|\mathbf{R}_i| r_s}{\lambda}\right) \tag{14}$$

then it follows that

$$\Omega^2 = g(\lambda)/r_s^3 \tag{15}$$

which is to be compared with Eq. (1). Evidently for a different set of variables r_s, T, B we find a different self-consistent solution and a different value of λ. The function $g(\lambda)$ is plotted in Figure 1 for the hexagonal structure, the functional dependence on λ subsuming the above variables. The calculations have also been carried out for the square lattice, and it is found that the curve in Figure 1 is relatively insensitive to structure. However the square lattice results are not plotted as this structure is known to be unstable to shear deformations in the classical limit[12]. The overlap parameter increases with increase of density and temperature, and Figure 2 shows plots of constant λ in the density-temperature plane at $B = 0$. In the classical limit r_s tends to infinity

$$\lambda^2 g(\lambda) \sim 2r_s/\beta \tag{16}$$

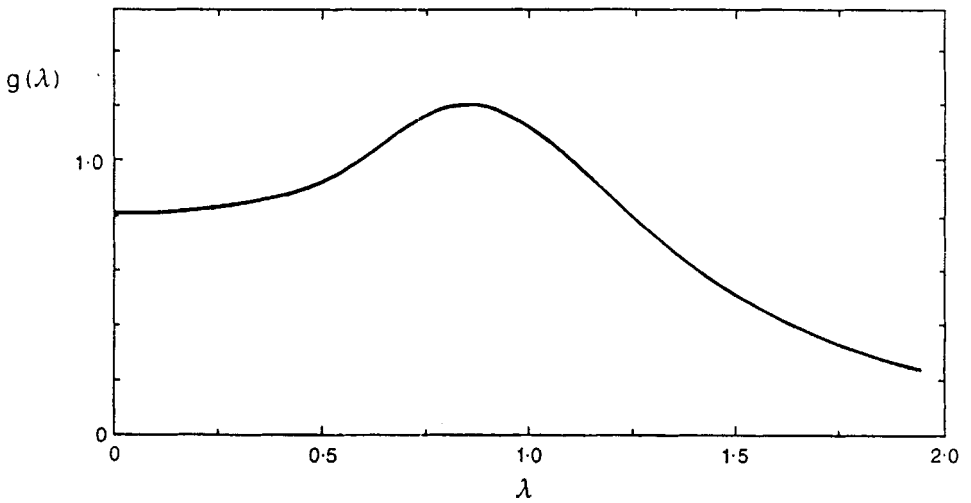

Figure 1 Spring constant characterized by $g(\lambda)$ in Eq. (1) as a function of the overlap parameter λ. Note that λ tends to zero is the classical limit corresponding to $g(0) = 0.81$ for the hexagonal lattice. The corresponding square lattice value differs by only about 1%. The large λ limit corresponds to the regime where tunnelling is important.

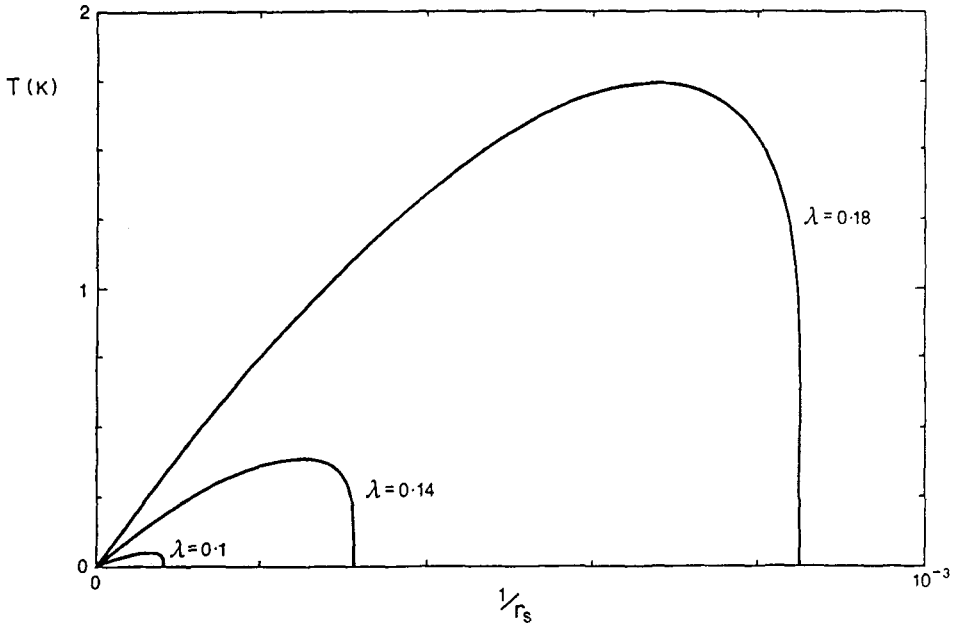

Figure 2 Shows curves of constant λ in the density-temperature plane for the case of zero magnetic field. (Actual plot is T vs. r_s^{-1} where r_s is related to the density n by Eq. (1)).

while in the limit T tends to zero the result is

$$\lambda^4 = \frac{\nu^2}{(1 + gr_s\nu^2)}. \tag{17}$$

In the case of zero field in fact one can write the implicit equation

$$\beta = \frac{r_s^{3/2}}{\{g(\lambda)\}^{1/2}} \ln\left[\frac{\lambda^2\{g(\lambda)\}^{1/2}r_s^{1/2} + 1}{\lambda^2\{g(\lambda)\}^{1/2}r_s^{1/2} - 1}\right]. \tag{18}$$

This is now the point to turn to the main focus of the paper; the influence of the Landau filling factor in relation to melting in high magnetic fields. There are various possible approaches; the one we have settled on after investigation is to utilize the experimental results of Glattli *et al.*[7] for the measured melting temperature T_m of the two-dimensional electron solid versus ν. Their melting temperature is normalized to the classical melting temperature T_{mc} given by

$$T_{mc} = e^2/\varepsilon r_s k_B \Gamma_m \tag{19}$$

where $\Gamma_m = 127 \pm 3$ has been found experimentally[13] for electrons on the surface of liquid helium. For GaAs/GaAlAs $\varepsilon = 13$ and $m = 0.067m_e$ where m_e is the free electron mass. The electron separation r_s is normalized to the Bohr radius $a_b = h^2\varepsilon\varepsilon_0/\pi e^2 m = 1.03 \times 10^{-8}$ m in this material. For a density of 10^{11}cm^{-2} this gives $r_s = 1.74$. Using the result of the present model for λ as a function of ν, T/T_{mc} and r_s,

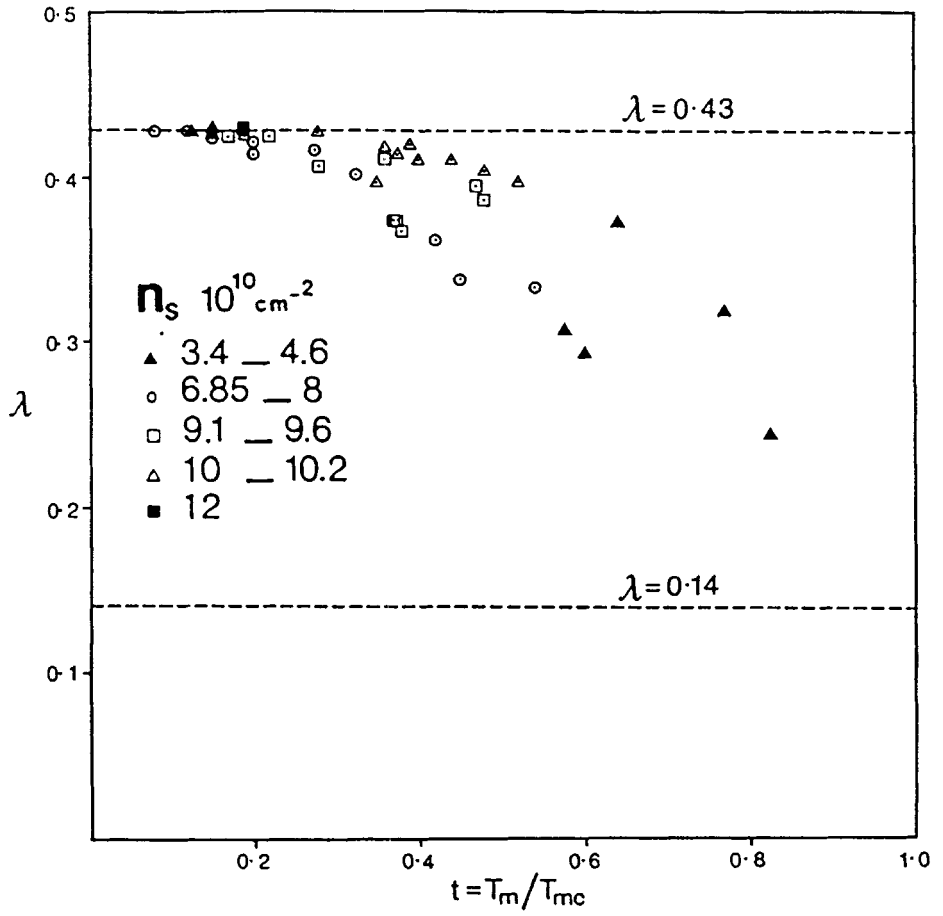

Figure 3 Shows critical overlap parameter λ_c versus reduced temperature T/T_{mc} as extracted from T versus Landau filling factor ν according to Glattli *et al*[7]. Different densities are recorded on the inset. The dashed line corresponds to the classical limiting value of 0.14 shown at $T/T_{mc} = 1$.

the critical value λ_c at melting can be derived from the phase diagram as determined by the experimental data. The classical limit, $\nu = 0$, corresponds to $\lambda_c = 0.14$; a rather low value. The definition of λ used here avoids the logarithmic singularity in the vibrational amplitude of two-dimensional crystals. Other values of λ_c derived from the work of Bedanov *et al.*[14] and Gann *et al.*[15] are 0.22 and 0.30 respectively, though the latter value may be enhanced by the logarithmic effects in their computer simulation. The melting here is thought to be a Kosterlitz–Thouless[16] transition, driven by the shear modulus and the thermal unbinding of dislocation pairs. The T_m tends to zero limit in a field occurs for $\nu = \nu_c = 0.192$ which corresponds to $\lambda_c = 0.43$. Evidently the critical λ is different for the melting of a two-dimensional classical crystal and its quantal counterpart where zero-point motion dominates. A similar conclusion was also reached by Lozovik *et al.*[17]. It is certainly worthy of note that

Ceperley's result[18] $r_W = 33$ for the melting of a two-dimensional quantal crystal in zero field also gives $\lambda_c = 0.44$ from Eq. (17). Figure 3 also shows the λ_c values obtained from the entire set of data of Glattli *et al*[7]. It can be seen that λ_c drops from the quantal value of 0.44 to the classical estimate of 0.14 as the magnetic field is increased. Hence Lindemann's Law must be transcended for two-dimensional melting in a magnetic field. It is probable that anharmonicity, not included here, plays an important role.

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