Single and Paired Point Defects in a 2D Wigner Crystal

Ladir Cândido, Philip Phillips, and D. M. Ceperley
Loomis Laboratory of Physics and NCSA, University of Illinois at Urbana-Champaign, 1100 West Green Street, Urbana, Illinois 61801-3080
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Using the path-integral Monte Carlo method, we calculate the energy to form single and pair vacancies and interstitials in a two-dimensional Wigner crystal of electrons. We confirm that the lowest energy point defects of a 2D electron Wigner crystal are interstitials, with a creation energy roughly 2/3 that of a vacancy. The formation energy of the defects goes to zero at melting, suggesting that point defects may be the melting mechanism and that the melting could be a continuous transition. In addition, we find that the interaction between defects is strongly attractive, so that most defects will exist as bound pairs.

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At sufficiently low densities, the ground state of a 2D electron gas is expected to be a Wigner crystal [1]. Quantum Monte Carlo calculations [2] predict Wigner crystal formation for $r_s \gtrsim 37$ at zero temperature where $r_s = a_W/a_0$ is the dimensionless parameter characterizing the ratio of potential to kinetic energy. QMC calculations also predict that disorder stabilizes the localized phase relative to that of the liquid [3], thereby shifting the melting boundary to higher densities, $r_s \approx 10$. In light of recent experimental observations [4–9,14–17] of a new conducting phase in 2D in the density range $10 < r_s < 37$, there is renewed interest in the properties of a dilute electron gas close to the Wigner crystal melting boundary. Yoon *et al.* [15] have observed a transition at $r_s \approx 40$ which they attribute to the melting of a Wigner crystal.

In this work, we calculate the energies of pointlike defects in a clean 2D electron Wigner crystal. The motivation for the study of defects is twofold. First, localized defects are present in a finite concentration at any nonzero temperature (they have even been speculated to exist at zero temperature as a super solid). Second, the melting process in 2D can be influenced or even determined by defect formation [18,19]. We investigate the energy of two kinds of point defects: a vacancy at one of the lattice sites or an interstitial centered in one of the triangular unit cells. We define N_{def} (the defect index) as the number of electrons minus the number of lattice sites. Using path-integral Monte Carlo (PIMC), we compute the energy to introduce defects into an N-electron crystal with $-2 \leq N_{\mathrm{def}} \leq 2$. We find that the lowest lying defect excitations are centered interstitials. Similar results have been obtained by Jain and Nelson [20] in hexagonal columnar crystals and by Cockayne and Elser [21] in the 2D Wigner crystal. This defect energy appears to vanish near melting, suggesting that the quantum melting could be continuous rather than first order. We then show that for $N_{\mathrm{def}} = \pm 2$, the defect creation energy increases as the defects are pulled apart. This indicates that the ground state for two defects is a bound pair.

The system being simulated is composed of electrons confined to two dimensions (2D) and interacting through a repulsive $1/r$ potential and immersed in a positive background with the same density. The Hamiltonian is

$$H = \frac{1}{r_s^2}\sum_{i=1}^{N}\nabla_i^2 + \frac{2}{r_s}\sum_{i<j}^{N}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + V_0\,, \qquad (1)$$

where energy is in units of the Rydberg $\hbar^2/2ma_0^2$, a_0 is the effective Bohr radius, and lengths are in units of the Wigner-Seitz radius $a_W = (\pi\rho)^{-1/2}$ and V_0 a constant.

At large values of r_s, the exchange contributions to the energy are small [2,22]. For sufficiently large r_s, $r_s > 75$, we consider distinguishable electrons and neglect antisymmetry but include it for $r_s \leq 75$. However, to keep the system stable, we forbid particle exchange by enforcing the condition $|\mathbf{r}_i - \mathbf{s}_i| < 1.1a$ where a is the nearest neighbor distance and $\mathbf{s_i}$ is the ith lattice site. Such a "tether" is realistic because in a quantum crystal exchanges are rare and the wave function is peaked around the lattice sites. We have verified the independence of our results by varying and removing this constraint. In these calculations we assumed a hexagonal lattice, shown to be the stable structure [22].

In the PIMC method [23], the density matrix

$$\rho(R_0, R_M; \beta) = \int\cdots\int dR_1\, dR_2\cdots dR_{M-1} \times \rho(R_0, R_1; \tau) \times \rho(R_1, R_2; \tau)\cdots\rho(R_{M-1}, R_M; \tau) \qquad (2)$$

for the quantum system is evaluated by sampling paths: $\{R_0, R_1\cdots R_{M-1}, R_M\}$, and $R_k = \{\mathbf{r}_{1,k}, \ldots, \mathbf{r}_{n,k}\}$ and $\mathbf{r}_{i,k}$, a bead, is the position of ith electron in the kth time slice and $\tau = \beta/M$ with $\beta = 1/k_BT$. The action $-\ln[\rho(R_{M-1}, R_M; \tau)]$ is evaluated by first splitting the potential into a long-ranged part and a short-ranged part. The long-ranged part (which is slowly varying) is handled in the primitive approximation, while the short-ranged action is the exact pair action of two electrons. To evaluate

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the $2NM$-dimensional integrals in Eq. (2), we employ the Metropolis bisection sampling technique [27]. Ewald [25] sums are used to calculate the long-ranged potential energy and pair action [26].

For lower densities where exchange is important ($r_s \leq 75$) we used restricted path integrals [10] to account for Fermi statistics. Only paths entirely in the positive region of the Slater determinant are allowed. Such a restriction is exact if the nodal surfaces of the trial density matrix are correct. For the nodes we used a Slater determinant of Gaussian orbitals $\exp[-c(\mathbf{r}_i - \mathbf{s}_j)^2]$ with $\mathbf{s}_i$ the lattice sites and c taken from [11] with a ferromagnetic spin arrangement. Calculation of the tunneling frequencies to determine the ground state magnetic ordering indicates that the magnetic energies are always much less than the defect energies [12], and that the system is nearly ferromagnetic in near melting. We find that the restriction also serves to stabilize the crystal against melting.

The energy to create N_{def} defects in a system with $N_l = N$ lattice sites is

$$\Delta E_{\text{def}} = [e(N + N_{\text{def}}) - e(N)](N + N_{\text{def}}), \quad (3)$$

where $e(n)$ is the energy per electron for a system containing n electrons with area $A = n/\rho$. The densities and temperatures studied were $r_s = 40$, 50, 75, 100, and 200 and $T = 5.0$, 2.5 and 1.25×10^{-5} Ry. We used 120 and 340 lattice sites. We performed independent PIMC calculations with a different number of particles rather than more efficient procedures where particles are inserted or removed [13]. Such differential procedures are difficult because of the combination of large relaxation of the lattice, the very large zero point motion, and the antisymmetry. Our calculations are very time consuming as the system gets larger because one needs high accuracy to obtain the energy difference, but the direct method allows better control over the systematic error.

To illustrate the types of defects of interest, we depict in Fig. 1 vacancy and centered-interstitial (CI) defects in a 2D hexagonal lattice. The initial configuration of the vacancy and CI defects have sixfold and threefold coordination, respectively. In PIMC all particles are dynamical variables, so that the surrounding lattice relaxes and may change the overall symmetry of the defect. However, the constraint makes such relaxation local. We find that the defect energy depends weakly on temperature. The following discussion concerns the defect energies for the temperature 1.25×10^{-5} Ry. This is significantly less than the melting temperature and the Debye temperature, but much greater than the magnetic energies [12].

Figure 2 demonstrates that the formation energy for an interstitial is consistently lower than creation energy for vacancies in 2D Wigner crystals at all densities. At $r_s = 75$ we find that $\Delta E_{\text{CI}} \approx 0.65 \Delta E_{\text{vac}}$. Simulations with 340 sites give agreement with the results for the smaller lattice. Jain and Nelson [20] and Cockayne and Elser [21] have obtained a similar result.

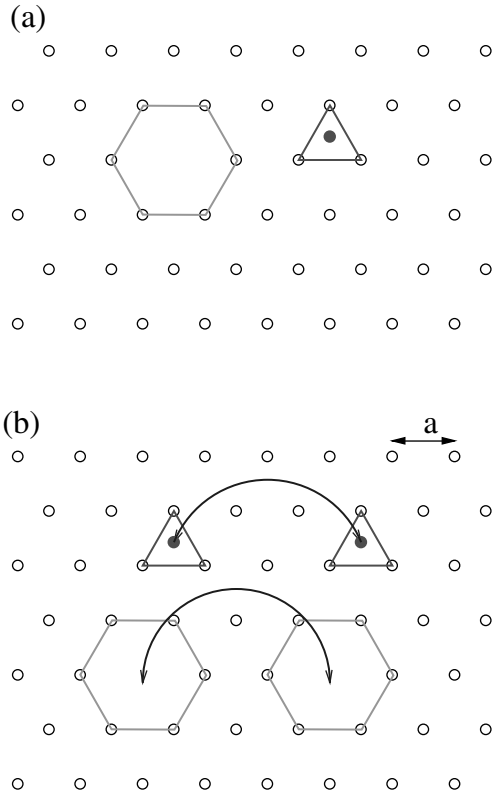

FIG. 1. a) Hexagonal 2D Wigner crystal with a single 6-coordinated vacancy and a threefold coordinated centered interstitial (CI) defect. (b) Pair vacancy and CI defects.

For a Coulomb system without fermion exchange, the energy of a defect can be expanded as

$$E_D = c_1 r_s^{-1} + c_{3/2} r_s^{-3/2} + c_2 r_s^{-2} \ldots . \quad (4)$$

The first term is the static potential energy of the defect, and the second is the harmonic energy of the defect. Cockayne and Elser [21] have done exact calculation of c_1 and $c_{3/2}$. Shown in the lower panel of Fig. 2 is the anharmonic contribution defined as the excess energy beyond the harmonic calculation. Anharmonic effects lower the defect energies to approximately half the harmonic value at $r_s = 50$. Cockayne and Elser find that the defect energy vanishes for CI defects at $r_s = 15 \pm 1$ and $r_s = 9 \pm 1$ for vacancies. We assume the exact values for c_1 and $c_{3/2}$ and fit c_2 to obtain $c_2(\text{vacancy}) = -2.8 \pm 0.2$ and $c_2(\text{CI}) = -1.85 \pm 0.15$. From these values we estimate that E_D vanishes for interstitials at $r_s = 35 \pm 2$ and $r_s = 29 \pm 2$ for vacancies. The proximity of the vanishing of the interstitial creation energy to the melting density is highly suggestive that interstitial defects play a role in the melting process. The proliferation of vacancies for $r_s < 40$ could result in a continuous rather than first order quantum melting, analogous to what happens for the classical 2D Wigner crystal. It is possible that the assumption of the ferromagnetic spin arrangement has stabilized the crystal with respect to interstitials for $35 \leq r_s \leq 40$.

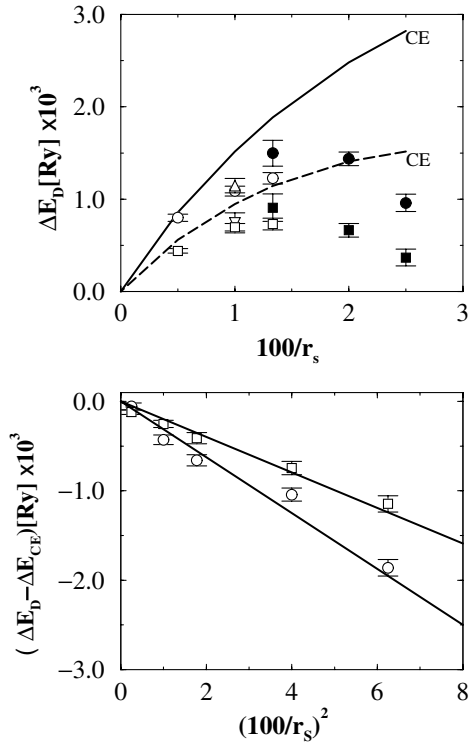

FIG. 2. Formation energy (top figure) for vacancy (circle) and CI (square) defects as a function of $1/r_s$ at a temperature of 1.25×10^{-5} Ry for a system of 120 lattice sites (open and solid symbols are for Boltzman and Fermi statistics, respectively). The triangles are results with 340 lattice sites. The lines (solid for vacancy and dashed for interstitial) are from harmonic calculations [21]. The anharmonic energy is shown on the bottom panel.

We have not considered the role of other defects such as dislocations.

We have also investigated the properties of pair defects as a function of the spacing between the defects. The geometry used for the study of the interaction energy between two defects is shown in Fig. 1b. Shown in Fig. 3 are the pair binding energies for vacancies and CI defects

$$E_{bp} = \Delta E_{\mathrm{def}}(N_{\mathrm{def}} = 2) - 2\Delta E_{\mathrm{def}}(N_{\mathrm{def}} = 1) \quad (5)$$

as a function of the separation between the defects. As expected, for large separations the binding energy goes to zero. For all separations studied, the pair-binding energy is negative, indicating an attraction between defects.

In fact, elasticity theory predicts that E_{bp} will decay as d^{-3}. For all separations studied, the pair-binding energy is negative. Similar results have been obtained by Frey, Nelson, and Fisher [28] for centered-interstitial defects in vortex crystals. The binding observed here is reminiscent of the phonon-induced electron attraction in the sense that it is more advantageous to add a defect nearby an existing defect, thereby sharing the strain field, rather than further away.

As is evident from Fig. 4, the interstitial pair binding becomes slightly positive at $r_s \approx 50$ indicating a possible weak unbinding near the melting transition. No such behavior was observed for vacancies. In two dimensions, any attraction is sufficient for the existence of a bound state of two defects. At $r_s = 100$, the binding energy for interstitials pairs is roughly 50 K, for vacancy pairs 125 K and the classical melting temperature is only 24 K (assuming the effective mass of the electrons and the dielectric constant are unity). The symmetry of this paired state will be determined by the magnetic order of the lattice and the relative exchange frequencies of the defects.

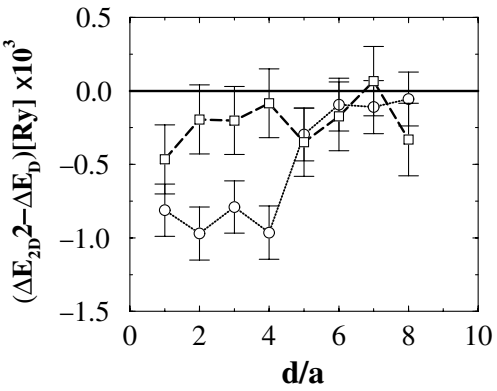

FIG. 3. Binding energy of pair defects at $r_s = 100$ and $T = 1.25 \times 10^{-5}$ Ry, computed for systems of 340 lattice sites. The geometry used to study such defects is shown in Fig. 1(b). Circles are for vacancies and squares for interstitials.

As seen in Fig. 5 the binding energy of the defect is much greater than the melting temperature, hence point defects are mainly interstitial pairs, which are likely to obey Bose statistics.

Assuming that this is the case, let us consider whether one could have a Bose condensation of defect pairs. The defect pairs are thermally activated so that their density is $\rho_{2D} = \rho_0 \exp(-E_{2D}/k_B T)$ with $\rho_0 = 1/\pi$ and E_{2D} the formation energy of a pair defect. The Brezinski-Kosterlitz-Thouless (BKT) transition occurs at a density

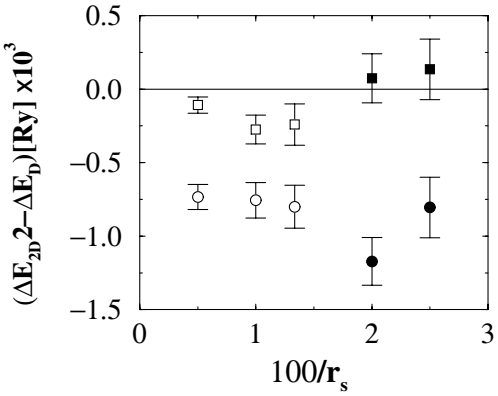

FIG. 4. Binding energy of pair defects separated by a single lattice site as a function of $1/r_s$ at $T = 1.25 \times 10^{-5}$ Ry, computed for systems of 120 lattice sites. Interstitials correspond to squares and vacancies to circles.

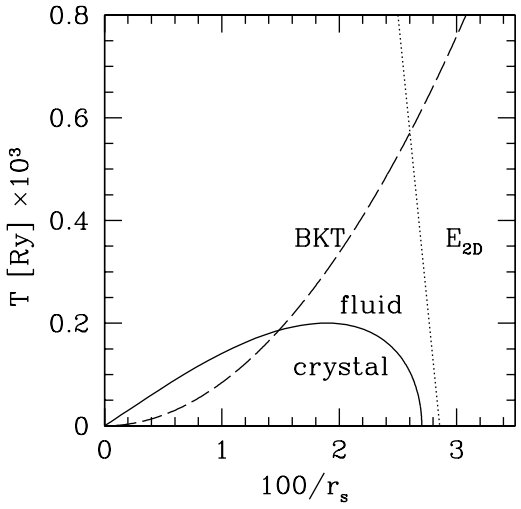

FIG. 5. Phase diagram. The solid line is an estimate of the stable region of the Wigner crystal. The dotted line indicates the energy of the paired interstitial, the dashed line the condition for the BKT transition, $E_{2D} < 0.84/r_s^2$.

$\rho_{2D}\lambda^*/k_BT \approx 0.28$ (this is scaled from the helium data [27]). A solution to these two equations exists provided that $E_{2D} < 0.42\lambda^*$. Here $\lambda^* = \hbar^2/(2m^*) < 2/r_s^2$ since the pair defects are heavier than two free electrons. Hence a necessary condition for the existence of a super-solid phase is that $E_{2D} < 0.84/r_s^2$. This condition is shown in Fig. 5. Our results indicate that the supersolid transition could occur only in the Wigner crystal very near melting and is likely to be precluded by the unbinding of pairs. Thus even making favorable assumptions, a supersolid is unlikely.

As mentioned above, we find that in a 2D Wigner crystal most defects will be bound pairs of interstitials. The conductivity is likely to be dominated by defect transport. This could explain the extreme sensitivity of the conductivity in the insulating phase [6] to an in-plane magnetic field which would cause unbinding of singlet pairs. Further simulations are needed to decide whether pairing persists in the melted phase as has been proposed by one of us [29].

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