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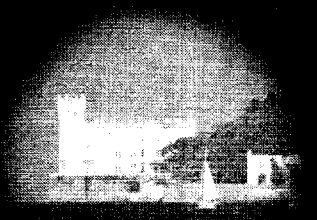

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Abstract

We estimate the formation energy of lattice vacancies in quantal Wigner crystals of charged particles near their melting point at zero temperature, in terms of the crystalline Lindemann parameter and of the static dielectric function of the fluid phase near freezing. For both 3D and 2D crystals of electrons our results suggest the presence of vacancies in the ground state at the melting density.

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It was predicted in early work of Wigner [1] that a degenerate system of electrons embedded in a uniform neutralizing background should crystallize at sufficiently low density. Such a transition has been reported from quantal Monte Carlo (QMC) simulations in dimensionality D = 3 by Ceperley and Alder [2] and in D = 2 by Tanatar and Ceperley [3] (see also Rapisarda and Senatore [4]). Most recently, Wigner crystallization in zero magnetic field has been reported for a 2D system of holes in an exceptionally clean semiconductor heterostructure [5], at a value of the carrier density which is quite close to the QMC predictions.

Theoretical studies of defects in Wigner crystals have been addressed to the triangular lattice of point charges in the extreme low-density limit [6 - 8]. The two leading terms of an expansion in inverse powers of the electron radius r_s have been obtained for the formation energy of a vacancy and of interstitial defects [8] (here r_s is the usual coupling-strength parameter, related to the particle density n and to the Bohr radius a_b by $r_s a_b = (\pi n)^{-1/2}$ in D = 2 and by $r_s a_b = (4\pi n / 3)^{-1/3}$ in D = 3). The leading term in the expansion, of order r_s^{-1} is the increase in the static Coulomb energy of the lattice upon creation of a defect, while the next term of order $r_s^{-3/2}$ derives from the change in the zero-point energy of harmonic phonons and is negative. Up to this order in the expansion there is, of course, no difference between charged bosons and electrons of equal charges and masses.

A drop in kinetic energy upon defect creation, which is evident for the 2D Wigner crystal from the above-mentioned sign of the zero-point energy change in the harmonic approximation, is a general feature of point defects in quantal solids. A kinetic energy gain is well established theoretically for vacancies in solid ^{4}He near the temperature-density melting curve, both from simple estimates of quantal fluctuations [9] and from refined variational calculations [10, 11]. These results are in accord with the appreciable concentration of vacancies which is observed in low-temperature He solids [12, 13]. Indeed, it was already proposed in the early work of Andreev and Lifshitz [14] that a vacancy in a quantal crystal should behave as a highly delocalized quasiparticle: delocalization causes the vacancy energy to spread into a band and may assist vacancy formation to the point where a finite concentration of these defects may be present even in the ground state. The dynamical consequences of a

propagating defect mode in a Bose supersolid have been elaborated in recent work by Bijlsma and Stoof [15].

In this letter we present some simple estimates of the vacancy formation energy E_v in Wigner crystals at the melting values of the coupling strength r_s. We also aim to assess the role of dimensionality (3D *vs* 2D) and statistics (electrons *vs* charged bosons). Anharmonicity of the crystal near melting is taken into account by a density functional (DF) approach invoking properties of the fluid phase near freezing, as previously developed in the study of freezing in quantal fluids [16], of lattice vibrations and elastic constants in Wigner crystals [17] and of vacancies in crystals of the two He isotopes [9].

In a DF approach the vacancy formation energy is given by the sum of an ideal kinetic energy contribution and an excess (Hartree plus exchange and correlation) energy contribution,

$$E_v = \Delta T_0 + \Delta E_{ex} \quad , \tag{1}$$

the quantities on the RHS being energy differences between the defective and the perfect crystal as determined by their respective particle density profiles.

We take the density profile of the perfect crystal as a superposition of Gaussian clouds centred on lattice sites [16] and treat its excess energy by a second-order functional expansion around the fluid phase at coexistence (see *e.g.* [17]). The expansion introduces an effective interparticle potential $v_{eff}(r)$ given in Fourier transform by

$$v_{eff}(k) = v(k)[1 - G(k)]f^2(k) \quad . \tag{2}$$

In equation (2) $v(k)$ is the bare Coulomb interaction (given by $4\pi e^2 / k^2$ in D = 3 and by $2\pi e^2 / k$ in D = 2), $G(k)$ is the so-called local field factor accounting for exchange and correlation in the static dielectric function of the fluid, and $f^2(k)$ is the Debye-Waller factor of the crystal. We have

$$f^2(k) = \exp(-k^2 < u^2 > / D) \tag{3}$$

in dimensionality D, where the mean square displacement $< u^2 >$ at melting can be expressed in terms of the Lindemann parameter L and of the first-neighbour distance d as $< u^2 >= L^2 d^2$. The QMC work on Wigner electron crystals [2 - 4, 18] yields $L \cong 0.30$; in the lack of similar data it is reasonable to assume the same value of L for charged bosons. Finally, the function $G(k)$ is known from QMC simulations for the 3D electron fluid [19], the 2D electron fluid in

both the spin-polarized (SP) and the paramagnetic (PM) state [20] and the 3D fluid of charged bosons [21]. Vacancies in the crystalline state of these systems are considered below.

We assume that the vacancy is created by extracting an atom from a site in the bulk crystal and reinserting it at a suitable surface site, where it experiences one-half of the effective interactions with its neighbours. This yields a crude estimate of ΔE_{ex} for a vacancy in a Bravais lattice structure [17],

$$\Delta E_{ex} = -\frac{1}{2}\sum_{\mathbf{G}\neq 0} n_s v_{eff}(G) \tag{4}$$

where n_s is the mean density of the crystal and $\mathbf{G}$ denotes a reciprocal lattice vector (RLV). Equation (4) should be an overestimate of the increase in excess energy on vacancy creation, since no account has been taken of the relaxation of the crystal.

A DF evaluation of the change in ideal kinetic energy would instead require solving a one-body Schrödinger equation in the self-consistent Kohn-Sham effective potential. We use again the Gaussian *Ansatz* and neglect relaxation and overlap of the Gaussian clouds to relate ΔT_0 to the average ideal kinetic energy of a particle before its extraction from a lattice site, with the result [16, 17]

$$\Delta T_0 = -\frac{\alpha \hbar^2}{2M < u^2 >} \tag{5}$$

where α = 9/4 in D =3 and 1 in D = 2. Again, equation (5) may be expected to overestimate the magnitude of the kinetic energy change, since it assumes complete delocalization of one atom per vacancy.

Our results are reported in Figure 1 and in Table 1. They have been obtained from the above mentioned data from QMC work except for the assumption $L = 0.3$ in the BCC lattice of charged bosons. We also show in the Table the magnetic state of the fluid and the value of r_s to which the data refer. These values are close to the melting density in each case.

Figure 1 presents a comparison between charged fermions and bosons in the 3D fluid state near freezing. It reports the effective potential $nv_{eff}(k)$ as a function of k, scaled by the respective lengths k_0 of the RLV's in the first star. In both cases the effective interaction in momentum space has an attractive region around the location of the first RLV star. This feature is a consequence of exchange and correlation between the charged particles and is responsible

for the fact that the values of ΔE_{ex} for vacancy formation in Table 1 are positive, in spite of the repulsive character of the bare interactions. It is also seen from the Figure that the effective interactions at the fluid-solid transition are comparatively stronger for fermions, in spite of the smaller value of their critical r_s.

Table 1 reports the numerical results for the energies involved in vacancy formation. Evidently, these estimates cannot be taken to have quantitative value. Nevertheless, they show some reasonable qualitative trends. It is seen that delocalization is comparatively more important for fermions than for bosons and in 2D than in 3D. This result is, of course, a consequence of the differences in the critical value of r_s at melting for the various Wigner crystals that we have evaluated. Therefore, given the stability of the solid phase down to the critical r_s which has been assessed from the QMC simulations for each of these systems, we should expect that lattice vacancies should be easier to form in a 2D crystal of charged fermions near melting. In fact, if we may take as significant a value of 2 or 3 for the ratio $|\Delta T_0 / \Delta E_{ex}|$ from our calculations, we would conclude that lattice vacancies are ground-state (*i.e.* zero-temperature) properties of the Wigner electron crystals near their melting density. For the BCC crystal of charged bosons instead we can only suggest that there should be a very substantial cancellation between the gain in kinetic energy and the loss in excess energy on vacancy formation. A similar result has been found for ^{4}He crystals [9 - 11].

A further feature of the numerical results in Table 1 is that there is only moderate sensitivity of the calculation of ΔE_{ex} to the input on the static dielectric function of the fluid phase. This is seen in particular from the similarity in the values of ΔE_{ex} for the triangular lattice from input on the spin-polarized or the paramagnetic fluid.

In summary, we have presented simple calculations of vacancy formation energies in quantal Wigner crystals near melting, which suggest that a finite concentration of vacancies may be a feature of the ground state at least for the triangular lattice of charged fermions. We feel that this suggestion would be worth testing by more accurate calculations in the DF approach and by quantal computer simulation studies. Experimentally, it may be possible to reveal the presence of a vacancy propagation mode by careful studies of excitation spectra and transport properties of the newly reported crystal of holes in high-quality heterojunctions. The

above-mentioned theoretical work of Bijlsma and Stoof [15] on defective Bose solids and the experimental study of Lengua and Goodkind [22] on sound waves in solid ^{4}He could be useful in this respect.

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Table 1. Energies of lattice vacancy formation in Wigner crystals near melting at T = 0

	r_s	ΔT_0 (K)	ΔE_{ex} (K)	E_v (K)
3D electrons (BCC, SP)	100	- 128	65	- 63
2D electrons (triangular, SP)	40	- 303	90	- 212
2D electrons (triangular, PM)	40	- 303	119	- 183
3D bosons (BCC)	160	- 50	44	- 6

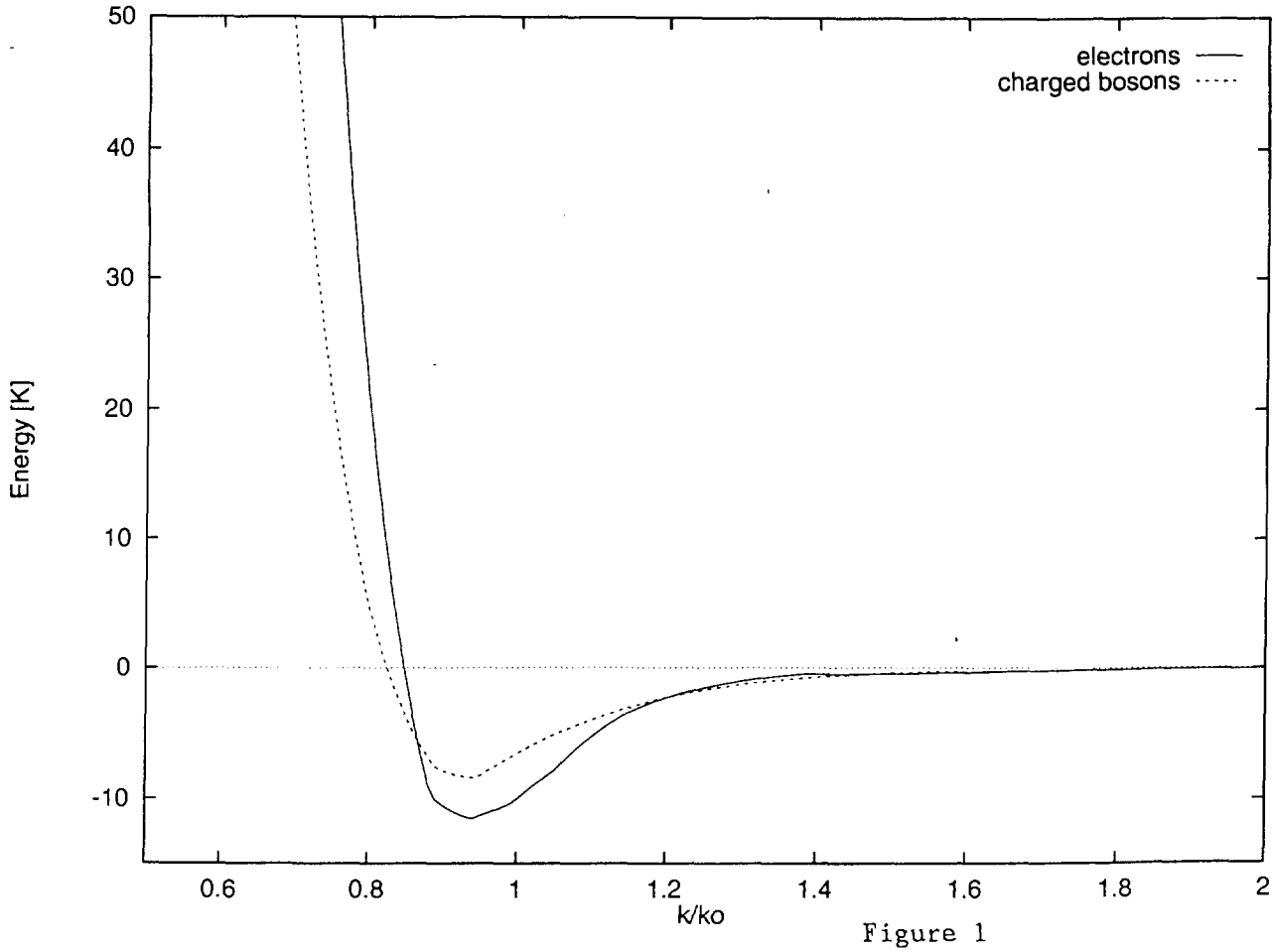

Figure 1

Effective pair potential $nv_{eff}(k)$ as defined in equation (2) (in Kelvin degrees), plotted against the reduced wave number k for the 3D electron fluid at r_s =100 (full curve) and for the 3D fluid of charged bosons at r_s = 160 (dashed curve). The wave number is scaled by the length k_0 of the first reciprocal lattice vectors in the respective BCC crystals.