Wigner Crystallization of Electrons in a One-Dimensional Lattice: A Condensation in the Space of States

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We study the ground state of a system of spinless electrons interacting through a screened Coulomb potential in a lattice ring. By using analytical arguments, we show that, when the effective interaction compares with the kinetic energy, the system forms a Wigner crystal undergoing a first-order quantum phase transition. This transition is a condensation in the space of the states and belongs to the class of quantum phase transitions discussed in [M. Ostilli and C. Presilla, J. Phys. A **54**, 055005 (2021).]. The transition takes place at a critical value r_{sc} of the usual dimensionless parameter r_s (radius of the volume available to each electron divided by effective Bohr radius) for which we are able to provide rigorous lower and upper bounds. For large screening length these bounds can be expressed in a closed analytical form. Demanding Monte Carlo simulations allow to estimate $r_{sc} \simeq 2.3 \pm 0.2$ at lattice filling $3/10$ and screening length 10 lattice constants. This value is well within the rigorous bounds $0.7 \leq r_{sc} \leq 4.3$. Finally, we show that if screening is removed after the thermodynamic limit has been taken, r_{sc} tends to zero. In contrast, in a bare unscreened Coulomb potential, Wigner crystallization always takes place as a smooth crossover, not as a quantum phase transition.

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The Wigner crystal (WC) [1], namely, the periodic arrangement of electrons that minimizes the Coulomb interaction energy in the presence of band motion effects [2], has been investigated in several long-range repulsive potential models [3–6]. Two dimensional [7–12] and one-dimensional [13,14] electron gases at zero temperature have been extensively studied from a theoretical point of view. A recent experiment succeeded in imaging an electronic WC in one-dimensional nanotubes [15].

The occurrence of a WC is often argued by comparing the typical kinetic and Coulomb energies involved. Roughly speaking, the kinetic energy can be evaluated as $\hbar^2/(2m^*r^2)$, where m^* is the effective electron mass and r the radius of the volume available to each electron, whereas the Coulomb energy can be taken as e^2/r, where e is the electron charge. These two energies have the same value when $r_s \equiv r/a_B$, a_B being the effective Bohr radius, is equal to the "critical value" $r_{sc} = 2$. Then one concludes that for $r_s > r_{sc}$ a WC must show up.

The above argument can be, however, misleading. Consider the case of the unscreened Coulomb potential in a d-dimensional space with a fixed value of r_s. For a gas of N_p electrons, the energy per particle of the *bare* d-dimensional Coulomb potential scales as ${N_p}^{d-1}$ for $d > 1$, and as $\ln N_p$ for $d = 1$ [16]. On the other hand, at any dimension d, the kinetic energy per particle is independent of N_p, so that the potential energy overwhelms the kinetic one for N_p large enough. In other words: in the thermodynamic limit (TD-lim), $r_{sc} \to 0^+$ and no quantum phase transition (QPT) takes place, the system being trivially a WC for any $r_s > 0$; for finite N_p, instead, the transition from free electron motion to WC obtained by increasing r_s is just a smooth crossover, not a QPT.

Screening is, therefore, an essential ingredient [2]: the ground-state (GS) energy per particle of the screened potential scales linearly with N_p and can fairly compete with the kinetic term. It is only in this case that we can hope to observe a QPT in the TD-lim by varying r_s.

We are not aware of any conclusive study on the phase transition nature of the Wigner crystallization, except for the work of Brascamp and Lieb on the $1d$ plasma in a neutralizing background [17]. Here, we study the ground state of a system of spinless electrons interacting through a screened $3d$ Coulomb potential in a lattice ring. By using analytical arguments, we demonstrate that, for any finite screening length, the Wigner crystallization is a QPT taking place at a finite critical value r_{sc} of the parameter r_s. For r_{sc} we provide rigorous upper and lower bounds, which can be cast in an analytical form in the limit of large screening length. The QPT that we find is of first order (according to Ehrenfest classification) and falls within the class of condensations in the space of states introduced in [18]. Demanding Monte Carlo (MC) simulations based on an advanced bias-free code [19] allow to estimate a value of

r_{sc}, which is well within the rigorous bounds. Finally, we show that, removing the screening after the TD-lim has been taken, we have $r_{sc} \to 0^+$, confirming that a nonzero minimal screening is necessary to have a realistic physical picture.

We briefly recall the mechanism of first-order QPT of [18]. To be specific, let us consider a lattice model with N sites and N_p particles described by a Hamiltonian

$$H = K + gV, \tag{1}$$

where K and V are Hermitian noncommuting operators, and g a free dimensionless parameter, which, without loss of generality, can be taken to be non-negative. Regardless of the details of K and V, we represent H in the eigenbasis of V and it is natural to call V the potential operator, and K the hopping operator. To exclude trivial behaviors, we suppose that the eigenvalues of K and V scale linearly with the number of particles N_p. Since in the two opposite limits $g \to 0$ and $g \to \infty$, the GS of the system tends to the GS of K and V, respectively, we wonder if, in the TD-lim, this transition occurs as a QPT taking place at some critical value g_c.

A quite general kind of QPT is the condensation in the space of states. We decompose the Hilbert space $\mathbb{F}$ of the system as the direct sum of two mutually orthogonal subspaces, denoted condensed and normal, namely, $\mathbb{F} = \mathbb{F}_{\rm cond} \oplus \mathbb{F}_{\rm norm}$. The definition of these subspaces is as follows. We write $\mathbb{F} = \text{span}\{|n\rangle\}_{n=1}^{M}$, where $\{|n\rangle\}$ (later on called configurations) is a complete orthonormal set of eigenstates of V, i.e., we have $V|n\rangle = V_n|n\rangle$, $n = 1, \ldots, M$, where we assume ordered, possibly degenerate, potential values $V_1 \le V_2 \le \ldots \le V_M$. Given an integer $M_{\rm cond} < M$, we then define $\mathbb{F}_{\rm cond} = \text{span}\{|n\rangle\}_{n=1}^{M_{\rm cond}}$ and $\mathbb{F}_{\rm norm} = \text{span}\{|n\rangle\}_{n=M_{\rm cond}+1}^{M} = \mathbb{F}_{\rm cond}^{\perp}$. This definition essentially relies on the choice of the dimension $M_{\rm cond}$, which, in view of the ordering of the potential values, marks the maximum potential value included in the condensed subspace

$$\max V_{\rm cond} = \max\{V_n : |n\rangle \in \mathbb{F}_{\rm cond}\} = V_{M_{\rm cond}}. \tag{2}$$

Consider the GS energies of the system, the condensed, and normal subspaces:

$$E = \inf_{|u\rangle \in \mathbb{F}} \langle u|H|u\rangle / \langle u|u\rangle, \tag{3}$$

$$E_{\rm cond} = \inf_{|u\rangle \in \mathbb{F}_{\rm cond}} \langle u|H|u\rangle / \langle u|u\rangle, \tag{4}$$

$$E_{\rm norm} = \inf_{|u\rangle \in \mathbb{F}_{\rm norm}} \langle u|H|u\rangle / \langle u|u\rangle. \tag{5}$$

We are interested in the situations where $M_{\rm cond}/M \ll 1$ and, as a consequence, $M_{\rm norm}/M \equiv (M - M_{\rm cond})/M \simeq 1$. This justifies the names *condensed* and *normal* assigned to the two subspaces and suggests the following dichotomy argument: since $\mathbb{F} \simeq \mathbb{F}_{\rm norm}$, we have $E \simeq E_{\rm norm}$—unless—it is energetically more convenient to "freeze" into the infinitely smaller subspace $\mathbb{F}_{\rm cond}$, where we get $E \simeq E_{\rm cond}$.

The above heuristic argument can be cast in rigorous terms as follows. The TD-lim is defined as the limit N, $N_p \to \infty$ with $N_p/N = \varrho$ constant. Consider the rescaled energies:

$$\epsilon(g) = \text{TD-lim } E(N, N_p, g)/N_p, \tag{6}$$

$$\epsilon_{\rm cond}(g) = \text{TD-lim } E_{\rm cond}(N, N_p, g)/N_p, \tag{7}$$

$$\epsilon_{\rm norm}(g) = \text{TD-lim } E_{\rm norm}(N, N_p, g)/N_p, \tag{8}$$

which are finite in view of the assumed scaling properties of K and V (dependence on ϱ is left understood). In [18] we have proved the following general theorem:

$$\text{if TD-lim } M_{\rm cond}/M = 0, \tag{9a}$$

$$\text{then } \epsilon = \min\{\epsilon_{\rm cond}, \epsilon_{\rm norm}\}. \tag{9b}$$

This theorem establishes the possibility of a QPT between a normal phase characterized by the energy per particle $\epsilon_{\rm norm}$, obtained by removing from $\mathbb{F}$ the infinitely smaller subspace $\mathbb{F}_{\rm cond}$, and a condensed phase characterized by the energy per particle $\epsilon_{\rm cond}$, obtained by restricting the action of H onto $\mathbb{F}_{\rm cond}$. The situation is particularly simple for systems characterized by a single parameter as in the case of Eq. (1). If Eq. (9a) holds and, moreover, the functions $\epsilon_{\rm norm}(g)$ and $\epsilon_{\rm cond}(g)$ are such that the equation

$$\epsilon_{\rm norm}(g) = \epsilon_{\rm cond}(g) \tag{10}$$

admits a unique *finite* solution $g = g_c$, Eq. (9b) provides

$$\epsilon(g) = \begin{cases} \epsilon_{\rm norm}(g), & g < g_c, \\ \epsilon_{\rm cond}(g), & g > g_c. \end{cases} \tag{11}$$

Equations (10) and (11) imply the existence of a first-order QPT at the critical point g_c. In fact, although in general $\epsilon_{\rm cond}(g)$ and $\epsilon_{\rm norm}(g)$ are separately analytic in $g = g_c$, on observing that $\epsilon_{\rm cond}(g)$ and $\epsilon_{\rm norm}(g)$ are different functions, we conclude that, while $\epsilon(g)$ is continuous at $g = g_c$, its first derivative undergoes the discontinuity $|\epsilon'_{\rm cond}(g_c) - \epsilon'_{\rm norm}(g_c)| > 0$.

Whereas Eq. (9a) can be checked easily, the existence of a finite solution to Eq. (10) can be difficult to prove. A practical approach can be as follows. For N, N_p finite with $N_p/N = \varrho$ constant, we evaluate $g_{\rm cross}(N, N_p)$ as the value of the parameter g, if any, solution of the equation

$$E_{\rm norm}(N, N_p, g) = E_{\rm cond}(N, N_p, g). \tag{12}$$

Assuming a smooth limiting behavior, we expect

$$g_c = \text{TD-lim } g_{\text{cross}}(N, N_p). \tag{13}$$

Even if this limit cannot be exactly evaluated, as in the case of numerical simulations, Eq. (13) can be used to provide strict upper and lower bounds to g_c as shown ahead.

To recapitulate, if we find a partition $\mathbb{F} = \mathbb{F}_{\text{cond}} \oplus \mathbb{F}_{\text{norm}}$ such that Eq. (9a) and Eq. (10) are satisfied, then a first-order QPT of the type introduced in [18] occurs at $g = g_c$. In general, such a partition is not unique. In fact, for Eq. (10) to admit a solution with condition (9a) satisfied, $\mathbb{F}_{\text{cond}}$ can invariantly be chosen provided that it is not too small and not too large in such a way that neither of the two restrictions of H, to $\mathbb{F}_{\text{cond}}$ and to $\mathbb{F}_{\text{norm}}$, have a QPT. In this case, ϵ_{cond} and ϵ_{norm} are both analytic functions of g at $g = g_c$, whereas ϵ is not. Note that, for finite sizes, different partitions of $\mathbb{F}$ lead, in general, to different values of both $E_{\text{cond}}(g)$ and $E_{\text{norm}}(g)$. Only in the TD-lim different invariant partitions of $\mathbb{F}$ lead to the same values of $\epsilon_{\text{cond}}(g)$ for $g > g_c$ and $\epsilon_{\text{norm}}(g)$ for $g < g_c$, namely, $\epsilon(g)$, as indicated by Eq. (11). We will exploit this invariance to get rigorous bounds to g_c.

We apply the above general strategy to a system of N_p electrons interacting in a ring of N sites. As usual, for simplicity and saving computational efforts, we consider spinless particles. The electronic Hamiltonian H_e cast in the dimensionless form (1) by $H_e/t = H = K + gV$, $t = \hbar^2/(2m^*a^2)$ being the hopping coefficient with m^* the effective electron mass and a the lattice constant [14], is given by

$$K = -\sum_{i=1}^{N} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i), \tag{14}$$

$$V = \sum_{i=1}^{N} \sum_{j=i+1}^{N} v_{i,j} c_i^\dagger c_i c_j^\dagger c_j, \tag{15}$$

where the fermionic annihilation operators obey the periodic condition $c_{i+N} = c_i$. We consider a screened Coulomb interaction [2]

$$v_{i,j} = \frac{1}{d_{i,j}} e^{-a d_{i,j}/R}, \tag{16}$$

R being the screening length and $d_{i,j} = \min(j - i, N + i - j)$, $j > i$, the dimensionless distance between sites i and j in the ring. Screening takes into account the many-body effects not explicitly considered in H and allows for the interaction energy to scale linearly with the number of particles N_p, as physically expected. The value of R depends on the microscopic details of the system considered. However, whereas the minimum of V has a logarithmic dependence on R, see later, the associated GS has a universal structure [2] under conditions on $v_{i,j}$ [3,4,6] that are fulfilled by Eq. (16) for any R. With the above choice for the potential, the dimensionless coupling g in Eq. (1) takes the form of the following Seitz radius [20]

$$g = 2a/a_B, \qquad a_B = \hbar^2/(m^* e^2). \tag{17}$$

Now we determine a partition $\mathbb{F} = \mathbb{F}_{\text{cond}} \oplus \mathbb{F}_{\text{norm}}$ which satisfies the conditions (9a) and (10). We recall that, according to Eq. (2), a partition is defined by specifying the maximum potential value allowed in $\mathbb{F}_{\text{cond}}$.

As we show in [21], in the TD-lim the distribution of the potential values (15) divided by N_p tends to a Dirac delta centered at $\overline{V}/N_p$, namely, the mean classical value of the potential per particle. This implies that, whenever $\max V_{\text{cond}}/N_p < \overline{V}/N_p$, we have $M_{\text{cond}}/M \to 0$ in the TD-lim, i.e., Eq. (9a) is satisfied.

To comply with Eq. (10), consider that E, E_{cond}, and E_{norm}, are monotonously increasing functions of g convex upward [21] and suppose that the critical point is unique. It follows that g_c is finite if and only if (i) $\epsilon_{\text{norm}}(0) < \epsilon_{\text{cond}}(0)$ and (ii) $\lim_{g\to\infty} \epsilon_{\text{cond}}(g)/g < \lim_{g\to\infty} \epsilon_{\text{norm}}(g)/g$.

Condition (i) is equivalent to saying that in the TD-lim $\min K_{\text{norm}}/N_p < \min K_{\text{cond}}/N_p$. Here and in the following, we use a notation as in Eq. (2), for example, $\min K_{\text{cond}}$ is the smallest eigenvalue of the operator K restricted to the condensed subspace, and so on. It's easy to prove [21] that, if Eq. (9a) is satisfied, the TD-lim of $\min K_{\text{norm}}/\min K$ is 1, therefore, condition (i) is satisfied if in the TD-lim $\max V_{\text{cond}}/N_p < \overline{V}/N_p$, i.e., $\max V_{\text{cond}} \le \overline{V} - \delta V$, with $\delta V > 0$ being an arbitrary $O(N_p)$ term.

Condition (ii) is equivalent to saying that in the TD-lim $\min V_{\text{cond}}/N_p = \min V/N_p < \min V_{\text{norm}}/N_p$. Since in the TD-lim we have $\min V_{\text{norm}}/N_p = \max V_{\text{cond}}/N_p$, the condition amounts to require $\max V_{\text{cond}}/N_p > \min V/N_p$, i.e., $\max V_{\text{cond}} \ge \min V + \delta V$, $\delta V > 0$ being an arbitrary $O(N_p)$ term.

In conclusion, the existence of any one of the partitions $\mathbb{F} = \mathbb{F}_{\text{cond}} \oplus \mathbb{F}_{\text{norm}}$ obtained choosing $\min V + O(N_p) \le \max V_{\text{cond}} \le \overline{V} - O(N_p)$ allows us to say that, provided the screening length R is finite, both Eqs. (9a) and (10) are satisfied. It follows that the Hamiltonian $H = K + gV$ of Eqs. (14)–(17) undergoes a Wigner crystallization in the form of a first-order QPT of the type introduced in [18], i.e., as a condensation in the space of states. About the critical parameter g_c, at this level we just know that it is finite. The following of the Letter is devoted to the construction of upper and lower bounds of g_c and, in order to do so, we shall exploit the invariance of the TD-lim (13) under different partitions of $\mathbb{F}$.

For finite N and N_p, since E_{cond} and E_{norm} are monotonously increasing functions of g convex upward, we have

$$g_{\text{cross}}^- \le g_{\text{cross}} \le g_{\text{cross}}^+, \tag{18}$$

where $g^+_{\rm cross}$ is the intersection point of two curves which are, respectively, a majorant of $E_{\rm cond}$ and a minorant of $E_{\rm norm}$, whereas $g^-_{\rm cross}$ is the intersection point of two curves which are, respectively, a minorant of $E_{\rm cond}$ and a majorant of $E_{\rm norm}$. Indicating with $g^\pm_c$ the TD-lims of $g^\pm_{\rm cross}$, we then have $g^-_c \le g_c \le g^+_c$. The more accurate are the approximations to $E_{\rm cond}$ and $E_{\rm norm}$, the tighter are the bounds $g^\pm_c$. However, we also want to choose these approximations to $E_{\rm cond}$ and $E_{\rm norm}$ sufficiently simple to allow for an analytical evaluation of the TD-lim of $g^\pm_{\rm cross}$.

Let us examine the following inequalities:

$$E_{\rm cond}(g) \le g \min\, V_{\rm cond}, \tag{19}$$

$$E_{\rm norm}(g) \ge \min\, K_{\rm norm} + g \min\, V_{\rm norm}, \tag{20}$$

and

$$E_{\rm cond}(g) \ge \min\, K_{\rm cond} + g \min\, V_{\rm cond}, \tag{21}$$

$$E_{\rm norm}(g) \le \min\, K_{\rm norm} + g \max\, V_{\rm norm}. \tag{22}$$

Equations (20), (21), and (22) are Weyl's inequalities [26] for the lowest eigenvalue of $H = K + gV$ restricted to the condensed and normal subspaces. Equation (19) follows from $E_{\rm cond} \le \langle u|H|u\rangle/\langle u|u\rangle, \quad \forall\, |u\rangle \in \mathbb{F}_{\rm cond}$, choosing $|u\rangle = |n\rangle$, where $|n\rangle$ is any GS of V, and observing that $\langle n|K|n\rangle = 0$. From the first and second pair of inequalities we obtain, respectively,

$$g^+_{\rm cross} = \frac{-\min\, K_{\rm norm}}{\min\, V_{\rm norm} - \min\, V_{\rm cond}}, \tag{23}$$

$$g^-_{\rm cross} = \frac{\min\, K_{\rm cond} - \min\, K_{\rm norm}}{\max\, V_{\rm norm} - \min\, V_{\rm cond}}. \tag{24}$$

Consider Eq. (23). We have $\min\, V_{\rm cond} = \min\, V$ relying only on the filling ϱ and the screening length R, the other quantities depend also on the choice of the condensed space. We choose $\mathbb{F}_{\rm cond}$ in order to make $g^+_{\rm cross}$ as small as possible. A way is to make the denominator, therefore $\min\, V_{\rm norm}$, as large as possible. We assume $\min\, V_{\rm norm}/N_p = \max\, V_{\rm cond}/N_p \to \overline{V}/N_p$. In the numerator of (23) we use $\min\, K_{\rm norm}/K_0 \to 1$ [21], where K_0 is the GS energy of K, namely,

$$K_0 \equiv \min\, K = -2\, \sin(\pi N_p/N)/\sin(\pi/N). \tag{25}$$

We thus obtain

$$g^+_c = \frac{-K_0/N_p}{\overline{V}/N_p - \min\, V/N_p}. \tag{26}$$

Consider Eq. (24). We have already discussed $\min\, V_{\rm cond}$, as for $\max\, V_{\rm norm} = \max\, V$, it is the potential corresponding to the configurations in which the N_p electrons are as tighter as possible, i.e., they occupy N_p consecutive lattice sites. Thus the denominator of Eq. (24) only depends on the filling ϱ and the screening length R. Now we choose $\mathbb{F}_{\rm cond}$ as small as possible, namely, $\max\, V_{\rm cond} \to \min\, V_{\rm cond}$. As before, $\min\, K_{\rm norm}/K_0 \to 1$. We can also put $\min\, K_{\rm cond}/N_p \to 0$ as the number of allowed hoppings in $\mathbb{F}_{\rm cond}$ is, with this choice of $\max\, V_{\rm cond}$, at most $O(1)$. Therefore

$$g^-_c = \frac{-K_0/N_p}{\max\, V/N_p - \min\, V/N_p}. \tag{27}$$

TABLE I. TD-lim of the energies entering Eqs. (26) and (27) and resulting bounds $g^\pm_c$ obtained at filling $\varrho = N_p/N = 3/10$ and screening length $R = 10a$ [27].

$\min\, V/N_p$	$\overline{V}/N_p$	$\max\, V/N_p$	K_0/N_p	g^+_c	g^-_c
0.3846	0.7056	2.3518	−1.7168	5.4	0.84

Equations (26) and (27) provide rigorous bounds to g_c. From Table I, it follows that, at filling $\varrho = 3/10$ and screening length $R = 10a$, a QPT takes place, in terms of the parameter r_s [20], at a critical value $r_{sc} = g_c/4\varrho$ in the range $0.7 \le r_{sc} \le 4.5$.

In principle, g_c could be estimated numerically by Eqs. (12)–(13), allowing also for a direct evidence of the invariance of the choice of $\mathbb{F}_{\rm cond}$. In fact, for different values of $\max\, V_{\rm cond}$ in the range allowed, we should observe different $g_{\rm cross}(N, N_p)$ converging to the same g_c in the TD-lim. However, due to the growing speed of the Hilbert space, this program appears hopeless by standard numerical methods unless one uses *ad hoc* MC simulations.

We wrote a highly parallelized version, see [21] for details, of the bias-free MC algorithm derived from an exact probabilistic representation of the quantum evolution operator [19,28], and run it in a computer farm with thousands of nodes. This allowed us to reach the remarkable size $N_p = 417$, $N = 1390$ with a computation time of several days per point, a point being the evaluation of $E_{\rm cond}(g)$ or $E_{\rm norm}(g)$ for a single value of g and for a chosen system size. The resulting values of $g_{\rm cross}(N, N_p)$, at constant filling $\varrho = N_p/N = 3/10$ and screening length $R = 10a$, are shown in Fig. 1 as a function of N_p for different choices of $\max\, V_{\rm cond}$. Despite the very slow convergence of $g_{\rm cross}(N, N_p)$ to g_c, note that the plot is shown in a log-log scale, all data sets appear to converge to a common g_c whose value is within the rigorous bounds given before. To estimate g_c, we fit the simple curve $A + B/N_p$ to the data obtained for large values of N_p, separately for each $\max\, V_{\rm cond}$. The found values of A suggest convergence to $g_c = 2.76 \pm 0.24$ (i.e., $r_{sc} = 2.3 \pm 0.2$). The first-order nature of the QPT is made evident in the inset of Fig. 1,

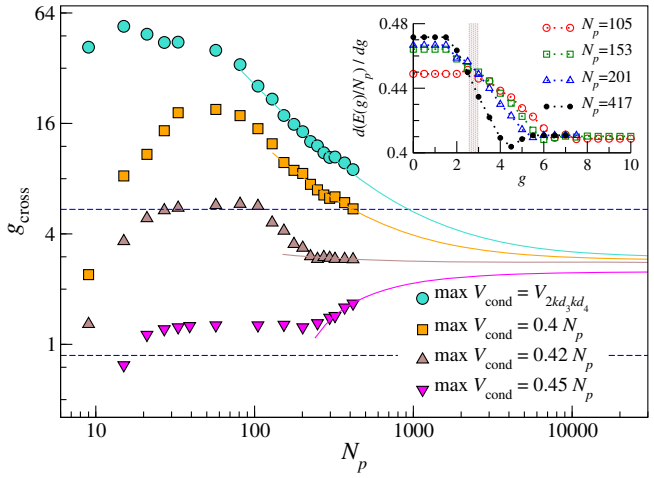

FIG. 1. Value of $g_{\rm cross}(N, N_p)$, solution of Eq. (12), as a function of N_p with filling $N_p/N = 3/10$ and screening length $R = 10a$. Four different condensed subspaces (different max $V_{\rm cond}$) are considered [30]. Numerical MC data (symbols) are extrapolated to $N_p \to \infty$ by fitting $A + B/N_p$ (solid lines) to the points with largest N_p. The horizontal dashed lines are the rigorous bounds of Eqs. (26) and (27). Inset: derivative of the GS energy per particle versus g for different values of N_p. The shaded column indicates the value of $g_c = 2.76 \pm 0.24$ extrapolated as explained above.

where we report $d(E(N, N_p, g)/N_p)/dg$ versus g for different values of N_p. By increasing N_p, we observe a developing discontinuity around the above estimate of g_c. As a further signal of consistency, the derivatives of the GS energy tend to intersect toward a common point g close to g_c [29].

Finally, we consider the limit $R \gg a$ in which screening becomes negligible. In this limit we are able to express the characteristic potential values, namely, $\min V/N_p$, $\max V/N_p$, and $\overline{V}/N_p$ in a closed analytical form [21]. We stress that these expressions are derived by first taking the TD-lim and then picking the leading term for $R \gg a$. By plugging these expressions together with $K_0/N_p \simeq -2\sin(\pi\varrho)/(\pi\varrho)$, obtained from Eq. (25) for $R \gg a$, into Eqs. (26) and (27), we find [20]

$$\frac{\sin(\pi\varrho)/(2\pi\varrho^2)}{\ln(R/a) - \varrho\ln(\varrho R/a)} \le r_{sc} \le \frac{\sin(\pi\varrho)/(2\pi\varrho^2)}{-\varrho\ln(\varrho)}. \quad (28)$$

Equation (28) allows us to estimate the dependence of r_{sc} on ϱ in the range $a/R < \varrho \le 1$, which, in virtue of the condition $R \gg a$, as a matter of fact coincides with the whole filling range.

In the limit $R/a \to \infty$, the lower bound of Eq. (28) vanishes whereas the upper bound remains finite. This is compatible with, but does not prove that $r_{sc} \to 0$ in the limit of infinitely large screening length. However, from Weyl's inequality $\min V(g + \min K/\min V) \le \min H \le \min V(g + \max K/\min V)$ and using the $R \gg a$ expressions of K_0 and $\min V$, we find

$$\lim_{R/a\to\infty} \text{TD-lim}\frac{E(g)}{N_p} = \begin{cases} +\infty, & g > 0, \\ -2\frac{\sin(\pi\varrho)}{\pi\varrho}, & g = 0. \end{cases} \quad (29)$$

We conclude that, if the TD-lim is taken first, the Wigner crystallization is always realized as a first-order QPT of the type [18] but the critical parameter $r_{sc} \to 0^+$ in the limit in which the potential becomes unscreened, $R/a \to \infty$.

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