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Ground state of a partially melted Wigner molecule

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Abstract. – We consider three spinless fermions free to move on $2d$ square lattice with periodic boundary conditions and interacting via a U/r Coulomb repulsion. When the Coulomb energy to kinetic energy ratio r_s is large, a rigid Wigner molecule is formed. As r_s decreases, we show that melting proceeds via an intermediate regime where a floppy two-particle molecule coexists with a partially delocalized particle. A simple ansatz is given to describe the ground state of this mesoscopic solid-liquid regime.

Ordered arrays of charged particles with long-range Coulomb repulsion have been a continuous subject of interest in various branches of physics, including colloidal suspensions, ion rings, atomic-ion Wigner crystals, quantum computers, biophysics, plasmas, electrons deposited on liquid-helium surfaces, charges created in semiconductor or organic field effect devices. These arrays can melt, exhibiting a transition from collective towards independent-particle motion, either as a function of the temperature (classical melting) or as a function of the charge density (quantum melting) at very low temperature. In principle, the quantum melting can be observed using electrons trapped in quantum dots [1,2] or cooled ions confined in radio frequency traps [3]. Very often, a parabolic confinement is imposed. When the confinement is weak and at a sufficiently low temperature, the Coulomb repulsion dominates the kinetic energy, the charges are ordered and a Wigner molecule is formed. If the confinement becomes stronger, the kinetic energy dominates the Coulomb repulsion, the molecule melts and one gets a Fermi system of weakly interacting particles. In a parabolic $2d$ trap, the molecule consists of well-separated shells. Both for the classical melting [4] (achieved by increasing the temperature for a given trap) and for the quantum melting [5] (achieved at zero temperature by reducing the size of the trap), it has been observed that melting proceeds in two stages: first, neighboring shells may rotate relative to each other while retaining their internal order; second, the shell broadening leads to radial melting. Wigner quantum crystallization in $2d$ electron dots is characterized by two distinct —radial and orientational— ordering transitions. However, a parabolic trap does not yield a uniform charge density, the low-density shells at the edges could order before the high-density part in the bulk, and this two-stage melting

could be an artifact due to the interplay between surface and bulk orderings. It is therefore interesting to study if a multi-stage melting persists in a system of uniform charge density, for instance when the charges are confined on a $2d$ torus. One has then to take into account the translational symmetry of a $2d$ torus instead of the rotational symmetry of a parabolic trap.

Another important issue can be mentioned, assuming that insights gained through investigations limited to small systems provide the foundations for understanding larger systems. Long ago, it was suggested by Andreev and Lifshitz [6] that low-temperature localized defects change into excitations that move practically freely through a crystal. As a result, the number of sites of a quantum crystal may be smaller than the total number of particles present in the system for intermediate couplings, such a crystal being neither a solid, nor a liquid. Two kinds of motion are possible in it; one possesses the properties of motion in an elastic solid, the second possesses the properties of motion in a liquid.

An intermediate regime of melting was detected using $N = 4$ spinless fermions in a $L \times L$ lattice, and it was observed [7, 8] that a combination of a few plane waves and site orbitals was able to describe it, suggesting a liquid-solid regime consistent either with a scenario *à la* Andreev-Lifshitz, or with a possible quantum liquid-crystal regime [9, 10]. This intermediate regime was shifted to lower ratios r_s when site disorder was included. Many signatures of a novel ground state (GS) were observed for intermediate couplings, considering the structure [11] of the persistent currents when the torus was pierced by an Aharonov-Bohm flux, the statistics [9] of its low-energy excitations, the failure [8] of the Hartree-Fock approximation to describe the persistent currents above a first ratio r_s^F , the suppression of the same currents above a higher ratio r_s^W , the GS magnetization [12] when the spin degrees of freedom were included. Moreover, it was noticed in ref. [11] that the ratios $r_s^F < r_s < r_s^W$, where the novel mesoscopic GS was observed, were consistent with those where transport measurements using dilute electron gases in $2d$ field effect devices [13, 14] indicate the puzzling possibility of a novel $2d$ metal.

The purpose of this work is to reveal the exact nature of the intermediate mesoscopic GS and to describe it with a simple wave function, considering $N=3$ spinless fermions with U/r Coulomb repulsion in a $L \times L$ square lattice with periodic boundary conditions. Using the operators $c_j^\dagger$ (c_j), c_k ($c_k^\dagger$) which create (destroy) a spinless fermion either at the lattice site $j = (j_x, j_y)$ or in a plane-wave state of momentum $k = (k_x, k_y)$ of this lattice, the Hamiltonian reads

$$H = -t \sum_{\langle j, j' \rangle} c_j^\dagger c_{j'} + \frac{U}{2} \sum_{\substack{j, j' \\ j \neq j'}} \frac{n_j n_{j'}}{d_{j, j'}} = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{k, k', q} U(q) c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k. \quad (1)$$

$n_j = c_j^\dagger c_j$, $d_{j, j'}$ is the shortest distance between sites j and j' , $\epsilon_k = -2t(\cos k_x + \cos k_y)$ and $U(q) = U/(2L^2) \sum_j \cos(qj)/d_{0, j}$. The Coulomb energy to kinetic-energy ratio $r_s = U/(2t\sqrt{\pi n_e})$ for a filling factor $n_e = N/L^2$. The operators c_k and c_j are related by the usual Fourier transform

$$c_k = \frac{1}{L} \sum_j e^{-i(kj)} c_j. \quad (2)$$

In the eigenbasis of the non-interacting system (eigenvectors $c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger |0\rangle$, $|0\rangle$ being the vacuum state), the Hamiltonian matrix is block-diagonal, each block being characterized by the same conserved total momentum $K = \sum_{i=1}^3 k_i$. Moreover, only the non-interacting states having in common one k out of three can be coupled by the interaction inside a K sub-block. Therefore, each K sub-block is a sparse matrix which can be exactly diagonalized using the Lanczos algorithm when L is small enough.

In the large-coupling limit ($r_s \rightarrow \infty$), the eigenstates correspond to rigid Wigner molecules. For a localized center of mass, the charges would be simply located on three lattice sites a, b and c , the location of those sites minimizing the electrostatic energy. However, translational invariance implies a delocalization of the center of mass in a plane-wave state of momentum K , and the Wigner molecule wave functions become

$$|\Psi\rangle = \frac{1}{L} \sum_j e^{i(Kj)} c_{j+a}^\dagger c_{j+b}^\dagger c_{j+c}^\dagger |0\rangle. \quad (3)$$

For a given shape (a, b, c) of the three-particle molecule, one has three well-defined inter-particle spacings $d_{\min} \leq d_{\text{int}} \leq d_{\max}$. The electrostatic energy becomes $U(d_{\min}^{-1} + d_{\text{int}}^{-1} + d_{\max}^{-1})$ while the kinetic energy $\propto t_{\text{eff}}$ (center-of-mass effective band width) $\rightarrow 0$ as $r_s \rightarrow \infty$. For some arbitrary values of K and for some molecular shapes of low electrostatic energy, we have decreased r_s and followed the corresponding levels, ignoring possible level crossings with other levels of different K and of different molecular shape. Two examples calculated using a $L = 8$ lattice are shown in fig. 1, revealing the generic scenario for the melting of a three-particle Wigner molecule. If one considers the change of the relative fluctuations $\Delta d / \langle d \rangle$ as one increases r_s , one can see both for $d_{\min}$ and $d_{\max}$ a crossover from a weak-coupling behavior where the fluctuations are large (the d are not well defined) towards a large-coupling behavior where the fluctuations become negligible (the d become well defined). The weak- (strong-) coupling limits can be described using U/t (t/U) perturbative expansions. For instance, the large-coupling behavior of the Wigner molecule is given at first order of a t/U expansion by

$$|\Psi(1)\rangle = |\Psi\rangle + \sum_{\substack{\alpha=1 \\ \alpha \neq 0}}^{12} \frac{t}{\Delta E_\alpha} |\Psi_\alpha\rangle, \quad (4)$$

where the $|\Psi_\alpha\rangle$ label the Wigner molecules of same K obtained by moving one of the sites a, b, c of $|\Psi\rangle$ by one lattice spacing, $\Delta E_\alpha \propto U$ being the corresponding changes of electrostatic energy. This gives the t/U decays of the three $\Delta d / \langle d \rangle$ indicated in fig. 1.

The main point to notice is the clear separation between the crossover ratios r_s^* (indicated by the arrows in fig. 1) characterizing $d_{\min}$ and $d_{\max}$. As one can see in the data, there are relatively large intervals of intermediate couplings where $d_{\min}$ is well defined while $d_{\max}$ is not, giving rise to an intermediate behavior for d_{int} . This tells us that the generic melting of a three-particle molecule proceeds also in two stages, if one considers a $2d$ system of uniform density, as had been shown using $2d$ parabolic traps. The intermediate regime of melting consists of a floppy two-particle molecule co-existing with a third delocalized particle.

We now study the ground states (GSs) of the three-body problem. The GS momenta and degeneracies depend on L , as the possible existence of GS level crossings. For simplicity, let us consider the case where L is even. At $U = 0$, one has a sixfold GS degeneracy which is partially removed by an infinitesimal U , the energy of a set of four states with momenta $K = (\pm 2\pi/L, \pm 2\pi/L)$ and $K = (\pm 2\pi/L, \mp 2\pi/L)$ becoming different to those of the two $K = 0$ states. Using a U/t expansion, one finds that the GSs remain in the first set for $L \leq 6$ while they go into the second set for $L \geq 8$. At $t = 0$, the low-energy Wigner molecules are L^2 triangles ($d_{\min} = d_{\text{int}} = L/2, d_{\max} = L/\sqrt{2}$) having $L^2/4$ different locations of their centers of mass and 4 different orientations. This L^2 degeneracy is removed when one turns on t . The energies $E_0(K)$ of the L^2 first levels are given when $t/U \rightarrow 0$ by

$$E_0(K) \approx A - 2t_{\text{eff}} (\cos K_x + \cos K_y) + 2r_{\text{eff}} (\cos(K_x L/2) + \cos(K_y L/2)), \quad (5)$$

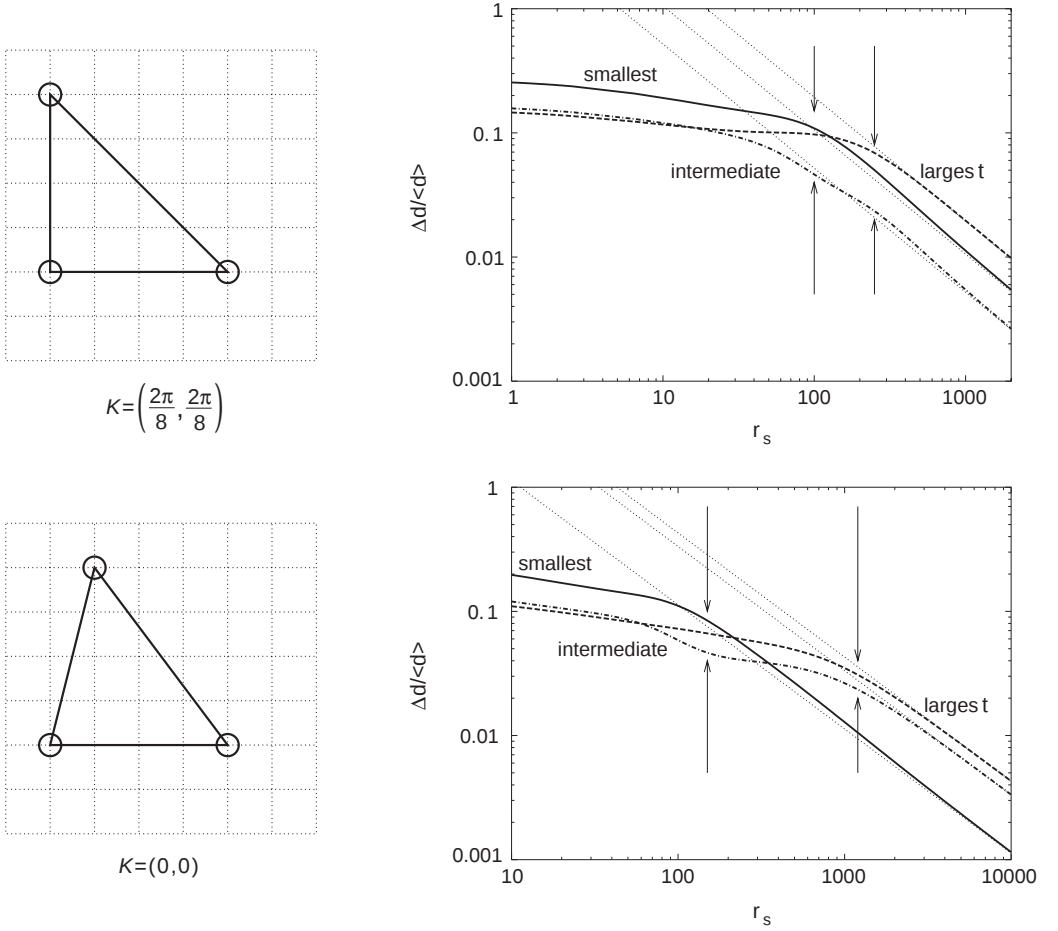


Fig. 1 – Left: scheme of two low-energy Wigner molecules in the limit $r_s \rightarrow \infty$ and of total momenta K for $L = 8$. Right: corresponding relative fluctuations $\Delta d / \langle d \rangle$ of the three particle spacings as a function of r_s . Smallest (continuous line), intermediate (dash-dotted line) and largest (dashed line) spacings. The thin dotted lines give the t/U perturbative behaviors. The arrows indicate the two crossover ratios r_s^* .

where A is a K -independent energy, $t_{\text{eff}} \propto t(t/U)^{N-1}$ is the effective center-of-mass band width while $r_{\text{eff}} \propto t(t/U)^{L/2-1}$ is the effective band width coming from single-particle motions which couple triangles of the same center of mass but of different orientations ($L/2$ one-particle hops). For $L \geq 8$, $t_{\text{eff}} \gg r_{\text{eff}}$, one has a non-degenerate $K = 0$ GS when $t/U \rightarrow \infty$, and consequently a GS level crossing as r_s increases inside the $K = 0$ subspace between the two weak-coupling GSs and the single large-coupling GS. For $L = 6$, r_{eff} and t_{eff} are both $\propto t^3/U^2$, the GSs keep as r_s varies their momenta $K = (\pm 2\pi/L, \pm 2\pi/L)$ and $K = (\pm 2\pi/L, \mp 2\pi/L)$ (fourfold degeneracy) and no GS level crossing occurs. Hereafter, we study the $L = 6$ GS of momentum $K = (2\pi/6, 2\pi/6)$. This allows us to avoid the complications coming from the GS level crossing for $L \geq 8$. However, as shown by the previous examples, our results will be relevant to generically describe the multi-stage quantum melting of a $N = 3$ low-energy Wigner molecule if one continuously follows a given level from large couplings towards weak couplings.

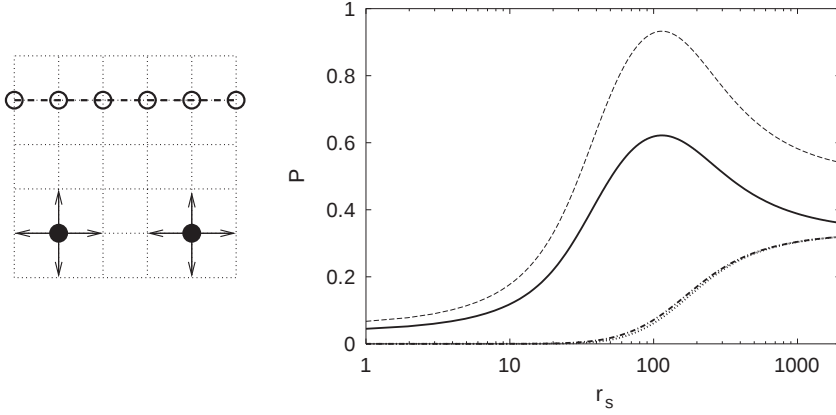


Fig. 2 – Left: scheme of an x -oriented partially melted triangular molecule (x -PMTM) for $L = 6$. The arrows give configurations allowed by a partial t/U expansion of the 2PWM. Right: GS projections $P_x(K, k_x = 0)$ (solid line) $P_x(K, k_x = 2\pi/3)$ (dash-dotted line), $P_x(K, k_x = -2\pi/3)$ (dotted line) over x -PMTMs of momentum k_x . $P(K, k_x = 0, k_y = 0)$ (upper thin dashed line) gives the total projection over the PMTM of momenta $k_x = 0$ and $k_y = 0$. Total momentum $K = (2\pi/6, 2\pi/6)$.

For $L = 6$, the degeneracy of the L^2 triangular molecules is broken when one turns on t . A t/U expansion gives for the $L^2 = 36$ low-energy levels

$$E_0(K) = A_2 - 2t_3 (\cos 2\pi K_x + \cos 2\pi K_y) + 2r_3 (\cos 2\pi 3K_x + \cos 2\pi 3K_y) + 0\left(\frac{t^4}{U^3}\right). \quad (6)$$

$A_2 = 0.9023U - 208.9(t^2/U)$, $t_3 = 1000(t^3/U^2)$ and $r_3 = 1660(t^3/U^2)$. This t/U expansion makes sense when both $d_{\min}$ and $d_{\max}$ are well defined, with small relative fluctuations of order t/U . This means $r_s \geq 200$ (see fig. 3 in the following). To describe lower r_s ($40 < r_s < 200$), where $d_{\min} \approx 3$ is well defined, while $d_{\max}$ has still large fluctuations, we propose a simple ansatz based on the concept of partially melted triangular molecules (PMTMs). An x -oriented PMTM (x -PMTM) is a rigid two-particle Wigner molecule (2PWM) with $d_{\min} = L/2$ combined with a third particle free to move with a wave vector k_x parallel to the 2PWM at a distance $L/2$, as sketched in fig. 2. The x -PMTM wave function of momentum K reads

$$|\Psi_x(K, k_x)\rangle = \frac{1}{6\sqrt{2}} \sum_j e^{i(K_x - k_x)j_x + K_y j_y} c_{j+a}^\dagger c_{j+b}^\dagger c_{k_x, j_y + c_y}^\dagger |0\rangle, \quad (7)$$

where $a = (0, 0)$, $b = (3, 0)$, $c = (0, 3)$, and

$$c_{k_x, j_y + c_y}^\dagger = \frac{1}{\sqrt{6}} \sum_{j_{x'}} e^{ik_x j_{x'}} c_{j_{x'}, j_y + c_y}^\dagger. \quad (8)$$

$(K_x - k_x) \cdot 6/(2\pi)$ must be odd, which leads to $k_x = 0, \pm 2\pi/3$ for $K = (2\pi/6, 2\pi/6)$. The y -oriented PMTM wave function $|\Psi_y(K, k_y)\rangle$ is defined in a similar way. The final PMTM ansatz of momentum K is a normalized combination of the x - and y -PMTMs, which reads

$$|\Psi(K, k_x, k_y)\rangle = \frac{|\Psi_x(K, k_x)\rangle - |\Psi_y(K, k_y)\rangle}{\sqrt{2 - 2\langle \Psi_x(K, k_x) | \Psi_y(K, k_y) \rangle}} = \sqrt{\frac{3}{8}} (|\Psi_x(K, k_x)\rangle - |\Psi_y(K, k_y)\rangle), \quad (9)$$

and the constraint $k_x = k_y$ makes it invariant under x - y permutation.

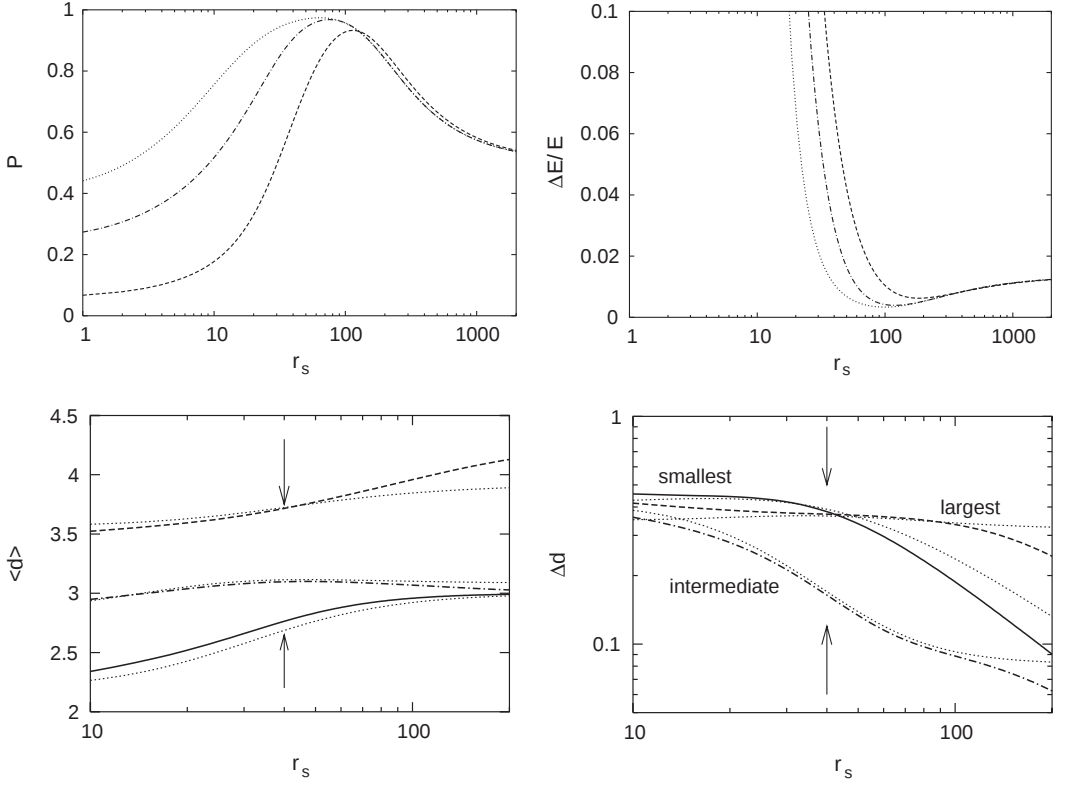


Fig. 3 – Upper left: GS projections over PMTM ansatz with k_x and $k_y = 0$. Upper right: relative errors $\Delta E/E$. The bare ansatz behaviors, corrected by a first-order or a second-order t/U expansion of 2PWM are given by dashed lines, dash-dotted lines and dotted lines, respectively. Lower left: average inter-particle spacings $\langle d \rangle$. Lower right: fluctuations Δd of the inter-particle spacings as a function of r_s . Exact behaviors (thick lines), and ansatz behaviors corrected by a second-order t/U expansion of 2PWM. $K = (2\pi/6, 2\pi/6)$.

In fig. 2, the three values $P_x(K, k_x) = |\langle \Psi_0(K) | \Psi_x(K, k_x) \rangle|^2$ taken by the projections of the exact GS $|\Psi_0(K)\rangle$ over the x -PMTMs $|\Psi_x(K, k_x)\rangle$ are given as a function of r_s , together with the GS projection $P(K, k_x, k_y) = |\langle \Psi_0(K) | \Psi(K, k_x, k_y) \rangle|^2$ over the PMTM of momenta $(K, k_x = 0, k_y = 0)$. Following the three projections over the x -PMTMs of different wave vector k_x , one can see how the third particle gets progressively localized in the x -direction as r_s increases, the rigid three-particle triangular molecule corresponding to $P_x(K, k_x) = 1/3$ for the three possible k_x . $P(K, k_x = 0, k_y = 0) \approx 93\%$ at $r_s \approx 100$. However, only the PMTMs with $k_x = k_y = 0$ contribute when $r_s \leq 50$. For those values of r_s , the third particle is fully delocalized in the direction parallel to the oriented PMWMs. However, it is likely that the PMTM ansatz overestimates the rigidity of the remaining 2PWM when r_s becomes smaller. This can be partly fixed using a t/U expansion for the 2PWM (as sketched in fig. 2, left) and keeping the third particle in its delocalized plane-wave state with $k_x(k_y) = 0$.

The improvements coming from this partial t/U expansion of the PMTM ansatz are given in fig. 3, where one can see the behaviors of the bare ansatz, of the ansatz corrected to first order and to second order of the t/U expansion of the 2PWM. In the upper panels, the GS projections and the relative errors $\Delta E(p)/E$ are shown, E denoting the exact GS

energy, $\Delta E(p) = E_A(p) - E$, $E_A(p)$ being the ansatz energy at the p -th order of the partial t/U expansion. Not only the GS description is improved, but lower values of r_s can now be reached. In the lower panels, the three GS inter-particle spacings $d_{\min}$, d_{int} and $d_{\max}$ are given, and compared to the corresponding values of the ansatz, after a second-order t/U expansion of the 2PWM. As underlined by the arrows, both the averages and the variances are now well described for $r_s \approx 40$.

However, let us underline that the mesoscopic melting process is not yet achieved at $r_s \approx 40$. From a study of the weak-coupling limit, we have obtained precursor behaviors of the formation of the Wigner molecule at smaller r_s . For instance, certain GS projections over low-energy non-interacting states which are close in energy to the non-interacting GS, but orthogonal to the large-coupling Wigner molecule, begin to decay when $r_s > 5$. Therefore, the PMTM ansatz, even improved by a t/U expansion of the 2PWM, fails to describe this precursor regime ($5 < r_s < 30$) where a floppy 2PWM takes place, but is not rigid enough to be described by a simple t/U expansion.

In summary, we have shown that the quantum melting of a three-particle Wigner molecule confined on a $2d$ torus proceeds via an intermediate regime which can be described by the simple concept of a partially melted Wigner molecule, built of a delocalized particle and of a floppy 2PWM. This is in agreement with the general multi-stage picture of mesoscopic quantum melting given by other works using $2d$ parabolic traps. At a mesoscopic scale, this gives a simple illustration of the quantum crystal with $k = 0$ defectons conjectured by Andreev and Lifshitz. Notably, one can see that the number of Wigner lattice sites is smaller than the total number of charges. This shows that the multi-stage melting is not a mesoscopic surface effect and suggests that dilute $2d$ electron gases of intermediate r_s could be more complicated than usually assumed.

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