

Absence of Wigner molecules in one-dimensional few-fermion systems with short-range interactions

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We study, by means of exact-diagonalization techniques, the ground state of a few-fermion system with strong short-range repulsive interactions trapped by a harmonic potential in one spatial dimension. Even when the ground-state density profile displays, at strong coupling, very well pronounced Wigner oscillations with a $4k_F$ periodicity, the pair-correlation function does not show any signature of Wigner-molecule-type correlations. For the sake of comparison, we present also numerical results for few-electron systems with Coulomb interactions, demonstrating that their ground state at strong coupling is, on the contrary, a Wigner molecule.

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I. INTRODUCTION

Understanding the nature of the ground state of strongly correlated few-fermion systems has attracted a great deal of interest. A large body of literature is available in the context of few-electron quantum dots, or “artificial atoms.”¹ In this case the relevant interaction potential is the long-range Coulomb force between electrons. It is by now well established that when Coulomb interactions are sufficiently strong, the ground-state of a quantum dot, either one-² or two-dimensional,³ is a “Wigner molecule” (WM). This jargon stems from the Wigner crystalline order that is displayed by an electron gas at ultralow densities.⁴ The WM state is not characterized by a spontaneous breaking of translational symmetry (which is absent to begin with due to the confining potential of the dot) but rather by strong short-range order that is evident in the density-density correlation function (the so-called pair-correlation function). The existence of WMs has been recently confirmed by inelastic light-scattering studies of few-electron circular quantum dots⁵ as well as by tunneling spectroscopies of quantum wires⁶ and carbon nanotubes.⁷

The ground state of one-dimensional (1D) systems of fermions trapped in a parabolic potential and interacting through a *short-range* potential has also been the subject of numerous analytical and numerical studies.^{8,9} The interest in these systems is not merely academic since gases of fermionic atoms trapped in “atomic quantum wires” can be realized experimentally¹⁰ and cooled to temperatures $T \sim 0.1 T_F$, where T_F is the Fermi temperature.¹¹ The relevant interaction potential in this case is a zero-range Fermi pseudopotential acting only between antiparallel-spin fermions,¹² $V(x) = g_{1D}\delta(x)$, with an amplitude g_{1D} which is controlled¹³ by the three-dimensional (3D) scattering length. Recent advances in atomic physics have made it possible also to confine only a few fermionic atoms with tunable short-range interactions in optical dipole traps.^{14,15}

In the noninteracting $g_{1D} \rightarrow 0$ limit the ground-state density profile of N fermions trapped in a parabolic potential displays, despite the smooth boundaries, “Friedel oscillations” with $N/2$ peaks,¹⁶ which are ultimately due to the Pauli

principle. In the noninteracting limit, indeed, the ground-state density $n_0(x)$ is obtained by occupying exactly $N/2$ harmonic-oscillator levels, each one with two fermions with antiparallel spin,

$$n_0(x) = 2 \sum_{n=0}^{N/2-1} |\phi_n(x)|^2, \quad (1)$$

where $\phi_n(x) = (2^n n! \pi^{1/2} \ell_{ho})^{-1/2} \exp(-\xi^2/2) H_n(\xi)$, with $\xi = x/\ell_{ho}$ and $\ell_{ho} = (\hbar/m\omega)^{1/2}$, are the eigenfunctions of a 1D harmonic oscillator with frequency ω . Here $H_n(\xi)$ is a Hermite polynomial of degree n . Straightforward mathematical manipulations yield the following approximate expression for $n_0(x)$ away from the trap edges:¹⁷

$$n_0(x) \approx n_{TF}(x) - \frac{(-1)^{N/2} \cos[2k_F(x)x]}{\pi L_{TF} (1 - x^2/L_{TF}^2)}, \quad (2)$$

where $n_{TF}(x) = (2L_{TF}/\ell_{ho}^2)[1 - (x/L_{TF})^2]^{1/2}$ is the Thomas-Fermi density profile, $L_{TF} = \ell_{ho}N^{1/2}$, and $k_F(0) = \pi n_{TF}(0)/2 = N^{1/2}/\ell_{ho}$ [the expression for $k_F(x)$ away from the trap center can be found in Ref. 17].

What happens to this simple single-particle physics when the strength of interparticle interactions is increased? In the limit $g_{1D} \rightarrow \infty$ the δ -function interaction imposes an effective Pauli principle between antiparallel-spin fermions. In this limit we thus expect oscillations in the ground-state density $n_\infty(x)$ with a bulk periodicity controlled by $4k_F(0)$. These have been dubbed in the literature as “Wigner oscillations.” The transition from the $2k_F(0)$ Friedel oscillations to the $4k_F(0)$ Wigner oscillations in a parabolic trap is a smooth crossover: see, for example, the extensive density-matrix renormalization group study by Söffing *et al.*¹⁷

Looking, however, at a one-body observable such as the ground-state density profile does not shed light on the nature of the ground state at strong coupling. Especially important in low-dimensional systems are, indeed, correlation functions. In the absence of the parabolic trapping, we know from bosonization¹⁸ that at strong coupling, i.e., when $K_\rho < 1/3$, K_ρ being the Luttinger liquid parameter in the charge sector,

1D interacting fermions are dominated by $4k_F$ charge-density-wave (CDW) correlations. Since in a Galilean invariant system $K_\rho = v_F/v_\rho$, where v_F is the bare Fermi velocity and v_ρ is the velocity of density excitations and $v_\rho \rightarrow 2v_F$ in the limit $g_{1D} \rightarrow \infty$,⁸ we expect that the ground state at strong coupling is completely dominated by $2k_F$ spin-density-wave correlations with no space for incipient CDWs. The situation changes dramatically in a system with long-range interactions, which stabilize $4k_F$ CDW correlations.^{18–20}

In this paper we analyze the nature of the ground state of a 1D few-fermion system at strong coupling in the presence of a parabolic potential, which breaks Galilean invariance. More precisely, inspired by the body of literature discussed above, we study both ground-state density profiles and pair-correlation functions. We focus on the strong-coupling regime, which is difficult to access with analytical techniques, and rely on accurate numerical calculations based on the exact-diagonalization method (also called “full configuration interaction”).²¹ We find that even when the ground-state density profile displays well-pronounced Wigner oscillations with a $4k_F(0)$ periodicity, the pair-correlation function does not show any signature of WM-type correlations. We then highlight the role of the interaction range by comparing these findings with those for a system of electrons interacting through the Coulomb potential. We demonstrate that the ground state of this system at strong coupling is a WM.

The structure of this paper is the following. In Sec. II, the model and the observables of interest are introduced. In Sec. III, we present our numerical results and discussions. Finally, a concluding section summarizes our results.

II. THE MODEL AND THE OBSERVABLES OF INTEREST

We consider a two-component Fermi gas with N atoms confined inside a strongly elongated harmonic trap. The two species of fermionic atoms are assumed to have the same mass m and different pseudospin $\sigma = \uparrow$ or \downarrow (hyperfine-state label). The trapping potential is axially symmetric and characterized by angular frequencies ω_\perp and ω in the radial and longitudinal directions, respectively, with $\omega \ll \omega_\perp$. Correspondingly, we introduce the harmonic-oscillator lengths $a_\perp = (\hbar/m\omega_\perp)^{1/2}$ and $\ell_{ho} = (\hbar/m\omega)^{1/2}$.

The gas is dynamically 1D if the anisotropy parameter of the trap is much smaller than the inverse atom number, $\omega/\omega_\perp \ll N^{-1}$. It can thus be described by an inhomogeneous Gaudin-Yang Hamiltonian,

$$\begin{aligned} \hat{\mathcal{H}} = \hat{\mathcal{T}} + \hat{\mathcal{V}} + \hat{\mathcal{W}} = & -\frac{\hbar^2}{2m} \sum_\sigma \int_{-\infty}^{+\infty} dx \hat{\Psi}_\sigma^\dagger(x) \partial_x^2 \hat{\Psi}_\sigma(x) \\ & + g_{1D} \int_{-\infty}^{+\infty} dx \hat{\Psi}_\uparrow^\dagger(x) \hat{\Psi}_\downarrow^\dagger(x) \hat{\Psi}_\downarrow(x) \hat{\Psi}_\uparrow(x) \\ & + \frac{1}{2} m \omega^2 \sum_\sigma \int_{-\infty}^{+\infty} dx \hat{\Psi}_\sigma^\dagger(x) x^2 \hat{\Psi}_\sigma(x), \end{aligned} \quad (3)$$

where $\hat{\Psi}_\sigma^\dagger(x)$ [$\hat{\Psi}_\sigma(x)$] is a field operator that creates (destroys) a fermion with spin σ at position x and $g_{1D} \simeq 4\hbar^2 a_{sc}/(ma_\perp^2)$ (in the limit $a_{sc} \ll a_\perp$) is a parameter that determines the strength

of interparticle repulsions.¹³ The 3D scattering length a_{sc} can be tuned by means of a magnetic field.¹⁰ The first term in Eq. (3) ($\hat{\mathcal{T}}$) is the kinetic energy, whereas the second term ($\hat{\mathcal{V}}$) describes two-body short-range interactions. Finally, the third term ($\hat{\mathcal{W}}$) is the parabolic trapping potential.

Choosing ℓ_{ho} as the unit of length and $\hbar\omega$ as the unit of energy, Hamiltonian (3) is governed by the dimensionless coupling parameter:

$$\lambda = \frac{g_{1D}}{\ell_{ho}\hbar\omega}. \quad (4)$$

In this paper we focus our attention on the dependence of two key quantities on λ for strong interparticle repulsions ($\lambda \gg 1$): (i) the local spin-resolved density,

$$n_\sigma(x) = \langle \hat{\Psi}_\sigma^\dagger(x) \hat{\Psi}_\sigma(x) \rangle / N_\sigma, \quad (5)$$

and (ii) the pair-correlation function (PCF),

$$\bar{g}_{\sigma\sigma'}(x) = \int_{-\infty}^{+\infty} dx' g_{\sigma\sigma'}\left(x' + \frac{x}{2}, x' - \frac{x}{2}\right), \quad (6)$$

which is defined in terms of the two-body correlator,

$$g_{\sigma\sigma'}(x, x') = \frac{\langle \hat{\Psi}_\sigma^\dagger(x) \hat{\Psi}_{\sigma'}^\dagger(x') \hat{\Psi}_{\sigma'}(x') \hat{\Psi}_\sigma(x) \rangle}{N_\sigma(N_{\sigma'} - \delta_{\sigma\sigma'})}, \quad (7)$$

with N_σ being the number of atoms with spin σ . We also introduce the total density, $n(x) = \sum_\sigma N_\sigma n_\sigma(x)/N$, and the total PCF, $\bar{g}(x) = \sum_{\sigma, \sigma'} N_\sigma(N_{\sigma'} - \delta_{\sigma\sigma'}) \bar{g}_{\sigma\sigma'}(x)/N(N-1)$. In all the definitions above $\langle \dots \rangle$ denotes the expectation value over the ground state of Hamiltonian (3). We recall that $g_{\sigma\sigma'}(x, x')$ measures the conditional probability of finding a fermion with spin σ' at position x' when another fermion of spin σ is known to be at position x , whereas $\bar{g}_{\sigma\sigma'}(x)$ provides the probability of finding two fermions at a relative distance x .

For the sake of comparison, we present also numerical results for another model interparticle potential, in the presence of the same trapping potential as in Eq. (3): we have studied a Hamiltonian identical to the one in Eq. (3), except for the term in the second line, which now reads

$$\begin{aligned} \hat{\mathcal{V}}_Y = & \frac{1}{2} \sum_{\sigma, \sigma'} \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx' \hat{\Psi}_\sigma^\dagger(x) \hat{\Psi}_{\sigma'}^\dagger(x') \\ & \times V_Y(|x - x'|) \hat{\Psi}_{\sigma'}(x') \hat{\Psi}_\sigma(x). \end{aligned} \quad (8)$$

As a model potential we use the following Yukawa interaction:

$$V_Y(|x - x'|) = \frac{e^2}{\kappa \sqrt{a^2 + (x - x')^2}} \exp(-|x - x'|/r), \quad (9)$$

where $a > 0$ regularizes $V_Y(|x - x'|)$ when $x' \rightarrow x$ and r is a tunable parameter that represents the range of $V_Y(|x - x'|)$. In the limit $r/\ell_{ho} \rightarrow \infty$, $V_Y(|x - x'|)$ reduces to a Coulomb potential, and the corresponding Hamiltonian $\hat{\mathcal{H}}_Y = \hat{\mathcal{T}} + \hat{\mathcal{V}}_Y + \hat{\mathcal{W}}$ describes few-electron quantum dots embedded, e.g., in a 1D quantum wire,² with κ being the relative dielectric constant of the wire. In the opposite limit, $r/\ell_{ho} \rightarrow 0$, $V_Y(|x - x'|)$ mimics a short-range interaction. Using the same dimensionless variables which have been used above for the inhomogeneous Gaudin-Yang Hamiltonian,

we find that the dimensionless coupling constant for $\hat{\mathcal{H}}_Y$ is given by

$$\lambda_Y = \frac{e^2}{\kappa \ell_{\text{ho}} \hbar \omega}. \quad (10)$$

Due to the presence of the parameters r and a in Eq. (9), the few-electron problem depends not only on λ_Y but also on the ratios r/ℓ_{ho} and a/ℓ_{ho} . The latter has been fixed to $a/\ell_{\text{ho}} = 10^{-1}$ for all our numerical calculations.²²

III. NUMERICAL RESULTS

In Fig. 1 we report numerical results for the spin-resolved density profiles $n_\sigma(x)$ of $N = 4$ and $N = 5$ fermionic atoms. All the data presented in Fig. 1 and in all the figures below have been calculated for $\lambda = 15$ and are qualitatively similar to those obtained for other values of N , whereas $N > 6$ is beyond our reach. In this ultrastrong coupling regime mean-field-like methods yield completely incorrect results (while we have checked that our numerical results at weak coupling can be explained very well by Bethe-Ansatz density functional theory⁹). In both panels of Fig. 1 we clearly see N distinct peaks in the total density profile $n(x)$, i.e., Wigner oscillations

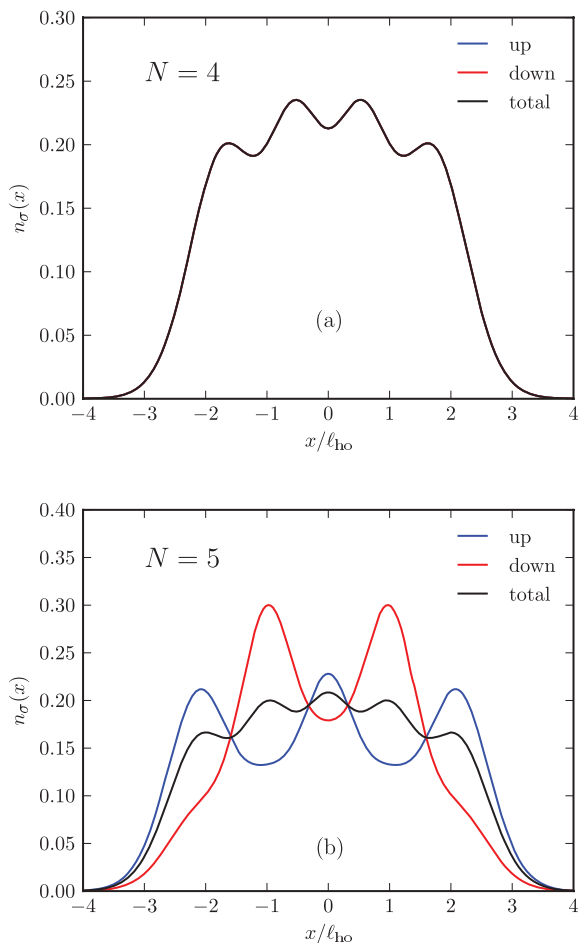


FIG. 1. (Color online) Spin-resolved and total ground-state density profiles (in units of ℓ_{ho}^{-1}) as functions of x/ℓ_{ho} for $\lambda = 15$. (a) Results for $N = 4$ particles (all curves overlap). (b) Results for $N = 5$.

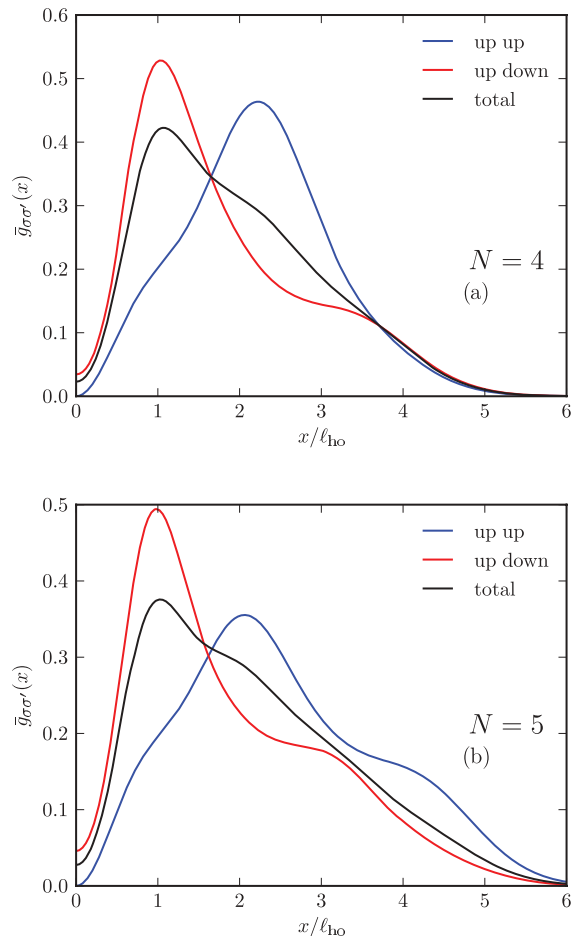


FIG. 2. (Color online) Pair-correlation function $\bar{g}_{\sigma\sigma'}(x)$ (in units of ℓ_{ho}^{-1}) vs x/ℓ_{ho} for the same system parameters as in Fig. 1. Note that $\bar{g}_{\uparrow\uparrow}(x=0) = 0$, a manifestation of Pauli's exclusion principle.

with a $4k_F(0)$ periodicity. Note also the “antiferromagnetic” spatial pattern of the spin-resolved densities $n_\sigma(x)$ in which $n_\downarrow(x)$ has a maximum in correspondence of every minimum of $n_\uparrow(x)$. Quite surprisingly, the PCFs corresponding to the density profiles in Fig. 1, which are plotted in Fig. 2, do *not* display any sign of WM-type short-range order. Despite the well-defined Wigner oscillations in the density profile, the ground state seems to display liquid-type correlations, without any sign of interaction-induced localization.

In Fig. 3 we compare the results reported in Fig. 1 with those for few electrons interacting through the Coulomb potential [$r/\ell_{\text{ho}} = \infty$ in Eq. (9)]. For the sake of comparison, in producing the data for Fig. 3 we have chosen $\lambda_Y = 15$, which is the same value used for the short-range coupling λ in Fig. 1. Also the total density profile in Fig. 3 is characterized by Wigner oscillations with a contrast that is much higher than in the case of fermions interacting through short-range forces.

Moreover, as is well known from the earlier literature,² at this large value of λ_Y the ground state of the few-electron system is definitely a WM. This is illustrated in Fig. 4, where we have presented the total PCFs corresponding to the density profiles in Fig. 3. In the case of Coulomb interactions (solid red line) we note that $\bar{g}(x)$ displays exactly $N - 1$

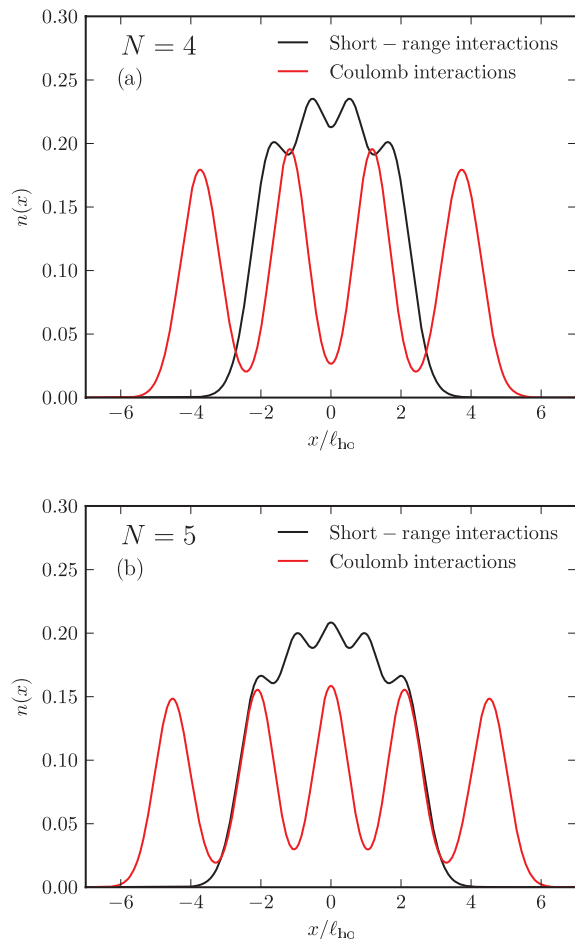


FIG. 3. (Color online) The total density profile $n(x)$ of a system of fermions interacting with short-range interactions is compared with that of electrons interacting through Coulomb interactions. The data for short-range interactions have been produced by setting $\lambda = 15$ (same data as shown in Fig. 1). The data for Coulomb interactions have been produced by setting $\lambda_Y = 15$ and $a/\ell_{ho} = 10^{-1}$.

well-defined peaks, a clear-cut signature of the WM nature of the ground state. Note also an “excluded-volume” region, i.e., a finite range of values of x close to the origin in which $\bar{g}(x) \sim 0$, which is typical of electronic systems at ultrastrong coupling.²³

In Fig. 4(b) we present also numerical results for the PCF of $N = 5$ fermions interacting through the Yukawa potential (9) for different values of the range r/ℓ_{ho} . Upon decreasing the range r/ℓ_{ho} , $\bar{g}(x)$ progressively loses structure, becoming identical to the one calculated with the Gaudin-Yang model (3) for $r/\ell_{ho} \sim 0.1$.

IV. CONCLUSION

In conclusion, we have studied density profiles and pair-correlation functions of few-fermion systems with short-range interactions at strong coupling. We have discovered that the nature of the ground state of these systems, at least in the regime of coupling constants we have investigated, is not a Wigner molecule, despite the well-defined Wigner oscillations displayed by the density profile. We believe that the ground state of this system is not localized into a Wigner molecule

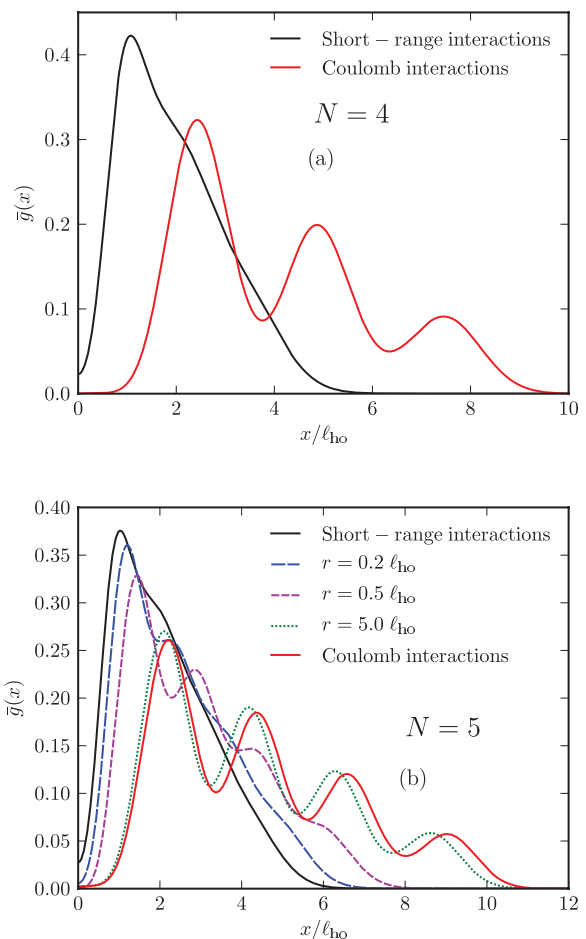


FIG. 4. (Color online) The total pair-correlation function $\bar{g}(x)$ of a system of fermions described by the Gaudin-Yang Hamiltonian (black solid lines in both panels) is compared with that of fermions interacting through the Yukawa potential with a variable range r (in units of ℓ_{ho}). The data labeled Coulomb interactions (red solid lines in both panels) correspond to $r/\ell_{ho} = \infty$ in Eq. (9). The parameters used to produce the data are identical to those in Fig. 3.

because of the short-range nature of the interatom interactions. Systems with identical statistics but long-range Coulomb forces, such as electrons trapped in a quantum dot embedded in a thin quantum wire, are Wigner molecules at similar coupling constants. Since one-dimensional few-fermion systems with tunable short-range interactions have been recently created,¹⁴ our predictions can be tested experimentally by using local probes that access both spatial density distribution and density-density correlation functions.

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- ²²We diagonalize exactly the Hamiltonians $\hat{\mathcal{H}}$ [Eq. (3)] and $\hat{\mathcal{H}}_Y$ [Eq. (9)] in the Hilbert space spanned by the Slater determinants obtained by filling in all possible ways N fermions in the orbitals $\phi_n(x)$, $n = 0, \dots, 24$. Different subsectors of this restricted Hilbert space are labeled by N , $N_\uparrow - N_\downarrow$, and symmetry under reflection $x \rightarrow -x$. The maximum subspace size considered is 1 233 804 for $N = 6$ (numerical results not shown here). Full details on the method are provided in Ref. 21.
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