Few ultracold spinor fermionic atoms with contact interaction in rotating traps: Probing spinfull fractional quantum-Hall-effect physics in the lowest Landau level with higher-order momentum correlations

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The fractional quantum Hall effect is theoretically investigated, with numerical and algebraic approaches, in assemblies of a few ultracold neutral fermionic atoms, interacting via repulsive contact potentials and confined in a single rapidly rotating two-dimensional harmonic trap. We consider spinor fermionic atom assemblies, where in addition to the two-dimensional orbital degree of freedom, each orbital within a degenerate Landau level state has also spin degrees of freedom. Going beyond the common theoretical approaches based on second-order correlations in the real configuration space, the methodology in this paper will assist the analysis of experimental observations by providing benchmark results for $N$-body spin-unresolved, as well as spin-resolved, momentum correlations that can be measured directly with time-of-flight protocols employing individual particle detection in the far-field region. Furthermore, our analysis shows that the few-body lowest-Landau-level (LLL) states with magic angular momenta exhibit intrinsic ordered quantum structures in the $N$-body correlations, similar to those associated with rotating Wigner molecules, familiar from the field of semiconductor quantum dots under high magnetic fields. Moreover, the application of a small perturbing stirring potential induces, in the neighborhood of the ensuing avoided crossings in the LLL energy spectra, symmetry-broken states (referred to as pinned Wigner molecules), exhibiting ordered structures which are manifested already at the lowest level of first-order correlations. This behavior portrays characteristics reminiscent of the ‘flea on the elephant’ concept familiar from the mathematical treatment of spontaneous symmetry breaking phenomena. A configuration-interaction-calculated LLL state, which is shown to be well-described by a corresponding Halperin (1,1,1) two-component orbital variational wave function, serves as an example of a rotating Wigner molecule in the context of a multi-component, spinfull fractional quantum Hall effect in a repulsively contact-interacting assembly of ultracold atoms confined in a rapidly rotating trap. Analysis of the calculated LLL wavefunction also allows a two-dimensional generalization of the Girardeau one-dimensional ‘fermionization’ scheme, originally invoked for mapping of bosonic-type wave functions to those of spinless fermions.

I. INTRODUCTION

The discovery [1] of the fractional quantum Hall effect (FQHE) in extended (bulk) electronic semiconductor samples of high purity, cooled down to low temperatures, and subjected to high perpendicular magnetic fields gave rise to a new subfield in condensed-matter physics, resulting in a large number of both experimental and theoretical investigations of correlated states of interacting electronic systems exhibiting emergent topological phases of matter. Among the theoretical approaches, we note in particular those based on the introduction of families of variational wave functions in the lowest Landau level (LLL) (see, e.g., Refs. [2–6]), following Laughlin’s seminal publications [2, 3].

The unprecedented experimental advances achieved recently in the area of trapped ultracold neutral atoms generated intense interest in finite-size bosonic analogs [7–14] of the FQHE, being embodied in clouds of a few ultracold atoms trapped in rotating harmonic traps, with the rotation acting as a synthetic (rotational gauge) magnetic field.

The expansion of the horizon of such LLL investigations to encompass the regime of a few ultracold spinor fermionic atoms is a natural undertaking. Theoretical investigations of such an endeavor, presented in this paper, are further supported by a growing number of recent experimental advances [15–19] in the deterministic control of assemblies of a few ($N$) trapped $^6$Li atoms, and in particular by the anticipated implementation [20] of a single rapidly rotating two-dimensional (2D) harmonic trap able to project the few-body wave functions within the LLL Hilbert space.

We use state-of-the-art computational tools based on exact diagonalization of the microscopic Hamiltonian with the use of the full configuration interaction (CI) methodology, as was adapted to two dimensions [21–25], in contrast to the familiar three-dimensional CI chemistry formalism [26]; indeed, this approach has been proved successful in previous studies of few bosons [11] or electrons [21, 22] in the LLL. Our approach will assist the analysis of experimental observations by providing benchmark results for $N$-body (spin-unresolved, as well as spin-resolved) momentum correlations that can be measured directly with time-of-flight (TOF) protocols employing individual particle detection through fluorescent imaging in free space [17, 19, 28]. Such research endeavors aim at revealing the microscopic structure of
the correlated FQHE states (here for contact-interacting spinor fermions), adding, supplementing, and going beyond the information gained from studies of bulk properties, e.g., Hall resistance. In this respect, the approach in this paper, demonstrated earlier for a few bosons in Ref. [11], goes beyond the common theoretical analyses that are based on second-order correlations in the real configuration space [9, 10, 21].

In addition, at the theoretical level, our paper shows that: (1) The few-body LLL states with magic angular momenta [29, 31] exhibit intrinsic ordered structures in the N-body correlations. Such ordered quantum structures, referred to commonly as rotating Wigner molecules (RWMs) [21, 31, 32], have been seen previously in the case of semiconductor quantum dots (electrons) under high magnetic fields. Here they are shown to appear even in the case of trapped fermions in a rotating trap interacting with a contact repulsion. (2) When a small perturbing stirring potential, \( V_P \), is applied to the rotating trap (needed in experimental protocols [9, 13, 14] in order to transit between good-total-\( L \) states), symmetry-broken states (referred to as pinned Wigner molecules [27, 33]) emerge in the neighborhood of ensuing avoided crossings, exhibiting the ordered structures already at the lowest level of the first-order correlations, i.e., the single-particle densities. (3) A CI-calculated LLL state, corresponding to Halperin’s (1,1,1) variational wave function [1], is shown to provide an example of both a rotating Wigner molecule and of a generalization to two dimensions of Girardeau’s one-dimensional “fermionization” scheme [16, 34], originally invoked for designating the mapping of bosonic-type wave functions to those of spinless fermions. The above theoretical predictions can be explicitly tested through analysis of experimentally determined momentum correlations; that is, including up to Nth-order correlation functions obtained for N fermionic atoms confined in the rotating trap via time-of-flight measurements.

As pointed out earlier [9, 13, 14, 20], rotating assemblies of a few ultracold atoms have become particularly promising for exploring the LLL physics due to experimental difficulties in reaching sufficiently dilute regimes (low filling fractions) with a large number of atoms [35, 36] in rotating traps; in the former experiment [35] high rotational rates of a BEC cloud of \(^{87}\)Rb atoms resulted in formation of ordered Abrikosov vortices, and similarly for the case of a large-number BEC cloud of \(^7\)Li atoms [36]. In this context, the raised level of understanding brought forth by consideration of the \( N \)-body correlations, compared to studies limited to examination of merely the 2nd-order ones, appears to be pivotal for making further progress in this field. This is the case in particular because the experimental window of fermionic LLL states is restricted to the lowest range of total angular momenta, up to values in the neighborhood of \( L(1,1,1) \) associated with the (1,1,1) Halperin wave function. Indeed for spin-balanced assemblies (with \( N \) particles), the total angular momentum value is \( L(1,1,1) = N(N-1)/2 \), which is smaller than the value of \( N(N-1) \) for the bosonic, and \( 3N(N-1)/2 \) for the fermionic, Laughlin states.

Traditionally, a \( V_P \) perturbation or its effects have not been considered in the literature of the electronic FQHE (see, e.g., Refs. [2–4]), with the exceptions of Refs. [27] and [33] in the context of disorder effects in the semiconductor sample and on the edge states in graphene quantum dots, respectively. A tunable \( V_P \) perturbation representing a multipole deformation of the shape of the rotating harmonic trap [see Eq. (6) below] has been proposed in Refs. [9, 13] as the building block of protocols for experimentally controlled assemblies of a few ultracold bosonic atoms enabling simulations of states characterized by well-known trial FQHE states, like the bosonic Laughlin ones. A proposal to use this type of perturbation in order to simulate well-known variational spinor FQHE states with ultracold \(^6\)Li atoms has been advanced in Ref. [20]. To this effect, consideration of energy spectra and spatial correlations up to second order was sufficient. By considering higher-order correlations (both spatial and momentum ones) beyond the second order, and investigating the spontaneous symmetry breaking induced by the \( V_P \) perturbation in the regions of the avoided crossings, the present paper focuses on previously unexplored fundamental properties of the many-body LLL states of a finite-size assembly of spinor, contact-interacting ultracold atoms, as recapit in points (1)-(3) above.

Before leaving the Introduction, we expatiate on the strong analogies with the field of semiconductor quantum dots. Indeed, in such parabolically confined (i.e., with a harmonic external potential), finite 2D strongly-interacting correlated electron-gas structures, the emergence of intrinsic quantum crystalline-like (or molecular-like) features (so-called Wigner molecules, WMs) is traditionally revealed through analysis of 2nd-order correlations in the CI [21, 31, 32], or center-of-mass separable [37], many-body wave functions, associated with spontaneous symmetry breaking at the mean-field unrestricted Hartree-Fock level [38, 40]. At zero magnetic field, formation of such ordered structures has been shown to be driven by competition between the crystallization inducing long-range repulsive Coulombic inter-electron interaction and the crystallization opposing electronic zero-point kinetic energy (due to single-particle orbital localization, that is reduced single-electron spatial uncertainty) [31, 38]. On the other hand, an applied magnetic field is acting as an independent factor inducing WM formation [6, 22, 31, 32]. The predicted occurrence of such WM electron structures in 2D electron dots under magnetic-field-free conditions, and in the presence of applied magnetic fields (where, as aforementioned, the magnetic-field-induced rotating molecular structures have been termed as rotating Wigner molecules [6, 31, 41], have been confirmed experimentally [12, 17]. Here we establish a broader viewpoint by showing that such RWMs emerge also in the case of ultra-
cold fermionic neutral atoms (e.g., $^6\text{Li}$ atoms) interacting via short-range contact interactions and confined in a rotating harmonic trap (that is emulating a magnetic field via implementation of a synthetic gauge).

A. Plan of paper

The plan of the paper is given below. Following this introductory section, we present in Sec. [II] theoretical preliminaries which aim at defining the problem, establishing notations, and giving a brief survey of the methodologies and techniques employed in this study. In more detail: Sec. [II A] presents the microscopic many-body Hamiltonian of ultracold fermionic atoms (here $^4\text{He}$ or $^6\text{Li}$) confined in a rapidly rotating (stirred up) trap, with or without a perturbation, $V_P$, that breaks the cylindrical symmetry of the trap. Sec. [II B] describes the configuration interaction method used to obtain numerical solutions of the Hamiltonian via exact diagonalization of the microscopic Hamiltonian, with illustrations of the effect of the perturbation, resulting in avoided crossings, depending on the strength of $V_P$, between neighboring eigenstates of the unperturbed Hamiltonian. Sec. [II C] discusses the tools of analysis used in this investigation, in particular, the spin-unsolved and spin-resolved correlation functions, that is, single-particle, first-order, correlation function (i.e., CI-single-particle density), and higher-order (up to 4th-order) correlation functions in real coordinate space, and Sec. [II D] describes these tools of analysis in the momentum space, that is, it discusses the Fourier transforms of the real-space correlation functions, as measured in TOF measurements of particle propagating in free space after confinement removal.

In Sec. [III] we discuss the LLL spectra and the concept of magic angular momenta and its group-theoretical geometrical-symmetry origins, including the combined effects of the rotational and spin degrees of freedom. Sec. [IV] is devoted to analysis of the properties of the ground-state in the spin sector ($S = 0, S_z = 0$) of the $^4\text{He}$ or $^6\text{Li}$ trapped and rotating atoms while traversing an avoided crossing, originating from the symmetry-breaking perturbation $V_P$. This includes illustration of the formation of a pinned crystalline-ordered (square) symmetry-broken single-particle density, revealed in the single-particle density, displayed in the single-particle density, and in the spin-resolved 2nd-order correlation functions (Sec. [IV B]) and in the spin-resolved 2nd-order correlation functions (Sec. [IV C]). These results signal the formation of a quantum ultracold rotating-Wigner-molecule (UC-RWM).

In Sec. [V] we address one of the main foci of this work, namely, examination of the generalization of the Laughlin wave function by Halperin to include FQHE spinor (non-spin-polarized) configurations. To this end, we concentrate our discussion on the spin sector ($S = 2, S_z = 0$) of the four $^6\text{Li}$ ultracold atoms in the rotating trap, and compare the predictions of our exact diagonalization CI calculations for the structure of the ground state in this sector with that of the Halperin (1,1,1) trial function. The discussion in Sec. [V] includes four subsections: Sec. [VA] The 4th order correlation and the molecular configuration predicted for the ground state of above spin sector by the CI calculation. Sec. [VB] Comparison between CI state and trial (1,1,1) Halperin wave function. Sec. [VC] Discussion of a fermionization analogy enabled by a derivation of an appropriate analytic expression for the calculated exact CI wave function. Sec. [VD] Examination of the limitations of analysis of the CI wave-function in the $(S = 2, S_z = 0)$ spin sector when using 2nd-order correlations [particularly for angular momenta corresponding to the (1,1,1) Halperin state], showing the advantages offered by the N-body correlation function (here $N = 4$).

In Sec. [VI] we pause to discuss a comparison between the Wigner parameter $R_W$ – specifying the interparticle interaction strength, and used to define the regime of formation of crystal-like-ordered geometric configurations (that is quantum Wigner-molecule formations) for confined particles interacting via sufficiently long-range interactions (such as Coulomb-interacting electrons in quantum dots, or the forces between trapped atoms interacting via dipolar interaction potentials) – and the parameter $R_6$ used as the strength of short-range contact interactions between trapped neutral ultracold atoms in fastly rotating traps (that is in the LLL regime). We summarize in Sec. [VII].

II. THEORETICAL PRELIMINARIES

A. Many-body Hamiltonian

The Fock-Darwin spectrum [48, 49] associated with the $(n,l)$ single-particle states in a rapidly rotating two-dimensional (2D) trap is given by

$$\epsilon_{n,l}^{\text{FD}} = \hbar[(2n + |l| + 1)\omega - l\Omega],$$

where $\omega$ is the trapping frequency of the harmonic confinement, $\Omega$ in the rotational frequency of the trap, $n$ is the number of nodes, and $l$ denotes the single-particle angular momentum. The projection on the LLL imposes $n = 0$ (Fock-Darwin single-particle states without radial nodes), and the associated many-body Hamiltonian without the perturbing contribution is [50]:

$$\frac{H_{\text{LLL}}}{\hbar \omega} = N + (1 - \frac{\Omega}{\omega})L + 2\pi R_6 \sum_{i<j}^{N} \delta(r_i - r_j),$$

where $N$ is the number of particles, and $L$ denotes the total angular momentum, $L = \sum_{i=1}^{N} l_i$, along the axis perpendicular to the 2D trap plane. The energies in Eq.
are in units of $\hbar \omega$ and the lengths in units of the oscillator length $\Lambda = \sqrt{\hbar / (M \omega)}$. Here, the first and second terms express the LLL kinetic-energy contribution, $H_K$, whereas the third term represents the contact-interaction contribution, $H_{\text{int}}$.

The dimensionless parameter

$$R_\delta = \frac{g}{2\pi \Lambda^2 \hbar \omega} = \frac{g M}{2\pi \hbar^2}$$

expresses the strength, $g$, of the contact interaction associated with an area $2\pi \Lambda^2$, relative to the zero-point energy, $\hbar \omega$, associated with the 2D harmonic trap; $M$ is the mass of the ultracold fermionic atoms. Naturally, the $\delta$-functions in Eq. (2) are two dimensional.

Another way for interpreting the parameter $R_\delta$ is that it equals the direct matrix element [see Eq. (1) below]

$$\epsilon_{\text{max}} = \langle l_1 = 0, l_2 = 0 | H_{\text{int}} | l_3 = 0, l_4 = 0 \rangle = R_\delta.$$

$\epsilon_{\text{max}}$ is in units of $\hbar \omega$ and the subscript ‘max’ indicates that this energy represents the maximum repulsion that two fermions with opposite spins can attain in the LLL.

For reasons of experimental convenience in transitioning from one LLL state to another, it has been shown [9, 13, 20] that the following perturbation (in second quantization), associated with a small multipole deformation of the rotating trap, is desirable:

$$\frac{V_P}{\hbar \omega} = C \left( \sum_l \frac{\sqrt{(l+m)!}}{2^{m/2} \sqrt{l!}} a_{l+m}^\dagger a_l^\dagger + h.c. \right),$$

where $m$ is the order of the multipole deformation, and $C$ is a dimensionless constant specifying the strength of the deformation. This perturbation can be introduced as a stirring potential. It couples the many-body solutions of $H_{\text{MB}}$ that differ by $m$ units in their total angular momenta $L$, and generates avoiding crossings, with an example given in Fig. 1. Note that in showing the spectra of $H_{\text{MB}}$, we limit ourselves to a particular spin sector; in Fig. 1 for $N = 4$, the spin sector is $(S = 0, S_z = 0)$, with the lowest-in-energy state within the spin sector termed “the relative ground state”.

For a small value of the parameter $C$ (e.g., $C = 0.0001$), $V_P$ couples mainly the two originally (when $V_P = 0$) crossing states with good total $L$ and $L + m$, or $L - m$ and $L$. In this case, the expectation value, $\langle L \rangle$, of the total angular momentum along the avoided crossing exhibits a sharp stepwise profile; see Fig. 2(a). A larger...
value of the parameter $C$ introduces additional contributions to $L \pm 2m$, $L \pm 3m$, etc., states, which may become non-negligible, and simultaneously the $(L)$-profile along the avoided crossing broadens and exhibits a slower variation rate; see Fig. 2(b) for the strong-coupling case of $C = 0.004$.

B. Configuration Interaction method

Denoting the spin degree of freedom by $\sigma$, in the CI method, one writes the many-body wave function $\Phi_{CI}(r_1\sigma_1, r_2\sigma_2, \ldots, r_N\sigma_N)$ as a linear superposition of Slater determinants $\Psi(r_1\sigma_1, r_2\sigma_2, \ldots, r_N\sigma_N)$ that span the many-body Hilbert space and are constructed out of the single-particle spatial orbitals

$$\chi_j(r) = \psi_j(r)\alpha, \quad 1 \leq j \leq K,$$

and

$$\chi_j(r) = \psi_j-K(r)\beta, \quad K < j \leq 2K,$$

where $\alpha(\beta)$ denote up (down) spins. Namely, the wave function of the $q$th CI state is given by

$$\Phi_{CI}^q(r_1\sigma_1, \ldots, r_N\sigma_N) = \sum_I c^q(I)\Psi_I(r_1\sigma_1, \ldots, r_N\sigma_N),$$

where

$$\Psi_I = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_{j_1}(r_1) & \cdots & \chi_{j_N}(r_1) \\ \vdots & \ddots & \vdots \\ \chi_{j_1}(r_N) & \cdots & \chi_{j_N}(r_N) \end{vmatrix},$$

and the master index $I$ counts the number of arrangements $\{j_1,j_2,\ldots,j_N\}$ under the restriction that $1 \leq j_1 < j_2 < \ldots < j_N \leq 2K$. Of course, $q = 1,2,\ldots$ counts the excitation spectrum, with $q = 1$ corresponding to the overall ground state for each total spin projection $S_z$.

Because we restrict the Hilbert space in the LLL, the single-particle spatial orbitals are nodeless and they are given in polar coordinates by the expression

$$\psi_l(r) = \frac{1}{\sqrt{\pi l!}} r^l e^{il\theta} e^{-r^2/2},$$

where $l \geq 0$ is the single-fermion angular momentum, and $r$ is in units of the oscillator length $\Lambda = \sqrt{\hbar/(M\omega)}$.

Next, the CI (exact) diagonalization of the many-body Schrödinger equation

$$H_{MB}\Phi_{CI}^q = E_{CI}^q\Phi_{CI}^q$$

transforms into a matrix diagonalization problem, which yields the coefficients $c^q(I)$ and the CI eigenenergies $E_{CI}^q$. Because the resulting matrix is sparse, we implement its numerical diagonalization employing the very efficient ARPACK solver [52] of large-scale eigenvalue problems with implicitly restarted Arnoldi methods [53].

The matrix elements $(\Psi_I|H_{MB}|\Psi_J)$ between the basis determinants [see Eq. (10)] are calculated using the Slater rules [26]. Naturally, an important ingredient in this respect are the two-body matrix elements of the contact interaction,

$$V_{1234} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dr_1 dr_2 \psi_1^*(r_1)\psi_2^*(r_2)\delta(r_1-r_2)\psi_3(r_1)\psi_4(r_2),$$

in the basis formed out of the single-particle spatial orbitals $\psi_i(r), i = 1,2,\ldots,K$ [Eq. (11)]. When the lengths are expressed in units of $\Lambda$, these matrix elements are dimensionless and are given analytically by [54]

$$V_{1234} = \frac{1}{2\pi} \delta_{l_1,l_2,l_3,l_4} (l_1 + l_2)! / 2^{l_1+l_2}.$$  (14)

The Slater determinants $\Psi_I$ [see Eq. (10)] conserve the third projection $S_z$, but not the square $S^2$ of the total spin. However, because $S^2$ commutes with the many-body Hamiltonian, the nondegenerate CI solutions are automatically eigenstates of $S^2$ with eigenvalues $S(S+1)$. After the diagonalization, these eigenvalues are determined by applying $S^2$ onto $\Phi_{CI}^q$ and using the relation

$$\hat{S}^2\Psi_I = \left( (N_\uparrow - N_\downarrow)^2/4 + N/2 + \sum_{i<j} \varpi_{ij} \right) \Psi_I,$$  (15)

where the operator $\varpi_{ij}$ interchanges the spins of fermions $i$ and $j$ provided that their spins are different; $N_\uparrow$ and $N_\downarrow$ denote the number of spin-up and spin-down fermions, respectively.

C. Tools of analysis: Real configuration space

The tools of analysis used in this paper are the single-particle densities (1st-order correlations), the spin-unresolved and spin-resolved 2nd-order correlations, as well as the higher-order $N$-body correlations (4th-order for $N = 4$ fermions).

The spin-unresolved CI single-particle densities (1st-order correlation functions) are given by

$$\rho_{CI}(r) = \langle \Phi_{CI} | \sum_{i=1}^{N} \delta(r_i - r) | \Phi_{CI} \rangle.$$  (16)

Here and in the following, it is understood that evaluation of expectation values over the many-body wave function $\Phi_{CI}(r_1\sigma_1, \ldots, r_N\sigma_N)$ involves integration over all the particles’ coordinates (including the spin ones).

We note that, in the case of a single Slater determinant, the above definition yields the simple formula of summation over the modulus square of the single-particle spatial orbitals.
The spin-unresolved 2nd-order correlations (pair correlations) are specified as

\[ 2 G^{\text{CI}}(r, r_0) = \langle \Phi_{\text{CI}} | \sum_{i \neq j} \delta (r - r_i) \delta (r_0 - r_j) | \Phi_{\text{CI}} \rangle, \]  

whereas the definition of the spin-resolved 2nd-order correlations (pair correlations) includes the spin degree of freedom as follows,

\[ 2 G_{\sigma \sigma_0}^{\text{CI}}(r, r_0) = \langle \Phi_{\text{CI}} | \sum_{i \neq j} \delta (r - r_i) \delta (r_0 - r_j) \delta_{\sigma \sigma_0} \delta_{\sigma_0 \sigma} | \Phi_{\text{CI}} \rangle. \]  

The spin-resolved \( 2 G_{\sigma \sigma_0}^{\text{CI}} \) is also referred to as conditional probability distribution (CPD) \cite{27, 31} because it gives the spatial probability distribution for finding a second fermion with spin projection \( \sigma \) under the condition that a first fermion with spin projection \( \sigma_0 \) is fixed at \( r_0 \); \( \sigma \) and \( \sigma_0 \) can be either up (\( \uparrow \)) or down (\( \downarrow \)). The first and second-order correlations defined above are calculated using the Slater rules \cite{55} for the matrix elements between determinants of one-body and two-body operators, respectively.

More importantly, here, we use in addition higher-order correlations, and in particular the \( N \)-body correlations (4th-order for \( N = 4 \) fermions which are the focus of this paper). To motivate our discussion, we start first with the case of 4 fully polarized fermions \( (S = 2 \text{ and } S_z = 2) \), whose spatial part is equivalent to the case of spinless fermions. For this case the CI wave function can be written as

\[ \Phi_{\text{CI}}(r_1, r_2, r_3, r_4) = F(r_1, r_2, r_3, r_4) \alpha(1) \alpha(2) \alpha(3) \alpha(4), \]  

the 4th-order correlation function is given simply by the modulus square of the spatial part, i.e.,

\[ 4 G_{\text{CI}}^{\text{un}}(r_1, r_2, r_3, r_4) = |F(r_1, r_2, r_3, r_4)|^2. \]  

The cases of non-spin-polarized configurations are more complicated, involving both spin-resolved and spin-unresolved correlations. In general, in the case of \( N \) spinor fermions (with \( N = N_\uparrow + N_\downarrow \)), the CI wave function \( \Phi_{\text{CI}} \) contains \( K = N!/(N_\uparrow N_\downarrow) \) primitive spin functions of the form

\[ \zeta_i(N_\uparrow, N_\downarrow) = \alpha \alpha ... \beta \beta. \]  

To be specific, for the case of \( N = 4 \) fermions with \( N_\uparrow = N_\downarrow = 2 \) \( (S_z = 0) \), there are \( K = 6 \) such spin primitives, namely

\[ \zeta_1 = \alpha(1) \alpha(2) \beta(3) \beta(4), \]
\[ \zeta_2 = \alpha(1) \alpha(3) \beta(2) \beta(4), \]
\[ \zeta_3 = \alpha(1) \alpha(4) \beta(2) \beta(3), \]
\[ \zeta_4 = \alpha(2) \alpha(3) \beta(1) \beta(4), \]
\[ \zeta_5 = \alpha(2) \alpha(4) \beta(1) \beta(3), \]
\[ \zeta_6 = \alpha(3) \alpha(4) \beta(1) \beta(2), \]  

where the arguments from 1 to 4 in the \( \alpha \)'s and \( \beta \)'s correspond to particle indices.

Considering the 4 spin orbitals \( u^{\uparrow \alpha}_i = \phi^{\uparrow \alpha}_i, u^{\uparrow \beta}_i = \phi^{\uparrow \beta}_i, u^{\downarrow \alpha}_i = \phi^{\downarrow \alpha}_i, u^{\downarrow \beta}_i = \phi^{\downarrow \beta}_i \) of the \( I \)-th determinant in the CI expansion [Eq. (9)], which (for a given determinant) are the same for all six \( \zeta_i \)'s listed in Eq. (22), the many-body CI wave function for \( N_\uparrow = N_\downarrow = 2 \) can be rewritten as

\[ \Phi_{\text{CI}} = \sum_{i=1}^{6} \mathcal{F}_i(r_1, r_2, r_3, r_4) \zeta_i, \]  

where

\[ \mathcal{F}_i = \sum_I c(I) \text{Det}^\uparrow [\phi^{\uparrow \alpha}_i(s^{\uparrow}_l), \phi^{\uparrow \beta}_i(s^{\uparrow}_l)] \text{Det}^\downarrow [\phi^{\downarrow \alpha}_i(s^{\downarrow}_l), \phi^{\downarrow \beta}_i(s^{\downarrow}_l)]. \]

where \( c(I) \) are the coefficients of the CI expansion and \( (s^{\uparrow}_1, s^{\uparrow}_2) \) and \( (s^{\downarrow}_1, s^{\downarrow}_2) \) coincide with the spatial coordinates associated with the particle indices for the up and down spins in the \( \zeta_i \) spin primitives defined in Eq. (22). For example, for \( i = 5 \), one has

\[ s^\uparrow_5 \rightarrow r_2, \]
\[ s^\downarrow_5 \rightarrow r_4. \]

The spin-unresolved 4th-order correlation is then given by

\[ 4 G_{\text{CI}}^{\text{un}} = \sum_{i=1}^{6} \mathcal{F}_i^\dagger \mathcal{F}_i. \]

The spin resolved 4th-order correlations are defined as a partial summation over the spin-primitive index \( i \) [Eq. (23)]. For example, the probability of finding the fourth fermion with spin down \( |\beta(4)\rangle \) in any \( \zeta_i \) spin primitive at a position \( r \), given the positions of the first three fermions with unresolved spins, is:

\[ 4 G_{\text{CI}}^{\text{res.1}} = \mathcal{F}_1^\dagger \mathcal{F}_1 + \mathcal{F}_2^\dagger \mathcal{F}_2 + \mathcal{F}_3^\dagger \mathcal{F}_3. \]

Other spin-resolved 4th-order correlations are possible: for example, finding the fourth fermion with spin down at position \( r \), given the positions of the first 3 fermions with the 2nd fermion having a spin up and the 1st and 3rd ones with unresolved spins is given by

\[ 4 G_{\text{CI}}^{\text{res.2}} = \mathcal{F}_1^\dagger \mathcal{F}_1 + \mathcal{F}_2^\dagger \mathcal{F}_2. \]

D. Tools of analysis: Momentum space

To channel our discussion about momentum-space correlation functions, we recall again that, usually, a CI
calculation (or other exact diagonalization schemes used for solution of the microscopic many-body Hamiltonian) yields a many-body wave function (e.g., \( \Phi_{\text{CI}} \)) in position coordinates \( (r_1 \sigma_1, r_2 \sigma_2, \ldots, r_N \sigma_N) \); see Eq. \( \text{(6)} \), which for the case of \( N = 4 \) fermions can take the form in Eq. \( \text{(23)} \).

The CI wave functions, \( \Phi_{\text{CI}} \), are particularly conducive for carrying out their mapping into the momentum-space ones, \( \Phi_{\text{CI}}^{\mathbf{M}} \); naturally the momentum space is spanned by the coordinates \( (k_1 \sigma_1, k_2 \sigma_2, \ldots, k_N \sigma_N) \), with \( k_j = p_j / \hbar \). Indeed it is sufficient to replace each LLL single-particle real-space orbital \( \psi_i(r) \) in the basis determinants \( \Psi_j \) [Eq. \( \text{(10)} \)] by its 2D Fourier transform, which is given by [compare to the real-space function in Eq. \( \text{(11)} \)]

\[
\psi_i(k) = \frac{i^j}{\sqrt{\pi \Lambda}} k^j e^{i \mu \varphi} e^{-k^2/2},
\]

where \( k \) is in units of the inverse of the oscillator length, \( 1/\Lambda \); see definition after Eq. \( \text{(11)} \).

Having obtained the many-body wave function in momentum space, all and each formula (in Sec. \( \text{III C} \)) specifying the tools of analysis in real space (1st, 2nd, and \( N \)th-order correlations) can be immediately translated in momentum space by simply replacing \( r_j \rightarrow k_j \) and \( \Phi_{\text{CI}} \rightarrow \Phi_{\text{CI}}^{\mathbf{M}} \). In addition, Eq. \( \text{(29)} \) shows that, apart from a phase \( i^j \), the LLL orbitals in momentum space retain the same form as the corresponding ones in configuration space, with the following substitutions: \( (r, \theta) \rightarrow (k, \varphi) \) and \( \Lambda \leftrightarrow 1/\Lambda \). Consequently: (i) All the expressions and final results, including the figure plots, for the 1st, 2nd, and 4th correlations calculated in real space represent also corresponding results in momentum space, the only change being the units of the axes (\( 1/\Lambda \) versus \( \Lambda \)). (ii) The TOF measurements in the far field \([8, 56]\) act as a microscope that magnifies directly the \( \textit{in situ} \) many-body wave function.

In deterministic time-of-flight measurements, the \( N \) trapped ultracold atoms expand subsequent to a sudden turn-off of the trapping potential, and a snapshot of the free-space traveling \( N \) atomic particles is taken in the far field after a time \( t_{\text{TOF}} \). This step is repeated several thousand times and the compilation of the ensuing snapshots reproduces the modulus square of the Fourier transform of the \( \textit{in situ} \) many-body wave function \([13]\). \( t_{\text{TOF}} \) is taken long enough so that the size of the compiled ensemble is much larger than its original (confined) size. The TOF far-field real-space coordinates of the particles at time \( t_{\text{TOF}} \) are given by \( r_j = \hbar k_j t_{\text{TOF}} / M \), with \( j = 1, 2, \ldots, N \), where \( \hbar k_j \) is the single-particle momentum at the source (the confining trap). From the above, we note that during the expansion the interatomic interactions can be neglected, whereas prior to the expansion the interactions play a key role in determining the properties of the trapped correlated LLL state \([8, 56]\). In this way, analyses of TOF measurements allow determination of the properties of the many-body state of the confined system via analyses of the all-order (1 to \( N \)) momentum-space correlation functions. These momentum correlation functions are indeed the focus of our study. As aforementioned, for the LLL case investigated here, the single-particle Fourier transform in Eq. \( \text{(29)} \) retains the same functional form on \( k \) as does \( \psi_i(r) \) in Eq. \( \text{(11)} \) on \( r \). As a result, apart of units, the \( \textit{in situ} \) real-space and momentum correlations coincide, and the TOF measurements act as a microscope of the \( \textit{in situ} \) many-body wave function.

### III. LLL SPECTRA AND MAGIC ANGULAR MOMENTA

A primary tool for the classification and for gaining a deeper understanding of the geometric aspects of the intrinsic correlations in the LLL many-body wave functions is the concept of magic angular momenta, introduced and extensively utilized in the treatments of semiconductor quantum dots \([21, 29, 32, 57, 61]\). An early \([29, 30]\) recognized signature of magic angular momenta was their forming sets of energetically advantageous states (referred to also as cusp states) in the LLL spectra of a few 2D fully spin-polarized electrons. According to subsequent \([21, 29, 32, 57, 61]\) findings from CI calculations in the field of semiconductor quantum dots (a few electrons confined in a harmonic potential), the 2D electrons under a perpendicular high magnetic field localize relative to each other and form ordered ring-like configurations \( (n_1, n_2, \ldots, n_r) \) (with \( \sum n_i = N \)). Such ordered ring configurations are not visible in the CI single-particle densities, which are azimuthally (rotationally) uniform, but are revealed by using higher-order correlations \([31]\). Furthermore, the CI total angular momenta must be compatible (i.e., satisfy) the \( C_n \) point group, etc., symmetries.
associated with the ring configurations \[21, 31, 32, 57-61\]. Similar magic angular momenta appear also in the LLL spectra and CI solutions for ultracold bosonic atoms \[11\]. The present paper demonstrates that magic angular momenta are pertinent as well to ultracold fermions in rapidly rotating harmonic traps.

Going beyond the fully spin-polarized case, previous investigations have found \[32, 59–61\] that the magic angular momenta depend in a nontrivial way on the value \(S\) of the total spin. In particular, for the case of \(N = 4\) fermions (which is the focus of this paper), the associated ring-like configuration is a square [denoted as (0,4)], and the series of magic angular momenta are as follows \[60, 61\]:

\[
S = 0 \rightarrow L = 4n \quad \text{or} \quad L = 4n + 2,
S = 1 \rightarrow L = 4n - 1 \quad \text{or} \quad L = 4n; \quad \text{or} \quad 4n + 1,
S = 2 \rightarrow L = 4n + 2,
\]

where \(n = 0, 1, 2, 3, \ldots\)

The relative ground states of \(H_{\text{LLL}}\) in each spin sector are associated with magic angular momenta. Indeed, the values of \(L = 2, 4, 8\) for \(S = 0\) listed in Eq. (30) corresponds to the ground states in the spin sector \((S = 0, S_z = 0)\), belong to the \(S = 0\) series listed in Eq. (30). Furthermore, in the spin sector \((S = 2, S_z = 0)\), the relative ground state has the magic angular momentum \(L = 6\) in agreement with the series in Eq. (30); see Fig. 3.

To further elaborate on the relation between magic angular momenta and LLL spectra, we display in Fig. 4 the restricted LLL spectra in each spin sector corresponding to the diagonalization of the contact-interaction term only, that is, to the last term in Eq. (2). These spectra are plotted as a function of the total angular momentum \(L\); for each value of \(L\), a tower of excited states is shown (upward standing triangles above the yrast-band line that connects the lowest-energy triangles). These excited LLL states display a highest-energy bound at \(2.5R_s\hbar\omega\). The number of states in each tower increases with increasing \(L\), and every newly appearing energy at a given \(L\) repeats itself at larger \(L\)’s. In this figure, the lowest-energies for each \(L\) (forming the so-called yrast band) are highlighted by passing a line through them. For the \((S = 0, S_z = 0)\) and \((S = 1, S_z = 0)\) spin sectors, the yrast bands involve successively lower energies and eventually they collapse to a horizontal line at vanishing energy. For the \((S = 2, S_z = 0)\), only the horizontal segment at zero energy is present. The zero-energy horizontal segment in Fig. 4 is a property connected to the zero range of the contact interaction; it is absent in the case of the long-range Coulomb interaction \[21, 31, 61\].

In Fig. 4, the magic angular momenta according to Eq. (30) are marked by an arrow. They are preceded by a sharp drop in energy relative to the previous angular momentum (as long as the previous \(L\) is non-magic or nonvanishing); as a result the associated LLL states are often referred to as cusp states \[31, 62\].

To enhance the brief historical overview in this Section, and to illustrate the role of the underlying geometric picture, we sketch here the derivation for the spin-dependent magic angular momenta in the simpler case of three localized fermions arranged in an intrinsic configuration of an equilateral triangle \[63\]. For \(N = 3\) fermions, both the \(S_z = 1/2\) and \(S_z = 3/2\) polarizations need to be considered. We start with the \(S_z = 1/2\) polarization, which is associated with three spin primitives \(|↓↑↑⟩, |↑↓↑⟩, \text{and } |↑↑↓⟩\). These primitives correspond to single Slater determinants which exhibit a breaking of both the total spin symmetry and of the continuous rotational symmetry. We first proceed with the restoration of the total
spin by noticing that the three spin primitives have a point-group symmetry lower than the $C_3$ symmetry of an equilateral triangle. The $C_3$ symmetry, however, can be readily restored by applying appropriate point-group projection operators according to group theoretical concepts \[64, 65\]. This yields the following two different three-determinantal combinations for the intrinsic part of the many-body wave function,

$$
\Phi_1^{\text{int}}(\gamma_0) = |\downarrow\uparrow\uparrow\rangle + e^{2\pi i/3}|\uparrow\downarrow\uparrow\rangle + e^{-2\pi i/3}|\uparrow\uparrow\downarrow\rangle,
$$

and

$$
\Phi_2^{\text{int}}(\gamma_0) = |\downarrow\uparrow\uparrow\rangle + e^{-2\pi i/3}|\uparrow\downarrow\uparrow\rangle + e^{2\pi i/3}|\uparrow\uparrow\downarrow\rangle.
$$

Here $\gamma_0 = 0$ denotes the azimuthal angle of the triangle vertex associated with the position of the original spin-down fermion in $|\downarrow\rangle$. We note that the intrinsic wave functions $\Phi_1^{\text{int}}$ and $\Phi_2^{\text{int}}$ are eigenstates of the square of the total spin operator $\hat{S}^2$ ($\hat{S} = \sum_{\alpha=1}^3 \hat{s}_\alpha$) with quantum number $S = 1/2$. This can be verified directly by applying to them the $\hat{S}^2$ as given in Eq. (15).

To restore the circular symmetry, one applies the continuous space projection operator $[31, 32],

$$
2\pi\mathcal{P}_L = \int_0^{2\pi} d\gamma \exp[-i\gamma(\hat{L} - L)],
$$

where $\hat{L} = \sum_{j=1}^N \hat{l}_j$ is the operator for the total angular momentum.

The resulting wave function, $\Xi$, has both good total spin and angular momentum quantum numbers; it is of the form,

$$
2\pi\Xi = \int_0^{2\pi} d\gamma \Phi_1^{\text{int}}(\gamma)e^{i\gamma L},
$$

where now the intrinsic wave function [given by Eq. (31) or Eq. (32)] has an arbitrary azimuthal orientation $\gamma$, which is integrated out.

The operator $\hat{R}(2\pi/3) \equiv \exp(-2\pi i\hat{L}/3)$ can be applied to $\Xi$ in two different ways, namely either on the intrinsic part $\Phi_1^{\text{int}}$ or the external part $\exp(i\gamma L)$. Using Eq. (31) and the property $\hat{R}(2\pi/3)\Phi_1^{\text{int}} = \exp(-2\pi i/3)\Phi_1^{\text{int}}$, one finds,

$$
\hat{R}(2\pi/3)\Xi = \exp(-2\pi i/3)\Xi,
$$

from the first alternative, and

$$
\hat{R}(2\pi/3)\Xi = \exp(-2\pi Li/3)\Xi,
$$

from the second alternative. Now if $\Xi \neq 0$, the only way that Eqs. (35) and (36) can be simultaneously true is if the condition $\exp[2\pi i(L-1)/3] = 1$ is fulfilled. This leads to a first sequence of magic angular momenta associated with total spin $S = 1/2$, i.e.,

$$
L = 3n + 1, \ n = 0, \pm 1, \pm 2, \pm 3, ...
$$

Using Eq. (32) for the intrinsic wave function, and following similar steps, one can derive a second sequence of magic angular momenta associated with good total spin $S = 1/2$, i.e.,

$$
L = 3n - 1, \ n = 0, \pm 1, \pm 2, \pm 3, ...
$$

In the fully polarized case, the spin primitive, $|\uparrow\uparrow\uparrow\rangle$, is already an eigenstate of $\hat{S}^2$ with quantum number $S = 3/2$. Thus only the rotational symmetry needs to be restored, that is, the intrinsic wave function is simply $\Phi_3^{\text{int}}(\gamma_0) = |\uparrow\uparrow\uparrow\rangle$. Since $\hat{R}(2\pi/3)\Phi_3^{\text{int}} = \Phi_3^{\text{int}}$, the condition for the allowed angular momentum is $\exp[-2\pi Li/3] = 1$, which yields the following magic angular momenta,

$$
L = 3n, \ n = 0, \pm 1, \pm 2, \pm 3, ...
$$

We mention again here that only non-negative angular momenta are present in the LLL.

IV. THE SPIN SECTOR ($S = 0$, $S_z = 0$): TRAVERSING THE AVOIDED CROSSING

In this Section, the properties of the relative-ground-state wave functions in the spin sector ($S = 0$, $S_z = 0$) and for $N = 4$ fermions will be investigated in detail along the avoided crossings highlighted in the insets (labeled as A and B) of Fig. 1. The tools used in this analysis are the single-particle densities (1st-order correlations) and the $N$-body correlations (4th-order for $N = 4$ fermions) defined in Sec. IIIC.

A. Single-particle densities

In Fig. 3 we plot the CI single-particle density for two different strengths of the perturbation $V_P$ [C = 0.004, top row (a-d) and C = 0.0001, bottom row (e-h)] and for two different values of the rotational frequency across the avoided crossing highlighted in the insets of Fig. 1, i.e., near the midpoint at $\Omega/\omega = 0.8855$ [Figs. 3(a,b)], or $\Omega/\omega = 0.8847$ [Figs. 3(e,f)], and after the crossing at $\Omega/\omega = 0.90$ [Figs. 3(c,d,g,h)]. As was the case in Fig. 1, $R_{\delta} = 0.4$ and $m = 4$.

As seen from Figs. 3(a-d), the value $C = 0.004$ is rather large and results in a symmetry broken solution even at the point $\Omega/\omega = 0.90$. Indeed, at this point, the associated expectation value of the total angular momentum, $\langle L \rangle = 8.0364$, is still rather different from the integer value of 8. On the contrary, the small value $C = 0.0001$ yields $\langle L \rangle = 8.00002$ at $\Omega/\omega = 0.90$, and the corresponding many-body wave function preserves the rotational symmetry for all practical purposes; see the single-particle density in Fig. 3(d).

This behavior conforms with the fact that the many-body wave functions, $\Phi_{gs}$’s, associated with Figs. 3(a,b),
FIG. 5. CI single-particle densities (both in real space and momentum space) of the relative ground state of $N = 4$ fermions in the spin sector with ($S = 0, S_z = 0$). 3D surfaces are plotted in (a), (c), (e), and (g). Corresponding cuts through the origin along the diagonals (solid line, violet) and perpendicular to the sides (dashed line, green) of the square configuration are displayed in (b), (d), (f), and (h), respectively. In (h) both curves overlap. (a,b) Calculation for $C = 0.004$ (strong perturbation) at the point $\Omega / \omega = 0.8855$. The expectation value of the total angular momentum is $\langle L \rangle = 7.189$, indicating that the plotted case is a state with broken rotational symmetry. (c,d) Calculation for $C = 0.004$ (strong perturbation) at the point $\Omega / \omega = 0.8855$. The expectation value of the total angular momentum is $\langle L \rangle = 7.189$, indicating that the plotted case is a state with broken rotational symmetry. (e,f) Calculation for $C = 0.0001$ (weak perturbation) at the point $\Omega / \omega = 0.8847$. The expectation value of the total angular momentum is $\langle L \rangle = 7.330$, and the single-particle density exhibits strong breaking of the rotational symmetry. (g,h) Calculation for $C = 0.0001$ (weak perturbation) at the point $\Omega / \omega = 0.8847$. The expectation value of the total angular momentum is $\langle L \rangle = 8.00002$, very close to integer 8, and the rotational symmetry is practically reestablished. $R_\delta = 0.4$ and the order of the multipole trap deformation $m = 4$. Because of the properties of the Fourier transform of the LLL orbitals [see Eq. (29)], both real-space and momentum densities are given by the same 3D numerical surface. For the spatial densities, the lengths along the $x$, $y$, and $r$ axes are given in units of $\Lambda$, and the vertical axes are in units of $1/\Lambda^2$. For the momentum densities, the momenta along the $k_x$, $k_y$, and $k_r$ axes are given in units of $1/\Lambda$, and the vertical axes are in units of $\Lambda^2$.

(c,d), and (e,f) contain significant contributions of basis determinants with total angular momenta other than $L = 8$, i.e., $L = 4$ and $L = 12$; see TABLES II - IV in the Appendix. In contrast, the many-body wave function, $\Phi_{gs}$, associated with Figs. 5(g,h) consists mainly of basis determinants each with total angular momentum $L = 8$ (with one exception of a basis determinant of $L = 4$ having a very small weight); see TABLE V in the Appendix.

It is remarkable that in all cases of symmetry breaking portrayed by the 3D surfaces in Figs. 5(a,c,e), the same underlying Wigner-molecule, square-ring configuration emerges. This $(0,4)$ ring configuration is further highlighted by plotting the corresponding cuts through the origin along the diagonals (solid line, violet) and perpendicular to the sides (dashed line, green) of the square configuration in Figs. 5(b,d,f,h), respectively. In Fig. 5(h), the reestablishment of rotational symmetry is reflected in the fact that both the solid and dashed cuts do overlap. Furthermore, the demonstrated here effect of $V_P$ at the avoided crossing upon the CI single-particle density is so profound and disproportionate to the smallness of the perturbation [compare, e.g., Figs. 5(e) and 5(g)] that it is appropriate to characterize the present results as a numerical example of the 'flea on the elephant' concept [66–68], developed in mathematical treatments of the phenomenon of spontaneous symmetry breaking [69].
that preserve the 2D rotational symmetry is gained by considering the 4th-order correlations defined in Sec. IIC. Fig. 6 displays the spin-unresolved 4th-order correlations [see Eq. (26)] associated with Fig. 5(d), i.e., for $C = 0.0001$ at the point $\Omega/\omega = 0.90$. The most natural way to analyze this quantity, that depends on 4 variables, is to fix three variables and plot $4G_{gs}$ as a function of the fourth variable. Motivated by the molecular ring configuration [usually denoted as (0,4)] of the broken-symmetry single-particle densities, we place the three fixed variables at the points $r_0 \exp(j \pi/2 + \Theta)$ (with $j = 1, 2, 3$), where $r_0 = 1.22\Lambda$ is the radius of the maxima of the 4 humps in Fig. 5(c), the angle $\pi/2$ reflects the square arrangement of these four humps, and $\Theta$ is an arbitrary reference angle. Two values of $\Theta = 0$ [Fig. 6(a)] and $\Theta = \pi/4$ [Fig. 6(b)] were used. In both cases, Fig. 6 shows that the conditional probability of finding the fourth fermion at a given point is localized around the apex point that completes the square of the (0,4) ring configuration.

Naturally, the fact that the intrinsic (0,4) molecular configuration contained in the $4G_{gs}$ correlation is independent of the reference angle $\Theta$ is consistent with the uniform (2D rotationally symmetric) single-particle density in Fig. 5(d); it is also the property that suggests the characterization of the associated many-body state as a “rotating Wigner molecule” in contrast to the term “pinned Wigner molecule” suggested by the broken-symmetry single-particle densities in Figs. 5(a), 5(b), and 5(c).

C. 2nd-order correlations

As described in Sec. IIC, 2nd-order correlations are a complementary tool in obtaining information regarding the intrinsic structure of the many-body wave function in the absence of symmetry breaking. The 2nd-order correlations [see Eqs. (17) and (18)] for the symmetry-preserving relative ground state in the $(S = 0, S_z = 0)$ spin sector at $\Omega/\omega = 0.90$ with $m = 4$ and $C = 0.0001$ [corresponding to the single-particle density in Fig. 5(d)] are displayed in Fig. 7. Specifically, taking the fixed point at $r_0 = (1.22\Lambda, 0, 0)$, Figs. 7(a) and 7(b) portray the up-up, $2G_{\uparrow\uparrow}$, and up-down, $2G_{\uparrow\downarrow}$, spin-resolved 2nd-order correlations, respectively, whereas Fig. 7(c) portrays the spin-unresolved one. Figs. 7(d) and 7(e) portray the up-up and up-down 2nd-order correlations, respectively, but with the fixed point taken to be at the origin. Lastly, Fig. 7(f) displays the difference between the two spin-resolved correlations, $2G_{\uparrow\downarrow} - 2G_{\uparrow\uparrow}$, when the fixed point is taken at the origin.

In addition to reproducing the relative single-particle localization of the four fermions in a square configuration (discussed in Sec. IVB using 4th-order correlations), the 2nd-order correlations in Figs. 7(a) and 7(b) can assist in the determination of the underlying spin structure.
FIG. 7. ↑↑ (a,d), ↑↓ (b,e), and spin-unresolved (c) 2nd-order correlations (both in real space and momentum space) of the relative CI ground state in spin sector \( \mathbf{S} = 0, S_z = 0 \) with \( L = 8 \) for \( N = 4 \) fermions at the trap angular frequency \( \Omega/\omega = 0.90 \). The strength of the \( V_p \) perturbation is weak, using \( C = 0.0001 \) with \( m = 4 \) and \( R_\delta = 0.4 \). These correlations correspond to the 2D rotationally symmetric single-particle density in Fig. 5(d). (d) The difference \( ^2G_{\uparrow\downarrow} - ^2G_{\uparrow\uparrow} \). The fixed points (see text) are placed at \((x_0 = 1.2, y_0 = 0)\) for the three top panels, and at the origin \((x_0 = 0, y_0 = 0)\) for the three bottom panels. Because of the properties of the Fourier transform of the LLL orbitals [see Eq. (29)], both real-space and momentum correlations are given by the same 3D numerical surface. For the space correlations, the lengths along the \( x \) and \( y \) axes are given in units of \( \Lambda \), and the vertical axes are in units of \( 1/\Lambda^4 \). For the momentum correlations, the momenta along the \( k_x \) and \( k_y \) axes are given in units of \( 1/\Lambda \), and the vertical axes are in units of \( \Lambda^4 \). In (a)-(c), the fixed point is denoted by a solid dot. The inset provides a graphical representation of the six \( \zeta_i \)'s spin primitives [see Eq. (22)], when associated with the Wigner-molecule square geometry.

According to Fig. 7(a), when the fixed spin-up fermion is placed at one corner of the square, the most probable locations of the other spin-up fermion are the two adjacent corners of the square, but not the opposite corner along the diagonal. This behavior is consistent with the graphical depictions of \( \zeta_1 \) and \( \zeta_3 \) (or \( \zeta_4 \) and \( \zeta_6 \)). In addition, it is straightforward to see that the ↑↓ 2nd-order correlation in Fig. 7(b) is consistent with the same graph-
ics for \(\zeta_1\) and \(\zeta_3\) (or \(\zeta_4\) and \(\zeta_6\)). Indeed, the most probable locations for the down-spin fermions are all three remaining corners, including the one across the diagonal. The higher probability at the corner across the diagonal is accounted for by the fact that this corner appears in both graphics as probable location of the down fermions. Taking into consideration that \(2G_{t\uparrow} = G_{t\uparrow}\) and \(2G_{t\downarrow} = G_{t\downarrow}\), one can conclude that the dominant contributions in the many-body wave function contain the spin configuration whose CI coefficients obey the following relations

\[
\begin{align*}
c(1) &= c(16) = 2c(4) = -2c(6) = -2c(9) = 2c(11) = c_1, \\
c(3) &= c(15) = c_2, \\
c(8) &= 2c(14) = -c_2, \\
c(5) &= c(13) = c_3, \\
c(7) &= c(12) = c_4, \\
c(10) &= c_5.
\end{align*}
\]

From TABLE [V] one can extract numerical values for the 5 constants \(c_i\) (with \(i = 1, \ldots, 5\)) in Eq. (41). However, as we will discuss below, the spin structure is independent of specific numerical values. Note that the coefficients grouped together in each line of Eq. (41) are associated with given (non-ordered) sets of single-particle angular momenta \(l_i\), i.e., with the six sets \((0,1,3,4), (0,2,2,4), (1,2,2,3), (0,3,2,3), (1,2,1,4)\), and \((1,3,1,3)\), respectively.

Using the relations (41) and the 15 Slater determinants in TABLE [V] and employing the MATHEMATICA algebraic language [70] we can write the CI wave function in the form of Eq. (23). The analytic expressions of the space parts, \(\Phi_{(z_1, z_2, z_3, z_4)}\) (with \(i = 1, \ldots, 6\) and \(z = x + iy = re^{i\theta}\)) are lengthy to be explicitly written in the text. However, the interested reader will find them as MATHEMATICA scripts in the Supplemental Material [71].

Before proceeding with the analysis, we recall here the form of the six spin eigenfunctions \(\tilde{\zeta}_i\) (with \(i = 1, \ldots, 6\)) having both good total spin \(S\) and a good spin projection \(S_z\). These spin eigenfunctions can be obtained by solving a 4-site Heisenberg Hamiltonian with the four spins arranged in a closed rectangular configuration, as was done in Appendix B of Ref. [72]. Taking all four Heisenberg exchange constants to be equal, the spin eigenfunctions (B13)-(B18) in Ref. [72] simplify to the following (relevant to the present paper) expressions:

\[
\begin{align*}
\tilde{\zeta}_1 &= \frac{1}{\sqrt{12}}(\zeta_1 + \zeta_3 + \zeta_4 + \zeta_6 - 2\zeta_2 - 2\zeta_5), & S = 0, \\
\tilde{\zeta}_2 &= \frac{1}{2}(\zeta_1 - \zeta_3 - \zeta_4 + \zeta_6), & S = 0, \\
\tilde{\zeta}_3 &= \frac{1}{\sqrt{2}}(\zeta_6 - \zeta_1), & S = 1, \\
\tilde{\zeta}_4 &= \frac{1}{\sqrt{2}}(\zeta_5 - \zeta_2), & S = 1, \\
\tilde{\zeta}_5 &= \frac{1}{\sqrt{2}}(\zeta_4 - \zeta_3), & S = 1, \\
\tilde{\zeta}_6 &= \frac{1}{\sqrt{6}}(\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 + \zeta_5 + \zeta_6), & S = 2.
\end{align*}
\]

D. Spin structure of the symmetry-preserving 
\(L = 8\) relative ground state

Motivated by the analysis of the 2nd-order correlations in Sec. IV.C, showing that the spin function displayed in Eq. (40) must be an important component of the many-body CI wave function \(\Phi_{C1}^{L=8, S=0, S_z=0}\), it is instructive to interrogate whether the complete spin function of this state can be determined from the microscopic CI wave function. To this end, we use the \(c(J)\) coefficients (rounded to the fourth decimal point) listed in TABLE [V] in the Appendix; naturally, we neglect the two orders-of-magnitude smaller \(c(2)\) coefficient. With the above, the CI wave function can be approximated by the sum of 15 Slater determinants (specified in TABLE [V]) by the single-particle angular momenta \(l_i\), with \(i = 1, \ldots, 4\)
where the $\zeta_i$’s (with $i = 1, \ldots, 6$) were defined in Eq. [22].

Solving the system of Eqs. [42-47] to obtain the spin primitives, $\zeta_i$ (with $i = 1, \ldots, 6$), as a function of the spin eigenfunctions, $\tilde{\zeta}_j$ (with $j = 1, \ldots, 6$), one can rearrange Eq. [23] for the many-body wave function as follows:

$$\Phi_{CI} = \sum_{i=1}^{6} F_i \zeta_i = \sum_{i=1}^{6} \tilde{F}_i \tilde{\zeta}_i,$$

(48)

where

$$\tilde{F}_1 = \frac{1}{\sqrt{12}} (F_1 + F_3 + F_4 + F_6 - 2F_2 - 2F_5), \quad S = 0,$$

(49)

$$\tilde{F}_2 = \frac{1}{2} (F_1 - F_3 - F_4 + F_6), \quad S = 0,$$

(50)

$$\tilde{F}_3 = \frac{1}{\sqrt{2}} (F_6 - F_1), \quad S = 1,$$

(51)

$$\tilde{F}_4 = \frac{1}{\sqrt{2}} (F_5 - F_2), \quad S = 1,$$

(52)

$$\tilde{F}_5 = \frac{1}{\sqrt{2}} (F_4 - F_3), \quad S = 1,$$

(53)

$$\tilde{F}_6 = \frac{1}{\sqrt{6}} (F_1 + F_2 + F_3 + F_4 + F_5 + F_6), \quad S = 2.$$  

(54)

We note that the arrangement of the $\tilde{F}_i$’s in Eqs. [49-54] coincide with that of the $\zeta_i$’s in Eqs. [42-47].

Using the analytic expressions [77] for the $F_i$’s, one can verify that $\tilde{F}_3 = \tilde{F}_4 = \tilde{F}_5 = \tilde{F}_6 = 0$, which is a confirmation of the fact that the CI wave function under consideration has total spin $S = 0$. Consequently, one obtains the following general form for the $L = 8$ ground state in the spin sector ($S = 0, S_z = 0$):

$$\Phi_{CI}^{L=8, S=0, S_z=0} = \tilde{F}_1 \tilde{\zeta}_1 + \tilde{F}_2 \tilde{\zeta}_2.$$  

(55)

From the analysis of 2nd-order correlations in Sec. [IV.C], it follows that the contribution of the first term in Eq. [55] must be less important than that of the second term. Indeed, this can further be confirmed by choosing the spatial coordinates to adhere to a square arrangement, i.e., by taking $z_1 = z_0$, $z_2 = 2z_0 e^{i\pi/2}$, $z_3 = z_0 e^{i\pi}$, and $z_4 = z_0 e^{i\frac{3\pi}{2}}$, with the point $z_0$ being arbitrary. In this case, the spin structure of $\Phi_{CI}^{L=8, S=0, S_z=0}$ agrees with Eq. [40], i.e., one finds

$$\tilde{F}_1 = 0,$$

$$\tilde{F}_2 = 3c_1 - 3\sqrt{6}c_2 + 2\sqrt{2}c_3 + 2\sqrt{3}c_4 - 4c_5 z_0^6 e^{-2z_0^6},$$

(56)

where of course $L = 8$ here.

We further note that neither $\tilde{F}_1$ or $\tilde{F}_2$ contain the associated Vandermonde determinant as a factor, unlike an assumption [73] used earlier in the description of quantal versions of skyrmions. The Fock antisymmetrization here is guaranteed by the fact that $F_{L=8, S=0, S_z=0}$ is the sum of Slater determinants.

V. THE SPIN SECTOR ($S = 2, S_z = 0$): AN ANALOG OF THE (1,1,1) HALPERIN STATE AND FERMIONIZATION IN TWO DIMENSIONS

Focusing now on the spin sector ($S = 2, S_z = 0$), we note that all the eigenvalues $E_{int}$ associated with the contact-interaction term of the $H_{LLL}$ Hamiltonian [third term in Eq. (3)] are vanishing [see Fig. 3(c)], so that the curves in Fig. 3 are non-intersecting straight lines, converging to zero for $\Omega/\omega = 1$. The relative ground state has a total angular momentum $L = 6$, which is of interest because it coincides with the angular momentum of the trial wave function [denoted as (1,1,1)] proposed by Halperin [41] for spinor fermions as a generalization of the celebrated Laughlin wave function [3] (applicable only for the case of fully spin-polarized fermions). Indeed the general $(p, p, q)$ Halperin wave function, where $p$ and $q$ are positive integers, is given by [41, 74, 75]

$$\Upsilon_{(p,p,q)}(z, w) = \prod_{i<j} (z_i - z_j)^p \prod_{k<l} (w_k - w_l)^p \prod_{i,k} (z_i - w_k)^q.$$  

(57)

In Eq. [57], $z_i = r_i e^{i\theta_i}$ and $w_k = r_k e^{i\theta_k}$ are the space coordinates (here in units of $\Lambda$) in the complex plane for the spin-up and spin-down fermions, respectively. Note further that the trivial Gaussian factors, $\exp[-\sum_{i=1}^{N_1} z_i^2 z_i^*/2] \exp[-\sum_{k=1}^{N_2} w_k^2 w_k^*/2]$, have been omitted in Eq. [57]. The total angular momentum associated with the wave function $\Upsilon_{(p,p,q)}(z, w)$ is

$$L_{(p,p,q)} = p \frac{N_1(N_1 - 1)}{2} + q N_1 N_2,$$  

(58)

which indeed for $N_1 = N_2 = 2$ and $p = q = 1$ gives $L_{(1,1,1)} = 6$.

Of significance is the fact that the original proposal for the $\Upsilon(z, w)$ wave functions did not include the spin variables. Below we will investigate the connection of the (1,1,1) Halperin wave function to the CI many-body wave function which is the relative ground state in the $(S = 2, S_z = 0)$ spin sector [77]; recall that the relative ground state is the lowest-in-energy state within each spin sector. Furthermore using this connection we will demonstrate a two-dimensional case of mapping from spinor to spinless fermions that is analogous to the fermionization mapping in one dimension [34].
A. The 4th order correlation and the molecular configuration

First in Fig. 8 we display the single-particle density [Fig. 8(a)] and the corresponding spin-unresolved 4th-order correlation [Fig. 8(b)] for the CI state with \( S = 2, S_z = 0 \) and \( L = 6 \). It is seen that the single-particle density is rotationally symmetric, but an intrinsic square geometrical configuration appears in the unresolved 4th-order correlation. This is similar to the behavior found for the CI relative ground state in the spin sector \( (S = 0, S_z = 0) \) at the point \( \Omega/\omega = 0.90 \). Common to these two states is the fact that the corresponding angular momenta, i.e., \( L = 6 \) and \( L = 8 \), respectively, are magic ones compatible with the \( C_4 \) point group symmetry; see Eq. (30).

B. Comparison between CI state and trial \((1,1,1)\)
Halperin wave function

Furthermore, in TABLE I we list the dominant CI coefficients, \( c(I) \), and the spin orbitals, \( (l_1 \uparrow,l_2 \uparrow,l_3 \downarrow,l_4 \downarrow) \), entering into the associated basis of Slater determinants (see Sec. III B). The criterion used for selection of the most dominant determinants in the CI solution was \( |c(I)| > 10^{-3} \). The CI calculation used 1296 basis determinants with all possible total angular momenta from 2 to 30. From TABLE I it is apparent that only six determinants with \( L = 6 \) and equal weighting coefficients, \( |c(J)| \), contribute to the CI LLL state with \( S = 2, S_z = 0 \); indeed \( \sum_{i=1}^{6} |c(J)|^2 = 0.99999475 \), i.e., the corresponding normalization constant differs from unity only in the sixth decimal point.

Taking into consideration that the numerical value of the \( |c(J)|'s \) in TABLE I equals \( 1/\sqrt{6} \), up to the sixth decimal point, and that the LLL single-particle orbitals [with lengths in units of \( \Lambda \), the harmonic confinement oscillator length, see text below Eq. (11)] are written as

\[
\exp[-z^2/2\sqrt{\pi\Lambda}],
\]

one can verify the following algebra.

![Figure 8: Structure of the relative CI ground state (in both real space and momentum space) in the spin sector \( (S = 2, S_z = 0) \) for \( N = 4 \) fermions at the trap angular frequency \( \Omega/\omega = 0.90 \). (a) Single-particle density. (b) Spin unresolved 4th-order correlation. The strength of the \( V_0 \) quantities, the momenta along the trap deformation \( m \) and the vertical axes are in units of the lengths along the same 3D numerical surface. For the spatial quantities, the lengths along the \( x \) and \( y \) axes are given in units of \( \Lambda \), and the vertical axes are in units of \( 1/\Lambda^2 \) for the density and \( 1/(\pi^4\Lambda^8) \) for the 4th-order correlation. For the momentum quantities, the momenta along the \( k_x \) and \( k_y \) axes are given in units of \( 1/\Lambda \), and the vertical axes are in units of \( \Lambda^2/\pi^2 \) for the the 4th-order correlation. The 2D single-particle density in (a) is rotationally symmetric. In (b), the three fixed points (denoted by solid dots) are placed at a radius \( r_0 = 0.90 \Lambda \), whereas the azimuthal angle between them is \( \pi/2 \), and the reference angle \( \Theta = \pi/4 \).

| \( I \) | \( J \) | \( c(J) \) | \( (l_1 \uparrow,l_2 \uparrow,l_3 \downarrow,l_4 \downarrow) \) | \( \sum_{i=1}^{4} |l_i| \) |
|---|---|---|---|---|
| 16 | 1 | -0.4082472 | \( (0,1,2,3) \) | 6 |
| 46 | 2 | 0.4082472 | \( (0,2,1,3) \) | 6 |
| 81 | 3 | -0.4082472 | \( (0,3,1,2) \) | 6 |
| 291 | 4 | -0.4082472 | \( (1,2,0,3) \) | 6 |
| 326 | 5 | 0.4082472 | \( (1,3,0,2) \) | 6 |
| 541 | 6 | -0.4082472 | \( (2,3,0,1) \) | 6 |
braic identity

\[ \Phi_{CI}^{S=2, S_z=0} = \sum_{j=1}^{6} \frac{\text{sgn}(J)}{\sqrt{4!}} \left( \prod_{i<j} (z_i - z_j) \right) \alpha(1) \alpha(2) \alpha(3) \alpha(4) \]

\[ = \frac{1}{2\sqrt{3} \times 4! \pi^2} \left( \prod_{i<j} (z_i - z_j) \right) \alpha(1) \alpha(2) \alpha(3) \alpha(4). \tag{59} \]

where \(\text{sgn}(J)\) is the + or − sign of the \(c(J)\) coefficients according to TABLE I. The \(J, J = 1, 2, \ldots, 6\) are defined in Eq. (22), and we omitted the trivial Gaussian factors.

Renaming the spatial coordinates of the spin-up fermions as \(z_3 \rightarrow w_1\) and \(z_4 \rightarrow w_2\), one sees immediately that the space part of the \(\Phi_{CI}^{S=2, S_z=0}\) wave function [see Eq. (59)] coincides with the \((1,1,1)\) Halperin function, i.e., with the expression for \(Y(z, w)\) in Eq. (57) when \(p = q = 1\). We recall here the possibility that in certain instances the LLL CI wave function may be expressed exactly in analytical form, as it has been noted in earlier publications [23] for the case of LLL ground states of a few spinless bosons in the range \(0 \leq L \leq N\). As a notable counterexample, we mention here the disagreement between the Moore-Read trial wave function [31], which consists mainly of a \((0,5)\) ring configuration, and the CI wave function, which contains mainly a \((1,4)\) ring configuration, in the case of the LLL ground state for \(N = 5\) spinless bosons and \(L = 8\) [32].

C. The fermionization analogy

The derivation of the exact CI analytic expression in Eq. (59) enabled us to make another important comparison. It is well known that the fully spin-polarized fermionic LLL CI state with \(L = N(N-1)/2 = L_{i=N_i}^{N,N_i}\) consists of only one Slater determinant constructed with the single-particle orbitals \(z^0, z^1, z^2, \ldots, z^{N-1}\alpha\) (again the Gaussian factors are omitted). For the case of \(N = 4\) fermions, this state is written as (considering that the space part is a Vandermonde determinant):

\[ \Phi_{CI}^{S=2, S_z=2} = \frac{1}{\sqrt{4!}} \text{Det}[\phi(1), \phi(2), \phi(3), \phi(4)] \]

\[ = \frac{1}{2\sqrt{3} \times 4! \pi^2} \left( \prod_{i<j} (z_i - z_j) \right) \alpha(1) \alpha(2) \alpha(3) \alpha(4). \tag{60} \]

One sees that, apart from a sign, the space part of the spinor \(\Phi_{CI}^{S=2, S_z=0}\) and the fully spin-polarized \(\Phi_{CI}^{S=2, S_z=2}\) wave functions are the same. This mapping between spinor and fully spin-polarized (equivalent to spinless fermions) many-body wave functions is analogous to the well-known mapping [34] in one dimension between the wave function of \(N\) hard bosons, i.e., bosons with strong interparticle contact interaction, and that of \(N\) spinless fermions; it can be described as a generalization of the “fermionization” concept [34] to two dimensions. We note that, because of the exchange hole, the contact interaction becomes inoperative in the case of fully polarized (or spinless) fermions, and as a result this fermionization mapping demonstrates that the intrinsic crystalline correlations portrayed in Fig. 8(b) can be generated, as a limiting case to the quantum Wigner molecule, by the Pauli exclusion principle alone [33].

D. What about the 2nd-order correlations?

Unlike the approach in this paper, and a handful of earlier publications [11, 20], the 2nd-order correlations have been traditionally considered sufficient (see, e.g., Refs. [3, 9, 10, 20, 32, 61]) for analyzing the intrinsic structure of the highly-correlated LLL states. The case of the \((S = 2, S_z = 0)\) CI LLL state for \(N = 4\) fermions and \(L = 6\) shows that the above supposition does not hold in general. Indeed, in Fig. 9, we display the up-up-\((\uparrow\uparrow)\) and up-down-\((\uparrow\downarrow)\) spin-resolved 2nd-order correlations for this CI state [which corresponds to the \((1,1,1)\) Halperin wave function]. Note that there is a 1-to-2 ratio between the \(\uparrow\uparrow\) and the \(\uparrow\downarrow\) 2nd-order correlations, because, for each spin-up fermion, there are one spin-up and two spin-down additional fermions.

As seen from Fig. 9 only the existence of the zero probability for finding two fermions at the same position is visible. Any signature of the square-rings intermediate molecular structure has been washed away in Fig. 9 due to the averaging performed through the double integrations over the coordinates of the third and fourth particles; see the definition of the 2nd-order correlations in Eq. (18). Revealing the intrinsic Wigner-molecule structure using 2nd-order correlations requires higher total angular momenta, as shown in Ref. [11] for the analogous cases of LLL bosons. However, it appears that the experimental window [21] for a few rapidly rotating ultracold fermions is restricted to the range of small \(L\)'s, up to values in the neighborhood of \(L_{(1,1,1)}\), corresponding to the \((1,1,1)\) Halperin states. Consequently, we conclude that consideration of the \(N\)-body correlations offers, as shown in this paper, essential additional information regarding the CI wave functions.

VI. DISCUSSION: THE ROLE OF THE WIGNER PARAMETER

The dimensionless parameter \(R_\delta\) [defined in Eq. (3)] enters naturally in the many-body LLL Hamiltonian in Eq. (6). This applies also for the many-body Hamiltonians for ultracold atoms in non-rotating traps, i.e.,
perturbation is weak with fermions at the trap angular frequency \( \Omega = 0 \). For the momentum correlations, the momenta along the \( x \) and \( y \) axes are given in units of \( \Lambda \). Note the different scales between (a) and (b).

When \( \Omega = 0 \); see, e.g., Ref. [39]. We note that, in the absence of a magnetic field and for a finite number of \( N \) trapped electrons in 2D semiconductor quantum dots, a corresponding parameter \([31, 37, 38]\) (usually referred to as the Wigner parameter) is defined as

\[
R_W = Q/(\hbar \omega),
\]

where \( Q = e^2/(\kappa l_0) \) is the Coulomb repulsive energy between two electrons at a distance equal to the oscillator length \( l_0 = \sqrt{\hbar/(m_e^* \omega)} \), \( \kappa \) is the dielectric constant of the semiconducting medium, \( m_e^* \) is the effective mass of the electron, and \( \omega \) is the frequency of the parabolic (harmonic) 2D potential confinement.

In the case of a high applied magnetic field \( B \) (LLL Hilbert space), \( l_0 \) in Eq. (61) is replaced by the magnetic length and \( \omega \) is replaced by the cyclotron frequency, that is, \( l_0 \rightarrow l_B \) and \( \omega \rightarrow \omega_e = eB/(m^*c) \), with \( l_B = \sqrt{\hbar/(m^*\omega_e)} \). As is the case with the contact interaction – i.e., the fact (discussed in Sec. III) that the LLL spectrum associated solely with the interaction term, \( H_{\text{int}} \) [third term in Eq. (2)], scales with \( R_3 \) – the LLL spectrum associated solely with the long-range Coulomb repulsion scales also with \( R_W \). As a result, the values \( R_3 \) and \( R_W \) do not influence the intrinsic structure of the LLL many-body wave functions. [Note that the eigenstates of \( H_{\text{int}} \) are also eigenstates of the LLL kinetic-energy Hamiltonian, \( H_K \); see second term in Eq. (2).] The only effect of the magnitude of \( R_3 \) is to determine the precise value of \( \Omega/\omega \) where the crossings in Fig. 1 occur. In contrast, for vanishing and small magnetic fields, or for a non-rotating trap, the emergence of the Wigner molecular structures does depend on the value of \( R_W \) and \( R_3 \), respectively, requiring values of these parameters larger than unity \([29, 25, 31, 37–40, 84]\).

The apparent above inconsistency concerning the qualitative role of the Wigner parameter motivates the following deeper insight. Indeed both the \( R_W \) and \( R_3 \) parameters at \( B = 0 \) and \( \Omega = 0 \), respectively, express the ratio

\[
R = \frac{\Delta E_{\text{int}}}{\Delta E_{\text{sp}}},
\]

where \( \Delta E_{\text{int}} \) is a representative amount of repulsive energy and \( \Delta E_{\text{sp}} \) is an average energy spacing in the single-particle spectrum. For \( B = 0 \), or \( \Omega = 0 \), the \( \hbar \omega \) used in Eqs. (3) and (61) reflects indeed the average energy gap between the single-particle states of the familiar 2D harmonic oscillator. In the case of the Landau-level spectrum (Fock-Darwin oscillator \([31, 38, 39]\)), \( \hbar \omega \), or \( \hbar \omega_e \), represents the energy spacing between Landau levels. However, the relevant many-body Hilbert space is restricted in the LLL where the energy gap between the single-particle states vanishes due to the well-known infinite degeneracy of the Landau levels; this is also referred to as single-particle kinetic-energy quenching. Thus with respect to the pertinent dimensionless parameter that controls Wigner-molecule formation in the LLL, the denominator in Eq. (22) must be taken to be precisely zero, which results in all instances in an infinite value for \( R \). Interestingly, the single-outcome value of \( R \rightarrow +\infty \) implies that the LLL many-body case is preset for favoring the emergence of Wigner molecules, independently of the strength or the type of the two-body

![Image](image_url)
interaction. In fact, in addition to the Coulombic and contact-interaction cases, this qualitative prediction has been confirmed by numerical calculations in the case of few fully spin-polarized LLL fermions interacting via a dipole-dipole potential [85].

VII. SUMMARY

The development and employment of both computational, numerical (two-dimensional configuration interaction [21, 22, 31] and algebraic (MATHEMATICA [70]), state-of-the-art methodological approaches were shown here to bring forth advanced tools (e.g., all-order momentum correlations) that boost and refine our ability to in-depth interogate the complex many-body physics underlying the fractional quantum-Hall effect in assemblies of a few ultracold neutral fermionic atoms, interacting via repulsive contact potentials and confined in a single rapidly rotating two-dimensional harmonic trap. We considered spinor fermionic atom assemblies, where in addition to the two-dimensional orbital degree of freedom, each orbital within a degenerate Landau level state has also spin degrees of freedom. Detailed results were given for the illustrative example of four spinfull ultracold fermions in a rapidly rotating trap (a case anticipated to be among the first to be experimentally explored in the near future).

Our analysis showed that the few-body LLL states with magic angular momenta exhibit intrinsic ordered quantum structures in the $N$-body correlations, similar to those associated with rotating Wigner molecules [21, 31], familiar from the field of semiconductor quantum dots under high magnetic fields.

The application of a small perturbing stirring potential $V_p$ [specifically a multipole deformation of the trap; see Eq. 6] induces, in the neighborhood of the ensuing avoided crossings in the global LLL energy spectra [see Fig. 1 associated with the $(S = 0, S_z = 0)$ spin sector], states with broken rotational symmetry (i.e., without good total angular momenta, referred to accordingly as pinned Wigner molecules). These structures, exhibit molecular-type (or crystalline-type) configurations which are manifested already at the lowest level of first-order correlations (i.e., in the single-particle CI spin-unresolved densities; see Fig. 5). This behavior portrays characteristics reminiscent of the 'flea on the elephant' concept [66–68], familiar from the mathematical treatment of spontaneous symmetry breaking phenomena [69].

Furthermore, our analysis identified a CI LLL state in the $(S = 2, S_z = 0)$ spin sector, which was shown to be well-described by a Halperin (1,1,1) two-component orbital variational wave function. Analysis of this CI LLL wavefunction enabled a two-dimensional generalization of the Girardeau one-dimensional 'fermionization' scheme [34], originally invoked for the mapping of bosonic-type wave functions to those of spinless fermions.

We stress that our systematic comparative analysis and investigations led us to conclude that in order to uncover the intrinsic geometrical structural characteristics of the symmetry-preserving ultracold rotating Wigner molecules that form in the rotating traps and exhibit magic angular momenta, it is imperative to carry out analysis that goes beyond second-order correlations in the real configuration space. To assist the design and analysis of experimental observations in 2D traps, we illustrate these findings through benchmark theoretical predictions for all-order spin-unresolved, as well as spin-resolved, all-order momentum correlations. These can be indeed directly measured [17, 18, 86] with time-of-flight protocols employing individual particle detection in the far-field region.

Our conclusions regarding all-order momentum correlations apply to the correlated FQHE states formed in ultracold neutral atom assemblies trapped in rotating traps on which we focused in the current study, as well as to future investigations, including interrogations of quantum magnetism in finite 2D systems (extending previous studies on 1D-trapped ultracold atoms [72, 87]), hole-pairing in 2D-plaquettes [88], and Mott-insulator to superfluid quantum phase transitions in finite 2D ultracold atom systems [89].

VIII. ACKNOWLEDGMENTS

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Appendix A: ADDITIONAL TABLES

This appendix lists the dominant contributions to the CI wave functions corresponding to Figs. 5(a,b), Figs. 5(c,d), Figs. 5(e,f), and Figs. 5(g,h).

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Table II. Dominant coefficients, $c(I)$, in the CI expansion of the relative LLL ground state (with $(L) = 7.189$) in the $(S = 0, S_z = 0)$ spin sector corresponding to the symmetry-broken state whose single-particle density portrayed in Figs. 5a,b. The CI expansion consists of $t_{total} = 1296$ basis determinants. The index $J$ is introduced to relabel the dominant coefficients, with the dominance criterion being $|c(I)| > 0.01$. 48 determinants with total angular momenta $J = 4$, 8, or 12 participate in this table. Note that $\sum_{I=1}^{48} |c(J)|^2 = 0.99843$, i.e., the corresponding contribution to the normalization constant differs from unity only in the third decimal point.

| $I$ | $J$ | $c(J)$ | $(l_1, l_2, l_3, l_4)$ | $\sum_{I=1}^{48} |c(J)|^2$ |
|-----|-----|--------|----------------------|-----------------|
| 3   | 1   | 0.1425510E+00 | (0, 1, 0, 3) | 4 | 303.25 |
| 9   | 2   | 0.1926172E+00 | (0, 1, 1, 2) | 4 | 304.26 |
| 13  | 3   | -0.1348374E-01 | (0, 1, 1, 6) | 8 | 328.27 |
| 22  | 4   | 0.2478987E+00 | (0, 1, 3, 4) | 8 | 332.28 |
| 26  | 5   | -0.2194019E-01 | (0, 1, 3, 8) | 12 | 334.29 |
| 29  | 6   | 0.1561250E+00 | (0, 1, 4, 7) | 12 | 338.30 |
| 38  | 7   | -0.3103776E+00 | (0, 2, 0, 2) | 4 | 363.31 |
| 42  | 8   | 0.1509984E+00 | (0, 2, 0, 6) | 8 | 369.32 |
| 53  | 9   | -0.3058820E+00 | (0, 2, 2, 4) | 8 | 433.33 |
| 57  | 10  | 0.2696752E+00 | (0, 2, 2, 8) | 12 | 478.34 |
| 64  | 11  | -0.1272792E+00 | (0, 2, 4, 6) | 12 | 507.35 |
| 73  | 12  | 0.1422510E+00 | (0, 3, 0, 1) | 4 | 513.36 |
| 83  | 13  | 0.1260992E+00 | (0, 3, 1, 4) | 8 | 543.37 |
| 87  | 14  | -0.1107325E+00 | (0, 3, 1, 8) | 12 | 547.38 |
| 92  | 15  | 0.2601536E+00 | (0, 3, 2, 3) | 8 | 549.39 |
| 96  | 16  | -0.1637189E+00 | (0, 3, 2, 7) | 12 | 578.40 |
| 118 | 18  | -0.1218950E+00 | (0, 4, 1, 3) | 8 | 687.42 |
| 182 | 19  | 0.1509984E+00 | (0, 6, 0, 2) | 8 | 722.43 |
| 197 | 20  | 0.1268128E+00 | (0, 6, 2, 4) | 12 | 757.44 |
| 232 | 21  | -0.1635275E+00 | (0, 7, 2, 3) | 12 | 831.45 |
| 262 | 22  | 0.1086994E+00 | (0, 8, 1, 3) | 12 | 901.46 |
| 289 | 23  | 0.1926172E+00 | (1, 2, 0, 1) | 4 | 974.47 |
| 299 | 24  | 0.2134452E+00 | (1, 2, 1, 4) | 8 | 1009.48 |

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TABLE III. Dominant coefficients, \( c(I) \), in the CI expansion of the relative LLL ground state (with \( \langle L \rangle = 8.0364 \)) in the \( (S = 0, S_z = 0) \) spin sector corresponding to the symmetry-broken state whose single-particle density portrayed in Figs. 5.b,c. The CI expansion consists of \( I_{\text{total}} = 1296 \) basis determinants. The index \( J \) is introduced to relabel the dominant coefficients, with the dominance criterion being \( |c(I)| > 0.01 \). 54 determinants with total angular momenta \( L = 4, 8, \) or 12 participate in this TABLE. Note that \( \sum_{i=1}^{4} |c(I)|^2 = 0.999912 \), i.e., the corresponding contribution to the normalization constant differs from unity only in the fourth decimal point.

| \( I \) | \( J \) | \( c(I) \) | \( \sum_{i=1}^{4} l_i \) | \( |c(I)|^2 \) | \( \sum_{i=1}^{4} l_i \) |
|---|---|---|---|---|---|
| 3 | 1 | -0.2252529E-01 | 0.1, 0, 3 | 4 | 332.0 |
| 9 | 2 | -0.2769987E-01 | 0.1, 1, 2 | 4 | 334.29 |
| 23 | 3 | -0.2782506E+00 | 0.1, 3, 4 | 8 | 338.30 |
| 26 | 4 | -0.2845012E-01 | 0.1, 3, 8 | 12 | 347.31 |
| 29 | 5 | -0.2007129E-01 | 0.1, 4, 7 | 12 | 363.32 |
| 38 | 6 | 0.4715954E-01 | 0.2, 0, 2 | 4 | 367.33 |
| 53 | 7 | 0.3406431E+00 | 0.2, 2, 4 | 8 | 369.34 |
| 57 | 8 | -0.3453988E-01 | 0.2, 2, 8 | 12 | 373.35 |
| 64 | 9 | 0.1613584E-01 | 0.2, 4, 6 | 12 | 443.36 |
| 73 | 10 | -0.2252529E-01 | 0.3, 0, 1 | 4 | 472.37 |
| 83 | 11 | -0.1395374E+00 | 0.3, 1, 4 | 8 | 478.38 |
| 87 | 12 | -0.1413700E-01 | 0.3, 1, 8 | 12 | 507.39 |
| 88 | 13 | -0.2935452E-00 | 0.3, 2, 3 | 8 | 513.40 |
| 92 | 14 | 0.2115172E-01 | 0.3, 2, 7 | 12 | 543.41 |
| 96 | 15 | -0.1388384E-01 | 0.3, 3, 6 | 12 | 547.42 |
| 118 | 16 | 0.1871866E+00 | 0.4, 1, 3 | 12 | 549.43 |
| 122 | 17 | -0.1001277E-01 | 0.4, 1, 7 | 12 | 578.44 |
| 197 | 18 | -0.1612048E-01 | 0.6, 2, 4 | 12 | 582.45 |
| 227 | 19 | 0.1005852E+00 | 0.7, 1, 4 | 12 | 687.46 |
| 232 | 20 | 0.2112242E-01 | 0.7, 2, 3 | 12 | 693.47 |
| 262 | 21 | -0.1409311E-01 | 0.8, 1, 3 | 12 | 722.48 |
| 289 | 22 | -0.2769878E-01 | 1.2, 0, 1 | 4 | 757.49 |
| 299 | 23 | -0.2401117E+00 | 1.2, 1, 4 | 8 | 802.50 |
| 303 | 24 | 0.2436981E-01 | 1.2, 1, 8 | 12 | 831.51 |
| 304 | 25 | -0.1691131E+00 | 1.2, 2, 3 | 8 | 901.52 |
| 308 | 26 | 0.1214360E-01 | 1.2, 2, 7 | 12 | 974.53 |
| 328 | 27 | 0.1387186E+00 | 1.3, 0, 4 | 8 | 1009.54 |

TABLE IV. Dominant coefficients, \( c(I) \), in the CI expansion of the relative LLL ground state (with \( \langle L \rangle = 7.330 \)) in the \( (S = 0, S_z = 0) \) spin sector corresponding to the symmetry-broken state whose single-particle density portrayed in Figs. 5.e,f. The CI expansion consists of \( I_{\text{total}} = 1296 \) basis determinants. The index \( J \) is introduced to relabel the dominant coefficients, with the dominance criterion being \( |c(I)| > 0.001 \). 20 determinants with total angular momenta \( L = 4 \) or 8 participate in this TABLE. Note that \( \sum_{i=1}^{4} |c(I)|^2 = 0.999939 \), i.e., the corresponding contribution to the normalization constant differs from unity only in the sixth decimal point.

| \( I \) | \( J \) | \( c(I) \) | \( \sum_{i=1}^{4} l_i \) | \( |c(I)|^2 \) | \( \sum_{i=1}^{4} l_i \) |
|---|---|---|---|---|---|
| 3 | 1 | 0.1255794E+00 | 0.1, 0, 3 | 4 | 299.11 |
| 9 | 2 | 0.1729051E+00 | 0.1, 1, 2 | 4 | 304.12 |
| 23 | 3 | 0.2555221E+00 | 0.1, 3, 4 | 8 | 328.13 |
| 38 | 4 | -0.2760651E+00 | 0.2, 0, 2 | 4 | 334.14 |
| 53 | 5 | -0.3130074E+00 | 0.2, 2, 4 | 8 | 363.15 |
| 73 | 6 | 0.1255794E+00 | 0.3, 0, 1 | 4 | 369.16 |
| 83 | 7 | 0.1278060E+00 | 0.3, 1, 4 | 8 | 543.17 |
| 88 | 8 | 0.2709799E+00 | 0.3, 2, 3 | 8 | 549.18 |
| 118 | 9 | -0.1277153E+00 | 0.4, 1, 3 | 8 | 578.19 |
| 289 | 10 | 0.1729051E+00 | 1.2, 0, 1 | 4 | 757.20 |

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| \( I \) | \( J \) | \( c(I) \) | \( (l_1 \uparrow, l_2 \uparrow, l_3 \downarrow, l_4 \downarrow) \) | \( \sum_{i=1}^{4} l_i \) | \( I \) | \( J \) | \( c(I) \) | \( (l_1 \uparrow, l_2 \uparrow, l_3 \downarrow, l_4 \downarrow) \) | \( \sum_{i=1}^{4} l_i \) |
|-----|-----|----------|----------------|--------|-----|-----|----------|----------------|--------|
| 22  | 1   | \(-0.2800321E+00\) | (0, 1, 3, 4) | 8      | 328 | 9   | \(0.1400283E+00\) | (1, 3, 0, 4) | 8      |
| 38  | 2   | \(0.1260197E-02\)  | (0, 1, 3, 4) | 4      | 334 | 10  | \(0.1400277E+00\) | (1, 3, 1, 3) | 8      |
| 53  | 3   | \(0.3429776E+00\)  | (0, 1, 3, 4) | 8      | 369 | 12  | \(-0.2425468E+00\) | (1, 4, 1, 2) | 8      |
| 83  | 4   | \(-0.2970589E+00\) | (0, 1, 3, 4) | 8      | 543 | 13  | \(-0.2970589E+00\) | (2, 3, 0, 3) | 8      |
| 118 | 6   | \(-0.2800727E+00\) | (0, 1, 3, 4) | 8      | 549 | 14  | \(-0.1417827E+00\) | (2, 3, 1, 2) | 8      |
| 299 | 7   | \(-0.2425213E+00\) | (0, 1, 3, 4) | 8      | 578 | 15  | \(0.3430137E+00\)  | (2, 4, 0, 2) | 8      |
| 304 | 8   | \(-0.1750686E+00\) | (0, 1, 3, 4) | 8      | 757 | 16  | \(-0.2800727E+00\) | (3, 4, 0, 1) | 8      |

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