Electron and boson clusters in confined geometries: symmetry breaking in quantum dots and harmonic traps

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We discuss the formation of crystalline electron clusters in semiconductor quantum dots and of crystalline patterns of neutral bosons in harmonic traps. In a first example, we use calculations for two electrons in an elliptic quantum dot to show that the electrons can localize and form a molecular dimer. The calculated singlet-triplet splitting (J) as a function of the magnetic field (B) agrees with cotunneling measurements with its behavior reflecting the effective dissociation of the dimer for large B. Knowledge of the dot shape and of J(B) allows determination of the degree of entanglement. In a second example, we study strongly repelling neutral bosons in two-dimensional harmonic traps. Going beyond the Gross-Pitaevskii (GP) mean-field approximation, we show that bosons can localize and form polygonal-ring-like crystalline patterns. The total energy of the crystalline phase saturates in contrast to the GP solution, and its spatial extent becomes smaller than that of the GP condensate.

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Wigner parameter $R_W$, defined as $R_W = Z^2e^2/\hbar \omega_0 l_0$, with $l_0 = \sqrt{\hbar/(m\omega_0)}$ being the characteristic harmonic-oscillator length of the confining potential. (The sub-
script $W$ in the case of a Coulomb force stands for “Wigner”, since the confined clusters of localized electrons may be viewed as finite-size precursors of the bulk Wigner crystal \cite{12}.) Formation of such “molecular structures” is a manifestation of spontaneous symmetry breaking associated with a quantum phase transition, occurring at zero magnetic field for circular 2D QDs for $R_W \geq 1$ and involving the crossover from a liquid-like state to a crystalline one. This crossover, described using symmetry breaking \cite{4}, was confirmed in other studies \cite{5, 7, 8, 9} using a variety of methods. The degree of electron localization, that underlies the appearance of crystalline patterns, has been described \cite{1} as a progression from “weak” to “strong” Wigner molecules as a function of increasing $R_W$ (or equivalently decreasing density). In high magnetic fields, the rotating electron molecules exhibit magic angular momenta \cite{12, 13, 14, 15, 16} corresponding to fractional quantum Hall effect (FQHE) fillings. This has led \cite{14, 15, 16} to the derivation of an analytic trial wave function that provides a better description of the finite-size analogs of the FQHE in comparison with the Laughlin \cite{17} and composite-fermion \cite{18} wave functions.

Because of the finite size, Wigner molecules are expected to show new behavior that differs from the classical Wigner crystal familiar from Solid State Physics. The limit of a classical Wigner crystal is expected to be reached for a higher number of electrons $N$ and very large $R_W$ \cite{4}. In the following we use the term “Wigner molecule” even in the case of only two localized electrons. For this case the WM exhibits close analogies to an H2 natural molecule, as described below.

Here we focus on a two-electron (2e) WM, in light of the current experimental effort \cite{21, 20} aiming at implementation of a spin-based \cite{21} solid-state quantum logic gate that employs two coupled one-electron QDs (double dot). We present an exact diagonalization (EXD) and an approximate (generalized Heitler-London, GHL) microscopic treatment for two electrons in a single elliptic QD specified by the parameters of a recently investigated experimental device \cite{22}. While formation of Wigner molecules in circular QDs requires weak confinement (that is small $\omega_0$ in the expression for $R_W$ given above), and thus large dots of lower densities (so that the interelectron repulsion dominates), we show that formation of such WMs is markedly enhanced in highly deformed (e.g., elliptic) dots due to their lower symmetry. The calculations provide a good description of the measured $J(B)$ curve (the singlet-triplet splitting) when screening \cite{23, 24} due to the metal gates and leads is included (in addition to the dielectric constant of the semiconductor, GaAs). In particular, our results reproduce the salient experimental findings pertaining to the vanishing of $J(B)$ for a finite value of $B \sim 1.3$ T [associated with a change in sign of $J(B)$ indicating a singlet-triplet (ST) transition], as well as the flattening of the $J(B)$ curve after the ST crossing. These properties, and in particular the latter one, are related directly to the formation of an electron molecular dimer and its effective dissociation for large magnetic fields. The effective dissociation of the electron dimer is most naturally described through the GHL approximation, and it is fully supported by the more accurate, but physically less transparent, EXD.

Of special interest for quantum computing \cite{21} is the degree of entanglement exhibited by the two-electron molecule in its singlet state. Entanglement is a purely quantum mechanical phenomenon in which the quantum state of two or more objects cannot be described independently of each other, even when the individual objects are spatially separated. The highest degree of entanglement occurs at full separation, as discussed in the celebrated EPR (Einstein, Podolsky, and Rosen) paper \cite{25}. Electrons confined in a quantum dot are not necessarily spatially separated from each other, and consequently their degree of entanglement may be lower than the maximal one, as shown by us below.

Here, in relation to the microscopic calculations, we investigate two different measures of entanglement. The first, known as the concurrence (C) for two indistinguishable fermions \cite{26, 27}, has been used in the analysis of the experiment in Ref. \cite{22} (this measure is related to the operational cycle of a two-spin-qubit quantum logic gate \cite{26, 27}). The second measure, referred to as the von Neumann entropy (S) for indistinguishable particles, has been developed in Ref. \cite{28} and used in Ref. \cite{29}. We show that the present wave-function-based methods, in conjunction with the knowledge of the dot shape and the $J(B)$ curve, enable theoretical determination of the degree of entanglement, in particular for the elliptic QD of Ref. \cite{22}. The increase in the degree of entanglement (for both measures) with stronger magnetic fields correlates with the dissociation of the 2e molecule. This supports the experimental assertion \cite{22} that cotunneling spectroscopy can probe properties of the electronic wave function of the QD, and not merely its low-energy spectrum. Our methodology can be straightforwardly applied to other cases of strongly-interacting devices, e.g., double dots with strong interdot-tunneling.

Clusters of neutral bosons in harmonic traps. Bose-Einstein condensates (BECs) in harmonic traps \cite{30, 31} are normally associated with weakly interacting neutral atoms, and their physics is described adequately by the Gross-Pitaevskii (GP) mean-field theory \cite{32}. Lately, however, experimental advances in controlling the interaction strength \cite{33, 34, 35, 36} permit the production of novel bosonic states in the regime of strong interparticle repulsions. Theoretical efforts motivated by this capability include studies of the Bose-Hubbard
model [37, 38], and investigations about the “fermionization” limit of an one-dimensional (1D) gas of trapped impenetrable bosons [39, 40, 41], often referred to as the Tonks-Girardeau (TG) regime [34, 42]. Here we address the problem of strongly repelling (impenetrable) bosons in higher dimensions. In particular, we discuss 2D interacting bosons in a circular harmonic trap, with the extension to 3D systems being straightforward. To this end, we use computational methods that go beyond the GP method.

We explore the transition from a BEC (diffuse cloud) state to a crystalline phase, in which the trapped localized bosons form crystalline patterns. At the mean-field level, these crystallites are static and are portrayed directly in the single-particle densities. After restoration of rotational symmetry, the single-particle densities are circularly symmetric, and thus the crystalline symmetry becomes “hidden”; however, it can be revealed in the conditional probability distribution (CPD, anisotropic pair correlation), $P(r, r_0)$, which expresses the probability of finding a particle at $r$ given that the “observer” (i.e., reference point) is riding on another particle at $r_0$.

**METHODS**

**Two-electron quantum dot: Microscopic treatment.** The Hamiltonian for two 2D interacting electrons is

$$\mathcal{H} = H(r_1) + H(r_2) + e^2/(\kappa r_{12}),$$

where the last term is the Coulomb repulsion, $\kappa$ is the dielectric constant, and $r_{12} = |r_1 - r_2|$. $H(r)$ is the single-particle Hamiltonian for an electron in an external perpendicular magnetic field $B$ and an appropriate confinement potential. When position-dependent screening is included, the last term in Eq. (1) is modified by a function of $r_{12}$ (see below). For an elliptic QD, the single-particle Hamiltonian is written as

$$H(r) = T + \frac{1}{2} m^* (\omega_x^2 x^2 + \omega_y^2 y^2) + \frac{g^* \mu_B B \cdot s}{\hbar},$$

where $T = (p - eA/c)^2/2m^*$, with $A = 0.5(-By, Bx, 0)$ being the vector potential in the symmetric gauge. $m^*$ is the effective mass and $p$ is the linear momentum of the electron. The second term is the external confining potential; the last term is the Zeeman interaction with $g^*$ being the effective $g$ factor, $\mu_B$ the Bohr magneton, and $s$ the spin of an individual electron.

The GHL method for solving the Hamiltonian consists of two steps. In the first step, we solve self-consistently the ensuing unrestricted Hartree-Fock (UHF) equations allowing for lifting of the double-occupancy requirement (imposing this requirement gives the restricted HF method, RHF). For the $S_z = 0$ solution, this step produces two single-electron orbitals $u_{L,R}(r)$ that are localized left ($L$) and right ($R$) of the center of the QD [unlike the RHF method that gives a single doubly-occupied elliptic (and symmetric about the origin) orbital]. At this step, the many-body wave function is a single Slater determinant $\Psi_{UHF}(1 \uparrow, 2 \downarrow) \equiv |u_L(1 \uparrow)u_R(2 \downarrow)|$ made out of the two occupied UHF spin-orbitals $u_L(1 \uparrow) \equiv u_L(r_1)\alpha(1)$ and $u_R(2 \downarrow) \equiv u_R(r_2)\beta(2)$, where $\alpha(\beta)$ denotes the up (down) $|\uparrow (\downarrow)|$ spin. This UHF determinant is an eigenfunction of the projection $S_z$ of the total spin $S = s_1 + s_2$, but not of $S^2$ (or the parity space-reflection operator).

In the second step, we restore the broken parity and total-spin symmetries by applying to the UHF determinant the projection operator $P^{s,t} = 1 \mp \sigma_{12}$, where the operator $\sigma_{12}$ interchanges the spins of the two electrons; the upper (minus) sign corresponds to the singlet. The final result is a generalized Heitler-London (GHL) two-electron wave function $\Psi^{s,t}_{GHL}(r_1, r_2)$ for the ground-state singlet (index $s$) and first-excited triplet (index $t$), which uses the UHF localized orbitals, $u_{L,R}(r)$ expanded in a real Cartesian harmonic-oscillator basis, i.e.,

$$u_{L,R}(r) = \sum_{j=1}^{K} C_j^{L,R} \phi_j(r),$$

where the index $j \equiv (m,n)$ and $\phi_j(r) = X_m(x)Y_n(y)$, with $X_m(Y_n)$ being the eigenfunctions of the one-dimensional oscillator in the $x(y)$ direction with frequency $\omega_x(\omega_y)$. The parity operator $\mathcal{P}$ yields $\mathcal{P}X_m(x) = (-1)^m X_m(x)$, and similarly for $Y_n(y)$. The expansion coefficients $C_j^{L,R}$ are real for $B = 0$ and complex for finite $B$. In the calculations we use $K = 79$, yielding convergent results.

In the exact-diagonalization method, the many-body wave function is written as a linear superposition over the basis of non-interacting two-electron determinants,
ψ(1; i) = \varphi_i(1 \uparrow) if 1 \leq i \leq K and ψ(1; i) = \varphi_{i-K}(1 \downarrow) if K + 1 \leq i \leq 2K [and similarly for ψ(2; j)]. The total energies \( E_{\text{EXD}}^{s,t} \) and the coefficients \( \Omega_{ij}^{s,t} \) are obtained through a “brute force” diagonalization of the matrix eigenvalue equation corresponding to the Hamiltonian in Eq. (1). The EXD wave function does not immediately reveal any particular feature in the context of two-component condensates, where each species is associated with a different space orbital \( \Phi_i \). We consider here one species of bosons, but allow each particle to occupy a different space orbital \( \phi_i(z) \). The permanent \( |\Phi_N\rangle = \text{Perm}[\phi_1(r_1), ..., \phi_N(r_N)] \) serves as the many-body wave function of the unrestrict Bose-Hartree-Fock (UBHF) approximation. This wave function reduces to the Gross-Pitaevskii form with the restriction that all bosons occupy the same orbital \( \phi_0(r) \), i.e., \( |\Phi_N^\text{GP}\rangle = \prod_{i=1}^N \phi_0(r_i) \), and \( \phi_0(r) \) is determined self-consistently at the restricted Bose-Hartree-Fock (RBHF) level via the equation \( 50 \)

\[ H_0(r_1) + (N-1) \int d^3 r_2 \phi_0^* \phi_0 \phi_0 \phi_0 \phi_0 \phi_0 \]

which is a maximally \( (C^t = 1) \) entangled state. Note that the analysis of the experiments in Ref. 22 is a conjecture that wave functions of the form given in Eqs. 4 and 7 describe the two electrons in the elliptic QD.

To compute the von Neumann entropy, one needs to bring both the EXD and the GHL wave functions into a diagonal form (the so-called “canonical form” 28-47), i.e.,

\[ \Psi_{\text{EXD}}^{s,t}(r_1, r_2) = \sum_{k=1}^M \zeta_k^{s,t} |\Phi(1; 2k - 1)\Phi(2; 2k)\rangle, \]

with the \( \Phi(i)'s \) being appropriate spin orbitals resulting from a unitary transformation of the basis spin orbitals \( \psi(j)'s \) [see Eq. (5)]; only terms with \( z_k \neq 0 \) contribute. The upper bound \( M \) can be smaller (but not larger) than \( K \) (the dimension of the single-particle basis); \( M \) is referred to as the Slater rank. One obtains the coefficients of the canonical expansion from the fact that the \( |z_k|^2 \) are eigenvalues of the hermitian matrix \( \Omega^i\Omega \) [28, see Eq. (5), is antisymmetric]. The von Neumann entropy is given by

\[ S = -\sum_{k=1}^M |z_k|^2 \log_2(|z_k|^2) \]

with the normalization \( \sum_{k=1}^M |z_k|^2 = 1 \). Note that the GHL wave functions in Eqs. (6) and (7) are already in canonical form, which shows that they always have a Slater rank of \( M = 2 \). One finds \( S_{\text{GHL}} = \log_2(1 + \eta^2) - \eta^2 \log_2(\eta^2)/(1 + \eta^2) \), and \( S_{\text{GHL}} = 1 \) for all \( B \). For large \( B \), the overlap between the two electrons of the dissociated dimer vanishes, and thus \( S \rightarrow 1 \) and \( S_{\text{GHL}} \rightarrow 1 \).

Neutral repelling bosons in harmonic traps: Symmetry breaking. We simplify the solution of the UBHF problem by considering explicit analytic expressions for the space orbitals \( \phi_0(r) \). In particular, since the bosons must avoid occupying the same position in space in order to minimize their mutual repulsion, we take all the orbitals to be of the form of displaced Gaussians, namely,
\[ \phi_i(\mathbf{r}_i) = \pi^{-1/2} \sigma^{-1} \exp[-(\mathbf{r}_i - \mathbf{a}_i)^2/(2\sigma^2)]. \]

The positions \( \mathbf{a}_i \) describe the vertices of concentric regular polygons, with both the width \( \sigma \) and the radius \( \alpha = |\mathbf{a}_i| \) of the regular polygons determined variationally through minimization of the total energy \( E_{\text{UBHF}} = \langle \Phi_N | H | \Phi_N \rangle / \langle \Phi_N | \Phi_N \rangle \), where \( H = \sum_{i=1}^N H_0(r_i) + \sum_{i<j}^N V(r_i, r_j) \) is the many-body hamiltonian.

With the above choice of localized orbitals, the unrestricted permanent \( |\Phi_N\rangle \) breaks the continuous rotational symmetry. However, the resulting energy gain becomes substantial for stronger repulsion. Controlling this energy gain (the strength of correlations) is the ratio \( R_\delta \) between the strength of the repulsive potential and the zero-point kinetic energy. Specifically, for a 2D trap, one has \( R_\delta = gm/(2\pi \hbar^2) \) for a contact potential.

Neutral repelling bosons in harmonic traps: Restoration of broken symmetry. Although the optimized UBHF permanent \( |\Phi_N\rangle \) performs exceptionally well regarding the total energies of the trapped bosons, in particular in comparison to the restricted wave functions (e.g., the GP anzatz), it is still incomplete. Indeed, due to its localized orbitals, \( |\Phi_N\rangle \) does not preserve the circular (rotational) symmetry of the 2D many-body hamiltonian \( H \). Instead, it exhibits a lower point-group symmetry, i.e., a \( C_2 \) symmetry for \( N = 2 \) and a \( C_5 \) one for the \((1,5)\) structure of \( N = 6 \) (see below). As a result, \( |\Phi_N\rangle \) does not have a good total angular momentum. This paradox is resolved through a post-Hartree-Fock step of restoration of broken symmetries via projection techniques \[22\, 51], yielding a new wave function \( |\Psi_{N,L}^{\text{PRJ}}\rangle \) with a definite angular momentum \( L \), that is

\[ 2\pi |\Psi_{N,L}^{\text{PRJ}}\rangle = \int_0^{2\pi} d\gamma |\Phi_N(\gamma)\rangle e^{i\gamma L}, \]

where \( |\Phi_N(\gamma)\rangle \) is the original UBHF permanent having each localized orbital rotated by an azimuthal angle \( \gamma \), with \( L \) being the total angular momentum. The projection yields wave functions for a whole rotational band. Note that the projected wave function \( |\Psi_{N,L}^{\text{PRJ}}\rangle \) in Eq. (11) may be regarded as a superposition of the rotated permanents \( |\Phi_N(\gamma)\rangle \), thus corresponding to a “continuous-configuration-interaction” solution.

Here, we are interested in the projected ground-state \((L = 0)\) energy, which is given by

\[ E_0^{\text{PRJ}} = \langle \Psi_{N,0}^{\text{PRJ}} | H | \Psi_{N,0}^{\text{PRJ}} \rangle / \langle \Psi_{N,0}^{\text{PRJ}} | \Psi_{N,0}^{\text{PRJ}} \rangle. \]

RESULTS AND DISCUSSION

Two-electron quantum dot. To model the experimental elliptic QD device, we take, following Ref. [22], \( \hbar \omega_x = 1.2 \text{ meV} \) and \( \hbar \omega_y = 3.3 \text{ meV} \). The effective mass of the electron is taken as \( m^* = 0.067 m_e \) (GaAs). Since the experiment did not resolve the lifting of the triplet degeneracy caused by the Zeeman term, we take \( g^\ast = 0 \).

Using the two-step method, we calculate the GHL singlet-triplet splitting \( J_{\text{GHL}}(B) = E_{\text{GHL}}^s(B) - E_{\text{GHL}}^t(B) \) as a function of the magnetic field in the range \( 0 \leq B \leq 2.5 \text{ T} \). Screening of the \( e-e \) interaction due to the metal gates and leads must be considered in order to reproduce the experimental \( J(B) \) curve. This screening can be modeled, to first approximation, by a position-independent adjustment of the dielectric constant \( \kappa \) \[52\]. Indeed, with \( \kappa = 22.0 \) (instead of the GaAs dielectric constant, i.e., \( \kappa = 12.9 \)), good agreement with the experimental data is obtained [see Fig. 2]. In particular, we note the singlet-triplet crossing for \( B \approx 1.3 \text{ T} \), and the flattening of the \( J(B) \) curve beyond this crossing.

We have also explored, particularly in the context of the EXD treatment, a position-dependent screening using the functional form, \( \left( e^2 / \kappa r_{12} \right) \left[ 1 - (4d^2 / r_{12}^2)^{1/2} \right] \), proposed in Ref. [24], with \( d \) as a fitting parameter. The \( J_{\text{EXD}}(B) \) result for \( d = 18.0 \text{ nm} \) is depicted in Fig. 2 (dotted line), and it is in very good agreement with the experimental measurement.

The singlet state electron densities from the GHL and the EXD treatments at \( B = 0 \) and \( B = 2.5 \text{ T} \) are displayed in Fig. 3. These densities illustrate the dissociation of the electron dimer with increasing magnetic field. The asymptotic convergence (beyond the ST point) of the energies of the singlet and triplet states, i.e., \( |J(B) \rightarrow 0 \text{ as } B \rightarrow \infty| \) is a reflection of the dissociation of the 2e

![Graph](image-url)
molecule, since the ground-state energy of two fully spatially separated electrons (zero overlap) does not depend on the total spin.

In contrast, the singlet-state RHF electron densities fail to exhibit formation of an electron dimer for all values of $B$. This underlies the failure of the RHF method to describe the behavior of the experimental $J(B)$ curve. In particular, $J_{\text{RHF}}(B = 0)$ has the wrong sign, while $J_{\text{RHF}}(B)$ diverges for high $B$ as is the case for the RHF treatment of double dots (see Ref. [43]).

For the GHL singlet, using the overlaps of the left and right orbitals, we find that starting with $\eta = 0.46$ ($C^s = 0.76$) at $B = 0$, the interaction parameter (singlet-state concurrence) increases monotonically to $\eta = 0.65$ ($C^s = 0.92$) at $B = 2.5$ T. At the intermediate value corresponding to the ST transition ($B = 1.3$ T), we find $\eta = 0.54$ ($C^s = 0.83$).

Our $B = 0$ theoretical results for $\eta$ and $C^s$ are in remarkable agreement with the experimental estimates of $\eta = 0.5 \pm 0.1$ and $C^s = 0.8$, which were based solely on conductance measurements below the ST transition (i.e., near $B = 0$). We note that, for the RHF, $C^s_{\text{RHF}} = 0$, since a single determinant is unentangled for both the two measures considered here.

Since the EXD singlet has obviously a Slater rank $M > 2$, the definition of concurrence is not applicable to it. The von Neumann entropy for the EXD singlet ($S^s_{\text{EXD}}$) is displayed in Fig. 4, along with that ($S^s_{\text{GHL}}$) of the GHL singlet. $S^s_{\text{EXD}}$ and $S^s_{\text{GHL}}$ are rather close to each other for the entire $B$ range, and it is remarkable that both remain close to unity for large $B$, although the maximum allowed mathematical value is $\log_2(K)$ [as aforementioned we use $K = 79$, i.e., $\log_2(79) = 6.3$]; this maximal value applies for both the EXD and GHL approaches. The saturation of the entropy for large $B$ to a value close to unity reflects the dominant (and roughly equal at large $B$) weight of two configurations in the canonical expansion [see Eq. (8) of the EXD wave function, which are related to the two terms ($M = 2$) in the canonical expansion of the GHL singlet [Eq. (6)]. This is illustrated by the histograms of the $|z^s_k|^2$ coefficients for $B = 1.3$ T at the top of Fig. 4. These observations support the GHL approximation, which is computationally less demanding than the exact diagonalization, and can be used easily for larger $N$.

Neutral repelling bosons in harmonic traps. In Fig. 5, we display as a function of the parameters $R_\delta$ the total energies for $N = 6$ bosons calculated at several levels of approximation. In both cases the lowest UBHF energies correspond to a $(1,5)$ crystalline configuration, namely one boson is at the center and the rest form a regular pentagon of radius $a$. Observe that the GPH total energies are slightly lower than the $P_{\text{UBHF}}$ ones; however, both exhibit an unphysical behavior since they diverge as $R_\delta \to \infty$. This behavior contrasts sharply with that of the unrestricted Hartree-Fock energies, $E_{\text{UHFB}}$ and PRJ (see below), which saturate as $R_\delta \to \infty$; in fact, a value close to saturation is achieved already for $R_\delta \sim 10$. We have checked that for all cases with $N = 2 - 7$, the total energies exhibit a similar behavior. For a repulsive
contact potential, the saturation of the UBHF energies is associated with the ability of the trapped bosons (independent of \(N\)) to minimize their mutual repulsion by occupying different positions in space, and this is one of our central results. For \(N = 2\), the two bosons localize at a distance \(2a\) apart to form an antipodal dimer. For \(N \leq 5\) the preferred UBHF crystalline arrangement is a single ring with no boson at the center [usually denoted as \((0,N)\)], \(N = 6\) is the first case having one boson at the center [designated as \((1,N-1)\)], and the \((0,6)\) arrangement is a higher energy isomer. The structural parameters (e.g., the width of the Gaussian orbitals and the radii of the polygonal ring, calculated via the UBHF method, show a saturation behavior similar to that illustrated above for the energy of the system \((6)\).

The transformation found here for 2D trapped bosons interacting through strong repelling contact potentials is an illustration of the “fermionization” analogies that appear in strongly correlated systems in all three dimensionalities. Indeed such energy saturation has been shown for the TG 1D gas \([34, 42]\) and has also been discussed for certain 3D systems (i.e., three trapped bosons \([35]\) and an infinite boson gas \([36]\)). Saturation of the energy and the length of the trapped atom cloud (and thus of the interparticle distance) has been measured recently for the 1D TG gas (see in particular Fig. 3 and Fig. 4 in Ref. \[36\]) and compare to the similar trends predicted here for the 2D case in Fig. 5).

For \(N = 6\) 2D bosons, Fig. 5 shows that the \(E_0^{\text{PRJ}}\) energies share with the UBHF ones the saturation property for the case of a contact-potential repulsion. However, the projection brings further lowering of the total energies compared to the UBHF ones. (The projected ground state is always lower in energy than the original broken-symmetry one \([55]\).) Thus, for strong interactions (large values of \(R_\delta\)) the restoration-of-broken-symmetry step yields an excellent approximation of both the exact many-body wave function and the exact total energy.

The transformations of the single-particle densities (displayed in Fig. 6 for \(N = 6\) neutral bosons interacting via a contact potential and \(R_\delta = 25\)) obtained from application of the successive approximations provide an illustration of the two-step method of symmetry breaking with subsequent symmetry restoration. Indeed, the GP single-particle density [Fig. 6(a)] is circularly symmetric, but the UBHF one [Fig. 6(b)] explicitly exhibits a \((1,5)\) crystalline configuration. After symmetry restoration [Fig. 6(c)], the circular symmetry is re-established, but the single-particle density is radially modulated unlike the GP density. In addition, the crystalline structure in the projected wave function is now hidden; however, it can be revealed through the use of the CPD \([14, 16]\) [see Fig. 6(d)], which resembles the (crystalline) UBHF single-particle density, but with one of the humps on the outer ring missing (where the observer is located). In particular, \(P(r_0, r_0) \approx 0\) and the boson associated with the observer is surrounded by a “hole” similar to the exchange-correlation hole in electronic systems. This is another manifestation of the “fermionization” of the strongly repelling 2D bosons. However, here as in the 1D TG case \([39, 42]\), the vanishing of \(P(r_0, r_0)\) results from the impenetrability of the bosons. For the GP condensate, the CPD is independent of \(r_0\), i.e., \(P_{\text{GP}}(r, r_0) \propto |\phi_0(r)|^2\), reflecting the absence of any space correlations.

It is of importance to observe that the radius of the

![Fig. 6: (a-c): Single-particle densities for \(N = 6\) 2D harmonically trapped neutral bosons with a contact interaction and \(R_\delta = 25\). (a) The single-orbital self-consistent GP case. (b) The symmetry broken UBHF case (static crystallite). (c) The projected case (symmetry-restored wave function, see Eq. \[13\]). The crystalline structure of the outer ring in this last case is “hidden”, but it is revealed in the conditional probability distribution \([14, 16]\) displayed in (d), where the observation point is denoted by a black dot (on the right). Lengths in units of \(l_0\).](image)
BEC [GP case, Fig. 6(a)] is significantly larger than the actual radius of the strongly-interacting crystalline phase [projected wave function, Fig. 6(c)]. This is because the extent of the crystalline phase saturates, while that of the GP condensate grows with no bounds as $R_\delta \rightarrow \infty$. Such dissimilarity in size (between the condensate and the strongly-interacting phase) has been also predicted for the trapped 1D Tonks-Girardeau gas and indeed observed experimentally. In addition, the 2D single-particle momentum distributions for neutral bosons have a one-hump shape with a maximum at the origin (a behavior exhibited also by the trapped 1D TG gas). The width of these momentum distributions versus $R_\delta$ increases and saturates to a finite value, while that of the GP solution vanishes as $R_\delta \rightarrow \infty$.

**SUMMARY**

In this paper, we explored symmetry-breaking transitions predicted to occur in confined fermionic and bosonic systems when the strength of the interparticle repulsive interactions exceeds an energy scale that characterizes the degree of confinement. For two electrons in an elliptic QD, we predicted formation and effective dissociation (with increasing magnetic field) of an electron dimer, which is reflected in the behavior of the computed singlet-triplet splitting, $J(B)$, that agrees well (Fig. 2) with measurements.

Furthermore, we showed that, from a knowledge of the dot shape and of $J(B)$, theoretical analysis along the lines introduced here allows probing of the correlated ground-state wave function and determination of its degree of entanglement. This presents an alternative to the experimental study where determination of the concurrence utilized conductance data. Such information is of interest to the implementation of spin-based solid-state quantum logic gates.

For the case of 2D trapped bosonic clusters, we found with increasing repulsive two-body interaction localization of the bosons in the trap, resulting in formation of crystalline patterns made of polygonal rings; while we have focused here on repulsive contact interactions, similar results were obtained also for a Coulomb repulsion.

These results provide the impetus for experimental efforts to access the regime of strongly repelling neutral bosons in two dimensions. To this end we anticipate that extensions of methodologies developed for the recent realization of the Tonks-Girardeau regime in 1D (using a finite small number of trapped $^{87}$Rb and optical lattices, with a demonstrated wide variation of $R_\delta$ from 5 to 200 and from 1 to 5) will prove most promising. Control of the interaction strength via the use of the Feshbach resonance may also be considered.

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