Cold Fermionic Atoms in Two-Dimensional Traps – Pairing versus Hund’s Rule

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The microscopic properties of few interacting cold fermionic atoms confined in a two-dimensional (2D) harmonic trap are studied by numerical diagonalization. For repulsive interactions, a strong shell structure dominates, with Hund’s rule acting at its extreme for the mid-shell configurations. In the attractive case, odd-even oscillations due to pairing occur simultaneously with deformations in the internal structure of the ground states, as seen from pair correlation functions.

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Quantum dots and related nanostructures appeared as the first “artificial atoms” [1], where semiconductor techniques allowed to design the quantum confinement of a few particles in the laboratory (see [2] for a review). In more recent years, artificial quantum confinement also became possible with ultracold trapped atomic gases [3]: Magneto-optical techniques allow to create very clean systems where the trapped particles can be bosons as well as fermions. Strength and sign of their interactions can be tuned, making them repulsive or attractive via Feshbach resonances, allowing for a variety of quantum many-body phenomena to be studied theoretically as well as experimentally. Cold atoms may be loaded into “deep” optical lattices, where the single sites may resemble harmonic confinement. With cold, trapped fermions, it became possible to experimentally study the crossover from a weakly attractive Fermi gas to the unitary limit of infinite scattering length, and beyond [4]. Attractive fermionic atoms in traps share many of their properties with nuclei, such as Bardeen-Cooper-Schrieffer (BCS) pairing and the occurence of shell structure [5].

The “Coulomb blockade” in the discrete charging and discharging of quantum dots leads to significant conductance oscillations. These are manifest in the “fundamental energy gap” \(\Delta_1(N) = \Delta_1(N+1) - \Delta_1(N)\), given by the difference between the modulus of the particle-removal and the addition energy, i.e., by the difference in the chemical potential of a quantum system confining \(N+1\) and \(N\) particles, \(\Delta_1(N) = E_0(N) - E_0(N-1)\), where \(E_0(N)\) is the \(N\)-body ground state energy. Very recently, Cheinet et al. [6] reported on the realization of a similar interaction blockade [7] in the transport of cold atoms through a double well in an optical lattice, observing discrete steps in the well population with increasing “bias” potentials [note that the atom number distribution as a function of the bias relates to \(\Delta_2(N)\)]. These findings indeed bring implementations of “atomtronics”, as suggested in the pioneering work of Seaman et al. [8], much closer to realization.

In this Letter, we thus investigate effects of interaction blockade for quantum dot-like, 2D fermionic atom traps. For repulsive interactions, a strong shell structure occurs and Hund’s rule acts at its extreme at half-filled shells. For attractive interactions, however, a pronounced odd-even staggering in the ground state energies (as recently discussed for 3D systems by Zinner et al. [9]) is accompanied by broken symmetries in the internal structure of the many-body states.

Let us now consider \(N\) atoms of spin 1/2 and equal masses \(m\) confined in a 2D harmonic trap, interacting through a contact potential,

\[
H = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega_0^2 r_i^2 \right) + \frac{1}{2} g' \sum_{i \neq j} \delta^{(2)}(r_i - r_j),
\]

where \(g'\) is the coupling constant. We use as energy unit \(\hbar \omega_0\) and as length unit \(\ell = (\hbar/m \omega_0)^{1/2}\). The dimensionless coupling constant is \(g = g'/(\hbar \omega_0 \ell^2)\). The few-body problem of Eq. (1) is solved by means of the full configuration interaction (CI) method [10]. In more than one spatial dimension, contact interactions do not allow to diagonalize the many-body Hamiltonian unless regularized properly. An approximate way to achieve this is a momentum-cutoff to a given subspace [11], effectively renormalizing the interaction strength [12].

Expanding the interacting \(N\)-body state on the given set of Slater determinants and diagonalizing [13], the CI method provides the many-body energies and wave functions of both ground states and (low-lying) excitations, which are eigenstates of the total spin \(S\) and \(z\)-projection of the orbital angular momentum \(M\). Figure 1 shows the fundamental gap \(\Delta_2(N)\) vs \(N\). In the upper panel, for repulsive interactions \(g > 0\), one clearly recognizes the distinctive features of a shell structure, strikingly similar to those observed for quantum dots [14] (confirming the earlier prediction by Capelle et al. [7]). The two peaks for \(N = 2, 6\) form when the first two energy shells of the 2D harmonic oscillator are completely filled by atoms as they...
are consecutively loaded into the trap. Since the height of the peaks is mainly dictated by the energy spacing ($\hbar \omega_0 = 1$) between neighboring shells, $\Delta_2(N = 2, 6) \approx 1$.

\[ \Delta_2(N) \text{ depends only weakly on the interaction strength } g, \text{ as it increases from } g = -0.3 \text{ (green curve) up to } g = 5 \text{ (black curve).} \]

The peak for $N = 4$ at mid-shell between $N = 2$ and $N = 6$ is a consequence of Hund’s rule acting at its extreme, where up to half-filling of the degenerate shell the Pauli principle eliminates the interactions.

The signatures of attractive interaction ($g < 0$) are dramatically different from the repulsive case of Fig. 1(a). Figure 1(b) shows that the non-interacting shell structure is gradually washed out as the magnitude of atom-atom attractive interaction is increased. As $g$ goes from $g = -0.3$ (green curve) up to $g = -5$ (black curve), $\Delta_2(N)$ develops a pronounced even-odd pattern, with $\Delta_2 > 0$ ($\Delta_2 < 0$) for even (odd) $N$, corresponding to $S = 0$ ($S = 1/2$). Pairing effects are likely to be the dominant mechanism behind these odd-even oscillations. If $N$ is even, all atoms form singlet pairs and a large amount of energy is required to add one unpaired atom. For odd $N$, $\Delta_2(N) < 0$ since energy is gained by pairing with an opposite-spin particle. However, the odd-even staggering of Fig. 1(b) could originate from either pairing or Jahn-Teller effects, as discussed for nuclei, metallic grains, clusters [17], and even for 2D systems [18].

In order to isolate effects from pairing we study the seniority model from nuclear physics (also called the method of ‘exact pairing’ [19]), applied to the 2D system. The model restricts the interactions in the 2D trap to be exclusively of the pairing type, that act only between particles in time-reversed orbits. Unpaired particles do not participate in the interaction beyond the mean-field level, except for blocking certain final states available for pairing. Using an attractive $\delta$-function pairing potential as for the full microscopic model above, we truncate the model space after the fourth oscillator shell. The results are shown in Fig. 1(c), comparing well with the full many-body calculations. For weak interactions, $g = -0.3$, $\Delta_2(N)$ displays the non-interacting shell structure. For stronger $g$, a pronounced odd-even staggering appears. We find large gaps between the ground and first excited state in even−, and the absence of a gap in odd-numbered systems. To discern between inter- and intra-shell pairing [20], we study the fraction of the pairing energy that comes from the off-diagonal Hamiltonian matrix elements, which involve pairs being moved between the oscillator shells. For smaller interaction strengths, this energy is a fraction of a percent. Increasing the coupling to $g = -5$, the off-diagonal contribution is larger than 20%. This was roughly the same for all particle numbers, though partially filled shells have higher contributions than particle numbers around closed shells.

Figure 2 shows the interaction energy $E_{\text{int}}$ for $2 \leq N \leq 20$ for small $g$ [20], where the non-interacting contribution was subtracted from the total energy, $E_{\text{int}} = E_0(N) - E_0(N, g = 0)$. In order to magnify the fine structure of $E_{\text{int}}$ in Fig. 2 we replace it with the scaled quantity $E_{\text{int}}/N^{3/2}$, since in the Thomas-Fermi approximation $E_{\text{int}} \sim N^{3/2}$. The plot clearly shows that in the case of repulsive interaction ($g = 0.3$) the energy gain is minimum for closed shells ($N = 2, 6, 12, 20$). Conversely, the energy gain is largest for the half-filled open shells at $N = 4, 9, 16$. In fact, in those cases the spin is maximized due to Hund’s rule ($S = 1, 3/2, 2$, respectively). In the attractive case, already for weak interactions the pattern of $E_{\text{int}}/N^{3/2}$ shows a marked even-odd alternation: the energetically favored ground states occur at even $N$ when all atoms are paired.

The key quantity for $g < 0$ is the pairing energy gap $\Delta$, measuring the interaction-energy gain (expense) by

\[ \Delta N^{3/2} \text{ vs } N \text{ for } g = \pm 0.3. \]
adding an atom to the \(N\)-body system if \(N\) is odd (even). We define \(\Delta\) as \(\Delta = [\Delta_1(N) - \Delta_1(N + 1)]/2\) with \(N\) odd. This is plotted in Fig. 3 vs \(g\) for the open-shell cases \(N = 3, 7\). Remarkably, the black \((N = 7)\) and red \((N = 3)\) curves almost overlap, showing that pairing is a generic feature of the few-body system.

Complementary information on the pairing energy \(\Delta\) is obtained by the analysis of the excitation spectrum for fixed even \(N\). Figure 3 focuses on the low-lying energy levels of \(N = 8\) as the magnitude of \(g\) increases, going from \(|g| = 0.3\) (top panel) up to \(|g| = 5\) (bottom panel). We resolve the six lowest-energy levels for orbital angular momenta \(0 \leq M \leq 4\). For small values of \(g\) \((g = \pm 0.3,\) top panel) the non-interacting low-lying sequence clearly emerges: three \(M = 0\) states, two \(M = 2\) states, and one \(M = 4\) state may be obtained by variously arranging two atoms with opposite spin in the third open shell of the 2D harmonic oscillator, while the remaining six atoms fill the two lowest shells. To have the lowest \(M = 1\) or \(M = 3\) excitations one particle (or hole) must be excited into the 4th (2nd) shell, whereas to have higher-energy states with even \(M\), one particle (hole) must be excited into the 5th (1st) shell or two into the 4th (2nd) shell. As \(|g|\) increases (center and bottom panels of Fig. 3), two fundamentally different types of excitation spectra appear for positive (blue curves) and negative (red curves) \(g\). For \(g < 0\), all excited states appear at some large energy related to the pairing gap \(\Delta\): A pair must be broken to excite the system, no matter the value of \(M\). As \(|g|\) increases, the gap becomes uniform with respect to \(M\), indicating the onset of internuclear pairing. The opposite holds for \(g > 0\), since excitation energies decrease for increasing \(g\), implying that several excited states become almost degenerate with respect to the ground state, as in strongly correlated quantum dots [2].

The lowest excitation energy, \(E_{\text{exc}}(N)\), may be used as an alternative definition of \(\Delta\) [21]. Such quantity is plotted in Fig. 4 for \(N = 4\) (blue line) and \(N = 8\) (green line) and may be compared with the previous evaluations of \(\Delta\) through the chemical potential. We see that all the different estimates basically coincide, independent of \(N\). A fair agreement is found also for cases other than open shells, provided \(|g|\) is sufficiently large. It is interesting to compare the curves for \(E_{\text{exc}}(N)\) in Fig. 4 with first-order perturbation theory in \(g\) (magenta curve). At small \(|g|\) all estimates of \(\Delta\) agree with the predicted value of \(-g/(4\pi)\), which is linear in \(g\). Around \(g \approx -1\), however, strong deviations from the perturbation-theory result arise, due to the non-linear behavior of \(\Delta\).

We finally investigate the internal structure of ground state wave functions, computing the conditional probability \(P_{\sigma_0}(\mathbf{r}, \mathbf{r}_0)\) of finding an atom with spin \(\sigma = \uparrow, \downarrow\) at \(\mathbf{r}\) provided another one is fixed at \(\mathbf{r}_0\) with spin \(\sigma_0\):

\[
P_{\sigma_0}(\mathbf{r}, \mathbf{r}_0) = A \sum_{i \neq j} \langle \delta(\mathbf{r} - \mathbf{r}_i) \delta_{\sigma \sigma_0} \delta(\mathbf{r}_0 - \mathbf{r}_j) \delta_{\sigma_0 \sigma} \rangle, \tag{2}
\]

where \(A\) is a normalization factor. The probability \(P_{\uparrow}(\mathbf{r}, \mathbf{r}_0)\) is plotted in Fig. 5 for even \(N\), with \(\mathbf{r}_0 = (x_0, 0)\) labeled by a black circle (for convenience, we scaled
the maximum height of $P_{g}(r, r_0)$ to the same value in each panel]. Figure 5 only shows correlations between opposite-spin atoms, since the parallel spin probability $P_{\sigma, \sigma}(r, r_0)$ is almost structureless, except the exchange hole around the fixed atom (the contact interaction does not scatter atoms with parallel spin).

Already for $N = 2$ (left column of Fig. 5), the difference between the repulsive (top panel, $g = 3$) and attractive (bottom panel, $g = -3$) case is manifest. In fact, whereas for $g > 0$ the $\uparrow$-atom may be found in the antipodal position with respect to the fixed $\downarrow$-atom, for $g < 0$ both atoms tend to overlap in space, suggesting the formation of a bound pair. The contour plots for $g = -3$ (bottom row) show a peak of the probability of finding an $\uparrow$-atom close to the $\downarrow$-atom, and they are rotated by $2\pi/N$ with respect to the repulsive case, as displayed in the upper panel. Intriguingly, whereas the overall spatial distribution for $P_{g}(r, r_0)$ tends to an isotropic distribution of atoms for $g = 3$, for $g = -3$ the distribution is strongly distorted in space. This distortion is particularly clear for $N = 4$ and $N = 6$, with six particles filling a shell in the non-interacting limit, which should maintain circular symmetry. The origin of the deformation seen in $P_{\downarrow\downarrow}(r, r_0)$ might be attributed to the Jahn-Teller effect or the seniority model lead to a significantly enhanced fundamental energy gap at closed-shell and mid-shell configurations. For attractive interactions on the BCS-side of unitarity, however, a pronounced odd-even staggering was found, where the ab-initio results agree well with the seniority model. Interaction blockade, as discussed here for 2D “quantum dots” with cold atoms, may experimentally be observed in atom-transport studies, as recently performed by Cheinet and coworkers [6] for bosons, and an extension to the fermionic case is called for.

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