Single-shot imaging of trapped Fermi gas

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Abstract – Recently developed techniques allow for simultaneous measurements of the positions of all ultra-cold atoms in a trap with high resolution. Each such single-shot experiment detects one element of the quantum ensemble formed by the cloud of atoms. Repeated single-shot measurements can be used to determine all correlations between particle positions as opposed to standard measurements that determine particle density or two-particle correlations only. In this paper we discuss the possible outcomes of such single-shot measurements in the case of cloud of ultra-cold noninteracting Fermi atoms. We show that the Pauli exclusion principle alone leads to correlations between particle positions that originate from unexpected spatial structures formed by the atoms.

Introduction. – Tremendous progress in experimental techniques for preparing, manipulating and probing ultracold gases has offered new possibilities of optical methods for monitoring atomic systems. Atomic fluorescence microscopes with resolution in the range of hundreds of nanometers became accessible [1–9]. The microscopes allow the observation of both boson and fermion atoms with resolution comparable to the optical wavelength. Single-shot pictures of such systems correspond to a single realization of the \( N \)-body probability density as opposed to a one-particle probability distribution. The difference between the two is tremendous, they differ by \( N \)-body correlations. The seminal work of [10] shows how interference fringes, visible in a simultaneous single-shot picture of \( N \) atoms, arise in the course of measurement. No fringes are observed in a single-particle detection instead. In a similar way the solitons emerge in a process of detection of \( N \)-particles prepared in a type-II excited state of a 1D system of bosons interacting via short-range potential described by the Lieb-Linger model [11]. Single-shot time-dependent simulations of many-body dynamics showing the appearance of fluctuating vortices and center-of-mass fluctuations of attractive BEC have been recently reported [12].

An \( N \)-body system is not a simple \( N \)-fold sum of systems of one particle. This is because of correlations between particles resulting from their mutual interactions. In quantum systems, correlations can be imposed not only by interactions, but also by the quantum statistics. Quantum mechanics gives a completely different meaning to the classical concept of identical objects [13]. They are identical not only because they share the same mass, spin, charge, etc., but also because they cannot be identified by tracing their history. Here we show yet another consequence of quantum indistinguishability: identical fermions confined by an external trapping potential arrange themselves in spectacular geometric structures even if no mutual interaction is present. This is because the indistinguishability of fermions, formulated in the language of the Pauli exclusion principle, prevents any two fermions from being at the same location. These unexplored geometric structures, Pauli crystals, emerge repeatedly in single-shot pictures of the many-body system.

Pauli crystals. – Here we study on a theoretical ground a manifestation of the quantum statistics, namely a high-order geometric correlations in a small system of ultra-cold spin-polarized fermions confined in space by an external binding potential. To this end we generate a single-shot picture of this noninteracting system. We limit our attention to the many-body ground state. Atoms are attracted towards the trap minimum, but, on the other hand, the Pauli exclusion principle does not allow any two fermions to be at the same position. These two competing effects lead to an equilibrium.

We limit our attention to a simple generic example of particles bound by a harmonic potential in two dimensions and frequency \( \omega_x = \omega_y = \omega \). One-particle states are the
standard harmonic-oscillator wave functions:

\[ \psi_{nm}(x, y) = N_{nm} e^{-(x^2+y^2)/2} \mathcal{H}_n(x) \mathcal{H}_m(y), \]  

where \( N_{nm} = (2^{n+m}n!m!/\sqrt{\pi})^{-1/2} \) is the norm, and \( \mathcal{H}_n(z) \) is the \( n \)-th Hermite polynomial. The positions \( x \) and \( y \) are expressed in the normal harmonic oscillator units, i.e., the unit of length being \( a = \sqrt{\hbar/M\omega} \), where \( M \) is the mass of the particle. Quantum numbers \( n \) and \( m \) enumerate excitations in the \( x \)- and \( y \)-direction, respectively. We consider an isotropic trap, therefore all states with the same total number of excitations, \( n + m \), are degenerated and all states of the same energy form an energy shell. These states have energy \( E_{nm} = \hbar \omega (n + m + 1) \). The ground state of a noninteracting \( N \)-body system is very simple, every particle occupies a different one-particle state. As a result the \( N \) lowest energy states, up to the Fermi energy are occupied. For \( N = 1, 3, 6, 10, 15 \) the ground state is uniquely defined because all states at the Fermi level are occupied. The many-body ground state is degenerated whenever the total number of particles does not coincide with the degeneracy of the energy shells.

The many-body wave function is given by the Slater determinant of the occupied one-particle orbitals:

\[ \Psi(r_1, \ldots, r_N) = \frac{1}{\sqrt{N!}} \det[\psi_{ij}(r_k)]. \]

The modulus square of the wave function \( |\Psi(r_1, \ldots, r_N)|^2 \) is the probability density of finding the particles at positions \( r_1, \ldots, r_N \).

In a single-shot measurement with a quantum gas microscope, a set of \( N \) positions of atoms can be determined. It is therefore legitimate to study the outcomes of such measurements on a theoretical ground. The positions are probabilistic variables, therefore the most probable ones are of special importance. To determine the configuration maximizing the \( N \)-body probability distribution \( |\Psi(r_1, \ldots, r_N)|^2 \) we used the Monte Carlo algorithm [14]. Starting from a randomly chosen configuration we shift the positions of all particles and check if the shifted configuration is more probable then the starting one. In case of failure another attempt is made. In fig. 1 we show the most probable configurations for a different number of fermions in a two-dimensional harmonic trap. We see that geometric structures do appear.

The patterns are universal if \( N \) corresponds to closed energy shells. For open shells (not shown here) the patterns depend on the occupied orbitals at the Fermi level. Concentrating on the closed shells we see the following crystalline structures: an equilateral triangle for 3 atoms; a pentagon at the outer shell and one atom located at the trap center for 6 atoms; two shells are seen for 10 atoms—an equilateral triangle forming the inner shell and a heptagon forming the outer shell; and finally, for 15 atoms, the third shell develops—one atom is located at the center, 5 atoms at the middle shell form a pentagon and the remaining 9 atoms are located in the outermost shell. Let us note that if the inner shell contains more than one atom it is generally not possible to match the discrete symmetries of the inner and outer shells. In this case the orientation of the inner shell with respect to the outer shell is fixed. Moreover the shells do not form regular polygons, i.e., distances of particles to the trap center vary slightly. The geometric shells are different from energy shells.

**Single-shot detection of a many-body system.** — The existence of geometrical structures maximizing the \( N \)-body probability is an unexpected consequence of the Fermi-Dirac statistics. Whether this fact belongs to a class of physical curiosities without any importance whatsoever depends upon the possibility of detection of Pauli crystals. Do they really exist in a sense that the probability distribution of different configurations is sharply peaked at the most probable one? Or, on the contrary, are they very elusive objects because probability distribution of different configurations is very flat and its maximum does not distinguish any particular geometric arrangement?

To answer these questions we have to analyze outcomes of single-shot measurements, each giving a collection of \( N \) values of particles’ positions. These values are unpredictable, have probabilistic character; however, the most probable configuration should emerge as the most frequently observed one in a series of measurements.

Consider an array of detectors, each one located at the position \( \mathbf{X} \). A single measurement of a particle at position \( \mathbf{x} \) (a click in the measuring device) means that the detector reacted to a particle. We introduce a function that takes values 0 if no particle is detected at \( \mathbf{X} \) and 1 if a particle is detected:

\[ \text{Click}(\mathbf{X}|\mathbf{x}) = \delta(\mathbf{X} - \mathbf{x}). \]  

Because the outcome of a single measurement is unpredictable, one has to repeat it many times to get a statistics. Repeated measurements allow to make a histogram defined as

\[ h_M(\mathbf{X}) = \frac{1}{M} \sum_{s=1}^{M} \text{Click}(\mathbf{X}|\mathbf{x}(s)), \]

where \( s \) refers to different measurements. It can be shown straightforwardly that in the limit of infinitely many measurements one gets the one-particle probability distribution:

\[ \lim_{M \to \infty} h_M(\mathbf{X}) = p(\mathbf{X}), \]

where

\[ p(\mathbf{X}) = \int d\mathbf{x}_2 \cdots d\mathbf{x}_N |\Psi(\mathbf{x}_2, \ldots, \mathbf{x}_N)|^2. \]
This quantity gives the probability distribution of finding one particle at a point \( \mathbf{X} \), without any information on the correlations between the particles.

Consider now a simultaneous detection of \( N \) particles in a single-shot measurement. Its result is given by

\[
\text{SingleShot} (\mathbf{X}|x_1, \ldots, x_N) = \sum_{i=1}^{N} \text{Click} (\mathbf{X}|x_i). \tag{6}
\]

The single shot is, in our case, a mapping of the 2\(N\)-dimensional configuration space on the 2-dimensional physical space. It contains information on the geometry of the detected configuration; however, it tells nothing about the probabilities of different configurations. Many repetitions are needed to get the probabilities and to construct a histogram of the particles’ positions:

\[
H (\mathbf{X}) = \frac{1}{M} \sum_{s=1}^{M} \text{SingleShot} (\mathbf{X}|x_1^{(s)}, \ldots, x_N^{(s)}) \tag{7}
\]

\[
= \frac{1}{M} \sum_{s=1}^{M} \sum_{i=1}^{N} \text{Click} (\mathbf{X}|x_i^{(s)}). \tag{8}
\]

Evidently, by changing order of summation in eq. (8), we get

\[
H (\mathbf{X}) = Nh_M (\mathbf{X}). \tag{9}
\]

The histogram however, does not contain any information about higher-order correlations, in particular about the geometry carried by a single-shot picture. Correlations are washed out by summation of different outcomes.

**Correlating configurations.** – Analysis of geometric configurations cannot be based on a simple histogram of particle positions. Some quantitative methods allowing to compare different configurations, not the positions of individual particles, are required. For a convenience we introduce a symbol \( \{ \mathbf{x} \} \) to denote the configuration \((x_1, \ldots, x_N)\). In order to compare an outcome of a measurement \( \{ \mathbf{x} \} \) to a given pattern, \( \{ \mathbf{x}^{(a)} \} \), we have to define a measure in the space of configurations defining the distance between them. To this end we use polar coordinates instead of the Cartesian ones, \((x_i) \rightarrow (r_i, \phi_i)\), \((r_0, i) \rightarrow (r_0, \phi_0, i)\), and assign to every particle \( x_i \) its unique partner \( r_0, \sigma(i) \), \((x_i) \rightarrow (r_0, \sigma(i))\) if the coordinates form a single shell then the transformation \( \sigma \) is a cyclic permutation of the set \( 1, \ldots, N \). We define the distance between the two configurations as

\[
d (\{ \mathbf{x} \}, \{ \mathbf{r}_0 \}) = \sum_{i=1}^{N} (\phi_{0, i} - \phi_{\sigma(i)})^2. \tag{10}
\]

The above definition is not the only possible one. In fact a problem of the good definition of a distance between polygons is one of the basic problems in all pattern recognition algorithms which inevitably must assume some knowledge about the pattern. However, we checked that our definition works very well in all cases studied here.

To observe the Pauli crystals one has to correlate outcomes of simultaneous measurement of all \( N \) positions. A single shot will never give a pure geometry of the Pauli crystal because of quantum fluctuations of the particle positions. The crystalline pattern has to be extracted from the measured noisy structure with the help of the image processing. Our goal is to compare different configurations leaving aside such details as the position of the center of mass and the orientation of the configuration in space, thus the geometry of a configuration depends only on the relative positions of particles. Therefore, we shift the center of mass of the configuration at hand to the origin of the coordinate system, \( x_i' = x_i - x_{CM} \) \((x_{CM} = (1/N) \sum x_i)\), and then apply rotations, \( \mathcal{R}_\alpha \), in the \( x-y \) plane by an angle \( \alpha \),

\[
x_i (\alpha) = \mathcal{R}_\alpha (x_i'). \tag{11}
\]

The “best alignment” of a given configuration \( \{ x(\alpha) \} \) is therefore the one which minimizes the distance:

\[
d (\{ x(\alpha) \}, \{ r_0 \}) = \min. \tag{12}
\]

Equation (12) determines the rotation angle \( \alpha \), which brings the given configuration to the “closest” distance to the pattern. Evidently this angle is different for every configuration. We checked that in order to ensure an elementary fairness in a treatment of all particles, the maximal angle of rotation has to be limited to \( 2\pi/k \) when the system has a \( k \)-fold axis of symmetry. Only then, all maxima of the configuration found, have similar heights and widths.

Our strategy of image processing is the following. Each configuration, selected according to the \( N \)-particle probability distribution, is optimally transformed by an isometric transformation \( \{{x}\} \rightarrow \{{x}(\alpha)\} \) to match the pattern according to eq. (12). To gain an insight into the geometric configuration we introduce the configuration probability density, \( C (\mathbf{X}) \) which is the histogram of configurations:

\[
C (\mathbf{X}) = \frac{1}{M} \sum_{s=1}^{M} \text{SingleShot} (\mathbf{X}|x_1^{(s)}(\alpha), \ldots, x_N^{(s)}(\alpha)). \tag{13}
\]

The configuration probability density \( C (\mathbf{X}) \) is seemingly not much different from the histogram of particles’ positions, \( H (\mathbf{X}) \). In fact the difference, related to the preprocessing of the measurement outcome, is tremendous. Contrary to \( H (\mathbf{X}) \) which is proportional to the one-particle probability density, the configuration probability density \( C (\mathbf{X}) \) contains information about the geometric \( N \)-order correlations of the particles.

**Ensemble of configurations.** – To generate an ensemble of configurations according to the many-body probability distribution we use the Metropolis algorithm. We generate a random Markov walk in the configuration space. The states belonging to the Markov chain
become members of the ensemble. The transition probability between subsequent configurations \( \{x^{(s)}\}_N \rightarrow \{y^{(s')}\}_N \) is given by the ratio of their probabilities \( p = |\Psi(\{y^{(s')}\}_N)|^2/|\Psi(\{x^{(s)}\}_N)|^2, \) [14]. If \( p > 1 \) the trial configuration is accepted: \( \{x^{(s+1)}\}_N = \{y^{(s)}\}_N \). If \( p < 1 \) there are two options chosen probabilistically: a) the trial step is accepted to the ensemble with the probability \( p \), \( \{x^{(s+1)}\}_N = \{y^{(s)}\}_N \); b) the old configuration is again included into the chain with the probability \((1 - p)\), \( \{x^{(s+1)}\}_N = \{x^{(s)}\}_N \). Typically we generate \( 2 \times 10^4 \) configurations, each being a set of \( N \) positions on a two-dimensional plane. Next we collect many realizations of the quantum state and after \( M \) realizations we have \( N \times M \) positions of particles. A histogram of such realizations, i.e., one-particle density, \( H(X)/N \), and the configuration density probability, \( C(X)/N \), for \( N = 3, 6, 10, 15 \) atoms, are shown in fig. 2. In all cases the one-particle distribution is a smooth function of the axial symmetry with some maxima in the radial direction. Clearly the one-particle distribution does not show any geometric structures resembling the Pauli crystals shown in fig. 1.

On the contrary, the configuration density probability \( C(X)/N \) shown in the left panels of fig. 2 shows the geometric structure of Pauli crystals. The agreement is amazing—compare with fig. 1. Quantum fluctuations lead to some smearing of the crystal vertices, fortunately the uncertainties of the atom positions are smaller than their separations, at least for small \( N \). For larger \( N \) several shells are formed. The outer shells are somewhat melted because of quantum fluctuations. A similar method of imaging of geometrical structures formed by interacting Rydberg atoms was recently realized in the experiment with ultra-cold atoms [15]. Evidently our image processing, thus the configuration density, \( C(X) \), depends on the pattern. To show how image-processed configurations are biased by the pattern used, in fig. 3 we compare two configuration densities obtained by the best matching to two different patterns, of the same ensemble of single-shot pictures. As an example we choose one of the lowest excited states of \( N = 6 \) particles, obtained by exciting one particle from the Fermi surface. In the Slater determinant we replaced the state \( n = 2, m = 0 \) by \( n = 2, m = 1 \).
To lift the degeneracy we assumed that in the ground-state \( H \) of three basis states. In fig. 4 we show the one-particle density has two maxima, both on the \( y \)-axis. The one-particle density does not depend on \( N \) and the configuration probability density, \( C(X)/N \), fig. 4(b), fit perfectly to the geometry of the Pauli crystal. The configuration density was obtained by our image processing method using rotations to align the configurations.

**Few-particle correlations.** – In this section we use an example of \( N = 6 \) particles to show to what extent the low-order correlation functions carry information on the Pauli crystalline structures. The Pauli crystal in this case forms two geometric shells with one particle in the trap center and five in the outer shell of the radius \( r_0 = 1.265 \), see fig. 1. The one-particle density does not depend on the azimuthal angle. This is expected because of the axial symmetry. But also a radial structure of the one-particle density does not indicate any geometrical arrangement of the atoms. The one-particle density has a sharp maximum at the center of the trap, a plateau at larger distances, and finally, at distance of the order of \( r \sim 1 \), it falls to zero quite rapidly, fig. 2(c). The one-particle density does not suggest the existence of the shell of radius \( r_0 = 1.265 \).

One might expect, however, that two-body correlations will disclose a geometric ordering. Figure 5(a) shows the conditional probability density of particle detection at position \( r_0 \) as a function of the azimuthal angle, provided that simultaneously another particle is found at the same distance \( r_0 \) and at the azimuthal angle \( \phi_0 = 2.705 \). Polar coordinates \( r_0 \) and \( \phi_0 \) correspond to the location of one of the vertices of the Pauli crystal in fig. 1. What is clearly seen is the effect of the Pauli exclusion principle — the probability of finding the second particle close to the first one is very small. Observation of this effect was reported recently [16,17]. In addition weak oscillations are seen; they are of the same type as the Friedel oscillations [18] known in the case of electron gas. No clear structure resembling a pentagon is visible in fig. 5(a); however four hardly distinguishable maxima of the correlation functions are seeds of the emerging structure. The second-order correlation function does not give enough evidence of the existence of the Pauli crystal. In contrast, the image processing procedure described above, showing \( N \)-order correlations, unveils the crystalline structure. To support
this statement we show in fig. 5(b) a cut through the config-

uration density function $C(X)$, fig. 2(d), along the circle

of radius $r_0 = 1.265$. Five distinct maxima indicate the

most probable positions of the particles arranged in a pen-

tagon —the Pauli crystal.

An alternative approach to the Pauli crystals is based

on the method of Javanainen [10]. In this approach the

Pauli crystal should emerge from the hierarchy of the con-

tional probability functions. The starting point of this

approach is to select a particle at position $x_1$, then use

the conditional probability to select the second particle at

position $x_2$, and continue this way through three, four etc.

conditional probabilities. One may expect that few parti-

cles will give a hint on the positions of all other particles.

We verified this approach using an example of 6 parti-

cles. In fig. 6 we show the result of this procedure. First,

fig. 6(a), we selected the first particle at the maximum of

the one-particle density. The corresponding one-particle conditional density shows a maximum along a ring with the radius of the Pauli crystal, fig. 6(b). This is the first signature of the emerging structure. Next, we chose the position of the second particle on this ring. In fig. 6(b) we plot the corresponding three-point conditional probability. Note a small structure appearing along the ring, fig. 6(c), in addition to a clearly visible Pauli hole. When the third particle is chosen at the maximum on the ring, the Pauli structure of $N = 6$ atoms system clearly emerges in higher-order conditional distributions, fig. 6(d)–(f). The conditional approach to the high-order correlation functions and emerging Pauli crystal structures is an independent test strengthening our confidence in the image processing method.

Comparison with other systems and experimental prospects. — Many other systems exist that contain atoms or molecules arranged in a regular geometric structure, like molecules, crystals, clusters. Also more exotic structures can be formed, e.g., Wigner [19] and Coulomb crystals [20–22]. In the context of ultra-cold trapped atoms interacting via a short-range contact potential, geometric crystalline structures such as “Wigner molecules” were predicted [23–25]. In all these cases, however, the geometry is determined by a balance between attractive interactions at large distances and repulsive ones at small distances. Quantum statistics plays a marginal role in the resulting geometry in all cases. It should be stressed that the geometry of Pauli crystals differs on the fundamental level from that of other crystals. It would be misleading to consider the anti-symmetry of the wave function as a simple kind of repulsion. The case of Pauli crys-
tals is truly unique. Observation of the Pauli crystals, as a result of the Pauli principle alone, can be possible only in ideal or very weakly interacting quantum systems. Stronger repulsive interactions might lead to a different geometry. Fermi-Dirac statistics leads to observable effects only when one-body wave functions of individual parti-
cles overlap. This is possible in the case of electrons in atoms. Electrons in atoms, however, are not good can-
didates for the envisaged experiments because of their Coulomb interactions. We rather have in mind systems of ultra-cold fermion atoms in optical traps. Lithium $^6$Li or potassium $^{40}$K atoms are good candidates. At densities of $10^{12}$ cm$^{-3}$ the wave functions describing atoms overlap at a temperature of the order of $T = 10^{-7}$ K. These are the conditions under which quantum statistics plays a crucial role [26–29].

There are many experimental imperfections which can destroy Pauli crystals. The nonzero temperature seems
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