

Pauli Crystals: hidden geometric structures of the quantum statistics

Mariusz Gajda, Jan Mostowski, Tomasz Sowiński, Magdalena Załuska-Kotur
Institute of Physics of the Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland
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The micro-world is governed by the laws of Quantum Theory. Although we cannot directly experience Quantum Mechanics in action, it imperceptibly enters our everyday life. It explains the structure of matter on the one hand and stands behind all modern technologies on the other. It also gives a completely different meaning to the classical concept of identical objects. Quantum identical particles are identical not only because they share the same mass, spin, charge, etc., but also because they cannot be identified by tracing their history. Indistinguishability results in a division of the world of elementary particles into fundamentally different families: fermions (e.g. electrons, protons, neutrons) and bosons (e.g. photons, gluons, Higgs boson). Identical fermions subjected to the Fermi-Dirac statistics cannot occupy the same quantum state. Here we show yet another, so far undiscovered, consequence of quantum indistinguishability. We show that identical fermions confined by an external trapping potential arrange themselves in spectacular geometric structures although 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 form a previously unknown form of particles' organization. Our results shed some light on the role of quantum statistics – one of the fundamentals of quantum mechanics of many-body systems.

Quantum statistics emerge from fundamental requirement of causality. Quantum theory of indistinguishable particles in four-dimensional space-time is consistent with relativistic theory only when operators of quantum fields fulfill commutation or anti-commutation relations for particles with integer (bosons) or half-integer (fermions) spins respectively [1]. In the nonrelativistic limit the commutation or anti-commutation relations pertain to the symmetry of the many-body wave function. The wave function of fermions is antisymmetric. Exchange of two fermions, including their spins, reverses the overall sign of the wave function. On the contrary, the wave function of bosons does not change at all if two bosons are exchanged.

The antisymmetry of the wave function prevents two identical fermions to be in the same quantum state (in-

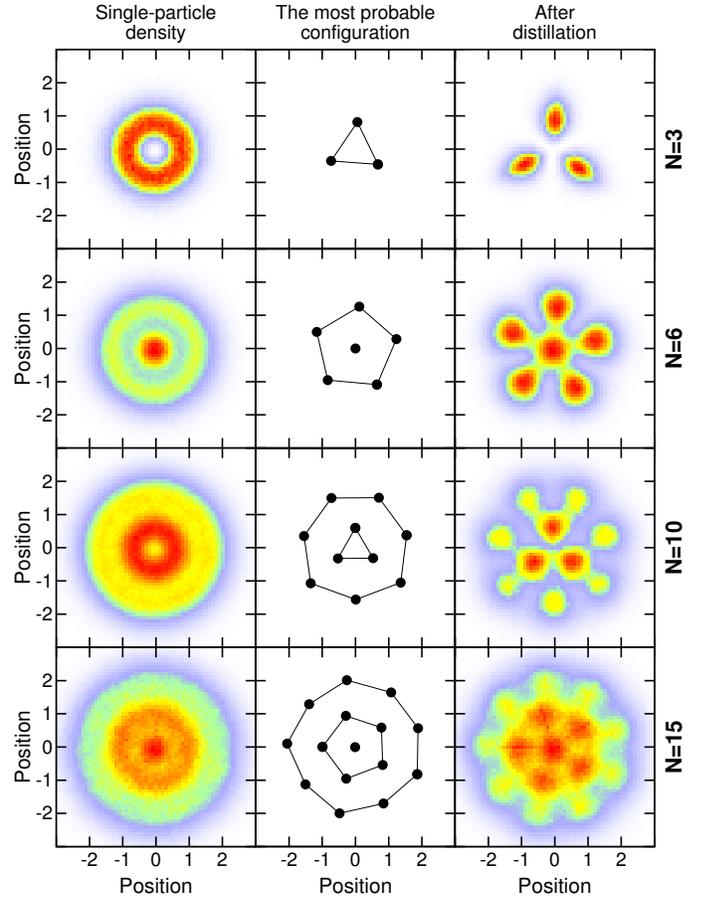


FIG. 1: **Pauli crystals in two-dimensional harmonic trap.** Left column: single-particle density distribution obtained with a direct collecting of particles' positions in many single-shot experiments. Middle column: the most probable configuration of N particles. Right column: distilled many-particle probability function. In all figures position is measured in natural units of harmonic oscillator.

cluding spin). This statement is known as the Pauli exclusion principle formulated by Wolfgang Pauli in 1925 in case of electrons [2]. The basic reason for this principle was the need to explain the structure of atoms. However, it was noticed very promptly that the principle plays a crucial role in determining the properties of all many-fermion systems (interior of nucleons and atomic nuclei, chemical molecules, superfluids, semi- and superconductors, and even more exotic systems like white dwarfs and neutron stars). On the contrary, the symmetry conditions imposed on the boson many-body wave function results in a tendency of particles to cluster in the same

state. Coherent laser light and Bose-Einstein condensates are the best examples.

In this letter we study a small system of non-interacting spin polarized fermions confined in space by an external binding potential. The particles are in the many-body ground state. The spatial part of the wave function is antisymmetric and there is no need to consider the spin. The particles 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.

We will illustrate the concept of the Pauli crystal using a simple generic example of particles in two dimensions bounded by a harmonic potential. The ground state of a non-interacting N -body system is very simple. According to the Pauli exclusion principle every particle occupies a different one-particle state. As a result the N lowest energy states are occupied, up to the Fermi energy. In the case studied, for $N = 1, 3, 6, 10, 15$ the ground state is uniquely defined because all states at or below the Fermi level are occupied and states above the Fermi level remain not occupied. Whenever the total number of particles does not coincide with the degeneracy of the energy shells the many-body ground state is degenerated. The many-body wave function is simply the Slater determinant (anti-symmetrized product) of the occupied one-particle orbitals. The latter are obviously products of the Hermite polynomials and Gaussian functions, since we consider particles in a harmonic trap.

A question arises what is the most probable configuration of the N particles in this state. One could naively think that the answer is trivial. Every particle occupies different quantum state. Obviously, since the state is axially symmetric, the single-particle density shown in the first column of Fig. 1 is smooth and does not exhibit any geometric structures. Suppose however, that it is possible to take single-shot measurements, i.e. determine positions of all the particles in one experiment. The outcome of such single-shot measurement is a collection of N positions. Their values are unpredictable, however the most probable configurations should emerge as the most frequently observed ones in a series of measurements.

To determine the configuration maximizing the N -body probability distribution we used the Monte-Carlo algorithm [3]. The probability distribution is equal to the square of the modulus of the Slater determinant of the occupied orbitals. In the middle column of Fig. 1 we show the configurations obtained for a different number of fermions in a two-dimensional harmonic trap. We see that the geometric structures do appear. If N corresponds to a closed energy shell, i.e. takes one of the magic values $N = 1, 3, 6, 10, 15$, the pattern is universal. For open shells (not shown here) the pattern depends on the occupied orbitals at the Fermi level. Concentrating on the closed shells we see the following crystalline structures: (1) an equilateral triangle for three atoms, (2) a pentagon at the outer shell and one atom located at the trap center for six atoms (3) two shells are developed for

ten atoms – an equilateral triangle forming the inner shell and a heptagon forming the outer shell, (4) finally for fifteen atoms the third shell starts to develop – one atom is located at the center, five atoms at the middle shell form a pentagon and the remaining nine atoms are located at 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 than energetic ones.

To observe the Pauli crystals one has to simultaneously detect all N particles. Such a detection, however, will never correspond to the pure geometry of the Pauli crystal because of quantum fluctuations of particle positions. The pattern has to be extracted from the measured noisy structure. To probe the N particle probability distribution we generate a large number ($M = 10^5 - 2 \times 10^6$) of N -particle configurations according to the probability given by the N particle ground state wave function. The configuration is 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. the function $h(x, y)$ which counts the number of realizations with a particle at the position (x, y) , if properly normalized, gives the probability of finding a particle at a given point. In this way the single-particle probability density is restored. Clearly the single-particle distribution does not show any geometric structure at all, as argued above. The reason is that the configuration of maximal probability, is not unique. The system we investigate has some symmetries and the same symmetries are enjoyed by the N -particle probability. In the case of closed energy shells the symmetries are rotations around the trap center, reflections and inversion. There are also other symmetries like permutations of particles and some specific symmetries depending on particle number N . This results in a huge degeneracy of configurations with maximal probability. All of them differ by some symmetry operation. The symmetries are broken differently in every single realization. Therefore the histogram based on the generated realizations of the system gives the single-particle distribution which restores all symmetries broken in a single detection. As a result the Pauli crystals are completely washed out.

The clue to overcome this difficulty is very simple. Before summing the results of every single realization to get the histogram, we have to correlate all single-shot pictures. The goal is to recognize a given pattern, the Pauli crystal, having at the disposal a collection of images, all of them rotated by a different angle. It is clear that to produce the histogram preserving geometric correlations we have to distill the image, i.e., to rotate every N -atom realization by some angle in order to make it

”the closest” to a given pattern.

In the right column panel of Fig. 1 we show joint N -body probability distribution of particles’ positions after the distillation mentioned above (see Methods). The maxima of this distribution correspond to the Pauli crystals shown in the middle column of Fig. 1. The agreement is amazing. Quantum fluctuations lead to some smearing of the crystal vertexes, fortunately the uncertainty of atom positions is smaller than their separation. The inner shells are much better visible than the outer shells. This analysis gives a hope for the experimental observation of the Pauli crystals. Similar method of imaging of crystalline structures in a few-body system of interacting Rydberg atoms was recently realized in experiment [4].

Our theoretical analysis is very general and can be adopted to any quantum many-body state of a few fermions. It is not limited to a particular form of external confinement or to two dimensions. For example, in Fig 2. we show Pauli crystals, i.e. the structures corresponding to the maximally probable configurations, in the case of particles in three dimensional isotropic harmonic trap. The number of particles is chosen to match the closed energy shells, i.e. equals to $N = 4, 10, 20, 35$. Regular crystalline structures are seen. Particles are located on several shells forming polyhedral structures of triangular walls: a tetrahedron for $N = 4$; one particle at the center of a polyhedron with 14 walls and 9 corners for $N = 10$. For larger N studied, the former structures form the inner shells while the outer shells contain the remaining particles. For $N = 20$, a tetrahedron is immersed inside the polyhedral structure of 28 triangular walls and 16 corners, while for $N = 35$ the crystalline similar to those obtained for $N = 10$ particles, is located inside a polyhedron with 25 corners and 46 triangular walls. The distillation procedure in this case is straightforward.

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 [5] and Coulomb crystals [6–8]. In all these cases, however, the geometry is determined by a balance between attractive interactions at large distances and repulsive 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 crystals is truly unique.

Observation of Pauli crystals can be possible only in ideal or very weakly interacting quantum systems. Fermi-Dirac statistic leads to observable effects only when one-body wave functions of individual particles overlap. This is possible in the case of electrons in atoms. Electrons in atoms, however, are not good candidates for the envisaged experiments because they interact and are hard to observe. We rather have in mind systems of ultra-

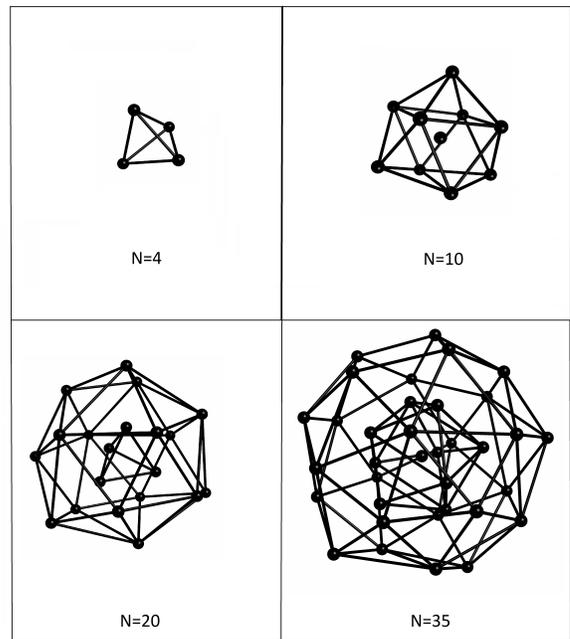


FIG. 2: **Pauli crystals in three dimensions.** The most probable configuration for $N = 4, 10, 20, 35$ fermions in a three-dimensional isotropic harmonic potential.

cold fermion atoms with tunable interactions in optical traps. At densities of 10^{12} cm^{-3} the wave functions describing atoms overlap at the temperature of the order of $T = 10^{-7} \text{ K}$. These are the conditions at which quantum statistics plays a crucial role, [9–12].

Tremendous progress of experimental techniques of preparing, manipulating and probing ultra-cold gases have opened new possibilities of optical methods of monitoring the atomic systems. Atomic fluorescence microscopes with resolution in the range of hundreds of nanometers became accessible, [13–16]. The microscopes allow for observation of both boson and fermion atoms with a resolution comparable to the optical wavelength. Therefore the observation of the Pauli crystals seems to be within the range of recent experimental techniques. The effect of the Pauli principle is already of the interest to experimentalists. Direct observation of the Pauli blocking in optical lattices has been recently reported [17].

Our finding shows that even such simple system as a noninteracting Fermi gas has some secret geometry deeply hidden in many-body correlations. This finding might suggest that geometric correlations are common in all Fermi systems. Interactions compete with quantum statistics and modify the geometric structures. For instance the Wigner crystals, resulting from minimization of the Coulomb potential energy, have different geometric structures than the Pauli crystals. Therefore, one can think of systems that will be somewhere between these two cases where both interactions and statistics play a role in determining the geometric structure. This may

suggests that the system may undergo some kind of 'geometric phase transition' from the one to the other crystalline structure. We can also imagine that attractive interactions between fermions are turned on gradually. Then the Pauli crystals will be modified, in particular the relative distances between particles should decrease. We can speculate therefore that crystalline structures will be melted because of quantum fluctuations. If this process is related to an appearance of the superfluid behavior of Fermi system remains an intriguing question.

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Methods

Numerical algorithms. N -body probability distribution is determined by a many-body wave function. The most probable configuration maximizes the distribution. We find this configuration using a Monte Carlo algorithm. At each step of the procedure we randomly deform the current configuration and select the one being the more probable. Iterating this procedure we arrive with the most probable configuration. The procedure spontaneously breaks the symmetry of the probability distribution and gives one configuration (out of multiply degenerated) maximizing the probability distribution.

To generate an ensemble of configurations according to the many-body probability distribution we use the Metropolis al-

gorithm. We generate a Markovian walk in the configuration space. The states visited in this walk become members of the ensemble. A transition probability between subsequent configurations is given by the ratio of their probabilities [3]. Typically we generate $10^5 - 2 \times 10^6$ configurations.

In order to distill the N -particle geometric correlations from the generated ensemble we use a simple image processing method. The algorithm we developed can be improved because it does not use all symmetries of the problem. Our idea is to give a proof of principles that geometric structures can be distilled from a collection of realizations. To correlate different configurations we use only rotations as the symmetry operations. Every single realization is rotated by an angle ranging from 0 to $2\pi/N$ and compared to the Pauli crystal pattern given by the most probable configuration. The 'best rotation' corresponds to the smallest distance between given single realization and the pattern. Only after such adjustment the histogram was calculated. The procedure is very sensitive to the definition of the distance between the Pauli crystal pattern and a single realization. In our case the distance is defined as follows. Every particle is assigned the nearest particle in the pattern. The angular distance to the nearest neighbor is then determined as the difference of azimuthal angles of the particles positions. The distance between the two configurations is defined as the sum of squares of all angular distances between neighboring particles. This way we get the distributions presented in the third column of Fig. 1.

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