Single shot imaging of trapped Fermi gas

Mariusz Gajda, Jan Mostowski, Tomasz Sowiński, and Magdalena Załuska-Kotur

Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, PL-02668 Warsaw, Poland

PACS 67.85.Lm – Degenerate Fermi gases

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 case of cloud of ultra-cold non-interacting 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 of preparing, manipulating and probing 2 ultra-cold gases have opened new possibilities of optical 3 methods of monitoring atomic systems. Atomic fluoresл cence microscopes with resolution in the range of hundreds of nanometers became accessible [1–7]. The micro-6 scopes allow for 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 10 as opposed to a one-particle probability distribution. Dif-11 ference between the two is tremendous, they differ by N12 body correlations. The seminal work of [8] shows how 13 interference fringes, visible in a simultaneous single shot 14 picture of N atoms, arise in the course of measurement. 15 No fringes are observed in a single particle detection in-16 stead. In a similar way the solitons emerge in a process 17 of detection of N-particles prepared in a type II excited 18 state of a 1D system of bosons interacting via short-range 19 potential described by the Lieb-Linger model [9]. Single 20 shot time-dependent simulations of many-body dynamics 21 showing appearance of fluctuating vortices and center-of-22 mass fluctuations of attractive BEC have been reported 23 recently [10]. 24

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 [11]. 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. Here we show yet another consequence of quantum indistinguishability. We show that 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.

32

33

34

35

36

37

38

39

40

41

42

43

44

Pauli crystals. – Here we study on a theoretical 45 ground a manifestation of the quantum statistics, namely 46 a high order geometric correlations in a small system of 47 ultra cold spin polarized fermions confined in space by an 48 external binding potential. To this end we generate a sin-49 gle shot picture of this noninteracting system. We limit 50 our attention to the many-body ground state. Atoms are 51 attracted towards the trap minimum, but on the other 52 hand, the Pauli exclusion principle does not allow any two 53 fermions to be at the same position. These two competing 54 effects might, in principle, lead to a kind of equilibrium. 55

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:

$$\psi_{nm}(x,y) = \mathcal{N}_{nm} \mathrm{e}^{-(x^2 + y^2)/2} \mathcal{H}_n(x) \mathcal{H}_m(y), \qquad (1)$$

where $\mathcal{N}_{nm} = (2^{n+m} n! m! \sqrt{\pi})^{-1/2}$ is the norm, and $\mathcal{H}_n(z)$ 56



Fig. 1: Pauli crystals in two-dimensional harmonic trap. Configurations maximizing N-particle probability: (a) -3 atoms, (b) -6 atoms, (c) -10 atoms, (d) -15 atoms.

is the *n*-th Hermite polynomial. The positions x and y are 57 expressed in the normal harmonic oscillator units, i.e. the 58 unit of length being $a = \sqrt{\hbar/M\omega}$, where M is the mass 59 of the particle. Quantum numbers n and m enumerate 60 excitations in x and y direction respectively. We consider 61 an isotropic trap, therefore all states with the same total 62 number of excitations, n + m, are degenerated. These 63 states have energy $E_{nm} = \hbar \omega (n + m + 1)$, all states of the 64 same energy form an energy shell. 65

The ground state of a non-interacting N-body system is 66 very simple, every particle occupies a different one-particle 67 state. As a result the N lowest energy states, up to the 68 Fermi energy are occupied. For N = 1, 3, 6, 10, 15 the 69 ground state is uniquely defined because all states at or 70 below the Fermi level are occupied and states above the 71 Fermi level remain not occupied. The many-body ground 72 state is degenerated whenever the total number of particles 73 does not coincide with the degeneracy of the energy shells. 74 The many-body wave function is simply the Slater 75 determinant of the occupied one-particle orbitals: 76 $\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N) = \sqrt{\frac{1}{N!}} \det[\psi_{ij}(\boldsymbol{r}_k)].$ The modulus square of the wave function $|\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)|^2$ is the probability 77 78 density of finding the particles at positions r_1, \ldots, r_N . 79

In a single-shot measurement with a fluorescence mi-80 croscope, a set of N positions of atoms can be deter-81 mined. It is therefore legitimate to study the outcomes 82 of such measurements on a theoretical ground. The posi-83 tions are probabilistic variables, therefore the most proba-84 ble ones are of special importance. To determine the con-85 figuration maximizing the N-body probability distribution 86 $|\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)|^2$ we used the Monte-Carlo algorithm [12]. 87 Starting from a randomly chosen configuration we shift 88 positions of all particles and check if the shifted config-89 uration is more probable then the starting one. In case 90 of failure another attempt is made. In Fig.(1) we show 91 the most probable configurations for a different number of 92 fermions in a two-dimensional harmonic trap. We see that 93 geometric structures do appear. 94

The patterns are universal if N corresponds to closed energy shells, i.e. takes one of the values N = 1, 3, 6, 10, 15. 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 three atoms; a pentagon at the outer shell and one atom located at the trap center for six atoms; two shells are seen for ten atoms – an equilateral triangle forming the inner shell and a heptagon forming the outer shell; and finally, for fifteen atoms, the third shell develops – 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 energy shells.

102

103

104

105

106

107

108

109

110

111

112

113

114

115

116

117

118

119

120

121

122

123

124

125

126

127

128

129

130

131

132

133

134

135

Single shot detection of many-body system. – Existence of geometrical structures maximizing the Nbody 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 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 object 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 such measurement gives a collection of values of N particle positions. These values are unpredictable, have probabilistic character, however the most probable configurations should emerge as the most frequently observed ones in a series of measurements. Let us now discuss detection of particle positions, such measurement is particularly important in discussion of the properties of the many-body system.

Consider an array of detectors, each one measures a particle 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 and 1 if a particle is detected.:

$$\operatorname{Click}(\mathbf{X}|\mathbf{x}) = \delta(\mathbf{X} - \mathbf{x}).$$
⁽²⁾

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:

$$h_M(\mathbf{X}) = \frac{1}{M} \sum_{s=1}^{M} \operatorname{Click}(\mathbf{X}|\mathbf{x}^{(s)}), \qquad (3)$$

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:

$$\lim_{M \to \infty} h_M(\mathbf{X}) = p(\mathbf{X}),\tag{4}$$

where

$$p(\mathbf{X}) = \int d\mathbf{x}_2 \cdots d\mathbf{x}_N |\Psi(\mathbf{X}, \mathbf{x}_2, \dots, \mathbf{x}_N)|^2.$$
(5)

This quantity gives the probability distribution of finding
one particle at a point 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:

SingleShot(
$$\mathbf{X}|\mathbf{x}_1, \dots, \mathbf{x}_N$$
) = $\sum_{i=1}^N \text{Click}(\mathbf{X}|\mathbf{x}_i).$ (6)

Single shot is, in our case, a mapping of the 2Ndimensional configuration space on the 2-dimensional
physical space. It contains information on the geometry of
the detected configuration, however it tells nothing about
probabilities of different configurations. Many repetitions
are needed to get the probabilities and to construct a histogram of particles' positions:

$$H(\mathbf{X}) = \frac{1}{M} \sum_{s=1}^{M} \text{SingleShot}(\mathbf{X} | \mathbf{x}_1^{(s)}, \dots, \mathbf{x}_N^{(s)}) \quad (7)$$

$$= \frac{1}{M} \sum_{s=1}^{M} \sum_{i=1}^{N} \operatorname{Click}(\mathbf{X} | \mathbf{x}_i^{(s)}).$$
(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 $\{\mathbf{x}\}_N$ to denote the configuration $(\mathbf{x}_1,\ldots,\mathbf{x}_N)$. In order to compare an outcome of a measurement $\{\mathbf{x}\}_N$ with a given pattern, i.e. with the Pauli crystal structure $\{\mathbf{r}_0\}_N$, 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, $(\mathbf{x}_i) \rightarrow (r_i, \phi_i), (\mathbf{r}_{0_i}) \rightarrow (r_{0_i}, \phi_{0_i}),$ and assign to every particle \mathbf{x}_i its unique partner $\mathbf{r}_{0_{\sigma(i)}}$, $(\mathbf{x}_i) \to (\mathbf{r}_{0_{\sigma(i)}})$. If the coordinates form a single shell then the transformation σ is a cyclic permutation of the set $1, \ldots, N$. We define the distance between the two configurations as:

$$d(\{\mathbf{x}\}_N, \{\mathbf{r_0}\}_N) = \sum_{i=1}^N \left(\phi_{0_i} - \phi_{\sigma(i)}\right)^2.$$
(10)



Fig. 2: Comparison of one-particle and configuration probability densities. (a), (b) – 3 atoms, (c), (d) – 6 atoms, (e), (f) – 10 atoms, (g), (h) – 15 atoms. For each pair of figures we show a one-particle density distribution obtained with a direct collecting of the particle positions in many single shot experiments $H(\mathbf{X})/N$ – left panels: (a), (c), (e), (g). In right panels – (b), (d), (f), (h), we show configuration probability density $C(\mathbf{X})/N$ resulting from the image processing. Position is measured in natural units of the harmonic oscillator. The same color scale is used for every pair of figures. Note that configuration distributions are strongly peaked around maximal values. This maxima dominate over relatively flat structures of the one-particle density.

The above definition is not the only possible. In fact a 150 problem of the good definition of a distance between poly-151 gons is one the basic problems in all pattern recognition 152 algorithms which inevitably must assume some knowledge 153 about the pattern. However, we checked that our defini-154 tion works very well in the case studied here. We checked 155 then when a system has a n-fold axis of symmetry, in or-156 der to ensure elementary fairness treatment of all particles, 157 the maximal angle of rotation has to be limited to $2\pi/n$. 158 Only then, all maxima of the pattern found have similar 159 heights and widths. 160

To observe the Pauli crystals one has to correlate outcomes of simultaneous measurement of all N positions. 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 relative positions of particles. Therefore we shift the center of mass of the configuration at hand to the origin of the coordinate system: $\mathbf{x}'_i = \mathbf{x}_i - \mathbf{x}_{CM} (\mathbf{x}_{CM} = (1/N) \sum_{i=1,N} \mathbf{x}_i)$ and then apply rotations in the x - y plane by an angle α ,

$$\mathbf{x}_{i}(\alpha) = \mathcal{R}_{\alpha} \left(\mathbf{x}_{i} - \mathbf{x}_{CM} \right). \tag{11}$$

The 'best alignment' of a given configuration $\{\mathbf{x}(\alpha)\}_N$ is therefore the one which minimizes the distance:

$$d\left(\{\mathbf{x}(\alpha)\}_N, \{\mathbf{r_0}\}_N\right) = \min..$$
(12)

Eq.(12) determines the rotation angle α, which brings the
given configuration to the 'closest' distance to the pattern.
Evidently this angle is different for every configuration.

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 $\{\mathbf{x}\}_N \to \{\mathbf{x}(\alpha)\}_N$ 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:

$$C(\mathbf{X}) = \frac{1}{M} \sum_{s=1}^{M} \text{SingleShot}(\mathbf{X} | \mathbf{x}_{1}^{(s)}(\alpha), \dots, \mathbf{x}_{N}^{(s)}(\alpha))$$
. (13)

The configuration probability density $C(\mathbf{X})$ is seemingly 171 not much different from the histogram of particles' posi-172 tions, $H(\mathbf{X})$. In fact the difference, related to the pre-173 processing of the measurement outcome, is tremendous. 174 Contrary to $H(\mathbf{X})$ which is proportional to one-particle 175 probability density, the configuration probability density 176 $C(\mathbf{X})$ contains information about the geometric N-order 177 correlations of the particles. 178



Fig. 3: Quality of pattern recognition. (a) Configuration density of the excited state of 6-particle system obtained after image processing based on a comparison with a *corresponding excited state* Pauli crystal pattern. (b) Configuration density of the state shown in (a) but obtained after processing of the same data as used in (a), but based on a comparison with the *ground state* pattern of 6-particle system. The patterns are marked by dots.

Ensemble of configurations. – To generate an 179 ensemble of configurations according to the many-body 180 probability distribution we use the Metropolis algorithm. 181 We generate a random Markov walk in the configura-182 tion space. The states belonging to the Markov chain 183 become members of the ensemble. The transition prob-184 ability between subsequent configurations $\{\mathbf{x}^{(s)}\}_N \rightarrow$ 185 $\{\mathbf{y}^{(s)}\}_N$ is given by the ratio of their probabilities p =186 $|\Psi({\mathbf{y}^{(s)}}_N)|^2 / |\Psi({\mathbf{x}^{(s)}}_N)|^2$, [12]. If p > 1 the trial con-187 figuration is accepted to the chain: $\{\mathbf{x}^{(s+1)}\}_N = \{\mathbf{y}^{(s)}\}_N$. 188 If p < 1 there are two options chosen probabilistically: (a) 189 the trial step is accepted to the ensemble with the proba-190 bility p, $\{\mathbf{x}^{(s+1)}\}_N = \{\mathbf{y}^{(s)}\}_N$, (b) the old configuration is 191 again included into the chain with the probability (1-p), 192 $\{\mathbf{x}^{(s+1)}\}_N = \{\mathbf{x}_N^{(s)}\}_N$. Typically we generate 2×10^6 configurations, each being a set of N positions on a two di-193 194 mensional plane. Next we collect many realizations of the 195 quantum state and after M realizations we have $N \times M$ 196 positions of particles. A histogram of such realizations, 197 i.e. one-particle density, $H(\mathbf{X})/N$, and configuration den-198 sity probability, $C(\mathbf{X})/N$, for N = 3, 6, 10, 15 atoms are 199 shown in Fig.(2). In all cases the one-particle distribution 200 is a smooth function of axial symmetry with some maxima 201 in the radial direction. Clearly the one-particle distribu-202 tion does not show any geometric structures resembling 203 the Pauli crystals shown in Fig.(1). 204

On the contrary, the configuration density probability 205 $C(\mathbf{X})/N$ shown in left panels of Fig(2) exhibits the geo-206 metric structure of Pauli crystals. The agreement is amaz-207 ing - compare Fig.(1). Quantum fluctuations lead to some 208 smearing of the crystal vertexes, fortunately the uncertain-209 ties of atom positions are smaller than their separations, at 210 least for small N. For larger N several shells are formed. 211 The outer shells are somewhat melted because of quan-212 tum fluctuations. A similar method of imaging geometri-213 cal structures formed by interacting Rydberg atoms was 214 recently realized in experiment with ultra cold atoms [13]. 215 Evidently our image processing, thus configuration den-216 sity, $C(\mathbf{X})$, depends on the pattern. To show how image-217

257

258

259

260

261

262

263

277

278

279

280

281

282

283

284

285

286

287

288

289

290



Fig. 4: Open shell Pauli crystalline structure for N=5 atoms. (a) – one-particle probability distribution $H(\mathbf{X})/N$, (b) – configuration probability distribution $C(\mathbf{X})/N$. Note that color scale is different in both panels to emphasize a small structure in the one-particle density. Maxima of one-particle distribution do not coincide with maxima of configuration distribution. The latter are marked by blue and black dots.

processed configurations are biased by the pattern used, 218 in Fig.(3) we show two configuration densities obtained by 219 the best matching of the same ensemble of single shot pic-220 221 tures to a two different patterns. As an example we choose the ensemble of configurations generated from the prob-222 ability distribution of the one of lowest excited states of 223 N = 6 particles, obtained by exciting the one at the Fermi 224 surface. In the Slater determinant we replaced the state 225 $n_x = 2, n_y = 0$ by $n_x = 2, n_y = 1$. In Fig.(3a) we show 226 the configuration density obtained by fitting the ensem-227 ble of configurations to the 'native' crystalline structure 228 of the excited state (marked by blue dots), while in the 229 right panel, Fig.(3b), the same set of images is adjusted 230 to the ground state Pauli crystal, marked by black dots. A 231 'quality' of agreement, favors the native structure. If, as 232 the pattern, a configuration similar to the native one were 233 used, the pattern recognition algorithm would have pro-234 duced a better agreement with the pattern. This however 235 is not surprising, similar patterns are hard to distinguish. 236

In the case studied here the configuration of maximal 237 probability is not unique. The system we investigate has 238 some symmetries. The same symmetries are enjoyed by 239 the N-particle probability. In the case of closed energy 240 shells the symmetries are rotations around the trap center, 241 reflections and inversion. There are also other symmetries 242 like permutations of the particles and some specific sym-243 metries depending on the particle number N. This results 244 in a huge degeneracy of configurations with maximal prob-245 ability. All of them differ by some symmetry operation. 246 The symmetries are broken differently in each single real-247 ization. This is an additional reason why the histogram 248 based on the generated single shot realizations washes out 249 the Pauli-crystal structure. 250

The above discussion might suggest that the problem of recognition of the crystalline structures is solely due the high symmetry of the system, and necessity of a proper alignment of single shot outcomes can be presumably overcame by choosing a trapping potential of a very low symmetry. One can hope then, that even one-particle density will show a number of maxima arranged in the geometry of Pauli crystals. Such small oscillations of one-particle density are in fact typical for small systems of noninteracting fermions as a result of the oscillatory character of one-particle wavefunctions – thus of one-particle densities too. We want to stress that this is not the case here, structures we found are different.

To show the effect of symmetry, we consider a case of 264 N = 5 particles, i.e. the open shell structure where we 265 have a freedom to choose two occupied orbital out of three 266 basis states. In Fig.(4) we show the one-particle den-267 sity $H(\mathbf{X})/N$ and the configuration probability density 268 $C(\mathbf{X})/N$ for the ground state system of N = 5 particles. 269 To lift the degeneracy we assumed that in the ground state 270 the orbitals n = 2, m = 0, and n = 1, m = 1 are occupied 271 and the orbital n = 0, m = 2 is empty. This choice is 272 equivalent to assumption that ω_x is 'a bit' smaller than 273 ω_y . The ground state has no rotational symmetry, the 274 only symmetry is the reflection with respect to the y-axis, 275 $y \rightarrow -y$. 276

There are two equivalent configurations maximizing the 5-particle probability. These are isosceles trapezoids differing by the reflection, see blue and black dots in Fig.(4a). These Pauli crystalline structures are drawn on top of the corresponding one-particle density. The structures are located in the region when the density is large, but evidently most of atoms forming the Pauli structure are not located at the maxima of the one-particle density. The one-particle density has two maxima, both on the *y*-axis. On the contrary, sharp maxima of the configuration density, $C(\mathbf{X})/N$, Fig.(4b), 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 291 an example of N = 6 particles to show to what extend the 292 low-order correlation function carry information on the 293 Pauli crystalline structures. The Pauli crystal in this case 294 forms two geometric shells with one particle in the trap 295 center and five at the outer shell of the radius $r_0 = 1.265$, 296 see Fig.(1). The one-particle density does not depend on 297 the azimuthal angle. This is expected because of the axial 298 symmetry. But also a radial structure of the one-particle 299 density does not indicate any geometrical arrangement of 300 atoms. The one-particle density has a sharp maximum at 301 the center of the trap, a plateau at larger distances, and 302 finally, at distance of the order of $r \sim 1$, it falls to zero 303 quite rapidly, Fig(2c). Nothing particular is happening at 304 the distance $r_0 = 1.265$. The one-particle density does not 305 suggest existence of the shell of the radius r_0 .

One might expect, however, that two-body correlations will disclose a geometric ordering. Fig.(5a) 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



Fig. 5: Probability density distribution functions. (a) -Two point correlation function - conditional probability density of detecting a particle at position $r_0 = 1.265$ (i.e. the radius of the Pauli crystal) as a function of the azimuthal angle, provided that another particle is found simultaneously at $(r_0, \phi_0 = 2.705)$. Black scattered points result from the Monte Carlo simulations while the blue line is the exact analytic curve. Pauli blocking and kind of the Friedel oscillations can be seen. These small four maxima in the correlation function indicate emerging Pauli crystal structure (b) - Configuration density as a function of the azimuthal angle at the distance $r = r_0$ obtained from the histogram of configurations generated by the Markovian random walk after our image processing (black line). Five maxima corresponding to the vertexes of the Pauli crystal are clearly seen. Note high contrast. Red line - the same function plotted for a thermal state corresponding to $k_B T = \hbar \omega$. Contrast is smaller.

coordinates r_0 and ϕ_0 correspond to the location of one of 313 the vertices of the Pauli crystal in Fig.(1). What is clearly 314 seen is the effect of the Pauli exclusion principle (Pauli 315 blocking) - the probability of finding the second particle 316 close to the first one is very small. In addition weak oscil-317 lations are seen; they are of the same type as the Friedel 318 oscillations [14] known in the case of electron gas. No 319 clear structure resembling pentagon is visible in Fig.(5a), 320 however four hardly distinguishable maxima of the cor-321 relation functions are seeds of emerging structure. The 322 second order correlation function does not give enough 323 evidence of existence of the Pauli crystal. In contrast, 324 the image processing procedure described above, showing 325 N-order correlations, unveils the crystalline structure. To 326 support this statement we show in Fig.(5b) a cut through 327 the configuration density function $C(\mathbf{X})$, Fig.(2d), along 328 the circle of the radius $r_0 = 1.265$. Five distinct maxima 329 indicate the most probable positions of particles arranged 330 in a pentagon - the Pauli crystal. The contrast is very 331 high. 332

An alternative approach to the Pauli crystals is based 333 on the method of Javanainen [8]. In this approach the 334 Pauli crystal should emerge from the hierarchy of the con-335 ditional probability functions. The starting point of this 336 approach is to select a particle at position $\mathbf{x_1}$, then use the 337 conditional probability to select the second particle at po-338 sition $\mathbf{x_2}$, continue this way through three, four etc. con-339 ditional probabilities. One may expect that few particles 340 will give hint on positions of all other particles. We veri-341 fied this approach using example of 6 particles. In Fig.(6)342 we show the result of this procedure. First, Fig. (6a) we se-343



Fig. 6: Emergence of a geometric structures in a course of a conditional measurement. Conditional density distributions of a ground state of a system of N = 6 particles. Reference particles are marked by white dots. In every panel we show a higher order correlation function by adding a consecutive reference particle at the maximum of the preceding correlation function. All densities are normalized to the number of 'not frozen' particles. (a) One-particle density. (b) Conditional two-point probability of the same system - reference particle frozen at maximum of the function in (a), i.e. at $\mathbf{r} = 0$. (c) Three-point correlation function – two reference particles. (d) Four-point correlation function – three reference particles. (e) Five-point correlation function – four reference particles. (f) Six-point correlation function – five reference particles. Note emergence of the Pauli crystalline structure. While consecutive particles are located in the vertices of the Pauli crystal, the corresponding conditional density distribution peaks more sharply around the positions of the remaining vertices of the structure.

lected the first particle at the maximum of the one particle 344 density. Corresponding one-particle conditional density 345 shows a maximum along a ring of the radius of the Pauli 346 crystal Fig.(6b). This is the first signature of the emerg-347 ing structure. Next we chose the position of the second 348 particle on this ring. In Fig.(6b) we plot a corresponding 349 three-point conditional probability. Note a small structure 350 appearing along the ring, Fig.(6c), in addition to clearly 351 visible Pauli hole. When the third particle is chosen at 352 the maximum on a ring, the Pauli structure of N = 6353 atoms system clearly emerges in higher order conditional 354 distributions, Fig.(6d)-Fig.(6f). The conditional approach 355 to the high order correlation functions and emerging Pauli 356 crystal structures is an independent test strengthening our 357 confidence in the image processing method. 358

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 [15] and Coulomb crystals [16–18]. In the context of ultra cold trapped atoms interacting via a short range contact potential, geometric

405

406

413

414

415

416

417

418

419

420

421

422

423

424

425

426

427

428

429

430

431

432

433

436

437

438

439

440

445



Fig. 7: Melting of the Pauli crystal at nonzero temperature. (a) Configuration distribution of the ground state of N = 6 particle system. (b) Configuration distribution of the same system at nonzero temperature $T = \hbar \omega / k_B$.

crystalline structures - "Wigner molecules" were predicted 366 [19–21]. In all these cases, however, the geometry is de-367 termined by a balance between attractive interactions at 368 large distances and repulsive at small distances. Quantum 369 statistics plays a marginal role in the resulting geometry 370 in all cases. It should be stressed that the geometry of 371 Pauli crystals differs on the fundamental level from that 372 of other crystals. It would be misleading to consider the 373 anti-symmetry of the wave function as a simple kind of 374 repulsion. The case of Pauli crystals is truly unique. Ob-375 servation of the Pauli crystals can be possible only in ideal 376 or very weakly interacting quantum systems. Fermi-Dirac 377 statistic leads to observable effects only when one-body 378 wave functions of individual particles overlap. This is pos-379 sible in the case of electrons in atoms. Electrons in atoms, 380 however, are not good candidates for the envisaged exper-381 iments because of their Coulomb interactions. We rather 382 have in mind systems of ultra-cold fermion atoms in opti-383 cal traps. Lithium ${}^{6}Li$ or Potassium ${}^{40}K$ atoms are good 384 candidates. At densities of $10^{12} \,\mathrm{cm}^{-3}$ the wave functions 385 describing atoms overlap at the temperature of the order 386 of $T = 10^{-7}$ K. These are the conditions at which quan-387 tum statistics plays a crucial role [22–25]. 388

Conclusions. – Our finding shows that even a simple 389 system of noninteracting Fermi gas has a geometry deeply 390 hidden in many-body correlations. This finding might sug-391 gest that geometric correlations are common in all Fermi 392 systems. Interactions compete with quantum statistics 393 and modify the geometric structures. For instance the 394 Wigner crystals have different geometric structures than 395 the Pauli crystals. Therefore, one can think of systems 396 that will be somewhere between these two cases where 397 both interactions and statistics play a role in determining 398 the geometric structure. This suggests that the system 399 may undergo some kind of 'geometric phase transition' 400 from one crystalline structure to another. We believe that 401 theoretical studies of high order geometric correlations in 402 ultra cold atomic systems, particularly in a view of exper-403 imental possibilities of single shot pictures, can bring to 404

light many interesting and unexpected information about the correlated many-body systems.

Acknowledgments. – M.G. acknowledges support 407 from the EU Horizon 2020-FET QUIC 641122. T.S. ac-408 knowledges financial support from the (Polish) Ministry of 409 Science and Higher Education, Iuventus Plus 2015-2017 410 Grant "Strongly correlated systems of a few ultra-cold 411 atoms" (No. 0440/IP3/2015/73). 412

REFERENCES

- [1] BAKR W. S. et al., Nature, 462 (2009) 74.
- [2]BAKR W. S. et al., Science, 329 (2010) 547.
- [3] SHERSON J. F. et al., Nature, 467 (2010) 68.
- [4]CHEUK L. W. et al., Phys. Rev. Lett., 114 (2015) 193001.
- [5] PARSONS M. F. et al., Phys. Rev. Lett., 114 (2015) 213002.
- [6]HALLER E. et al., Nature Phys., 11 (2015) 738.
- [7]EDGE G. J. A. et al., Phys. Rev. A, 92 (2015) 063406.
- JAVANAINEN J. et al., Phys. Rev. Lett., 76 (1996) 161. [8]
- SYRWID A. et al., Phys. Rev. A, 92 (2015) 032110. [9]
- [10]SAKMANN K. et al., Nat. Phys., 12 (2016) 451.
- [11] WEINBERG S., The Quantum Theory of Fields, Vol. 1 1995 (Cambridge University Press, Cambridge).
- METROPOLIS N. et al., J. Chem. Phys., 21 (1953) 1087. [12]
- SCHAUSS P. et al., Science, 347 (2015) 1455. [13]
- FRIEDEL J., Nuovo Cimento Suppl., 7 (1958) 287. [14]
- [15]WIGNER E., Phys. Rev. A, 46 (1934) 1002.
- MOSTOWSKI J. et al., Acta Phys. Pol. A, 67 (1985) 783. [16]
- [17]
- DIEDRICH F. et al., Phys. Rev. Lett., 59 (1987) 2931.
- WINELAND D. J. et al., Phys. Rev. Lett., 59 (1987) 2935. [18]
- YANNOULEAS C. et al., Rep. Prog. Phys., 70 (2007) [19]434 20672148. 435
- [20] BAKSMATY L. O. et al., Phys. Rev. A, 75 (2007) 023620.
- BRANDT B. B. et al., Nano Lett., 15 (2015) 7105. [21]
- [22] ANDERSON M. H. et al., Science, 269 (1995) 198.
- [23] DAVIS K. B. et al., Phys. Rev. Lett., 75 (1995) 3969.
- [24] DEMARCO B. et al., Science, **285** (1999) 1703.
- [25] LEWENSTEIN M., SANPERA A., and AHUFINGER V., Ul-441 tracold Atoms in Optical Lattices: Simulating quantum 442 many-body systems (Oxford University Press, Oxford) 443 2012.444
- [26] OMRAN A. et al., Phys. Rev. Lett., 115 (2015) 263001.