Detailed study of an ultra-small Pauli crystal

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Abstract

Particular geometric arrangements, called Pauli crystals, have been conjectured to exist in a two-dimensional system of free fermions under harmonic confinement. The fermions are neutral fermionic atoms with frozen spins. The question whether such crystalline structures do really exist is open for discussion. We adopted an effective statistical interaction potential approach to study such structures in the past, but without conducting a detailed analysis of their stability. In this work, we point out the fact that the smallest Pauli crystal that contains three fermions can be studied exactly within the framework of our approach. This means that we can predict the structure, size and geometry at any temperature where the Pauli crystal, presumably, emerges. Our results for three fermions appear to be in good quantitative agreement with the reported values of Pauli crystals seen in single-shot imaging data at a specific temperature. However, it is remarked that the size of the crystal is temperature-dependent in our approach. This feature seems to have gone unobserved and/or unnoticed in earlier work.

Keywords: Pauli crystals, Confined fermions, Few-body system.

I. INTRODUCTION

The Pauli exclusion principle states that two fermions cannot have the same values for all their quantum numbers [1]. The Pauli exclusion principle has countless important applications in quantum mechanics [2, 3] and helps explain an extensive range of physical phenomena that are relevant to many disciplines [4–11]. For example, given that electrons are fermions, one particularly important consequence of the Pauli exclusion principle is the elaborate electron shell structure of atoms. In turn, this helps us explain the structure of the periodic table of elements. Based on our current knowledge, the conventional understanding is that a system of free fermions (in the sense that they are non-interacting with each other) should behave as a quantum gas.

However, recent work [12–14] focused on confined systems of free fermions in a two-dimensional (2D) harmonic trap has conjectured the possible existence of crystalline structures, called Pauli crystals. Emergence of such structures in total absence of interaction between fermions is a very surprising scenario that has stimulated few other studies including some work ruling out their existence [15]. The idea of formation of crystalline structures would have been acceptable and not controversial if there were interactions, no matter how weak, between fermions. There are precedents for systems of interacting fermions stabilizing into a crystallline state in the form of Wigner crystals of electrons [16, 17] or Coulomb crystals of ions [18]. However, in the case of Pauli crystals, it is remarked that there is no interaction between fermions. This means that Pauli crystals, should they exist, have a different origin.

The present authors have been the first to introduce a theoretical model for the description of a Pauli crystal with an arbitrary number of fermions, at an arbitrary temperature, for a model of free fermions in a 2D harmonic trap [19, 20]. We used the statistical interaction potential approach [21] to treat a quantum system of free fermions (that abides to the Pauli exclusion principle) as an ensemble of classical particles interacting with the above-mentioned interaction potential. In simple words, the statistical interaction potential tends to mimic the quantum statistics of the fermions. Having adopted this model, we carried out numerical work to calculate the minimum energy configuration that would correspond to various systems of fermions at a limited number of selected temperatures. In this work, we focus our attention on an ultra-small Pauli crystal consisting of only $N = 3$ fermions. Such a system caught our attention, not only because it is the simplest Pauli crystal that potentially may exist, but because it seems to be the only one that allows a fully exact analytical treatment within the framework of the statistical interaction potential approach.

The results that we obtain for the Pauli crystal of $N = 3$ fermions show that the minimum energy configurations in this model is an equilateral triangle consistent with the symmetry of the system, as expected. However, the crucial point of our findings is the clear temperature-dependence of the equilibrium parameters of the crystalline structure. One may, casually, choose a specific temperature and find that the size of the crystal obtained is in quite good quantitative agreeement with the original work reported in Ref.[12, 13]. However, change of

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the temperature, in our model, would lead to a change of the size of the Pauli crystal in a predictable way. Such an effect, in our view, should have been noticed in recent quantum experiments that presumably showed existence of a Pauli crystal [22]. Absence of it, in our view, raises questions that, hopefully will be fully answered in future work.

II. GENERAL APPROACH

Let us consider a system of N free identical fermions with mass, m and frozen spins. They can be thought as, typically, a cloud of neutral fermionic atoms. The fermions do not interact with each other, but they are confined in a 2D isotropic harmonic trap with angular frequency, ω. The center of the trap corresponds to the origin of the system of coordinates. It is straightforward to write down an expression for the quantum Hamiltonian of the system of N fermions as:

$$\hat{H} = \frac{1}{2\,m}\sum_{i=1}^{N}\left(\hat{p}_{ix}^2 + \hat{p}_{iy}^2\right) + \frac{m}{2}\,\omega^2\sum_{i=1}^{N}\left(x_i^2 + y_i^2\right)\,, \qquad (1)$$

where $\hat{\vec{p}} = (\hat{p}_x, \hat{p}_y)$ is the 2D linear momentum operator and $\vec{r} = (x, y)$ is the 2D position vector of the fermions. The one-particle wave functions that solve the stationary Schrödinger equation for such a case are well known:

$$\phi_{n_x n_y}(x,y) = N_{n_x n_y}\,\exp\Big(-\frac{x^2+y^2}{2\,l_0^2}\Big)\,H_{n_x}\Big(\frac{x}{l_0}\Big)\,H_{n_y}\Big(\frac{y}{l_0}\Big)\,, \qquad (2)$$

where $N_{n_x n_y}$ is a normalization constant, $H_n(x)$ is a Hermite polynomial, $n_{x,y} = 0, 1, \ldots$ are the allowed quantum numbers and

$$l_0 = \sqrt{\frac{\hbar}{m\,\omega}}\,, \qquad (3)$$

is the harmonic oscillator length. The corresponding energies for a quantum state labeled as (n_x, n_y) are:

$$E_{n_x n_y} = (n_x + n_y + 1)\,\hbar\,\omega \quad ; \quad n_{x,y} = 0, 1, \ldots\,. \qquad (4)$$

The allowed discrete energies, $\hbar\,\omega$, $2\,\hbar\,\omega$, $3\,\hbar\,\omega$, can also be written as: $E_n = (n+1)\,\hbar\,\omega$ where $n = n_x + n_y = 0, 1, 2, \ldots$. Each energy value, E_n is $(n+1)$ times degenerate. At absolute zero temperature ($T = 0$), the system of N fermions fills the quantum states starting from $n = 0$ to a maximum, n_{max}. If all quantum states corresponding to an energy level are occupied, that energy shell is completely filled. It easy to estimate for fermions with frozen spins, that systems where the number of particles is $N = 1, 3, 6, 10, 15, 21, \ldots$ correspond to filled energy shells. As long as the fermions are not interacting with each other, a (normalized) many-body ground state wave function consistent with Pauli exclusion principle can be written as a Slater determinant wave function of occupied one-particle states,

$$\Psi(\vec{r}_1, \ldots, \vec{r}_N) = \frac{1}{\sqrt{N!}}\,Det\Big\{\phi_{n_{ix} n_{iy}}(\vec{r}_j)\Big\}\,, \qquad (5)$$

where (n_{ix}, n_{iy}) represents the quantum state and $\vec{r}_j = (x_j, y_j)$ is a 2D position vector for each of the $j = 1, \ldots, N$ particles. For a system of $N = 3$ particles, one fermion has an energy, $\hbar\,\omega$ and occupies the state $(0, 0)$ while the two other ones have an energy, $2\,\hbar\,\omega$ and occupy, respectively, the states, $(1, 0)$ and $(0, 1)$.

In the single-shot measurements where Pauli crystals were detected, one attempts to determine the position configuration of N fermions that maximizes the value of $|\Psi(\vec{r}_1, \ldots, \vec{r}_N)|^2$ at a given nonzero temperature, $T > 0$. It was found that the most probable configurations observed had a distinct crystalline nature if the number N of fermions corresponds to filled shells [12]. For the case of $N = 3$ particles, a Wigner crystal with the geometry of an equilateral triangle was observed [12–14]. The temperature considered was $T = 1\,\hbar\omega/k_B$ where k_B is Boltzmann's constant.

At temperatures, $T > 0$, fermions occupy the quantum states according to the Fermi-Dirac distribution. If temperature is high, the system can be treated as a non-degenerate ideal gas with Boltzmann statistics. The first quantum correction to the classical partition function of an ideal gas can be rigorously calculated by following a recipe developed by Uhlenbeck et al. [21]. The central notion of the method is the mapping of non-interacting fermions into a classical interacting system via the so-called Uhlenbeck's effective temperature-dependent statistical interaction potential. This correction has the same effect as endowing the particles with an inter-particle effective statistical interaction potential, $v_s(r)$ and treating the system classically. The statistical potential between quantum particles (case of fermions) that arises from the symmetry properties of the N-particle wave function can be written as:

$$v(r) = -k_B\,T\,\ln\Big[1 - \exp\Big(-2\,\pi\,r^2/\lambda^2\Big)\Big]\,, \qquad (6)$$

where λ represents the mean thermal wavelength parameter defined as:

$$\lambda = \sqrt{\frac{2\,\pi\,\hbar^2}{m\,k_B\,T}}\,. \qquad (7)$$

If λ is small relative to a typical interparticle separation, the system of fermions is approximately classical at that temperature. One can easily verify that the statistical interaction potential between two of fermions is highly "repulsive" at short separation distances.

This approach allows one to map the system of N non-interacting fermionic quantum particles (that obey quantum statistics) to a system of N interacting classical particles whose total energy under an isotropic 2D harmonic confinement can be written as:

$$E_N = \sum_{i<j}^{N} v(r_{ij}) + \frac{m}{2}\,\omega^2\sum_{i=1}^{N} r_i^2, \qquad (8)$$

where $v(r_{ij})$ is given from Eq.(6), $r_{ij} = |\vec{r}_i - \vec{r}_j|$ represents the 2D inter-particle separation distance and $\vec{r}_i$ are 2D position vectors. The energy of the system can be conveniently expressed in units of $\hbar\omega$ and the distances in units of l_0. In these units, the total energy of the classical system of N interacting particles in the given 2D harmonic trap reads:

$$\frac{E_N(\alpha)}{\hbar\omega} = -\alpha \sum_{i<j}^{N} \ln\Big[1 - \exp\Big(-\alpha\,\frac{r_{ij}^2}{l_0^2}\Big)\Big] + \frac{1}{2}\sum_{i=1}^{N}\frac{r_i^2}{l_0^2}\ , \quad (9)$$

where

$$\alpha = \frac{k_B\,T}{\hbar\,\omega}\ , \quad (10)$$

is a dimensionless temperature parameter and l_0 is the harmonic oscillator length defined in Eq.(3). It is easy to verify, by comparing Eq.(7), Eq.(10) and Eq.(3), that

$$\frac{2\,\pi}{\lambda^2} = \frac{\alpha}{l_o^2}\ , \quad (11)$$

which explains the form of the argument of the exponential function in Eq.(9). Furthermore, note that we denoted the total energy in Eq.(9) as $E_N(\alpha)$ in order to draw attention to the fact that the value of this quantity depends on the parameter α (thus, temperature).

III. RESULTS AND DISCUSSION

The lowest energy crystalline configuration found for $N = 3$ fermions is an equilateral triangle with its center corresponding to the center of the harmonic trap as we thoroughly checked through Monte Carlo calculations with the simulated annealing method. This geometric arrangement is the same as one reported in Ref. [12].

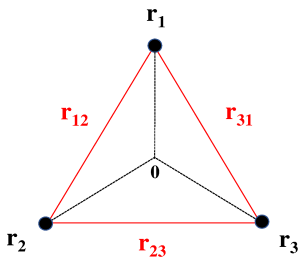

FIG. 1: An equilateral triangle represents the minimum energy configuration for a system of $N = 3$ fermions under 2D harmonic confinement.

The importance of the $N = 3$ model is that we can proceed and calculate exactly all the quantities of interest at any given temperature as a function of the parameters that characterize the system. The geometry of the $N = 3$ Pauli crystal is shown in Fig. 1. The distances of each of the three fermions at the vertices of the equilateral triangle from the center of the 2D harmonic trap are written as:

$$r_1 = r_2 = r_3 = r\ . \quad (12)$$

It is easy to verify that, for an equlaterial triangle, the separation distances, $r_{ij} = |\vec{r}_i - \vec{r}_j|$ can be expressed in terms of r as:

$$r_{12} = r_{23} = r_{31} = \sqrt{3}\,r\ . \quad (13)$$

For the case of the equilateral triangle configuration, the total energy of the system for the $N = 3$ fermions reads:

$$\frac{E_{N=3}(\alpha, r)}{\hbar\omega} = -3\,\alpha\,\ln\Big[1 - \exp\Big(-3\,\alpha\,\frac{r^2}{l_o^2}\Big)\Big] + \frac{3}{2}\frac{r^2}{l_o^2}\ , \quad (14)$$

where the argument of the energy shows explicitely the dependence on the variable r after one has used the results in Eq.(12) and Eq.(13).

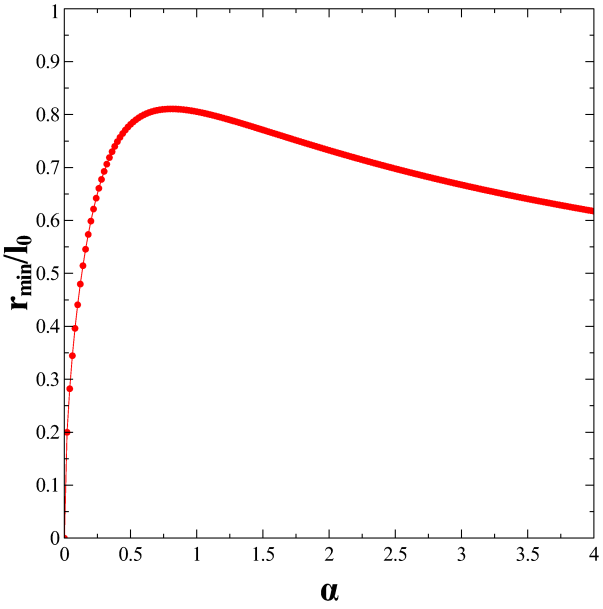

FIG. 2: Dependence of r_{min}/l_0 as a function of α for the case of the equilateral triangular crystal where r_{min} is the distance of each fermion from the center of the harmonic trap that gives rise to a minimum of total energy and $\alpha = k_B\,T/(\hbar\omega)$ is the dimensionless temperature parameter. Distances are expressed in units of the harmonic oscillator length, l_0.

To find the lowest energy configuration at any given temperature, we minimize the energy $E_{N=3}(\alpha, r)/(\hbar\omega)$ with respect to r which is the only parameter to optimize.

This way one obtains the optimal distance, r that gives rise to the minimum energy. We denote this quantity as r_{min} and we calculate it analytically as a function of α. The final result reads:

$$\frac{r_{min}}{l_0} = \sqrt{\frac{\ln\left(6\,\alpha^2+1\right)}{3\,\alpha}}\ . \tag{15}$$

The dependence of r_{min}/l_0 as a function of the dimensionless temperature parameter, α is shown in Fig. 2.

By subsituting the value of r_{min} from Eq.(15) into Eq.(14) one can calculate the corresponding minimum energy, $E_{N=3}(\alpha, r_{min})$ as a function of parameter, α. The result found is:

$$\frac{E_{N=3}(\alpha, r_{min})}{\hbar\,\omega} = \frac{\ln\left(6\,\alpha^2+1\right)}{2\,\alpha} - 3\,\alpha\,\ln\left(1-\frac{1}{6\,\alpha^2+1}\right)\ . \tag{16}$$

The dependence of $E_{N=3}(\alpha, r_{min})/(\hbar\,\omega)$ as a function of the dimensionless temperature parameter, α is shown in Fig. 3. The dependence of total minimum energy as

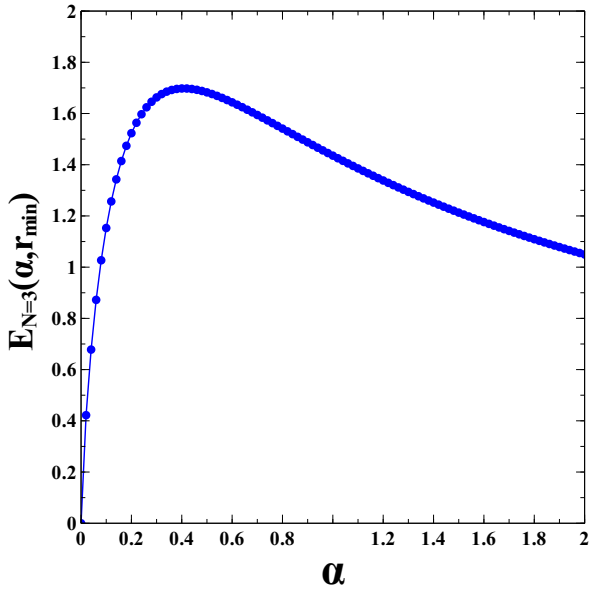

FIG. 3: Dependence of $E_{N=3}(\alpha, r_{min})$ (in units of $\hbar\,\omega$) as a function of $\alpha = k_B\,T/(\hbar\,\omega)$.

a function of α is qualititively similar to that of r_{min} in terms of α. Since r_{min} measures the size of the triangular crystal, the most striking conclusion is that the largest of such crystals will be observed at temperatures that, crudely, correspond to values of α between 0.5 and 1.0. In our opinion, the question of the nature of the Pauli crystals should have a relatively clear answer for the case of $N = 3$ fermions. In other words, a triangular Pauli crystal can be distinguished from its triangular Wigner counterpart (case of three point charges under the same type of 2D harmonic confinement) for manifesting its peculiar non-monotonic dependence of its size as a function of temperature.

IV. CONCLUSIONS

The key objective of this work is to investigate analytically the properties of a possible ultra-small Pauli crystal consisting of only $N = 3$ fermions. The reason why we studied such a small N in this work is to generate results that can be fully analytically checked. We adopted an effective statistical interaction potential approach [21] that captures both qualitatively and quantitatively the physics of a Pauli crystal and can be solved exactly. It is found that the lowest energy structure for a system of $N = 3$ fermions under 2D harmonic confinement calculated at an arbitrary temperature is an equilateral triangle with center corresponding to the center of the harmonic trap. This is in agreement with the Pauli crystal structure recently reported [12]. It appears that the model considered in our work, despite its simplicity, is able to capture both qualitatively and quantitatively the essential features of few-body Pauli crystals.

Our results for three fermions show that the size of the triangular Pauli crystal is heavily dependent on the temperature. This is consistent with the fact that the effective statistical potential, to start with, involves a temperature-dependent characteristic length, namely, the mean thermal wavelength, λ. Obviously, the approach has limitations in its applicability since, after all, it is a classical approximation at the pair level to high-order quantum correlations. Nevertheless, we believe that the observation that the size of the crystal must be temperature-dependent should be a feature associated with real quantum Pauli crystals, too. From our understanding of earlier work, this feature seem to have gone unobserved or not studied in detail. We believe that size, geometry, shape of a Pauli crystal, should this crystal indeed exist, must manifest some form of temperature dependence. This observation would be consistent, at least qualitatively, with the findings of the current work.

The general expression for the energy of $N = 3$ fermions, for an arbitrary α, depends only on one variable that determines its size. Therefore, one can minimize the energy exactly to determine the optimal size of the triangular Pauli crystal at any given arbitrary temperature, namely, obtain r_{min}/l_0 as a function of the variable α. The plot of the dependence r_{min}/l_0 as a function of α indicates that there is a specific temperature that leads to the formation of the largest possible triangular crystal. For any other temperature, the size of the structures is smaller than this specific one. This means that the findings of our work may be tested experimentally by analyzing the size of the $N = 3$ triangular Pauli crystal as a function of the temperature in the appropriate temperature range specified by our model. Results for Pauli crystals reported in previous work [12, 13] typically involve the choice of parameter $\alpha = 1$. Such results, when extended to different values of α, should show variations of the size of the triangular structure in the vicinity of the value of α for whom the largest Pauli crystal is observed within the framework of the statistical interaction

model adopted in this work.

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Conflict of interest

The authors declare no conflict of interest.

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