Supersolid under rotation and sphere packing problem

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We use the model proposed by Josserand, Pomeau, Rica [6] to prove properties on the ground state of a supersolid crystal and relate it to a sphere packing problem. This allows us to find, in the limit of small rotation, an approximate theoretical value for the reduction of the moment of inertia of a supersolid set in rotation, with respect to its classical value.

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I. INTRODUCTION

The theory of the supersolid phase of matter has raised a lot of interest recently due to new experimental observation on solid helium [1, 2]. Different microscopic mechanisms have been used to describe the supersolidity of a crystal (see the review paper of Prokof'ev [3]). But presently, there is no established theoretical framework to explain the experimental data.

Leggett [4] suggested that the property of nonclassical rotational inertia possessed by superfluid helium may be shared by solids: a supersolid under rotation has a response different from a normal solid, in the sense that there is a reduction of the moment of inertia of the solid sample with respect to its classical value. Josserand, Pomeau, Rica [5, 6] proposed a model to account for this phenomenon. Their model is based on the fact that the complex valued wave function common to all particles of mass m minimizes the Gross-Pitaevskii energy with an integral term that can be viewed as a 2-body potential in a first Born approximation:

$$\int \frac{\hbar^2}{2m}|\nabla\psi(\boldsymbol{r})|^2\ d\boldsymbol{r} + \frac{1}{4}\iint \tilde{U}(\boldsymbol{r}'-\boldsymbol{r})|\psi(\boldsymbol{r}')|^2|\psi(\boldsymbol{r})|^2\ d\boldsymbol{r}\ d\boldsymbol{r}'$$

where $\tilde{U}(\cdot)$ is a two body potential depending on the distance, chosen as $\tilde{U}(|\boldsymbol{r}|) = U_0\theta(a-|\boldsymbol{r}|)$, with $\theta(.)$ the Heaviside function. The normalisation condition is $\nu = \int|\psi|^2/V$ where V is the volume of the region $\mathcal{D}$ occupied by the solid. We define $g = U_0\frac{ma^2}{\hbar^2}na^3$ and rescale distances by a so that the rescaled energy E_g is given by

$$\int \frac{1}{2}|\nabla\psi(\boldsymbol{r})|^2\ d\boldsymbol{r} + \frac{g}{4}\iint U(\boldsymbol{r}'-\boldsymbol{r})|\psi(\boldsymbol{r}')|^2|\psi(\boldsymbol{r})|^2\ d\boldsymbol{r}\ d\boldsymbol{r}' \tag{1}$$

where $U(|\boldsymbol{r}|) = \theta(1-|\boldsymbol{r}|)$ and $\int|\psi|^2 = V$. For small g, the ground state is $|\psi| = 1$, and for large g, computations in [5, 6] indicate the presence of a crystal phase with a periodic modulation in density and some supersolid-like behaviour under rotation. The aim of this paper is to use this model to prove properties on the ground state of a supersolid crystal and relate it to a sphere packing problem. We derive an approximate theoretical value for the reduction of the moment of inertia of a supersolid, which is linked to a variational problem that we describe.

We are going to relate the crystal phase to a sphere packing problem: if $\mathcal{D}$ is the sample of a supersolid, the sphere packing problem [7, 8] provides a number $m(\mathcal{D},r) := \max\{k : \exists x_1,\dots,x_k \in \mathcal{D} \text{ s. t. } |x_i - x_j| \geq r \ \ \forall i \neq j\}$. When this number is large, the optimal location of the x_i is proved [7, 8] to be close to a hexagonal lattice in 2D. In 3D, various configurations are optimal: body centered cubic close packing and face centered close packing. Our interest is in the number $n(\mathcal{D}) := \max\{k : \exists x_1,\dots,x_k \in \mathcal{D} \text{ s.t. } |x_i - x_j| > 1 \ \ \forall i \neq j\}$. In particular, $n(\mathcal{D}) = \lim_{r\to 1,\ r>1} m(\mathcal{D},r)$. For most sets $\mathcal{D}$, in fact $n(\mathcal{D})$ and $m(\mathcal{D},1)$ are equal. If ever they differ, by extending $\mathcal{D}$ slightly, they can be made equal, which we will assume here for simplicity.

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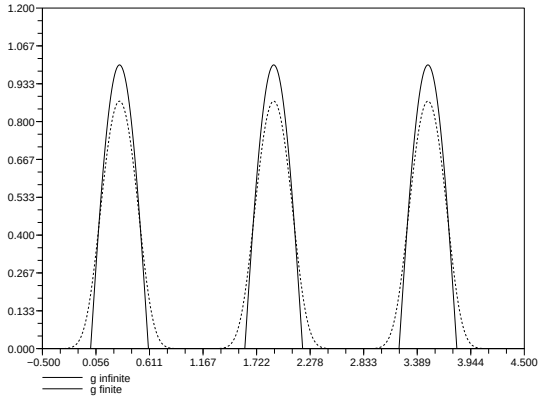

FIG. 1: Ground state of E_g (dashed line), and its limiting profile ψ_0 (solid line) when g is large. The bumps are of size l and separated by a distance 1.

When g is large, the two terms in (1) are of different order, hence the ground state ψ_g is very close to a function ψ_0 that is found by minimizing the kinetic energy within the space of functions that minimize the interaction term, which is dominant. We are going to prove that such a function is supported in sets A_i which are at distance at least one and whose number is $n(\mathcal{D})$. The sets A_i are determined by the minimization problem

$$\inf_{A_i,\ \mathrm{dist}(A_i,A_j)>1} \left\{ \sum_{i=1}^{n(\mathcal{D})} \lambda_1(A_i) \right\} \tag{2}$$

where λ_1 is the first eigenvalue of $-\Delta$ in A_i:

$$\lambda_1(A_i) = \inf_{u, \int_{A_i}|u|^2=1, u_{|\partial A_i}=0} \left\{ \int_{A_i} |\nabla u|^2 \right\}.$$

The expected configuration is illustrated in figure 2. The function ψ_0 corresponds to the ground state of $-\Delta$ in each A_i and vanishes outside the A_i's. A ground state of E_g will be very close to ψ_0 in the sets A_i, and exponentially small away from the A_i's, except on a boundary layer. In dimension 1, that is if we have an interval $\mathcal{D} = (0, L)$, then $n(\mathcal{D}) = [L]+1$ (if L is not an integer), and the A_i's are intervals $(x_i, x_i + l)$, with $l = L/n - 1 + 1/n$ and $x_i = i(l+1)$. Then $\psi_0(x) = \sqrt{(2L/nl)}\sin(\pi(x - x_i)/l)$ if $x \in (x_i, x_{i+1})$ and 0 otherwise (see figure 1). If L is an integer, then $n(\mathcal{D})$ and $m(\mathcal{D}, 1)$ are not equal and the situation is slightly more involved; one has to take $n = L$ in the function ψ_0. Nevertheless, this example allows to see that the size l of the bumps gets very small as L gets close to an integer, and decreases at least like $1/L$ when L gets large.

When the sample is set under rotation Ω about the z axis, the free energy of the system is defined as

$$e(\Omega) = \inf_{\psi} \{E_g(\psi) - \Omega\langle\psi, L_z(\psi)\rangle\} \tag{3}$$

where $L_z(\psi) = i\mathbf{r} \times \nabla\psi$ and E_g is the energy defined in (1). When Ω is small, $e(\Omega)$ can be expanded as $e_0 - (1/2)I\Omega^2$ where I is the effective moment of inertia of the system. Leggett [4] suggested as a criterion for superfluidity the non classical rotational inertia fraction (NCRIF) which is defined as $(I_0 - I)/I_0$, where I_0 is the classical moment of inertia of the crystal phase and is equal to $\int |\psi_g|^2 r^2$ where ψ_g is a ground state of E_g. The point of this analysis is to find an estimate for the non classical rotational inertia fraction (NCRIF), computed numerically in [6], and prove that it is non zero for small values of the rotational velocity.

The paper is organized as follows: first, we study the ground state of the crystal phase with no rotation and derive (2). Then, we present some more refined computations in the 1D case, and finally we derive an estimate for the NCRIF.

II. CRYSTAL PHASE WITH NO ROTATION

We first describe the minimization of the second term of (1) which provides a class of functions ψ such that $\rho = |\psi|^2$ has mass located in disjoint sets A_i, at distance at least the range of the potential, which is 1. When one wants to minimize $\int |\nabla\psi|^2$ in this class, this provides a constraint (2) on the shape of the sets A_i that we explain.

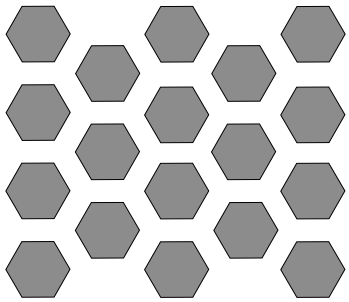

FIG. 2: The expected configuration of sets A_i in 2D.

We denote by $(U * \rho)(\mathbf{r}) = \int U(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$ and $F(\rho) = \int\int U(\boldsymbol{r}' - \boldsymbol{r})\rho(\boldsymbol{r}')\rho(\boldsymbol{r})\ d\boldsymbol{r}\ d\boldsymbol{r}'$. Recall that $n(\mathcal{D})$ was defined in the introduction and is related to the sphere packing problem.

Theorem 1 *A measure ρ with $\int \rho = V$ minimizes $F(\rho)$ if and only if there exist $n(\mathcal{D})$ pairwise disjoint sets $A_1, \ldots, A_{n(\mathcal{D})}$, such that*

$$\mathrm{dist}(A_i, A_j) \geq 1 \text{ if } i \neq j, \text{ and } \int_{A_i} \rho = \frac{V}{n(\mathcal{D})}. \tag{4}$$

Moreover, $\min F = V^2/n(\mathcal{D})$.

We prove this result in the appendix.

We call $\mathcal{M}$ the set of densities ρ satisfying (4). We want to prove properties of the ground states ψ_g of E_g and in particular that for large g, ψ_g is close to a function ψ_0 such that $\rho_0 = |\psi_0|^2$ minimizes F and the A_i's satisfy (2).

If ψ_g is a ground state of E_g and ψ_0 such that $\rho_0 = |\psi_0|^2$ minimizes F, then $F(|\psi_0|^2) \leq F(|\psi_g|^2)$ and $E_g(|\psi_g|^2) \leq E_g(|\psi_0|^2)$. This implies $F(|\psi_0|^2) \leq F(|\psi_g|^2) \leq F(|\psi_0|^2) + (1/g)\int |\nabla\psi_0|^2 - |\nabla\psi_g|^2$. For g large, we deduce that $|\psi_g|^2$ is an almost minimizer of F, and that the limit of $|\psi_g|^2$ as g is large, $\rho_0 = |\psi_0|^2$ satisfies the conclusion of Theorem 1. In addition, the kinetic energy term may be seen as a perturbation of the interaction term, and thus ψ_0 should minimize the kinetic energy $\int |\nabla\psi|^2$ among all ψ_g such that $|\psi_g|^2$ is a ground state of F. This implies that the support of ψ_g is the union of n connected sets A_i, $1 \leq i \leq n$, which satisfy (2).

In dimension 2, there is no complete determination of the A_i's, except that once the sphere packing problem is known to provide a hexagonal lattice, the A_i's are sets whose centers are located on an almost hexagonal lattice. Since minimizing $\lambda_1(A_i)$ over A_i with fixed volume implies that A_i is a ball (see [9]), condition (2) implies that A_i "looks like" a ball to some extent. However, $\lambda_1(A_i)$ is increasing with respect to A_i, which implies that A_i cannot be exactly a ball, but is closer to a hexagon (see figure 2).

When g is large, the Euler-Lagrange equation satisfied by a ground state ψ of E_g reads $-\Delta\psi + g\left(U * |\psi|^2 - \lambda\right)\psi = 0$, where λ is the Lagrange multiplier for the mass constraint. Since ψ is close to ψ_0, this equation can be approximated by

$$-\Delta\psi + g\left(U * |\psi_0|^2 - \lambda_0\right)\psi = 0, \tag{5}$$

where $\lambda_0 = F(\psi_0^2)/V = V/n$. Next, according to the proof of Theorem 1 in the appendix, if $\mathrm{dist}(x, A_j) \geq \delta$ for all j, we have $U * |\psi_0|^2(x) - \lambda_0 \geq a_\delta > 0$ for some a_δ. The behaviour of a_δ may be computed for δ small using the fact that near the boundary of A_i, ψ_0 is a linear function of the distance to the boundary. Hence, $a_\delta \propto \delta^{(D+5)/2}$ for small δ, where D is the dimension. Going back to the equation for ψ, we find $-\Delta\psi + g a_\delta \psi \leq 0$, which implies that ψ is exponentially small between the A_i's: $|\psi(x)| \leq e^{-\delta\sqrt{g a_\delta}}$ if $\mathrm{dist}(x, A_i) > \delta$, $\forall i$. In the experiments, it is likely that eventually g is not large to the point of having tiny density.

III. MORE SPECIFIC COMPUTATIONS IN 1D

In dimension 1, that is if $\mathcal{D} = (0, L)$, it is possible to compute explicitly the ground state in the large g limit. More precisely, let ψ be such that $\rho = |\psi|^2$ minimizes $F(\rho)$, with the constraint $\int \rho = V$. Then, $\int |\psi'|^2$ is minimal if and only if $\psi = \psi_0$ up to translation, where

$$\psi_0(x) = \sqrt{\frac{2L}{ln}} \sin\left(\frac{\pi(x - i(1+l))}{l}\right)$$

if $x \in [i(1+l), i(1+l)+l]$, and $\psi_0 = 0$ otherwise, where $l = (L-n+1)/n$. Moreover, $E_0(\psi_0) = \pi^2 L/2l^2$. Indeed, the ground state of F provides n sets A_i separated from one another by distance at least 1. Hence $A_i \subset [a_i, b_i]$ for all i, and $b_i + 1 \leq a_{i+1}$ for $i = 1, \ldots, n-1$. Then, since (4) implies that $\int_{a_i}^{b_i} |u|^2 = \frac{L}{n}$ for every i, $\int |u'|^2 = \sum_{i=1}^n \int_{a_i}^{b_i} |u'|^2 \geq \sum_{i=1}^n \frac{\pi^2}{(b_i-a_i)^2} \int_{a_i}^{b_i} |u|^2 = \frac{L}{n} \sum_{i=1}^n \frac{\pi^2}{(b_i-a_i)^2}$, with equality if and only if the restriction of u to each interval (a_i, b_i) is a scaled and normalized sine function multiplied by a constant of modulus 1. Moreover, Jensen's inequality implies that $\sum \frac{1}{(b_i-a_i)^2} \geq \frac{n}{(n^{-1}\sum (b_i-a_i))^2} \geq n/l^2$, with equality if and only if $b_i - a_i = l$ for every i.

As pointed out above, one expects a boundary layer around each A_i. In this one-dimensional setting, it is possible to compute it explicitly. In order to do so, we assume that ψ is a dilation of the limit ψ_0, namely

$$\psi(x) = \sqrt{\frac{2L}{(l+k)n}} \sin\left(\frac{\pi(x - i(l+1))}{l+k}\right)$$

if $x \in [i(1+l) - k/2, i(1+l) + l + k/2]$, and $\psi = 0$ otherwise. The energy of this trial function is computed explicitly, in the limit of small k: $E_g(\psi) \approx \frac{\pi^2 L}{2(l+k)^2} + \frac{gL^2}{4n} + \frac{g}{4} A \left(\frac{k}{l+k}\right)^6$, where $A = 13L^2\pi^6/(90n)$. Minimizing this expression with respect to k yields $k = \left((2L\pi^2 l^3)/(3A)\right)^{1/5} g^{-1/5}$. Inserting this in the expression of the energy, we find

$$E_g(\psi) \approx \frac{\pi^2 L}{2l^2} + \frac{gL^2}{4n} - \frac{5}{6}\left(\frac{60L^4\pi^6 n^2}{13 l^{12}}\right)^{1/5} g^{-1/5},$$

as g is large.

The above computation indicates that the boundary layer around each bump of the limit function ψ_0 is of order $g^{-1/5}$ and if x denotes the scaled distance to the boundary, then the matching between ψ_0 and 0 in the boundary layer is described by the solution of $u'' = cx^3 u$. This boundary layer decreases the energy by an amount of order $g^{-1/5}$.

IV. SMALL ROTATION

When the sample is set under rotation Ω about the z axis, the free energy of the system is defined by (3) and E_g is the energy defined in (1). We assume that the ground state ψ of (3) is of the form $\psi(x) = \psi_g(x) e^{i\Omega S(x)}$ for small Ω, where ψ_g is a ground state of E_g, that is for $\Omega = 0$. This corresponds to expanding the phase in terms of Ω and assuming that the first order variation in the phase is not sensitive to the variations in density in terms of Ω. Then, the phase S should minimize $\int |\psi_g|^2 |\nabla S - \mathbf{e}_z \times \mathbf{r}|^2$ among all possible test functions. This provides an expansion of $e(\Omega)$ for small Ω and hence a value for I which allows to compute

$$NCRIF = \frac{\inf_S \int |\psi_g|^2 |\nabla S - \mathbf{e}_z \times \mathbf{r}|^2}{\int |\psi_g|^2 r^2}.$$

Two limiting cases are easily identifiable: when $\psi_g = 1$ (i.e when g is small), this ratio is 1, and when ψ_g has all its mass localized in the center of the cell, this ratio tends to 0. Our aim is to estimate this ratio in the large g limit, where ψ_g is periodic but not completely localized in the center of the cell, and find that the NCRIF is non zero. This complements the results of [6]. As we have seen earlier, when g is large, ψ_g is significant in sets A_i determined by (2), and ψ_g is close to ψ_0. Hence, we may replace ψ_g by ψ_0 in the expression of $NCRIF$. Moreover, in each A_i, we can define local coordinates $\mathbf{r}_i$ with respect to a point in A_i whose coordinate is $\mathbf{x}_i$. Then $\mathbf{r} = \mathbf{r}_i + \mathbf{x}_i$ and the phase S can be defined as a local phase S_i in each A_i through $\nabla S = \nabla S_i + \mathbf{x}_i^\perp$ where $\mathbf{x}_i^\perp = \mathbf{e}_z \times \mathbf{x}_i$. The function S_i for which the infimum is achieved in each A_i is such that div $(|\psi_0|^2(\nabla S_i - \mathbf{e}_z \times \mathbf{r}_i)) = 0$. Using this decomposition, we thus have

$$NCRIF \approx \frac{\sum_{i=1}^{n(\mathcal{D})} \inf_{S_i} \int_{A_i} |\psi_0|^2 |\nabla S_i - \mathbf{e}_z \times \mathbf{r}_i|^2}{\int |\psi_0|^2 r^2}.$$

Assuming that each A_i is the translation of a reference set A_0, the numerator is proportional to $n(\mathcal{D})$ times the infimum of the cell problem. Note that this cell problem depends on the volume since the size of A_0 depends on $n(\mathcal{D})$. If V is large, a coarse-grained approximation for ψ_0 yields that $\int |\psi_0|^2 r^2 \approx \int r^2$. Hence the denominator is proportional to V^2.

Let us point out that this behaviour contrasts to the 1D case, where, in the large g asymptotic, the NCRIF is zero: indeed a similar computation yields that is equal to $L^2/(\int |\psi_g|^2 \int 1/|\psi_g|^2)$ (see also [4]). In the large g case, this tends to 0 since ψ_g tends to ψ_0 which is compactly supported and thus $\int 1/\psi_0^2 = \infty$.

Conclusion: We have estimated the ground state of the energy in the large g limit and found that its modulus is significant in sets A_i given by (2). The number and location of these sets is related to the number $n(\mathcal{D})$ introduced for the sphere packing problem. This allows us to estimate the NCRIF fraction when the rotational velocity is small and find that it is not zero, hence this model proves the supersolid property of the crystal. For g moderate, we expect the wave function to be still strongly localized in A_i, but with tails in between which are not too small, and still a higher NCRIF.

Appendix: *Proof of Theorem 1. Step 1.* We find the Euler-Lagrange equation for the minimization problem: we claim that if ρ minimizes F, then $F(\rho)/V = \min_{\mathbf{r}} \int U(\boldsymbol{r}' - \boldsymbol{r})\rho(\boldsymbol{r}')d\boldsymbol{r}'$ and the infimum is achieved for all $\mathbf{r}$ except on a set S such that $\rho(S) = 0$. Indeed let $\rho_\alpha = \alpha V\delta_x + (1-\alpha)\rho$ for every $\alpha \in [0,1]$, then $0 \le \lim_{\alpha\to 0} \frac{1}{\alpha}(F(\rho_\alpha) - F(\rho)) = \int_{\mathcal{D}} U * \rho(V\delta_x - \rho)$. Therefore $\inf U * \rho \ge V^{-1}F(\rho)$. Also, note that $\int (VU * \rho - F(\rho))\rho = VF(\rho) - F(\rho)\int \rho = 0$. However, we have shown above that $U * \rho - V^{-1}F(\rho) \ge 0$, so we deduce the result.

Step 2. We want to prove the upper bound: $\inf F \le V^2/n(\mathcal{D})$. In fact, we prove more, that for any test function ρ which satisfies the property (4) for the sets A_i, then $F(\rho) = V^2/n$. We claim that for every j, if $x \in A_j$, then $B_x \cap (\cup_{k=1}^n A_k) = A_j$, where B_x is the ball of radius 1 centered at x. Indeed, it is clear from (4) that if $x \in A_j$ then $B_x \cap (\cup_{k=1}^n A_k) \subset A_j$. The opposite inclusion can be deduced from the definition of n. Since (4) implies that $\rho(\mathcal{D} \setminus \cup A_j) = 0$, we conclude that if $x \in A_j$, then $U * \rho(x) = \rho(B_x) = \rho(A_j) = V/n$. In particular $U * \rho(x) = V/n$ in $\cup A_j$, which is a set of full ρ measure, and it then follows that $F(\rho) = V^2/n$. In particular, $\inf F \le V^2/n$.

Step 3. We are going to prove the lower bound $\inf F \ge V^2/n$. Let ρ be a ground state for F. We claim that there exist points $x_1, \dots, x_n$ such that

$$|x_i - x_j| \ge 1 \text{ and } U * \rho(x_i) = \inf F/V \tag{6}$$

Indeed, let $T := \{x \ : \ U * \rho(x) = \inf_x U * \rho = \inf F/V\}$ (the last equality follows from the Euler-Lagrange equation, step 1). T is nonempty, so we can find some point $x_1 \in T$. If we have found $x_1, \dots, x_{j-1}$, for $j \le n$, then $V = \rho(\mathcal{D}) > V(j-1)/n \ge \sum_{i=1}^{j-1} U * \rho(x_i) = \sum_{i=1}^{j-1} \rho(B_{x_i}) \ge \rho(\cup_{i=1}^{j-1} B_{x_i})$. Thus $\rho(\mathcal{D} \setminus (\cup_{i=1}^{j-1} B_{x_i}) > 0$, so we can find $x_j \in T \setminus (\cup_{i=1}^{j-1} B_{x_i})$. Together with the induction hypothesis, this implies that $\{x_1, \dots, x_j\}$ satisfy (6). This completes the induction proof and hence establishes the claim.

The definition of n implies that if $x_1, \dots, x_n$ are any points such that $|x_i - x_j| \ge 1$ for all $i \ne j$, then $\cup B_{x_i} = \mathcal{D}$. So for the points $x_1, \dots, x_n$ found above satisfying (6), we find that $V = \rho(\cup_{i=1}^n B_{x_i}) \le \sum_{i=1}^{\bar{n}} \rho(B_{x_i}) = \sum_{i=1}^n U * \rho(x_i) = \frac{n}{V} \inf F$. Thus $\min F = V^2/n$.

Step 4. We assume that ρ minimizes F and we prove that (4) holds. Let $x_1, \dots, x_n$ be points satisfying (6), which in view of Step 3 can now be rewritten

$$|x_i - x_j| \ge 1 \text{ whenever } i \ne j, \text{ and } \rho(B_{x_i}) = V/n. \tag{7}$$

Define $A_j = \{x \in B_{x_j} \cap \text{supp}\, \rho\}$. Then by the Euler-Lagrange equation, $U * \rho(x) = V/n$. This implies that $\rho(A_i) = V/n$. We must check that the sets A_j satisfy the first condition of (4). We first claim that $\rho(B_{x_i} \cap B_{x_j}) = 0$ whenever $i \ne j$. Since, as remarked above, (6) and the definition of n imply that $\mathcal{D} \subset \cup B_{x_i}$, it implies in particular that $\rho(\cup A_i) = \sum \rho(A_i)$, hence $\rho(A_i \cap A_j) = 0$. So the claim holds, as well as the property $A_j \cap B_{x_i} = \emptyset$.

Note that if $y_i \in A_i$, then $U * \rho(y_i) = \rho(B_{y_i}) = V/n$. Hence the points $(\{x_1, \dots, x_n\} \cup \{y_i\}) \setminus \{x_i\}$ again satisfy (7). Thus, repeating the reasoning that led to the previous claim, we find that $A_j \cap B_{y_i} = \emptyset$ for all $j \ne i$, ie $|y_i - y_j| \ge 1$ for any $y_j \in A_j, j \ne i$. Since y_i was an arbitrary point in A_i, this proves (4).

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