ENERGY MINIMIZATION OF REPELLING PARTICLES ON A TORIC GRID

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Abstract. With the work by Bouman, Draisma, and Leeuwaarden [1], we aim to study the most efficient configuration that minimizes the total energy of repelling particles distributed in a grid. Supposing that the force is a completely monotonic function of the Lee distance between two particles, we claim that the particles should be distributed equally among locations on the grid. In this paper, we look at a special case when the number of particles is half of the number of all locations, and also the sizes of the torus are either two or a multiples of four in all dimensions.

1. Introduction

The problem of finding the best configuration to minimize the energy is presented as a tool for use in information theory. To visualize it, we suppose that there are points in the space such that there is a repelling force between these points. We try to maximize the number of points and also minimize the total of force between any two of them. This problem has been explored by Bouman, Draisma, and Leeuwaarden in [1].

We consider a case in which every particle is set on a toric grid which we define as a d-dimensional grid that the boundaries are wrapped around in each dimension. In the other words, if n_i be the size of the grid in dimension i, then each location on the toric grid will be in the form $(a_1, a_2, \dots, a_d) \in \mathbb{Z}/n_1 \times \mathbb{Z}/n_2 \times \dots \times \mathbb{Z}/n_d$.

Each particle will be placed in one of those locations on the toric grid. We will calculate force between any two particles p_i, p_j as $f(\delta(p_i, p_j))$ depending on the distance between those two particles. For this paper, we use the Lee distance to represent a distance between two particles, i.e. for locations $(a_1, a_2, \dots, a_d)$ and $(b_1, b_2, \dots, b_d)$, the distance between these two locations is

$$\sum_{i=1}^{d} \min(|a_i - b_i|, n_i - |a_i - b_i|).$$

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We study a case where f is a decreasing function. For more convenience, our function f can be looked as $f(x) = x^{-\alpha}$ with $\alpha > 0$, and this problem can be looked as a behaviour of forces between electrical charge in physics.

Let a positive integer n be a number of particles. Denote the locations of n particles by $p_1, p_2, \ldots, p_n$. The energy that we concern is defined as the sum of all the force between every particles or $\sum_{1\leq i<j\leq n} f(\delta(p_i, p_j))$. We investigate the case when n is equal to half of all locations in the grid. In order to minimize the energy of the system, we claim that the best configuration has to be *checkerboard configuration* where there is exactly one particle placed in any two neighboring locations.

In this paper we prove the claim in one dimensional case, and when each n_i is either two or a multiple of four. In section 2, we introduce the useful theorem in linear algebra and representation theory that we use in this paper. After that, in section 3, we start with the one dimensional case which can be proved by pure combinatorics and inequality without the use of algebra. For the higher dimension, we formulate the problem into a linear algebra problem in section 4 by constructing the matrix from the force and the positions of the particle. Later on, we can find the condition of the best configuration which depends on the eigenvector, so it becomes the problem of finding the eigenvector corresponding to the smallest eigenvalue which is simplified in section 5. Finally, we show the proof of the strongest result by assuming that f is completely monotonic.

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2. Background

Through out this paper, we will make a proof based on the understanding of linear algebra. Moreover, we also use the idea from representation theory to make a claim for the proof in this paper. Thus, it should be useful to introduce notations and definitions of linear algebra and representation theory for the same understanding.

For this paper, we call a vector with dimension n as an $n \times 1$ matrix V, and we use V_k represents the term in k^{th} row of a vector V. For an $m \times n$ matrix M, we also use $M_{i,j}$ represents the term in i^{th} row and j^{th} column of a matrix M.

First, we will state the theorem from linear algebra that is useful in this paper.

Theorem 2.1. (see Chapter 6.4 in [2]) *A symmetric matrix has only real eigenvalues, and the eigenvectors can be chosen orthonormal.*

Next, we will introduce the representation theory that is used as a fundamental idea for many proof in this paper. The statement and proof can be found in [3].

Definition 2.2. A matrix representation of a group G is a group homomorphism

$$X : G \to GL_d.$$

Equivalently, to each $g \in G$ is assigned $X(g) \in Mat_d$ such that

(1) $X(\epsilon) = I$ the identity matrix, and

(2) $X(gh) = X(g)X(h)$ for all $g, h \in G$,

where Mat_d stands for the set of all $d \times d$ matrices with entries in $\mathbb{C}$, and GL_d is the group of all all invertible matrix in Mat_d.

Definition 2.3. Let V be a vector space and G be a group. Then V is a $G-$*module* of there is a group homomorphism

$$\rho : G \to GL(V).$$

Equivalently, V is a $G-$*module* if there is a multiplication, gv, of elements of V by elements of G such that

(1) $gv \in V$,

(2) $g(cv + dw) = c(gv) + d(gw)$,

(3) $(gh)v = g(hv)$, *and*

(4) $\epsilon v = v$

for all $g, h \in G; v, w \in V$; and scalars $c, d \in C$, where $GL(V)$ stands for the set of all invertible linear transformations of V to itself.

Definition 2.4. Let V be a vector space with subspaces U and W. Then V is the direct sum of U and W, written $V = U \oplus W$, if every $v \in V$ can be written uniquely as a sum

$$v = u + w, u \in U, w \in W.$$

Theorem 2.5. (Maschke's Theorem) *Let G be a finite group and let V be a nonzero G-module. Then*

$$V = W^{(1)} \oplus W^{(2)} \oplus \cdots \oplus W^{(k)},$$

where each $W^{(i)}$ is an irreducible G-submodule of V.

Definition 2.6. Let $X(g)$, $g \in G$, be a matrix representation. Then the *character of X* is

$$\chi(g) = \mathrm{tr}X(g),$$

where tr denotes the trace of a matrix. Otherwise put, χ is the map

$$G \xmapsto{\mathrm{tr}\,X} \mathbb{C}.$$

If V is a $G-$*module*, then its character is the character of a matrix representation X corresponding to V.

Proposition 2.7. (see chapter 1.8 in [3]) *X be a matrix representation of a group G of degree d with character* χ.

(1) $\chi(\epsilon) = d$.

(2) If K is a conjugacy class of G, then

$$g, h \in K \Rightarrow \chi(g) = \chi(h).$$

Definition 2.8. Let χ and ψ be any two functions from a group G to the complex numbers $\mathbb{C}$. The inner product of χ and ψ is

$$(\chi, \psi) = \frac{1}{|G|}\sum_{g \in G} \chi(g)\overline{\psi(g)}$$

Theorem 2.9. (Character Relations of the First Kind) *Let χ and ψ be irreducible characters of a group G. Then*

$$(\chi, \psi) = \begin{cases} 1 & \text{if } \chi = \psi; \\ 0 & \text{otherwise} \end{cases}$$

Corollary 2.10. (see Chapter 1.9 in [3]) *Let X be a matrix representation of G with character χ. Suppose*

$$X \cong m_1 X^{(1)} \oplus m_2 X^{(2)} \oplus \cdots m_k X^{(k)},$$

where the $X^{(i)}$ are pairwise inequivalent irreducibles with characters $\chi^{(i)}$.

(1) $\chi = m_1\chi^{(1)} + m_2\chi^{(2)} + \ldots + m_k\chi^{(k)}$.

(2) $(\chi, \chi^{(j)}) = m_j$ *for all j.*

(3) $(\chi, \chi) = m_1^2 + m_2^2 + \ldots + m_k^2$.

(4) X is irreducible if and only if $(\chi, \chi) = 1$.

3. The One Dimensional Case

First, we look at the one dimensional case where every point is placed on a grid in circle. We will use an inequality on the distance between each of them to find a minimum of the energy, and we find a configuration that minimize the energy to complete the proof.

Definition 3.1. Let $x_1, x_2, \ldots, x_k$ be the locations of the k particles in a loop G with a total of n equally spaced vertices, with x_1 to x_k in clockwise order. For convenience sake, we will take the indices of the particles mod k, such that particle $x_{k+i} = x_i$ for all integers i.

We define $\delta(g, h)$ to be the Lee distance between 2 particles g and h, where the Lee distance is the length of the shortest path, in terms of number of edges, between the vertices g and h of this graph.

We define d_i for $i \in \mathbb{Z}$ to be the distance of the shortest clockwise path, in terms of edges, from particle x_i to x_{i+1}. Furthermore, we also define $d_{i,j}$ to be shortest clockwise path, in terms of number of edges, from particle x_i to x_j. We see that either $d_{i,j} = \delta(x_i, x_j)$ or $d_{i,j} = n - \delta(x_i, x_j)$, depending on the relative position of the two points.

Further, we have $f : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}$ to be a decreasing strictly convex function, with $f(x)$ defined for $x \in [1, n/2]$. In this problem, we will try to place the k particles in the n nodes such that the "energy" $E = \sum_{1 \le i < j \le k} f(\delta(x_i, x_j))$ of the system is minimized. Note that we can extend the definition of function f to be valid for the range $[n/2, n-1]$ by setting $f(x) = f(n - x)$ for all $x > n/2$, and we can use the equivalent definition $E = \sum_{1 \le i < j \le k} f(d_{i,j})$ instead. The function f now becomes a strictly convex function (no longer a decreasing function).

Theorem 3.2. *If there exists a certain configuration of k particles satisfying*

$$d_{i,j} = \left\lfloor \frac{(j-i)\,n}{k} \right\rfloor \ \textit{or} \ \left\lceil \frac{(j-i)\,n}{k} \right\rceil \qquad \text{for all } i, j \in \mathbb{Z} \text{ with } 1 \le j - i < k,$$

then this configuration must have the minimum energy. Furthermore, all other configurations with the same minimal energy will have to satisfy this criteria as well.

Proof. We note that

$$E = \sum_{1\le i<j\le k} f(d_{i,j}) = \frac{1}{2}\sum_{1\le i\neq j\le k} f(d_{i,j}) = \frac{1}{2}\sum_{1\le j\le k}\sum_{1\le i\le k} f(d_{i,j}) = \frac{1}{2}\sum_{1\le j\le k}\sum_{1\le i\le k} f(d_{i,i+j}).$$

First, we will prove that

$$\sum_{1\le i\le k} f(d_{i,i+j}) \ge \left(k\left(\left\lfloor\frac{jn}{k}\right\rfloor+1\right)-jn\right) f\left(\left\lfloor\frac{jn}{k}\right\rfloor\right) + \left(jn-\left\lfloor\frac{jn}{k}\right\rfloor k\right) f\left(\left\lceil\frac{jn}{k}\right\rceil\right).$$

We know that

$$\begin{aligned}\sum_{1\le i\le k} d_{i,i+j} &= \sum_{1\le i\le k} d_i + d_{i+1} + \ldots + d_{i+j-1}\\ &= j\sum_{1\le i\le k} d_i\\ &= jn\end{aligned}$$

We will use Karamata's inequality on a convex function f with the fact that $(d_{1,j+1}, d_{2,j+2}, \ldots, d_{k,j+k})$ majorizes a tuple $(\left\lceil\frac{jn}{k}\right\rceil, \left\lceil\frac{jn}{k}\right\rceil, \ldots, \left\lceil\frac{jn}{k}\right\rceil, \left\lfloor\frac{jn}{k}\right\rfloor, \left\lfloor\frac{jn}{k}\right\rfloor, \ldots, \left\lfloor\frac{jn}{k}\right\rfloor)$ which $jn - \left\lfloor\frac{jn}{k}\right\rfloor k$ of these are $\left\lceil\frac{jn}{k}\right\rceil$'s, and $k\left(\left\lfloor\frac{jn}{k}\right\rfloor+1\right) - jn$ of these are $\left\lfloor\frac{jn}{k}\right\rfloor$'s.

So, we will get the desired result where equality holds when $(d_{1,j+1}, d_{2,j+2}, \ldots, d_{k,j+k})$ only consists of $\left\lceil\frac{jn}{k}\right\rceil$ and $\left\lfloor\frac{jn}{k}\right\rfloor$

Therefore, if there exists a certain configuration of k particles satisfying

$$d_{i,j} = \left\lfloor\frac{(j-i)\,n}{k}\right\rfloor \; or \; \left\lceil\frac{(j-i)\,n}{k}\right\rceil \quad \text{for all } i, j \in \mathbb{Z} \text{ with } 1 \le j-i < k$$

then this configuration must have the minimum energy. Moreover, other configurations with the same minimal energy will have to satisfy this criteria because Karamata's inequality described above has to be held.

□

Theorem 3.3. *There exists a configuration of k particles that satisfies the criteria stated in Theorem 3.2*

Proof. We construct the configuration as follows: Starting from the first particle x_1, we pick subsequent particles x_2 to x_k in order such that at each step, when we are picking the particle x_{i+1}, d_i satisfies

$$\frac{n\,i}{k} - \frac{1}{2} < d_1 + \ldots + d_i \le \frac{n\,i}{k} + \frac{1}{2}.$$

We first note that this results in one and only one unique choice for x_{i+1} for all i, since the difference between the upper and lower bounds is exactly 1.

Next, we want to show that any configuration that satisfies these inequalities will satisfy the criteria in Theorem 3.2 as well. Before this, we notice that when the above inequality is satisfied for $1 \le i \le k-1$, it will also be satisfied for all positive integers i since for $i \geq k$, we have $d_1 + \ldots + d_k = n$ and hence $d_1 + \ldots + d_i = n + d_1 + \ldots + d_{i-k}$, giving

$$\frac{n\,(i-k)}{k} - \frac{1}{2} + n < d_1 + \ldots + d_i \leq \frac{n\,(i-k)}{k} + \frac{1}{2} + n,$$

which after simplification becomes the same as the original inequality.

Hence,

$$d_{i,j} = d_i + \ldots + d_{j-1} = (d_1 + \ldots + d_{j-1}) - (d_1 + \ldots + d_{i-1}) \ < \frac{n\,(j-i)}{k} + 1$$

and

$$d_{i,j} = (d_1 + \ldots + d_{j-1}) - (d_1 + \ldots + d_{i-1}) \ > \frac{n\,(j-i)}{k} - 1$$

and it is clear that the only possible values of $d_{i,j}$ that satisfies these bounds are $\left\lfloor \frac{(j-i)\,n}{k} \right\rfloor$ and $\left\lceil \frac{(j-i)\,n}{k} \right\rceil$.

□

Theorem 3.4. *Every other configuration of k particles that minimizes the energy of the system is a rotation of the configuration described in the proof of Theorem 3.3*

Proof. We assume on the contrary that there are two different configurations P and Q that produce the same minimal energy. For this proof only, we will let the locations of the k particles in P be $x(P)_1, \ldots, x(P)_k$ while the particles in Q be $x(Q)_1, \ldots, x(Q)_k$. We also redefine the clockwise distances in configuration P to be $d(P)_i$ and $d(P)_{i,j}$ instead of d_i and $d_{i,j}$ respectively, and those in Q to be $d(Q)_i$ and $d(Q)_{i,j}$.

Now for each configuration, we define a "sequence" s to be the list of values $(d_{1,2}, d_{1,3}, \ldots, d_{1,k})$. Since we can set x_1 to be any of the k vertices and renumber accordingly, there are k different possible such sequences depending on which of the k particles we pick x_1 to be. From the k different sequences, we rank them first based on the largest first value $(d_{1,2})$, and if there is a tie, we break tie by looking at the second value $d_{1,3}$, and so on, and we define the top ranking sequence as the "max_sequence". We see that if P and Q have the same max_sequence, then they are essentially the same configuration (just a rotation of each other), and hence we assume they are different and let the max_sequence of P be $s(P)_{max} = (d(P)_{1,2}, \ldots, d(P)_{1,k})$ and the max_sequence of Q be $s(Q)_{max} = (d(Q)_{1,2}, \ldots, d(Q)_{1,k})$.

Suppose that the max_sequences for P and Q have a difference $d(P)_{1,i} \neq d(Q)_{1,i}$, and without loss of generality we let $d(P)_{1,i} + 1 = d(Q)_{1,i}$ (we can do this because the two values can only differ by at most 1, by Theorem 3.2). Consider configuration P, from Theorem 3.2, there exist $j \in 1, 2, \ldots, k$ such that $d(P)_{j,j+i-1} = d(P)_{1,i} + 1$ because if there is no such j,

$$(i-1)n = \sum_{1 \leq m \leq k} D(P)_{m,m+i-1} \leq n \cdot D(P)_{1,i} < (n-1) \cdot D(P)_{1,i} + D(Q)_{1,i} \leq \sum_{1 \leq m \leq k} D(Q)_{m,m+i-1} = (i-1)n$$

which is a contradiction.

Hence, there exists another possible sequence for configuration P which gives $s(P)' = (d'(P)_{1,2}, \ldots, d'(P)_{1,i}, \ldots, d'(P)_{1,k})$ with $d'(P)_{1,i} = d(P)_{1,i} + 1$ (This sequence is obtainable by setting the $x(P)_j$ vertex in the max_sequence configuration to be the new $x(P)_1$).

However, since we know that the sequence $s(P)_{max}$ has a higher ranking than $s(P)'$, there must also exist some integer $z < i$ such that $d(P)_{1,z} \geq d'(P)_{1,z} + 1$. Hence, we have

$$d(P)_{1,i} - d(P)_{1,z} \leq d'(P)_{1,i} - d'(P)_{1,z} - 2$$

$$d(P)_{i,z} \leq d'(P)_{i,z} - 2$$

and this contradicts the criteria in Theorem 3.2 ◻

4. Formulating the Problem

For higher dimension, we will transform our energy minimization problem into a linear algebra problem with help of basic understanding of representation theory. We then change the problem from finding the optimized position of the particles to be finding an eigenvector of the least eigenvalue which will be shown in the following sections. We claim that such an eigenvector will prove us the checkerboard conjecture.

Definition 4.1. Let $x_1, x_2, \ldots, x_N$ be all N locations. We have a function $f : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}$ as a repelling force between two positions that depends on the Lee distance between those. We define an $N \times N$ matrix A such that

$$A_{i,j} = \begin{cases} f(\delta(x_i, x_j)) & \text{if } i \neq j; \\ 0 & \text{if } i = j \end{cases}$$

for all $i, j \in \{1, 2, \ldots, N\}$.

Let n be a natural number which is less than or equal to N. Let S be a set of locations of our particles. Thus, S will be a subset of $\{x_1, x_2, \ldots, x_N\}$ of cardinality n.

We also define an N-dimensional vector V as follows

$$V_i = \begin{cases} 1 & \text{if } x_i \in S; \\ 0 & \text{otherwise} \end{cases}$$

for all $i \in \{1, 2, \ldots, N\}$.

Remark. For this problem, N will be even number, and n will be equal to $\dfrac{N}{2}$

Proposition 4.2. *The energy of the system is equal to* $\dfrac{1}{2}V^T AV$

Proof.

$$\begin{aligned} \frac{1}{2}V^T AV &= \frac{1}{2}\sum i = 1^N \sum_{j=1}^{N} V_i A_{i.j} V_j \\ &= \frac{1}{2}\sum_{x_i \in S}\sum_{x_j \in S} A_{i,j} \\ &= \frac{1}{2}\sum_{x_i \in S}\sum_{x_j \in S} f(\delta(x_i, x_j)) \end{aligned}$$

which is the energy of the system. ◻

Lemma 4.3. *If space is a toric grid, then a vector e where every element is* 1 *is an eigenvector of A.*

Proof. First, we will prove that $(Ae)_i$ is a constant λ for all $i \in \{1, 2, \ldots, N\}$. Because every point on a toric grid is equivalent in terms of distance to other points, so we have

$$(Ae)_i = \sum_{k=1}^{N} A_{i,k} = \sum_{k=1}^{N} f(\delta(x_i, x_k)) = \sum_{k=1}^{N} f(\delta(x_1, x_k)) = \sum_{k=1}^{N} A_{1,k} = (Ae)_1$$

which is a constant for all $i \in \{1, 2, \ldots, N\}$. Thus, $Ae = \lambda e$ as desired. □

Proposition 4.4. $V^T e = n$

Proof.

$$V^T e = \sum_{k=1}^{N} V_k = \sum_{x_k \in S} 1 = n$$

□

Proposition 4.5. $V^T V = n$

Proof.

$$V^T V = \sum_{k=1}^{N} V_k^2 = \sum_{x_k \in S} 1 = n$$

□

Theorem 4.6. *Let λ_N be the smallest eigenvalue of matrix A, and λ_1 be eigenvalue associated with the eigenvector e, an all 1's vector, of matrix A. Then, the energy of the system is not less than*

$$\frac{n^2}{N}\lambda_1 + (n - \frac{n^2}{N})\lambda_N.$$

Equality holds when $V = \frac{n}{N}e + \sqrt{n - \frac{n^2}{N}}e_N$, where e_N is the unit eigenvector corresponding to λ_N.

Proof. From Lemma 4.3, we know that $Ae = \lambda_1 e$. We define e_1 as $\frac{1}{\sqrt{N}}e$, then we have

$$Ae_1 = \frac{1}{\sqrt{N}}Ae = \frac{1}{\sqrt{N}}\lambda_1 e = \lambda_1 e_1.$$

Thus, e_1 is a unit eigenvector corresponding to an eigenvalue λ_1.

Let $e_1, e_2, \ldots, e_N$ be basis consisting of orthonormal eigenvectors of A such that e_i is associated with λ_i for all $i \in \{1, 2, \ldots, N\}$. There are such eigenvectors because of Theorem 2.1 and the fact that A is a symmetric matrix. Therefore, there are real numbers $u_1, u_2, \ldots, u_N$ such that V can be written as $\sum_{i=1}^{N} u_i e_i$. From Proposition 4.4, we have

$$n = V^T e = V^T \sqrt{N} e_1 = \sqrt{N}(\sum_{i=1}^{N} u_i e_i^T) e_1 = \sqrt{N} u_1.$$

Thus,

$$u_1 = \frac{n}{\sqrt{N}}. \quad (*)$$

From Proposition 4.5, we have

$$n = V^T V = (\sum_{i=1}^{N} u_i e_i^T)(\sum_{i=1}^{N} u_i e_i) = \sum_{i=1}^{N} u_i^2 = \sum_{i=2}^{N} u_i^2 + \frac{n^2}{N}$$

Therefore,

$$\sum_{i=2}^{N} u_i^2 = n - \frac{n^2}{N}. \tag{**}$$

We will use these relations to prove the lower bound of the energy which is represented by $V^T AV$

$$\begin{aligned} V^T AV &= V^T A(\sum_{i=1}^{N} u_i e_i) \\ &= V^T (\sum_{i=1}^{N} u_i A e_i) \\ &= V^T (\sum_{i=1}^{N} u_i \lambda_i e_i) \\ &= (\sum_{i=1}^{N} u_i e_i^T)(\sum_{i=1}^{N} u_i \lambda_i e_i) \\ &= \sum_{i=1}^{N} u_i^2 \lambda_i \end{aligned}$$

From (*), (**), and the fact that λ_i is real number for all $i \in \{1, 2, \ldots, N\}$ which is true because of Theorem 2.1, we get

$$V^T AV = \sum_{i=1}^{N} u_i^2 \lambda_i = \frac{n^2}{N}\lambda_1 + \sum_{i=2}^{N} u_i^2 \lambda_i \geq \frac{n^2}{N}\lambda_1 + (\sum_{i=2}^{N} u_i^2)\lambda_N = \frac{n^2}{N} + (n - \frac{n^2}{N})\lambda_N,$$

and equality holds when $(u_1, u_2, \ldots, u_{N-1}, u_N) = (\frac{n}{\sqrt{N}}, 0, \ldots, 0, \sqrt{n - \frac{n^2}{N}})$ which is equivalent to $V = \frac{n}{N} e + \sqrt{n - \frac{n^2}{N}} e_N$ as desired. □

5. Finding The Eigenvalues

In this section, we will state all the eigenvalues of a matrix A as mentioned in Definition 4.1. By using the idea from representation theory, we can create a basis consisting of eigenvectors of A, so we can find the eigenvalues corresponding to those eigenvectors.

Definition 5.1. Let a positive integer d the dimension of our toric grid. Let positive integers $n_1, n_2, \ldots, n_d$ be the size for each dimension respectively. Thus, each position in our toric grid will be labeled as $(i_1, i_2, \ldots, i_d) \in \mathbb{Z}/n_1 \times \mathbb{Z}/n_2 \times \ldots \mathbb{Z}/n_d$.

Define a function $l : \{x_1, x_2, \ldots, x_N\} \mapsto \mathbb{Z}/n_1 \times \mathbb{Z}/n_2 \times \ldots \mathbb{Z}/n_d$ such that $l(x)$ is a label of location x, and l has an addition property which satisfies $(a_1, a_2, \ldots, a_d) + (b_1, b_2, \ldots, b_d) = (a_1 + b_1, a_2 + b_2, \ldots, a_d + b_d)$.

Proposition 5.2. *For each $i, j \in \{1, 2, \ldots, d\}$, there exists $k \in \{1, 2, \ldots, d\}$ such that $l(x_i) + l(x_j) = l(x_k)$.*

Proof. Let $a_1, a_2, \ldots, a_d, b_1, b_2, \ldots, b_d$ be integers such that $l(x_i) = (a_1, a_2, \ldots, a_d)$ and $l(x_j) = (b_1, b_2, \ldots, b_d)$.Then, we have $l(x_i) + l(x_j) = (a_1 + b_1, a_2 + b_2, \ldots, a_d + b_d)$. However, from ..., there exists $k \in \{1, 2, \ldots, N\}$ such that $l(x_k) = (a_1 + b_1, a_2 + b_2, \ldots, a_d + b_d)$. Thus, there we have $l(x_i) + l(x_j) = l(x_k)$ as desired. □

Definition 5.3. Let $g : \mathbb{C}^d \times \{x_1, x_2, \ldots, x_{n_1 n_2 \ldots n_d}\} \mapsto \mathbb{C}$ be a function that satisfies

$$g((c_1, c_2, \ldots, c_d), x_k) = c_1^{i_1} c_2^{i_2} \ldots c_d^{i_d} \text{ where } l(x_k) = (i_1, i_2, \ldots, i_d)$$

In the following part, we will present a set of $n_1 n_2 \ldots n_d$ vectors and prove that they are linearly independent to each other. Therefore, we will get a basis consisting of eigenvectors of A and all eigenvalues respectively.

Definition 5.4. For each $i \in \{1, 2, \ldots, d\}$, let R_i be a set of n_i^{th} root of unity, so $\|R_i\| = n_i$ for all i. We define a set $\{y_1, y_2, \ldots, y_{n_1 n_2 \ldots n_d}\} = R_1 \times R_2 \times \ldots R_d$.

We will create a set of vectors $\{v_1, v_2, \ldots, v_{n_1 n_2 \ldots n_d}\}$ as follows

$$(v_i)_k = g(y_i, x_k) \text{ for all } i, k \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}$$

Theorem 5.5. *Vectors $v_1, v_2, \ldots, v_{n_1 n_2 \ldots n_d}$ are linearly independent to each other.*

Proof. We will prove by contradiction by first let n be the smallest number of vectors from $\{v_1, v_2, \ldots, v_{n_1 n_2 \ldots n_d}\}$ such that these vectors are linearly dependent. Assume now that $v_1, v_2, \ldots, v_n$ and complex numbers $c_1, c_2, \ldots, c_n$, not all of them are 0, satisfy the condition for case n vectors. We have $c_1 v_1 + c_2 v_2 + \ldots + c_n v_n$ is equal to a vector consisting only 0.

Thus, we have

$$(*) \qquad c_1(v_1)_k + c_2(v_2)_k + \ldots c_n(v_n)_k = 0 \text{ for all } k \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}.$$

Since $v_n \neq v_1$, there is $m \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}$ such that $(v_n)_m \neq (v_1)_m$. From Proposition 5.2, we know that for each k, there is $p \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}$ such that $l(x_k) + l(x_m) = l(x_p)$. Then, we have $(v_i)_p = g(y_i, x_p) = g(y_i, x_k) \cdot g(y_i, x_m) = (v_i)_k \cdot (v_i)_m$. Substituting k with p, we get

$$(**) \qquad c_1(v_1)_k(v_1)_m + c_2(v_2)_k(v_2)_m + \ldots c_n(v_n)_k(v_n)_m = 0 \text{ for all } k \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}.$$

Now we multiply (*) by $(v_n)_m$:

$$(***) \qquad c_1(v_1)_k(v_n)m + c_2(v_2)_k(v_n)_m + \ldots c_n(v_n)_k(v_n)_m = 0 \text{ for all } k \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}.$$

Subtracting (***) from (**), we get

$$c_1((v_1)_m - (v_n)_m)(v_1)_k + c_2((v_2)_m - (v_n)_m)(v_2)_k + \ldots + c_{n-1}((v_{n-1})_m - (v_n)_m)(v_{n-1})_k = 0$$

for all $k \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}$. This is a linear dependence relation of $n - 1$ vectors. By the definition of n, we have $c_i((v_i)_m - (v_n)_m) = 0$ for all $i \in \{1, 2, \ldots, n - 1\}$. To be specific, $c_1((v_1)_m - (v_n)_m) = 0$. Since $(v_n)_m \neq (v_0)_m$, we must have $c_1 = 0$. By arguing in the similar way, we get $c_1 = c_2 = \ldots = c_{n-1}$, which makes $c_n = 0$. It contradicts the definition of $c_1, c_2, \ldots, c_n$. Therefore, there is no such n and hence the theorem is proved. □

Theorem 5.6. *For each $i \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}$, a vector v_i is an eigenvector of a matrix A corresponding to an eigenvalue $\lambda_i = \sum_{j=2}^{n_1 n_2 \ldots n_d} f(\delta(x_j, 0))g(y_i, x_j)$ where 0 is x_1, i.e. $Av_i = \lambda_i v_i$.*

Proof. We have to prove that for each $k \in \{1, 2, \ldots, (n_1 n_2 \ldots n_d)\}, (Av_i)_k = (\lambda_i)_k$. Consider $(Av_i)_k$ is the product of row k of A with the vector v_i, so we have

$$\begin{aligned}
(Av_i)_k &= \sum_{l=1}^{n_1 n_2 \ldots n_d} A_{k,l}(v_i)_l \\
&= \sum_{l=1, l\neq k}^{n_1 n_2 \ldots n_d} f(\delta(x_k, x_l))g(y_i, x_l) \\
&= \sum_{m=1, m\neq k}^{n_1 n_2 \ldots n_d} f(\delta(x_k, x_m))g(y_i, x_m) && \text{where } l(x_m) = l(x_k) + l(x_l) \text{ (from Proposition 5.2)} \\
&= \sum_{l=2}^{n_1 n_2 \ldots n_d} f(\delta(0, x_l))g(y_i, x_l)g(y_i, x_k) && \text{(from Definition of } l, g \text{ and } \delta) \\
&= (\sum_{l=2}^{n_1 n_2 \ldots n_d} f(\delta(x_l, 0))g(y_i, x_l))(v_i)_k \\
&= \lambda_i (v_i)_k \\
&= (\lambda_i v_i)_k
\end{aligned}$$

as desired. □

Because there are only $n_1 n_2 \ldots n_d$ eigenvectors of a matrix A that are linearly independent, so our set of eigenvectors as we mentioned in Definition 5.4 is a basis. Thus, set of all eigenvalues of A is $\{\lambda_1, \lambda_2 \ldots, \lambda_{n_1 n_2 \ldots n_d}\}$. In following sections, we will find a tuple $y \in R_1 \times R_2 \times \ldots R_d$ that gives us the smallest eigenvalue of A, so we can find the position of all particles that minimize the energy of the system from the result in Theorem 4.6.

6. Main Results

This section will be the summary of solution for this paper in cases when each n_i, as mentioned in Definition 5.1, is either two or a multiple of four which is proved in [1].

For this result, we assume that our function $f : \mathbb{R}^+ \mapsto \mathbb{R}^+$ as mentioned in Definition 2. is a strictly completely monotonic, i.e., $(-1)^k f^{(k)}(x) > 0$ for all $x \in \mathbb{R}^+$ and for all k.

Theorem 6.1. *Assume that each of $n_1, n_2, \ldots, n_d$ is either 2 or a multiple of 4, then the energy of the system is minimized when the position of particles is a checkerboard configuration.*

From Theorem 4.6, it suffices to find the eigenvector corresponding to the smallest eigenvalue of a matrix A, so that V, the vector that represents the position of particles on the toric grid, will be equal to $\frac{1}{2}e + \frac{\sqrt{N}}{2}e_N$ because $N = n_1 n_2 \ldots n_d = 2n$.

Lemma 6.2. *The function $R_1 \times R_2 \times \ldots R_d \mapsto \mathbb{R}$ sending y to*

$$\sum_{j=2}^{n_1 n_2 \ldots n_d} f(\delta(x_j, 0))g(y, x_j)$$

has a unique minimum at $(-1, \ldots, -1)$.

Proof. From Bernstein's theorem (see Chapter IV, Theorem 12b in [5]) on monotone functions, the completely monotonic function f can be written as

$$f(x) = \int_0^\infty e^{-xt} dh(t)$$

where h is nondecreasing and the integral converges for $0 < x < \infty$. Thus, we have to find a minimum point of

$$\sum_{j=2}^{n_1 n_2 \dots n_d} f(\delta(x_j, 0)) g(y, x_j) = \int_0^\infty \left(\sum_{j=2}^{n_1 n_2 \dots n_d} e^{-\delta(x_j,0)t} g(y, x_j) \right) dh(t).$$

It is sufficient to prove that $(-1, \dots, -1)$ is a unique minimum for the function

$$y \mapsto \sum_{j=2}^{n_1 n_2 \dots n_d} e^{-\delta(x_j,0)t} g(y, x_j) \text{ for each fixed } t.$$

which is equivalent to the function

$$y \mapsto \sum_{j=1}^{n_1 n_2 \dots n_d} a^{-\delta(x_j,0)} g(y, x_j), \text{ where } a = e^t,$$

where we include $x_1 = 0$ to the sum because it is just a constant term 1 independently to y.

We know that $\delta(x_j, 0)$ is the sum of the distance from x_j to 0 in each dimension. Thus, we can write $\delta(x_j, 0) = \delta_1(x_j, 0) + \delta_2(x_j, 0) + \ldots + \delta_d(x_j, 0)$, where $\delta_i(x_j, 0)$ is the distance from x_j to 0 in i^{th} dimension. Let y be $(c_1, c_2, \dots, c_d)$, and $l(x_j) = (x_j^{(1)}, x_j^{(2)}, \dots, x_j^{(d)})$ for all $j \in \{1, 2, \dots, n_1 n_2 \dots n_d\}$. We have

$$\sum_{j=1}^{n_1 n_2 \dots n_d} a^{-\delta(x_j,0)} g(y, x_j) = \sum_{j=1}^{n_1 n_2 \dots n_d} a^{-(\delta_1(x_j,0)+\delta_2(x_j,0)+\ldots+\delta_d(x_j,0))} c_1^{x_j^{(1)}} \dots c_d^{x_j^{(d)}}$$

Since $x_1, x_2, \dots, x_{n_1 n_2 \dots n_d}$ cover all the positions on the toric grid, and $\delta_i(x_j, 0) = \min(x_j^{(i)}, n_i - x_j^{(i)})$, we can factorize the previous function as the product of the factors

$$\sum_{j=0}^{n_i - 1} a^{-\min(j, n_i - j)} c_i^j$$

for $i = 1, 2, \dots, d$. Therefore, it is sufficient to prove that each of these factors is positive for all $c_i \in \mathbb{R}_i$, and has its minimum at $c_i = -1$.

We will simplify notation by fixing i and writing n_i, c_i as n, c respectively. We have two cases when n is either two or a multiple of four. Consider the case when $n = 2$, the sum becomes $1 + a^{-1}c$ where c can be either 1 or -1. Because $a > 1$, we can see that this sum is positive and have its minimum at -1 as desired. Next, we have to prove the case when n is a multiple of four. Consider the sum

$$\begin{aligned}
\sum_{j=0}^{n-1} a^{-\min(j,n-j)} c^j &= 1 + \sum_{j=1}^{n/2-1} a^{-j}(c^j + c^{-j}) + a^{-n/2} c^{n/2} \\
&= -1 + \sum_{j=0}^{n/2-1} a^{-j}(c^j + c^{-j}) + a^{-n/2} c^{n/2} \\
&= \frac{1 - a^{-n/2} c^{n/2}}{1 - a^{-1} c} + \frac{1 - a^{-n/2} c^{-n/2}}{1 - a^{-1} c^{-1}} - (1 - a^{-n/2} c^{n/2}).
\end{aligned}$$

Because c is an n^{th} root of unity, $c^{n/2}$ is either 1 or -1. If it equals to 1, then the sum is reduced to

$$(1 - a^{-n/2})\left(\frac{1}{1 - a^{-1}c} + \frac{1}{1 - a^{-1}c^{-1}} - 1\right) = (1 - a^{-n/2})\left(\frac{1 - a^{-2}}{|1 - a^{-1}c|^2}\right).$$

Since $a > 1$, so the sum is positive. In order to get its minimum, $|1 - a^{-1}c|$ has to get its maximum when it is furthest away from 1 which is when $c = -1$ since n is a multiple of four. Next, if $c^{n/2}$ is equal to -1, then the sum is reduced to

$$(1 + a^{-n/2})\left(\frac{1}{1 - a^{-1}c} + \frac{1}{1 - a^{-1}c^{-1}} - 1\right) = (1 + a^{-n/2})\left(\frac{1 - a^{-2}}{|1 - a^{-1}c|^2}\right),$$

which is positive since $a > 1$. And its minimum is when c is the furthest one from 1 in the complex plane.

We have to compare those two minimum point from each case. Note that the factor $1 - a^{-n/2}$ is less than $1 + a^{-n/2}$, and -1 is the furthest away from 1 than any other c. Thus, the minimum is at $c = -1$ as desired. □

Back to our Theorem 6.1, we can conclude from Lemma 6.2 that the eigenvector corresponding to the smallest eigenvalue is generated by $y = (-1, -1, \dots, -1)$ as mentioned in Definition 5.4. Thus, from Definition 5.4 and Theorem 4.6, we have

$$V_i = \begin{cases} 1 & \text{if } a_1 + a_2 + \dots + a_d \text{ is divisible by 2, where } l(x_i) = (a_1, a_2, \dots, a_d); \\ 0 & \text{otherwise,} \end{cases}$$

which is according to the checkerboard configuration as desired. This concludes the proof of Theorem 6.1.

References

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