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ENERGY MINIMIZATION OF REPELLING PARTICLES ON A TORIC GRID*

NIEK BOUMAN[†], JAN DRAISMA[‡], AND JOHAN S. H. VAN LEEUWAARDEN[§]

Abstract. We explore the minimum energy configurations of repelling particles distributed over n possible locations forming a toric grid. We conjecture that the most energy-efficient way to distribute $n/2$ particles over this space is to place them in a checkerboard pattern. Numerical experiments validate this conjecture for reasonable choices of the repelling force. In the present paper, we prove this conjecture in a large number of special cases—most notably, when the sizes of the torus are either two or multiples of four in all dimensions and the repelling force is a completely monotonic function of the Lee distance between the particles.

Key words. energy minimization, repelling particles, discrete Fourier transform, wireless networks

AMS subject classifications. 90C27, 05B30, 05E18

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1. Introduction. The problem of distributing particles uniformly over a metric space has proved an inspiring question for mathematicians, and has also attracted the attention of biologists, chemists, and physicists working on crystallography, molecular structures, and electrostatics.

We consider an interacting particle system with a repelling force between the particles. Under influence of the force, the particles arrange themselves in the most energy-efficient manner (one that minimizes the total amount of energy in the system). The intuition is that repelling particles tend to spread apart until there is as much distance between them as possible, which results in some sort of “uniform distribution” of the particles.

We investigate the case in which the repelling force between any pair of particles is given by a function f of their distance. This function f can take the form $f(x) = x^{-\alpha}$ with $\alpha > 0$. This is a generalization of the *inverse square law* that is well known in physics, where it describes the behavior of forces like electrical charge. It also describes the reduction in power density of an electromagnetic wave as it propagates through space, known as *path loss*. Path loss plays a crucial role in the design of wireless networks, for which the exponent α normally ranges from 2 to 4 (where 2 is for propagation in free space, and 4 is for relatively lossy environments [ARY95]). Note that, since f is a decreasing function, we assume that the repelling force becomes stronger when the particles move closer to each other.

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[†]Department of Mathematics and Computer Science, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands (n.bouman@tue.nl). This author’s work was supported by Microsoft Research through its Ph.D. Scholarship Programme.

[‡]Department of Mathematics and Computer Science, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands and Centrum Wiskunde & Informatica, Amsterdam, The Netherlands (j.draisma@tue.nl). This author’s work was supported by a Vidi grant from The Netherlands Organization for Scientific Research (NWO).

[§]Department of Mathematics and Computer Science, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands (j.s.h.v.leeuwaarden@tue.nl). This author’s work was supported by an ERC starting grant and a TOP grant from The Netherlands Organization for Scientific Research (NWO).

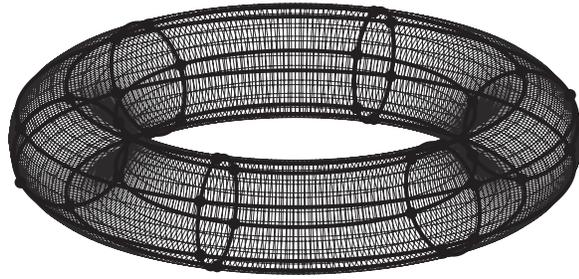


FIG. 1.1. An embedding of a 6×6 grid on a two-dimensional torus.

Denote the locations of the N particles by x_1, \dots, x_N . The f -energy experienced by particle x_i is defined as $\sum_{j \neq i} f(\delta(x_i, x_j))$, where δ denotes the metric. Our original motivation stems from the area of wireless networks, in which particles are mobile users, and the f -energy of a user is its interference with all other users. When experiencing too much interference, a user is unable to transmit data [BB09, GK00]. For a given maximal sustainable interference level T , a natural question is to find the maximal packing of users that can be active simultaneously without violating the threshold T , i.e., while maintaining f -energy at most T for each user. In the case that we will deal with, this question is intimately related to the problem of minimizing the total energy among all pairs of particles; see section 2.

A lot of research in energy minimization focuses on spheres. In dimension one, the uniform distribution on the circle is simply given by the N equally spaced points (roots of unity in the complex plane), but in higher dimensions it becomes less obvious on what type of patterns the particles arrange themselves, and this presents all sorts of mathematical challenges [CK07, HS04, KS97].

In this paper, rather than spheres or other continuous metric spaces, we consider a d -dimensional grid as possible locations for the particles. Further, to avoid boundary effects, we wrap around the boundaries. This grid has a natural embedding on a d -dimensional torus (see Figure 1.1), which is why we call it the d -dimensional *toric grid*.

Let n_i be the size of the grid in dimension i , so that we have a total of $n = n_1 \cdots n_d$ possible locations for the particles. It seems reasonable to expect that the best way, in terms of minimal energy, to distribute $n/2$ particles over this space is to place them in a *checkerboard pattern*, by which we mean a pattern in which exactly one particle is placed at any two neighboring points. Of course, because of the wrapping around, such a pattern exists only when all n_i are even.

For any toric grid, regardless of its dimensions, there are only two such configurations (see Figure 1.2), and the checkerboard pattern is a natural “uniform distribution” on a toric grid. It is also a maximal-size *independent set* in the graph whose vertices are the possible locations and whose edges connect locations differing by ± 1 in one coordinate and not at all in the remaining coordinates. The Lee distance between two locations is defined as the length of the shortest path, in terms of edges, between the corresponding vertices on this graph. The following conjecture formalizes, to some extent, our intuition that checkerboard patterns are optimal.

CONJECTURE 1.1 (checkerboard conjecture). *For any toric grid with n_1, \dots, n_d all even, and for any reasonable function f of the Lee distance, the arrangements of $N = n/2$ particles that minimize the maximal f -energy experienced by any of the particles are the two checkerboard patterns, and only these.*

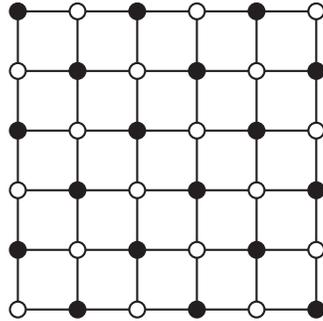


FIG. 1.2. A 6×6 grid, the black and white points denote the checkerboard configurations.

Of course, the validity of this conjecture depends on what *reasonable* means. It will certainly imply *decreasing*, but more conditions will be necessary.

For the example of wireless networks the checkerboard conjecture has the following implication. When the threshold T is increased slowly, an increasing number of users are allowed to be active simultaneously, and there will be a critical value $T = T^*$ at which this number becomes precisely $n/2$. At that critical threshold, we then know that $n/2$ active users can only be arranged in a checkerboard pattern—a phenomenon that we have first observed in simulations of wireless networks. For a large toric grid it is of course infeasible to prove the checkerboard conjecture by exhaustive search through all $\binom{n}{N}$ possible configurations.

In this paper we prove the checkerboard conjecture in a large number of special cases. We first derive a continuous relaxation of our energy minimization problem in section 2. Then, as a first (and known) special case, we prove the checkerboard conjecture for the one-dimensional toric grid and $f(x) = 1/x$ in section 3. In section 4 we prove the checkerboard conjecture for the toric grid that has size two in any dimension and functions f whose k th forward difference has sign $(-1)^k$. Section 5 then gives our strongest result (which however does not immediately imply any of the previous two results): a proof for the checkerboard conjecture in the case where each n_i is either two or a multiple of four, now assuming that f is completely monotonic; see section 5 for this notion. Finally, in section 6 we discuss some problems open for future research.

2. Framework. In this section we formulate a general version of our energy minimization problem, which belongs to the realm of discrete optimization. We then derive a continuous relaxation of that problem. If all optimal solutions of the relaxation happen to be feasible for the discrete problem, then they are also the optimal solutions for the discrete problem. This is our strategy for proving special cases of the checkerboard conjecture in the following sections.

Let d be a positive integer, the *dimension* of our toric grid. Let n_1, \dots, n_d be positive integers, and set $G := \prod_{i=1}^d (\mathbb{Z}/n_i)$, a finite Abelian group. Let $\Delta := \{(g, g) \mid g \in G\}$ be the diagonal in $G \times G$. Let u be a function $(G \times G) \setminus \Delta \rightarrow \mathbb{R}$ that is *symmetric* ($u(g, h) = u(h, g)$ for all $g, h \in G$) and *G -invariant* ($u(k + g, k + h) = u(g, h)$ for all $g, h, k \in G$). Later we will add the restriction on u that it is a suitable (and in particular decreasing) function of some G -invariant distance on G , so that we may think of $u(g, h)$ as a repelling force between particles located at g and h . But for deriving our relaxation this restriction is not needed.

Next let p be a natural number less than or equal to $|G|$. Let S be a subset of G of cardinality p ; this is the set of locations of our particles. Given $h \in S$ we define

$$E_h(S) := \sum_{g \in S \setminus \{h\}} u(h, g),$$

called the *energy of S experienced by h* , and

$$E_{\max}(S) := \max_{h \in S} E_h(S),$$

called the *maximal energy of S* . The checkerboard conjecture concerns the following optimization problem with $p = |G|/2$.

PROBLEM 2.1 (maximal energy minimization). *Minimize the maximal energy $E_{\max}(S)$ over all subsets $S \subseteq G$ of cardinality p .*

Further we define

$$E_{\text{tot}}(S) := \sum_{h \in S} E_h(S),$$

called the *total energy of S* . We can now formulate a second optimization problem.

PROBLEM 2.2 (total energy minimization). *Minimize the total energy $E_{\text{tot}}(S)$ over all subsets $S \subseteq G$ of cardinality p .*

An important relation between these two optimization problems is the following. If a set S^* minimizes the total energy and happens to have the property that $E_h(S^*) = E_g(S^*)$ for all $h, g \in S^*$, then S^* also minimizes the maximal energy—indeed, any S with $E_{\max}(S) < E_{\max}(S^*)$ would necessarily have $E_{\text{tot}}(S) < E_{\text{tot}}(S^*)$. The condition that $E_h(S^*)$ does not depend on $h \in S^*$ is satisfied, in particular, when S^* is a coset of a subgroup G' of G . Indeed, the set $S^* \setminus \{h\}$ is then equal to G' for all $h \in S^*$, and hence $E_h(S) = \sum_{g \in G'} u(h, h+g) = \sum_{g \in G'} u(0, g)$, independently of $h \in S^*$, by the G -invariance of u . Checkerboard patterns S are examples of cosets. In view of this relation between maximal energy minimization and total energy minimization, most of our paper focuses on total energy minimization.

We proceed to derive a continuous relaxation, which uses the space $V = \mathbb{R}^G$ of real-valued functions on G . We represent a subset $S \subseteq G$ by its *characteristic vector* $x_S \in V$ defined by

$$x_S(g) = \begin{cases} 1 & \text{if } g \in S, \\ 0 & \text{if } g \notin S. \end{cases}$$

The space V has two important additional structures. First, it is equipped with a G -action defined by $(gx)(h) = x(h-g)$ for $g, h \in G$ and $x \in V$; here the minus sign is customary but not strictly necessary since G is Abelian. Second, it has a natural inner product $(x|y) := \sum_{g \in G} x(g)y(g)$ that is G -invariant in the sense that $(hx|hy) = (x|y)$ for all $h \in G$.

Now we define the key quantity in this paper: the *energy kernel*

$$A := \sum_{g \in G, g \neq 0} u(g, 0)g,$$

which lives in the group algebra $\mathbb{R}G$ and acts by a linear map on V :

$$(Ax)(h) = \sum_{g \in G, g \neq 0} u(g, 0)x(h-g).$$

Alternatively, one may think of A as the symmetric $G \times G$ -matrix whose (g, h) -entry equals $u(g, h)$, and perhaps this conceptually simplifies the following computations.

For any subset S of G we have

$$\begin{aligned} (x_S | Ax_S) &= \sum_{h \in G} x_S(h)(Ax_S)(h) = \sum_{h \in S} (Ax_S)(h) = \sum_{h \in S} \sum_{g \in G, g \neq 0} u(g, 0)x_S(h - g) \\ &= \sum_{h \in S} \sum_{g \in G, g \neq h} u(h - g, 0)x_S(g) = \sum_{h \in S} \sum_{g \in S, g \neq h} u(h - g, 0) \\ &= \sum_{h \in S} \sum_{g \in S, g \neq h} u(h, g) = E_{\text{tot}}(x_S). \end{aligned}$$

Thus we have identified the total energy of a set S as the inner product of x_S with its image under the energy kernel. Moreover, if S has cardinality p , then x_S has the further properties $(x_S | x_S) = (x_S | \mathbf{1}) = p$, where $\mathbf{1}$ is the all-one vector in V . This motivates the following optimization problem.

PROBLEM 2.3 (fractional energy minimization). *Minimize the “fractional total energy” $(x | Ax)$ over all $x \in V$ satisfying the constraints $(x | x) = (x | \mathbf{1}) = p$.*

Note that if we add the additional constraint that x be a 0/1-vector, then this problem is just total energy minimization. Thus a feasible solution of the relaxation can be thought of as a “fractional” solution to the original problem, though this is slight abuse of language for two reasons. First, the optimal solution to the problem just stated may very well have irrational coordinates, so that it is not a “fraction.” Second, it may have coordinates that are not in the interval $[0, 1]$ —indeed, we do not even impose that the coordinates be nonnegative—so that it cannot be “rounded” to an actual solution of the original problem. We could have added the additional constraint that all coordinates lie in that interval. This would have led to a more general *quadratically constrained quadratic program*. However, as we describe next, the formulation just given allows for a simple solution once the eigenvalues of A are known. But first we discuss an example to make all notions more concrete.

Example 2.4. Let $d = 2$ and $n_1 = n_2 = 4$, so that $G = (\mathbb{Z}/4) \times (\mathbb{Z}/4)$. We depict a vector $x \in V$ as a 4×4 -matrix of real numbers, with rows and columns labeled by the elements 0, 1, 2, 3 of $\mathbb{Z}/4$ and entry $x(k, l)$ at position (k, l) . Here is an example of the action of G on V (“shift 1 down and 2 to the right”):

$$(1, 2) \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{bmatrix} = \begin{bmatrix} 15 & 16 & 13 & 14 \\ 3 & 4 & 1 & 2 \\ 7 & 8 & 5 & 6 \\ 11 & 12 & 9 & 10 \end{bmatrix}.$$

In this case the Lee distance δ on G is given by

$$\delta((j, k), (l, m)) = |l - j| + |m - k|,$$

where $|a|$ is the smallest nonnegative integer in $(a + 4\mathbb{Z}) \cup (-a + 4\mathbb{Z})$. Define $u(g, h) = \frac{1}{\delta(g, h)}$, so that particles situated at g and h repel each other with a force inversely proportional to the Lee distance between g and h . Take $p = 4$ and $S =$

$\{(0, 0), (0, 1), (0, 2), (0, 3)\}$. Then the energy kernel A satisfies

$$Ax_S = A \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \\ = \begin{bmatrix} 0 + 1 + \frac{1}{2} + 1 & 1 + 0 + 1 + \frac{1}{2} & \frac{1}{2} + 1 + 0 + 1 & 1 + \frac{1}{2} + 1 + 0 \\ 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{2} & \frac{1}{2} + 1 + \frac{1}{2} + \frac{1}{3} & \frac{1}{3} + \frac{1}{2} + 1 + \frac{1}{2} & \frac{1}{2} + \frac{1}{3} + \frac{1}{2} + 1 \\ \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{3} & \frac{1}{3} + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} & \frac{1}{4} + \frac{1}{3} + \frac{1}{2} + \frac{1}{3} & \frac{1}{3} + \frac{1}{4} + \frac{1}{3} + \frac{1}{2} \\ 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{2} & \frac{1}{2} + 1 + \frac{1}{2} + \frac{1}{3} & \frac{1}{3} + \frac{1}{2} + 1 + \frac{1}{2} & \frac{1}{2} + \frac{1}{3} + \frac{1}{2} + 1 \end{bmatrix},$$

where the contributions from the elements of S are listed in order. For instance, the expression $0 + 1 + \frac{1}{2} + 1$ for the $(1, 1)$ -entry of Ax_S reflects that the elements of S have Lee distances $0, 1, 2, 1$ to $(0, 0)$, respectively. We find that $(x|Ax)$ equals $4(0 + 1 + 1/2 + 1) = 10$, which is indeed the total energy of S . Note that one could represent A by a symmetric 16×16 -matrix.

The geometric intuition behind what follows is that, to minimize $(x|Ax)$ over the sphere defined by the constraints $(x|x) = (x|\mathbf{1}) = p$, we have to maximize the component of x in the eigenspace of A corresponding to the smallest eigenvalue of A . Indeed, since A “is” a symmetric matrix, or, equivalently, a self-adjoint linear map with respect to $(\cdot|\cdot)$, we know beforehand that all of its eigenvalues on V are real. Nevertheless, to determine those eigenvalues it is convenient first to complexify V to $V_{\mathbb{C}} := \mathbb{C} \otimes V = \mathbb{C}^G$, because this allows us to simultaneously diagonalize all group elements g in their action on V . As a consequence, their linear combination A is then also diagonalized.

We use basic terminology from the representation theory of finite Abelian groups, for which we refer to [SS03, Chapter 7]. Since G is Abelian, $V_{\mathbb{C}}$ splits as a direct sum of simultaneous eigenspaces of all $g \in G$, that is, we have

$$V_{\mathbb{C}} = \bigoplus_{\chi \in G^{\vee}} V_{\chi},$$

where χ runs over the set G^{\vee} of group homomorphisms $(G, +) \rightarrow (\mathbb{C}, \cdot)$ (called the *character group* of G), and where V_{χ} is the subspace of V defined as

$$V_{\chi} := \{v \in V_{\mathbb{C}} \mid gv = \chi(g)v \text{ for all } g \in G\}.$$

Distinct V_{χ} are orthogonal with respect to the complexification of $(\cdot|\cdot)$ to a Hermitian inner product, and as $V_{\mathbb{C}}$ is isomorphic to the *regular representation* of G , each V_{χ} is one dimensional. More explicitly, being a group homomorphism, $\chi \in G^{\vee}$ is determined by its values ζ_1, \dots, ζ_d on the generators $(1, 0, \dots, 0), \dots, (0, \dots, 0, 1)$ of G . Each ζ_i is an n_i th root of unity, and the space V_{χ} is spanned by the element of $V_{\mathbb{C}}$ whose value at (g_1, \dots, g_d) equals $\zeta_1^{-g_1} \cdots \zeta_d^{-g_d}$. Note that this function is just the multiplicative inverse χ^{-1} of χ , which equals the complex conjugate $\bar{\chi}$ since the ζ_i lie on the unit circle.

Since A is a linear combination of the group elements, it acts by scalar multiplication on each V_{χ} , and the scalar equals

$$\lambda(\chi) := \sum_{g \neq 0} u(g, 0)\chi(g).$$

Note that this is the (discrete) *Fourier transform* of the function $G \rightarrow \mathbb{C}$, $g \mapsto u(g, 0)$. As noted before, this is a real number, since

$$\overline{\lambda(\chi)} = \sum_{g \neq 0} u(g, 0) \overline{\chi(g)} = \sum_{g \neq 0} u(g, 0) \chi(-g) = \lambda(\chi),$$

where the second equality follows from the fact that $\overline{\chi(g)} = \chi(g)^{-1} = \chi(-g)$, and where we have used the symmetry and G -invariance of u in the last step. This computation also shows that $\lambda(\overline{\chi})$ equals $\lambda(\chi)$. Thus the real vector space V splits as a direct sum

$$V = \bigoplus_{\{\chi, \overline{\chi}\}} V_{\{\chi, \overline{\chi}\}}$$

over unordered pairs of a character and its conjugate (which may coincide), where $V_{\{\chi, \overline{\chi}\}}$ is the real space of real-valued vectors in the complex space $V_\chi + V_{\overline{\chi}}$. Here the direct sum is in fact orthogonal, each summand is one dimensional or two dimensional according to χ being real or nonreal, and each summand has corresponding A -eigenvalue $\lambda(\chi)$. As a special case, the trivial character $\mathbf{1}$ sending every element of G to 1 is real, and the vector space $V_{\{\mathbf{1}\}}$ is spanned by the all-one vector $\mathbf{1}$. Now we can solve fractional energy minimization as follows.

PROPOSITION 2.5. *Let λ_{\min} be the smallest value of $\lambda(\chi)$ as χ ranges over the nontrivial characters. Then the set of optimal solutions of fractional energy minimization consists of all vectors of the form $\frac{p}{|G|}\mathbf{1} + y$, where y belongs to the eigenspace of A in V with eigenvalue λ_{\min} , is perpendicular to $\mathbf{1}$, and satisfies $(y|y) = p - p^2/|G|$.*

Note that the condition that y be perpendicular to $\mathbf{1}$ is automatic if $\lambda_{\min} < \lambda(\mathbf{1})$, because eigenvectors corresponding to distinct eigenvalues are perpendicular. In this case the set of optimal solutions forms a sphere whose dimension equals the multiplicity of λ_{\min} minus one, embedded in the affine hyperplane where $(x|\mathbf{1}) = p$. If λ_{\min} happens to equal $\lambda(\mathbf{1})$, then the dimension of that sphere of optimal solutions equals the multiplicity of λ_{\min} minus two.

Proof. Consider any feasible solution x . The condition $(x|\mathbf{1}) = p$ means that x can be written as $\frac{p}{|G|}\mathbf{1}$ plus y with y in the direct sum of all $V_{\{\chi, \overline{\chi}\}}$ with χ nontrivial. The condition that $(x|x) = p$ translates into the condition $(y|y) = p - p^2/|G|$ on the norm of y . Let $y_{\{\chi, \overline{\chi}\}}$ be the component of y in $V_{\{\chi, \overline{\chi}\}}$. Then, by orthogonality,

$$(x|Ax) = \left(\frac{p}{|G|}\mathbf{1} + y \middle| A \left(\frac{p}{|G|}\mathbf{1} + y \right) \right) = \lambda(\mathbf{1}) \frac{p^2}{|G|} + \sum_{\{\chi, \overline{\chi}\} \text{ nontrivial}} \lambda(\chi) \|y_{\{\chi, \overline{\chi}\}}\|^2.$$

For this expression to be minimal among all y with squared norm $p - p^2/|G|$ it is necessary and sufficient that all components $y_{\{\chi, \overline{\chi}\}}$ for which $\lambda(\chi)$ is not equal to λ_{\min} are zero. This proves the proposition. \square

Example 2.6 (continuation of Example 2.4). In this case a character $\chi \in G^V$ is determined by its values $\zeta_1 := \chi(1, 0)$ and $\zeta_2 := \chi(0, 1)$, and these complex numbers must satisfy $\zeta_1^4 = \zeta_2^4 = 1$. Conversely, any such pair determines a character, which maps the pair $(g_1, g_2) \in (\mathbb{Z}/4)^2$ to $\zeta_1^{g_1} \zeta_2^{g_2}$. The eigenvalue $\lambda(1, i)$ of A , for instance,

equals

$$\begin{aligned} \lambda(1, i) &= \sum_{(g_1, g_2) \in (\mathbb{Z}/4)^2 \setminus \{(0,0)\}} \frac{1}{\delta((0,0), (g_1, g_2))} 1^{g_1} \cdot i^{g_2} \\ &= \left(0 + i - \frac{1}{2} - i\right) + \left(1 + \frac{i}{2} - \frac{1}{3} - \frac{i}{2}\right) \\ &\quad + \left(\frac{1}{2} + \frac{i}{3} - \frac{1}{4} - \frac{i}{3}\right) + \left(1 + \frac{i}{2} - \frac{1}{3} - \frac{i}{2}\right) \\ &= \frac{13}{12}. \end{aligned}$$

All further eigenvalues of the energy kernel A are recorded in the following table:

		ζ_2			
	$12 \cdot \lambda(\zeta_1, \zeta_2)$	1	i	-1	$-i$
ζ_1	1	103	13	-9	13
	i	13	-9	-19	-9
	-1	-9	-19	-25	-19
	$-i$	13	-9	-19	-9

This shows that $\lambda(1, 1)$ is the maximal eigenvalue, with a one-dimensional eigenspace spanned by $\mathbf{1}$; and $\lambda(-1, -1)$ is the minimal eigenvalue, with a one-dimensional eigenspace spanned by

$$z = ((g_1, g_2) \mapsto (-1)^{g_1} \cdot (-1)^{g_2}) = \begin{bmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{bmatrix}.$$

Hence fractional energy minimization has two optimal solutions (forming a zero-dimensional sphere). For $p = 4$ these are $\frac{1}{4}\mathbf{1} \pm \frac{\sqrt{3}}{4}z$. Both of these solutions have irrational, and even negative, entries, so we cannot conclude anything for the total energy minimization problem from this. Of course, a brute-force computer search over all configurations of $p = 4$ particles on G is possible in this case. Such a search reveals that, up to translations, the following three characteristic vectors are the ones minimizing the total energy:

$$\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

Note that the first two are each other's images under swapping rows and columns, and that they represent the cyclic subgroups of G generated by $(2, 1)$ and $(1, 2)$, respectively. The last one is not a coset of a subgroup, but still has the property that the energies experienced by all particles are the same. This means that these configurations also minimize the maximal energy. We conclude that for $p = 4$ the optimal solution to the fractional energy minimization problem has little bearing on the original discrete optimization problem, and it would be very interesting to find a strengthening of our relaxation that does give the optimal solutions for $p = 4$.

On the other hand, consider now $p = 8 = |G|/2$. Then the optimal solutions for fractional energy minimization are $\frac{1}{2}\mathbf{1} \pm \frac{1}{2}z$, and these are exactly the characteristic vectors of the two checkerboard patterns. Since fractional energy minimization is a

relaxation of total energy minimization, this proves that the checkerboard patterns also minimize total energy E_{tot} . And since they are cosets of a subgroup, the argument given after the introduction of E_{tot} shows that the checkerboard patterns are also the (unique) minimizers of E_{max} . We have thus *proved* our first instance of the checkerboard conjecture.

In the following three sections we follow exactly the same strategy: we determine the minimal eigenvalue of the energy kernel, use Proposition 2.5 to derive the optimal solutions of fractional energy minimization, and when these are the checkerboard patterns, then we are done. This works in quite a number of cases—in particular, when each n_i is either two or a multiple of four; see section 5—but not in general; see section 6.

We conclude this section by relating our techniques and results to existing literature on energy minimization. The most relevant reference is [CK07], which is primarily concerned with energy minimization of repelling particles on high-dimensional spheres. There are close parallels between our approach and the techniques there. In particular, both papers make essential use of the representation theory of the natural symmetry group of the problem. In our case this is the group G itself, while in the spherical case it is the orthogonal group. The fact that G is Abelian (and hence diagonalizable) makes the representation theory much easier than that required for the spherical problem. On the other hand, there are also important distinctions. First of all, [CK07] makes essential use of the fact that the symmetry group acts distance transitively, while our group G acts only simply transitively on itself. Second, while [CK07] deals with continuous optimization problems, our optimization problem is inherently of a discrete nature. It could be strengthened into a continuous problem by letting $\frac{n_1 \cdots n_d}{2}$ particles move on the continuous torus $\mathbb{R}^d / (n_1 \mathbb{Z} \times \cdots \times n_d \mathbb{Z})$. If the energy-minimizing configurations for that problem are (unique up to translation and) equal to our checkerboard configurations, then that implies our results (provided that one uses the 1-norm, which is the continuous analogue of the Lee distance). It would be interesting to know if the techniques from [CK07] can be used to prove such a stronger statement. Note that the preimage in \mathbb{R}^d of the particles' positions form a periodic set. The paper [CK07] does discuss optimization problems for such sets, but in the context where the lattice of periodicity is allowed to vary, as well. In our case, the lattice is fixed to $n_1 \mathbb{Z} \times \cdots \times n_d \mathbb{Z}$.

Another, more recent reference is [CZ12], which deals with energy minimization for a large class of error-correcting codes. One of the main differences with our work is that [CZ12] uses the Hamming distance rather than the Lee distance. Again, this results in a non-Abelian, but distance-transitive symmetry group.

Our minimization problem is also reminiscent of certain instances of the *quadratic assignment problem* that are studied in [BÇRW98]. In that paper it is proved that the class of those instances is NP-complete. In view of this, minimality of checkerboard configurations is an interesting result. On the other hand, in [BÇRW98] the corresponding *maximization* problem is proved to be solvable in polynomial time. In our setting, this would correspond to taking for u some *increasing* function of the distance, which has an interpretation in terms of *attracting* particles rather than repelling ones. This problem, in turn, resembles the problem of *how to build an optimal city* [BBDF04]. Our attention, however, is focused entirely on the setting where u is some *decreasing* function of the Lee distance.

3. The one-dimensional case. The first special case that we consider is the one-dimensional toric grid. That is, we consider $G = (\mathbb{Z}/n)$, with n a positive integer,

and define a graph on G by connecting elements that differ by ± 1 . One can think of this as n equally spaced points on a circle. Further we define the function $u : G \times G \setminus \Delta \rightarrow \mathbb{R}_+$ as $u(g, h) := f(\delta(g, h))$, where $\delta(g, h)$ denotes the Lee distance between g and h and $f : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a decreasing strictly convex function. In [Göt03] the continuous problem of letting particles move on a circle is considered and it is shown that total energy is minimized if and only if the particles are equally spaced. This validates the checkerboard conjecture for this special case.

The proof in [Göt03] is based on a direct comparison between the total energy in the configuration with equally spaced particles (i.e., the checkerboard configuration and its translations) and the total energy in any other configuration. To get a better feeling for the technique of section 2 we now assume $f(x) = x^{-1}$ and prove that fractional energy is uniquely minimized as well by the checkerboard vectors. That is, we will prove the following result.

THEOREM 3.1. *Assume that n is a multiple of 2, set $G := \mathbb{Z}/n$, and assume that $f(x) = x^{-1}$. Then the fractional energy $(x|Ax)$ over all $x \in V = \mathbb{R}^G$ with $(x|x) = (x|\mathbf{1}) = n/2$ is minimized by the characteristic vectors $x_{S_{\text{even}}}$ and $x_{S_{\text{odd}}}$ of the checkerboard configurations*

$$S_{\text{even/odd}} := \{g \in G \mid g \text{ even/odd}\},$$

and only by these. As a consequence, both the total energy and the maximal energy among all subsets $S \subseteq G$ with $|S| = n/2$ are uniquely minimized by S_{even} and S_{odd} .

By Proposition 2.5 we know that the set of optimal solutions of the fractional energy minimization problem is determined by the smallest eigenvalue of the energy kernel A . As discussed in section 2 the eigenvalues are functions on the dual group $G^\vee = C_n$, with C_n the group of complex n th roots of unity. And the fractional energy is uniquely minimized by the checkerboard vectors if the eigenvalue has a unique minimum at -1 , which lives in G^\vee as n is even. Thus the following proposition implies Theorem 3.1.

PROPOSITION 3.2. *The function $\lambda : G^\vee \rightarrow \mathbb{R}$,*

$$\lambda(\chi) = \sum_{g \neq 0} \delta(g, 0)^{-1} \chi^g$$

has a unique minimum at $\chi = -1$.

Proof. As n is even we can write

$$\lambda(\chi) = \sum_{k=1}^{n/2-1} \frac{1}{k} (\chi^{-k} + \chi^k) + \frac{2}{n} \chi^{n/2}.$$

Now note that the n elements of the group C_n can be represented by $e^{2\pi i j/n}$ for $j \in \mathcal{J} = \{0, \dots, n-1\}$. With a slight abuse of notation we can thus write

$$\lambda(j) = \sum_{k=1}^{n/2-1} \frac{1}{k} 2 \cos\left(\frac{2\pi j k}{n}\right) + \frac{2}{n} (-1)^j.$$

So, we need to prove that $\operatorname{argmin} \lambda = \frac{n}{2}$. To this end, define $\kappa : [0, n) \rightarrow \mathbb{R}$ by

$$\kappa(x) = \sum_{k=1}^{n/2-1} \frac{1}{k} 2 \cos\left(\frac{2\pi x k}{n}\right) + \frac{2}{n} \cos(\pi x);$$

this equals $\lambda(x)$ when x lies in \mathcal{J} , so $\operatorname{argmin} \kappa = \frac{n}{2}$ implies $\operatorname{argmin} \lambda = \frac{n}{2}$. To prove

that $\operatorname{argmin} \kappa = \frac{n}{2}$, we differentiate κ and obtain

$$\kappa'(x) = \frac{-4\pi}{n} \sum_{k=1}^{n/2-1} \sin\left(\frac{2\pi x k}{n}\right) - \frac{2\pi}{n} \sin(x\pi).$$

To simplify this expression note that

$$\sum_{k=1}^m \sin(kx) = \frac{\cos\left(\frac{x}{2}\right) - \cos\left(\left(m + \frac{1}{2}\right)x\right)}{2 \sin\left(\frac{x}{2}\right)},$$

as can be proved using the prosthaphaeresis formula

$$\sin\left(\frac{x}{2}\right) \sin(kx) = \frac{\cos\left(\left(k - \frac{1}{2}\right)x\right) - \cos\left(\left(k + \frac{1}{2}\right)x\right)}{2}.$$

We thus find

$$\begin{aligned} \kappa'(x) &= \frac{-4\pi}{n} \frac{\cos\left(\frac{\pi x}{n}\right) - \cos\left(\frac{(n-1)\pi x}{n}\right)}{2 \sin\left(\frac{\pi x}{n}\right)} - \frac{2\pi}{n} \sin(\pi x) \\ &= \frac{-4\pi}{n} \frac{\cos\left(\frac{\pi x}{n}\right) - (\cos(\pi x) \cos\left(\frac{\pi x}{n}\right) + \sin(\pi x) \sin\left(\frac{\pi x}{n}\right))}{2 \sin\left(\frac{\pi x}{n}\right)} - \frac{2\pi}{n} \sin(\pi x) \\ &= \frac{2\pi}{n} (\cos(\pi x) - 1) \frac{\cos\left(\frac{\pi x}{n}\right)}{\sin\left(\frac{\pi x}{n}\right)}. \end{aligned}$$

Hence, $\kappa'(x) \leq 0$ for $x \in (0, \frac{n}{2})$ and $\kappa'(x) \geq 0$ for $x \in (\frac{n}{2}, n)$. Further, by l'Hôpital's rule, $\lim_{x \rightarrow 0} \kappa'(x) = 0$. Also, $\kappa'(x) < 0$ for $x \in (\frac{n}{2} - 1, \frac{n}{2})$ and $\kappa'(x) > 0$ for $x \in (\frac{n}{2}, \frac{n}{2} + 1)$. Thus κ has a unique minimum at $\frac{n}{2}$, which completes the proof. \square

4. The Hamming cube. In the previous section we considered the one-dimensional toric grid with an arbitrary number of points. In this section we consider the d -dimensional toric grid, but now we will assume that the grid has size two in all dimensions. That is, we consider $G := \prod_{i=1}^d (\mathbb{Z}/2) = \{0, 1\}^d$. Further we define a graph on G by connecting two elements if they differ by $(0, \dots, 0, 1, 0, \dots, 0)$ for some position of the 1. One can think of this graph as the d -dimensional unit hypercube; the corners of this hypercube are the points of the toric grid. In fact, one should construct a d -torus from the d -dimensional hypercube, but this only connects corners that are connected already, as our grid has size two in every dimension.

Let $f : \mathbb{Z}_+ \rightarrow \mathbb{R}_+$ be such that its m th forward difference has sign $(-1)^m$, i.e., we assume that

$$(4.1) \quad (-1)^m \Delta^m [f](x) > 0$$

for all $x \in \mathbb{Z}_+$. Here Δ denotes the forward difference, $\Delta[f](x) = f(x + 1) - f(x)$.

We now define the function $u : G \times G \setminus \Delta \rightarrow \mathbb{R}_+$ as $u(g, h) := f(\delta(g, h))$, where $\delta(g, h)$ denotes the Lee distance between g and h (which in this case equals the Hamming distance). We will validate the checkerboard conjecture for this case. That is, we will prove the following theorem.

THEOREM 4.1. *Set $G := (\mathbb{Z}/2)^d$ and assume that f satisfies (4.1). Then the fractional energy $(x|Ax)$ over all $x \in V = \mathbb{R}^G$ with $(x|x) = (x|\mathbf{1}) = |G|/2 = 2^{d-1}$ is*

minimized by the characteristic vectors $x_{S_{\text{even}}}$ and $x_{S_{\text{odd}}}$ of the checkerboard configurations

$$S_{\text{even/odd}} := \{(g_1, \dots, g_d) \in G \mid \sum_i g_i \text{ even/odd}\},$$

and only by these. As a consequence, both the total energy and the maximal energy among all subsets $S \subseteq G$ with $|S| = 2^{d-1}$ are uniquely minimized by S_{even} and S_{odd} .

To prove Theorem 4.1 we again capitalize on Proposition 2.5 and determine the smallest eigenvalue of the energy kernel A . As the toric grid has size two in all dimensions we know by the discussion in section 2 that the eigenvalues are functions of the dual group $G^\vee = \{-1, 1\}^d$. We further know that the fractional energy is minimized by the checkerboard vectors if the eigenvalue has a unique minimum at $(-1, \dots, -1) \in G^\vee$. This we prove in the following proposition, which thus implies Theorem 4.1.

PROPOSITION 4.2. *The function $\lambda : G^\vee \rightarrow \mathbb{R}$,*

$$\lambda(\chi) = \sum_{g \neq 0} f(\delta(g, 0)) \prod_{i=1}^d \chi_i^{g_i}$$

has a unique minimum at $\chi = (-1, \dots, -1)$.

Proof. Because of symmetry it suffices to prove that if $\chi, \tilde{\chi} \in \{-1, 1\}^d$ are characters that differ only in the first position, where $\chi_1 = 1, \tilde{\chi}_1 = -1$, then $\lambda(\chi) > \lambda(\tilde{\chi})$. We therefore compute

$$\begin{aligned} \lambda(\chi) - \lambda(\tilde{\chi}) &= \sum_{g \neq 0} f(\delta(g, 0))(1 - (-1)^{g_1})\chi_2^{g_2} \cdots \chi_d^{g_d} \\ &= 2 \sum_{g=(g_2, \dots, g_d)} f(\delta(g, 0) + 1)\chi_2^{g_2} \cdots \chi_d^{g_d}. \end{aligned}$$

Write q for the number of ones among the χ_2, \dots, χ_d , use dummy variable $l \in \{0, \dots, q\}$ for the number of indices j with $\chi_j = g_j = 1$, and use dummy variable $k \in \{0, \dots, d-1-q\}$ for the number of indices j with $\chi_j = -1$ and $g_j = 1$. Then the product $\chi_2^{g_2} \cdots \chi_d^{g_d}$ equals $(-1)^k$; $\delta(g, 0)$ equals $l+k$; and grouping together terms with equal k and l the above expression becomes

$$\begin{aligned} &2 \sum_{l=0}^q \binom{q}{l} \sum_{k=0}^{d-1-q} f(l+k+1) \binom{d-1-q}{k} (-1)^k \\ &= 2 \sum_{l=0}^q \binom{q}{l} (-1)^{d-1-q} (\Delta^{d-1-q} f)(l+1) \\ &> 0, \end{aligned}$$

where the last inequality follows from the conditions on f and the last equality follows from the formula

$$\Delta^m[f](x) = \sum_{k=0}^m \binom{m}{k} (-1)^{m+k} f(x+k);$$

see, for instance, [Rio79, p. 203, equation 1a]. This proves the proposition. \square

5. Multiples of four. In this section we prove our strongest result about the checkerboard conjecture, concerning $(n_1 \cdots n_d)/2$ particles on the Abelian group $G = (\mathbb{Z}/n_1\mathbb{Z}) \times \cdots \times (\mathbb{Z}/n_d\mathbb{Z})$ when each n_i is either two or a multiple of four. Define a

graph on G by connecting two elements if they differ by $\pm(0, \dots, 0, 1, 0, \dots, 0)$ for some position of the 1. The Lee distance is the shortest-path distance between $g, h \in G$ in that graph, and denoted by $\delta(g, h)$. The energy will be measured with a function $f : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ that we assume to be (strictly) *completely monotonic*, i.e., C^∞ and with $(-1)^k f^{(k)}(x) > 0$ for all $x \in \mathbb{R}_+$ and for all k .

Remark 5.1. Typical examples of completely monotonic f are $f(x) = x^{-\alpha}$ for α a positive real number. These functions appear prominently in the paper [CK07], as well. Moreover, as mentioned in the introduction, these function generalize the inverse square law in physics, and describe the path loss for electromagnetic waves.

Remark 5.2. Note that if $g : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is completely monotonic, then so is $-\Delta g$ because

$$(-1)^k (-\Delta g)^{(k)}(x) = (-1)^k (g^{(k)}(x) - g^{(k)}(x+1)) = (-1)^{k+1} \int_x^{x+1} g^{(k+1)}(t) dt > 0$$

for all $x > 0$. Iterating, we find that $(-\Delta)^k g$ is a positive function, so that the restriction of g to \mathbb{Z}_+ satisfies the condition on f . In particular, Theorem 4.1 implies the special case of the upcoming Theorem 5.3 where all n_i are equal to 2.

Define the function $u : G \times G \setminus \Delta \rightarrow \mathbb{R}_+$ as $u(g, h) := f(\delta(g, h))$. The maximal energy E_{\max} , the total energy E_{tot} , the energy kernel A , and the fractional energy are defined using this function u .

THEOREM 5.3. *Assume that each of n_1, \dots, n_d is either 2 or a multiple of 4. Then the fractional energy $(x|Ax)$ over all $x \in V = \mathbb{R}^G$ with $(x|x) = (x|\mathbf{1}) = |G|/2$ is minimized by the characteristic vectors $x_{S_{\text{even}}}$ and $x_{S_{\text{odd}}}$ of the checkerboard configurations*

$$S_{\text{even/odd}} := \{(j_1, \dots, j_d) \mid \sum_i j_i \text{ even/odd}\},$$

and only by these. As a consequence, both the total energy and the maximal energy among all subsets $S \subseteq G$ with $|S| = |G|/2$ are uniquely minimized by S_{even} and S_{odd} .

By Proposition 2.5 it suffices to find the smallest eigenvalue of the energy kernel A . Recall that the eigenvalues are functions on the dual group G^\vee , which in our present setting we may identify with $G^\vee = C_{n_1} \times \dots \times C_{n_d}$, where C_a is the group of complex a th roots of unity. Since all n_i are even, G^\vee contains the real character $-\mathbf{1} = (-1, \dots, -1)$, with character space $V_{\{-1\}}$ spanned by the vector z defined by $z(j_1, \dots, j_d) = (-1)^{j_1 + \dots + j_d}$. The checkerboard configurations have characteristic vectors $\frac{1}{2}\mathbf{1} \pm \frac{1}{2}z$. Thus the following proposition implies Theorem 5.3.

PROPOSITION 5.4. *The function $G^\vee \rightarrow \mathbb{R}$ sending χ to*

$$\sum_{g \neq 0} f(\delta(g, 0)) \chi(g)$$

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

Proof. The completely monotonic function f can be written as

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

where α is nondecreasing and the integral converges for $0 < x < \infty$ (for this theorem of Bernstein see [Wid41, Chapter IV, Theorem 12b]). Thus, after interchanging the

integral and (finite) sum the function that we seek to minimize is seen to equal

$$\chi \mapsto \int_0^\infty \left(\sum_{g \neq 0} e^{-\delta(g,0)t} \chi(g) \right) d\alpha(t).$$

For this function to have a unique minimum at $\chi = (-1, \dots, -1)$ it suffices that for each fixed $t > 0$ the function

$$G^\vee \rightarrow \mathbb{R}, \chi \mapsto \sum_{g \neq 0} e^{-\delta(g,0)t} \chi(g)$$

has a unique minimum at $\chi = (-1, \dots, -1)$. At this point, there is no harm in including $g = 0$ in the sum, which adds a constant term 1 independently of χ . Writing $a := e^t > 1$, we want to minimize

$$\sum_g a^{-\delta(g,0)} \chi(g)$$

over all characters χ . Write $g = (g_1, \dots, g_d)$; then the Lee distance $\delta(g, 0)$ equals $\delta(g_1, 0) + \dots + \delta(g_d, 0)$, where we use the notation d also for the Lee distance in the individual $\mathbb{Z}/n_i\mathbb{Z}$. Hence we have

$$\sum_g a^{-\delta(g,0)} \chi(g) = \sum_{(g_1, \dots, g_d)} a^{-(\delta(g_1,0) + \dots + \delta(g_d,0))} \chi_1(g_1) \cdots \chi_d(g_d),$$

which factorizes as the product of the factors

$$\sum_{g_i \in \mathbb{Z}/n_i} a^{-\delta(g_i,0)} \chi_i(g_i)$$

for $i = 1, \dots, d$. Thus we are done if we can show that each of these factors is positive for all χ_i , and minimal at $\chi_i = -1$.

What remains is an easy calculation. Simplify notation by fixing i and writing $n := n_i$. As a warm-up, consider the case where $n = 2$. Then the trivial character 1 of $\mathbb{Z}/2\mathbb{Z}$ is mapped to $1 + a^{-1}$, while the character -1 of $\mathbb{Z}/2\mathbb{Z}$ is mapped to $1 - a^{-1}$. The latter value is smaller than the former, as desired. Next assume that n is divisible by 4, and consider the function $\lambda : C_n \rightarrow \mathbb{R}$ sending an n th root of unity ζ to

$$\begin{aligned} & \sum_{g \in \mathbb{Z}/n\mathbb{Z}} a^{-\delta(g,0)} \zeta^g \\ &= 1 + \sum_{g=1}^{n/2-1} a^{-g} (\zeta^g + \zeta^{-g}) + a^{-n/2} \zeta^{n/2} \\ &= -1 + \sum_{g=0}^{n/2-1} a^{-g} (\zeta^g + \zeta^{-g}) + a^{-n/2} \zeta^{n/2} \\ &= \frac{1 - a^{-n/2} \zeta^{n/2}}{1 - a^{-1} \zeta} + \frac{1 - a^{-n/2} \zeta^{-n/2}}{1 - a^{-1} \zeta^{-1}} - (1 - a^{-n/2} \zeta^{n/2}). \end{aligned}$$

Now $\zeta^{n/2}$ equals ± 1 . If it equals 1, then this expression reduces to

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

Since $a > 1$, this is a positive number for any ζ , and its smallest value is attained for the $n/2$ th root of unity ζ_0 furthest away from 1 in the complex plane, which equals -1

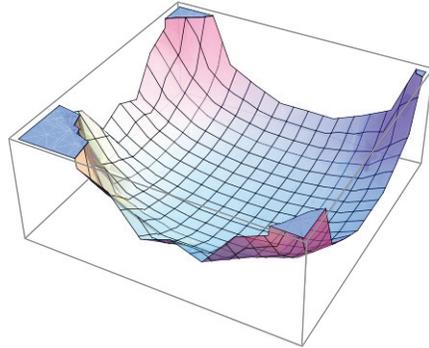


FIG. 5.1. Eigenvalues of the energy kernel (interpolated to make an easily interpretable surface, and truncated near the corners).

since n is a multiple of 4. Next, if $\zeta^{n/2}$ equals -1 , then the expression above reduces to

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

which is again positive for all ζ with $\zeta^{n/2} = -1$ and minimal for the ζ_1 furthest away from 1 in the complex plane (which equals $-e^{\pm 2\pi i/n}$).

It remains to compare $\lambda(\zeta_0)$ and $\lambda(\zeta_1)$. For this, note that the factor $(1 - a^{-n/2})$ in the expression for $\lambda(\zeta_0)$ is smaller than the factor $(1 + a^{-n/2})$ in the expression for $\lambda(\zeta_1)$, while moreover ζ_0 is further away from 1 than ζ_1 . Hence the minimum is attained at $\zeta = \zeta_0 = -1$, as desired. This concludes the proof of the proposition, and hence the proof of Theorem 5.3. \square

Remark 5.5. The problem in extending this argument to the case of general even n_i is that in the proof of the proposition, when $n/2$ is odd and at least 3, $\lambda(\zeta_1) = \lambda(-1)$ can very well be *larger* than $\lambda(\zeta_0)$. In other words, Proposition 5.4 does not extend to that situation for general completely monotonic functions f . Extensive numerical evidence with $d = 2$ and n_1, n_2 up to 100 suggests that the proposition *does* extend to the case where $f(x) = 1/x$ (and probably even for $f(x) = x^{-\alpha}$ with $\alpha > 0$), in which case also Theorem 5.3 extends.

Of course, the checkerboard conjecture may still very well hold for general completely monotonic f and general even n_i , even when Proposition 5.4 does not. To prove this, one would like to have a combinatorial/algebraic argument why the eigenspaces corresponding to characters χ having some entries equal to the relevant $-\exp(2\pi i/n)$ with $n/2$ odd are no good for finding 0/1-vectors. At this moment we have no such argument.

Remark 5.6. Note that the table of eigenvalues of A contains $|G|$ entries, and evaluating each individually involves a summation over $|G|$, so that a straightforward implementation would require $\mathcal{O}(|G|^2)$ (floating-point) operations. However, the table of eigenvalues is nothing but the *Fourier transform* of the table of values $f(\delta(g, 0))$, so that algorithms for (d -dimensional) *fast Fourier transform* may be used to compute the table of eigenvalues more efficiently. We have used Mathematica's built-in function `Fourier` in our numerical experiments. For instance, Figure 5.1 shows the eigenvalues of the energy kernel for $d = 2$ and $n_1 = n_2 = 10$ and $f(x) = x^{-0.3}$ as a function of (j, k) , standing for the character $(e^{\frac{2\pi i j}{10}}, e^{\frac{2\pi i k}{10}})$. The “rough edges” are related to the

even/odd effect in the proof above, but they smooth out in the middle, so that the minimum is attained at $j = k = 5$, which corresponds to the character $(-1, -1)$.

6. Open problems. In this paper we have proved the checkerboard conjecture for toric grids and energy functions f for which the unique minimal eigenvalue of the energy kernel A is uniquely attained at the character $(-1, \dots, -1)$ in the dual group. Indeed, the minimal eigenvalue of A *always* governs the solution to fractional energy minimization (Proposition 2.5), and if it is uniquely attained at $(-1, \dots, -1)$, then the minimizers of fractional energy minimization are 0/1-vectors and hence minimizers of the original problem. This motivates the following open problems.

6.1. Generalizing Theorem 5.3. One would like to extend the results of section 5 to the case where some of the n_i are larger than 2 but equal to 2 modulo 4. Computer experiments with two-dimensional grids up to 100×100 suggest that for $f(x) = 1/x$ (and perhaps for general inverse power laws) the minimal eigenvalue of the energy kernel is still uniquely attained at $(-1, \dots, -1)$. However, a proof of this fact would require more sophisticated analytical methods than the factoring into one-dimensional instances that we used there. Alternatively, one might try and find a combinatorial argument why the minimizers of total energy minimization are necessarily perpendicular to the eigenspaces of A corresponding to the “undesirable” characters, thus sharpening the relaxation.

6.2. Euclidean or other metrics. The question remains for which metrics, other than the Lee distance, the checkerboard conjecture will hold. For the Euclidean metric the analogue of Proposition 5.4 does not hold for general completely monotonic functions f . The first steps of its proof go through when one replaces the Lee distance with the square of the Euclidean distance. This holds in particular for the all-important factorization step. One is then lead to minimize

$$\sum_{g \in \mathbb{Z}/n} a^{-\delta(g,0)^2} \zeta^g$$

over the n th roots ζ of unity, where δ stands for the Euclidean metric on the one-dimensional toric grid, and where a is a real number greater than 1. However, for a close to 1 the minimum is *not* in general attained at -1 ; see Figure 6.1. On the other hand, extensive numerical evidence for two-dimensional grids up to 100×100 suggest that the analogue of Proposition 5.4 does hold when the energy is given by an

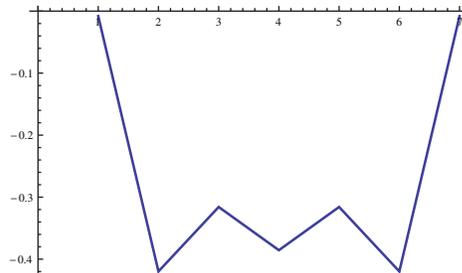


FIG. 6.1. Values (vertical axis) of $\sum_{g \in \mathbb{Z}/8} (1.05)^{-\delta(g,0)^2} \zeta^g$ for $\zeta = \exp(\frac{2k\pi i}{8})$, $k = 1, \dots, 7$ (horizontal axis); $k = 0$ is excluded to make it clear where the minimum is attained: at $k = 2, 6$ rather than $k = 4$.

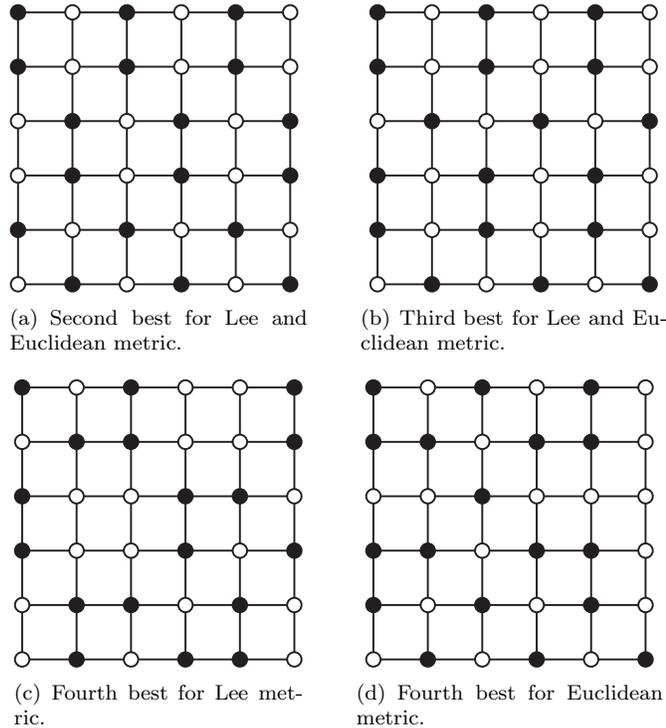


FIG. 6.2. The black nodes denote the nearly optimal configurations for E_{\max} in a 6×6 grid for $f(x) = \frac{1}{x}$.

inverse power law of the Euclidean distance (and if these computations were done in suitable interval arithmetic, they would *prove* the checkerboard conjecture for those grids). Perhaps one can prove such a statement by bounding the contribution, in the Bernstein expansion of these inverse power laws, of the bit where a is small.

The checkerboard conjecture is not true for *every* metric however. For example, for the Chebyshev (or L_∞) metric one can compute that the maximal energy of the patterns in Figures 6.2(a) and 6.2(b) is lower than the maximal energy of the checkerboard pattern in a 6×6 grid. It is unknown what properties a metric should have in order for the checkerboard conjecture to be true.

6.3. Nearly optimal configurations. It is also interesting to consider *nearly optimal* configurations of $n/2$ particles in toric grids. When considering *total energy* E_{tot} , these configurations are probably given by small perturbations of checkerboard patterns. However, nearly optimal configurations for *maximal energy* E_{\max} seem to exhibit beautiful, regular patterns. For example, for a 6×6 grid we have computed the maximal energy of all possible $\binom{36}{18}$ configurations for the function $f(x) = \frac{1}{x}$ and for both the Lee metric and the Euclidean metric. This computation shows not only that the checkerboard conjecture holds (a fact that one can prove more efficiently using the discrete Fourier transform as in Remark 5.6), but also that the second and third best configurations agree for the Lee and Euclidean metrics (see Figures 6.2(a) and 6.2(b)). The fourth best configurations are different for the two metrics though; see Figures 6.2(c) and 6.2(d). It is a widely open question how to prove that certain configurations are second or third best.

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