Formally dual configurations in Euclidean space and in abelian groups

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$$E_f(x) = \sum_{y \in \mathcal{P}, y \neq x} f(|x - y|)$$

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Remark: We usually take $f$ to be a completely monotonic function of squared distance.
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[Cohn-K-Schürmann ’09]: computer simulations for $f(r) = e^{-cr^2}$ for various $c$, dimension $n \leq 8$, number of translates $N \leq 10$. Gradient descent on the space of periodic configurations with fixed number of translates.

We observed very interesting phenomena for $n \geq 5$. For instance, in dimensions 5 and 7, the limit of the energy minimizers for $c \gg 0$ is not the densest lattice packing, but rather a periodic packing! (Disproving a conjecture of Torquato and Stillinger).
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For instance, let $D_n^+$ be $D_n \cup (D_n + (1/2, \ldots, 1/2))$, where $D_n$ is the checkerboard lattice. Let $D_n^+(\alpha)$ be obtained by scaling the last coordinate of every point of $D_n^+$ by the positive real number $\alpha$.

Then $D_n^+(\alpha)$ is formally dual to $D_n^+(1/\alpha)$. 
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Then $D_n^+ (\alpha)$ is formally dual to $D_n^+ (1/\alpha)$.

For $n = 5$, and for $c$ not too close to 1, the global minimum seems to be some $D_5^+ (\alpha)$. 
For any lattice $\Lambda$, we have its dual lattice $\Lambda^* = \{ y \in \mathbb{R}^n \mid \langle x, y \rangle \in \mathbb{Z} \quad \forall x \in \Lambda \}$.

We know $\operatorname{vol}(\mathbb{R}^n / \Lambda^*) = 1 / \operatorname{vol}(\mathbb{R}^n / \Lambda)$, $(\Lambda^*)^* = \Lambda$, etc.
Dual lattices and Poisson summation

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**Poisson summation formula**: For any nice function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ (e.g. Schwartz function),

$$\sum_{x \in \Lambda} f(x) = \frac{1}{\text{vol}(\mathbb{R}^n/\Lambda)} \sum_{y \in \Lambda^*} \hat{f}(y)$$

where $\hat{f}(y) = \int_{\mathbb{R}^n} f(x) e^{2\pi i \langle x, y \rangle} dx$
Can the same hold for periodic configurations $\mathcal{P}$ and $\mathcal{Q}$? i.e. Can we have

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But we’re really only interested in $\mathcal{P} - \mathcal{P} = \{x - y : x, y \in \mathcal{P}\}$, since if

$$
\Sigma(f, \mathcal{P}) := \frac{1}{N} \sum_{i,j} \sum_{x \in \Lambda} f(x + v_i - v_j)
$$

then $E_f(\mathcal{P}) = \Sigma(f, \mathcal{P}) - f(0)$. 
Say $\mathcal{P}$ and $\mathcal{Q}$ are formal duals if $\Sigma(f, \mathcal{P}) = \delta(\mathcal{P})\Sigma(\hat{f}, \mathcal{Q})$ for every Schwartz function $f : \mathbb{R}^n \to \mathbb{R}$ (we do not omit the diagonal).
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Note: this implies (and is stricter than) the “classical” notion of a formal dual:

For binary codes, the weight enumerators are related by MacWilliams identities.
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For periodic configurations, the average theta functions are related by the modular transformation $z \rightarrow -1/z$. This follows by analytic continuation from

$$E_f(\mathcal{P}) + 1 = \delta \cdot (1 + E_{\hat{f}}(\mathcal{Q}))$$

when $f(x) = \exp(-\pi c|x|^2)$, $\hat{f}(y) = \exp(-\pi |y|^2/c)$.
Theorem (Cohn-K-Schürmann)

$D_n^+(\alpha)$ is formally self-dual when $n$ is odd or $n$ is a multiple of 4. If $n \equiv 2 \pmod{4}$, then $D_n^+$ is formally dual to an isometric copy of itself.
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**Theorem (Cohn-K-Schürmann)**

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**Corollary**

\[ D_n^+(\alpha) \text{ is formally dual to an isometric copy of } D_n^+(1/\alpha). \]

So if \( f \) is radially symmetric, the Gaussian potential energies of these periodic configurations at parameters \( c \) and \( 1/c \) respectively are related.
Remark: if $\mathcal{P}$ and $\mathcal{Q}$ are formally dual, then so are $\phi(\mathcal{P})$ and $\phi^{-1}(\mathcal{Q})$ for any affine transformation $\phi$ of $\mathbb{R}^n$. 
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Poisson summation tells us that

$$\sum(f, \mathcal{P}) = \delta(\mathcal{P}) \sum_{y \in \Lambda^*} \hat{f}(y) \left| \frac{1}{N} \sum_{i=1}^{N} e^{2\pi i \langle v_j, y \rangle} \right|^2.$$
Combinatorial description

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So formal duality really is only a combinatorial property of the group structure and cosets involved. Namely, if $\mathcal{P} = \Lambda + \{v_1, \ldots, v_n\}$ and $\mathcal{Q} = \Gamma + \{w_1, \ldots, w_n\}$, we need for every $y \in \Lambda^*$:

$$
\sum_{y \in \Lambda^*} \left| \frac{1}{N} \sum_{i=1}^{N} e^{2\pi i \langle v_j, y \rangle} \right|^2 = \frac{1}{M} \# \{(x, j, k) \in \Gamma \times [M] \times [M] : y = x + w_j - w_k\}.
$$
We can reformulate everything now in terms of abelian groups. Letting \( Q \) be \( M \) translates \( w_1, \ldots, w_M \) of a lattice \( \Gamma \), it is not hard to check that \( v_1, \ldots, v_N \) lie in \( \Gamma^* \).
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Let $G = \Gamma^*/\Lambda$ and its dual $\hat{G} = \Lambda^*/\Gamma$. We are then looking for subsets $S$ of $G$ and $T$ of $\hat{G} = \text{Hom}(G, \mathbb{C}^*)$ such that

$$\left| \sum_{v \in S} \langle v, y \rangle \right|^2 = \frac{N^2}{M} \# \{ (w, w') \in T \times T : y = w - w' \}$$

for every $y \in \hat{G}$.

It automatically follows that duality is a symmetric relation.
The simplest example is of course $G = \hat{G} = \{0\}$ and $S = T = \{0\}$.

The next simplest example, from which $D_n^+$ arises by a taking a product with $n - 1$ copies of the first example, is the following:

Take $G = \hat{G} = \mathbb{Z}/4\mathbb{Z}$ and $S = T = \{0, 1\}$. 
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The relevant calculations are:

\[
\begin{align*}
|1 + 1|^2 &= 4 = 2 \cdot \#\{(0, 0), (1, 1)\} \\
|1 + i|^2 &= 2 = 2 \cdot \#\{(1, 0)\} \\
|1 - i|^2 &= 2 = 2 \cdot \#\{(0, 1)\} \\
|1 - 1|^2 &= 0 = 2 \cdot \#\{\} 
\end{align*}
\]

Call this example **TITO** (two-in-two-out).
Cyclic case

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We can show that when $M = N$ is squarefree and odd, there only solutions are the trivial ones, i.e. $S = H$ a subgroup of $G$, and $T = H^\perp$ its annihilator in $\hat{G}$. 
Quadratic examples and Gauss sums

We will now give some examples with $G = \hat{G} = (\mathbb{Z}/p\mathbb{Z})^2$, with the pairing

$$\langle (a, b), (c, d) \rangle = \zeta_p^{ac+bd},$$

where $\zeta_p$ is some fixed primitive $p$-th root of unity.
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Recall that

$$\left| \sum_{n=1}^{p} \zeta_p^{cn^2+dn} \right|^2 = \begin{cases} p^2 & \text{if } p|c, d \\ 0 & \text{if } p|c, p \nmid d \\ p & \text{if } p \nmid c. \end{cases}$$
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Proof is an easy exercise using the basic Gauss sum \( \left| \sum_{n=1}^{p} \zeta_p^{n^2} \right|^2 = p \) and completing squares.
Proposition

\[ S = \{(n^2, n) : 1 \leq n \leq p\} \text{ and } T = \{(n, n^2) : 1 \leq n \leq p\} \text{ are formally dual to each other.} \]
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Proof.

We need to show for every \((c, d) \in [p] \times [p]\) that

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\left| \sum_{n=1}^{p} \sum_{n=1}^{p} \zeta_p^{cn^2+dn} \right|^2 = \frac{p^2}{p} \# \{(j, k) : c = j - k, d = j^2 - k^2\}
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For \(p|c\) this is trivial.

For \(p \nmid c\) it easily follows from the previous page that the LHS is \(p\). So enough to show there is a unique solution \((j, k)\) to \(c = j - k, d = j^2 - k^2\). This is trivial once we observe that \(j + k = d/c\).
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- Conway and Sloane asked whether the Best packing in 10 dimensions has a formal dual. We can at least show it doesn’t have a formal dual in our stronger sense.
- Understanding which Barlow packings may have a formal dual (work in progress).
Thank you!