One-Dimensional Crystals and Quadratic Residues

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The main problem in crystallography is recovering the electronic density from the diffraction peak intensities. The one-dimensional model leads to recover a discrete Fourier series in $\mathbb{Z}_n$ with integral coefficients from its absolute value, which has arithmetical implications. In this paper we prove that the constant absolute value of Gaussian sums determines them among a class of exponential sums. This implies that if diffraction peak intensities are constant except for one of them, then, modulo translations, we obtain a quadratic residue molecule.

1. INTRODUCTION

The spatial configurations of crystallized molecules are usually obtained via x-ray diffraction data. As was first suggested by M. von Laue, when the intensities of the diffracted rays are registered on a flat screen, high peaks appear in a discrete set, revealing the symmetries of the crystal. The standard interpretation assigns diffraction peak intensities to absolute values of the Fourier transform $\hat{\rho}$ of the electron density $\rho$. The phase problem asks for the reconstruction of $\rho$ from the knowledge of $|\hat{\rho}|$. In certain interesting cases this leads naturally to problems of factorization in suitable rings of polynomials (see [6]). For example, if we have a density $\rho = \sum \delta_n$ where $\delta_n$ denotes Dirac’s delta function placed at the integer $n$, then $|\hat{\rho}|$ determines (modulo translations or reflections) $\rho$ if the polynomial $\sum x^n$ is irreducible in $\mathbb{Z}[x]$. This leads to the study of irreducible polynomials with 0, 1 coefficients. In [4] the conjecture that most of these polynomials are irreducible is stated and some other related results are quoted. On the other hand, in general, if the polynomial $\sum x^n$ is not irreducible there is a lack of uniqueness, showing that in general terms the phase problem is not well posed (the first practical example of nonuniqueness was considered in 1930 by Pauling and Shappell [5] who were studying crystals of bixbyte). A rather interesting question is which kind of “chemical,”
“geometric,” or “arithmetic,” information about \( \rho \) is relevant to ensure the reconstruction (see \([3]\) and \([6]\)). A plausible model for the electronic density of one-dimensional (periodic) crystals is given by infinite sums of Dirac’s delta functions (cf. \([2]\))

\[
p = \sum_{j=1}^{N} b_j \sum_{n=-\infty}^{\infty} \delta \left( x_j + n \right),
\]

where \( b_j \in \mathbb{Z}^+ \) are positive integers and \( 0 \leq x_j < 1 \).

In this context, the phase problem seeks to locate the positions \( \{x_j\} \) (modulo translations or reflections \( x_j' = 1 - x_j \)) knowing the absolute values

\[
F(v) = \left| \sum_{j=1}^{N} b_j e^{2\pi i x_j v} \right|, \quad v \in \mathbb{Z}.
\]

The result presented in this paper consists of a new observation about Gaussian sums, i.e., roughly speaking, they are determined by their absolute value among a class of exponential sums. In this way we obtain a nontrivial case in which the phase problem can be solved.

**Notation.** Throughout this paper we shall write \( e(x) \) as an abbreviation of \( e^{2\pi i x} \), and \( (n/p) \), \( p \) prime, will denote the usual Legendre symbol (i.e., +1 if \( n \) is a quadratic residue and \(-1\) if \( n \) is a quadratic nonresidue modulo \( p \)).

### 2. STATEMENT AND PROOF OF THE RESULT

Our result reads as follows:

**Theorem 2.1.** Let \( 0 = x_1 < x_2 < \ldots < x_N < 1 \) be real numbers and assume that there exists a prime number \( p \) such that the sum

\[
S(m) = \sum_{j=1}^{N} b_j e(m x_j), \quad b_j \in \mathbb{Z}^+,
\]

is of constant modulus \( |S(m)| = \Gamma \) if \( p \) is not a divisor of \( m \) and \( |S(m)| = \sum b_j \) otherwise. Then \( px_j \in \mathbb{Z}, 1 \leq j \leq N \), and either

\[
S(m) = A T(m) + B e \left( \frac{m k}{p} \right) G(m) \quad \text{or} \quad S(m) = A T(m) + B e \left( \frac{m k}{p} \right),
\]
where $A, B, k \in \mathbb{Z}$ and

$$T(m) = \sum_{n=0}^{p-1} e\left(\frac{nm}{p}\right), \quad G(m) = \sum_{n=1}^{p-1} e\left(\frac{nm}{p}\right).$$

The proof will be based on the following lemma.

**Lemma 2.2.** If all the algebraic conjugates of $x \in \mathbb{Q}(\zeta)$, $\zeta = e(1/p)$, are complex numbers of equal modulus, then either $x = B\zeta^k$ or $x = B\zeta^{k}$.

**Proof.** Let $\sigma$ be a generator of the Galois group of the extension $\mathbb{Q}(\zeta)/\mathbb{Q}$. Using the hypothesis of the lemma we can write $\sigma(x)/x = e(x)$, for some $x \in \mathbb{Q}$ (if $x \notin \mathbb{Q}$ then $\sigma(x)$ is not an algebraic number [1], i.e., $\sigma(x)/x = \zeta^k$, where $\zeta_k = e(1/b), a, b \in \mathbb{Z}^+$, $(a, b) = 1$.

Taking $a^*$ such that $a^*a \equiv 1 \mod b$ we get that $\zeta_b = (\zeta^a)^{a^*} \in \mathbb{Q}(\zeta)$. We have two cases:

(i) If $p \mid b$, then $[\mathbb{Q}(\zeta) : \mathbb{Q}(\zeta_b)] = \phi(p)/\phi(b)$ yields $b = p$ or $b = 2p$.

(ii) If $p \nmid b$, then $\mathbb{Q}(\zeta) = \mathbb{Q}(\zeta, \zeta_b) = \mathbb{Q}(\zeta, b)$ yields $pb = p$ or $pb = 2p$.

Therefore we have that $b = 1, 2, p, 2p$ and $\zeta^a_b = \pm \zeta^l$ for some integer $l$, $0 \leq l \leq p - 1$.

Let us assume that $\sigma(\zeta) = \zeta^r$, and take $k$ such that $(g - 1) k \equiv l \mod p$, then since $\sigma(x)/x = \pm \zeta^l$, we get

$$\frac{\sigma(\zeta^{-k}x)}{\zeta^{-k}x} = \pm 1, \quad \frac{\sigma^2(\zeta^{-k}x)}{\sigma(\zeta^{-k}x)} = \pm 1.$$

Therefore $\sigma^2(\zeta^{-k}x) = \zeta^{-k}x$.

The subfield invariant under $\sigma^2$ is

$$M = \{a(\sigma^2(\zeta) + \sigma^4(\zeta) + \cdots + \sigma^{p-1}(\zeta)) + b(\sigma(\zeta) + \sigma^2(\zeta) + \cdots + \sigma^p(\zeta)), a, b \in \mathbb{Q}\},$$

hence

$$\zeta^{-k}x = a \sum_{n \in \mathbb{Z}} \zeta^n + b \sum_{n \in \mathbb{Z}} \zeta^n, \quad a, b \in \mathbb{Q},$$

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where $\mathbb{R}$ and $\mathbb{N}$ denote, respectively, the set of quadratic and nonquadratic residues mod $p$.

If $\sigma(\zeta^{-k}x) = \zeta^{-k}x$, $\zeta^{-k}x \in \mathbb{Q}$, if $\sigma(\zeta^{-k}x) = -\zeta^{-k}x$, then we have $b = -a$ and that $\zeta^{-k}x$ is a rational multiple of a Gauss sum.

**Proof of the Theorem.** The identity $|S(p)| = \sum b_j$ implies $e(px_1) = e(px_2) = \cdots = e(px_n)$ and since we have fixed $x_1 = 0$ then we must have $x_j = n_j/p$ for some integers $n_j$, $0 \leq n_j < p$. Therefore $x = S(1)$ is in the hypothesis of the lemma and we get either

$$S(1) = Be\left(\frac{k}{p}\right) G(1) \quad \text{or} \quad S(1) = Be\left(\frac{k}{p}\right).$$

For $m$ prime with $p$ we obtain by conjugation in $\mathbb{Q}(\zeta)$ either

$$S(m) = Be\left(\frac{mk}{p}\right) G(m) \quad \text{or} \quad S(m) = Be\left(\frac{mk}{p}\right).$$

Finally, let us observe that $T(m)$ vanishes if and only if $p \mid m$. Therefore there exists $A \in \mathbb{Q}$ such that either

$$S(m) = AT(m) + Be\left(\frac{mk}{p}\right) G(m) \quad \text{or} \quad S(m) = AT(m) + Be\left(\frac{mk}{p}\right).$$

for every $m \in \mathbb{Z}$.

Identifying coefficients, we deduce easily that $A$ and $B$ are integers.

**REFERENCES**