The Theta Series of the 2D Lattices

Haina Wang*

Department of Chemistry Torquato Lab, Princeton University, Princeton, USA

E-mail: hainaw@princeton.edu

Introduction

The lattice sum is a function that takes the form of a power series whose terms are related to the position of points on a perfect lattice Λ. It has wide applications in crystal physics, *e.g.* facilitating the calculation of lattice energy. The Madelung's constant of an ionic lattice is a special form of lattice sum.[1]

This report considers the *theta series* of a 2D square lattice Λ with the origin O at an arbitrary lattice point. The theta series is given by

$$\Theta_\Lambda(z) = \sum_{m=1}^{\infty} N(m)\mathrm{e}^{\pi i z m} \tag{1}$$

Where z is a complex variable with $\mathrm{Im}(z) > 0$. m runs through all positive integers.[2 3] (Some texts include the term where $m = 0$.) $N(m)$ is the number of lattice points whose distance to O is $\sqrt{m}$. For example, if we assign the nearest-neighbor distance of the square lattice to be 1, *i.e.* if $\Lambda = \mathbb{Z}^2$, then $N(m)$ is simply the number of different integer pairs (k, l) such that $k^2 + l^2 = m$.

We will present the algorithm to generate the theta series of $\mathbb{Z}^2$ and visualize this series as a complex function. Then we will briefly discuss how to treat other primary 2D lattices.

Algorithm

To find $N(m)$ of the lattice $\mathbb{Z}^2$, we examine all integers k such that $0 \le k \le \sqrt{\frac{m}{2}}$. If $m - k^2$ is a square number, we let l to be the integer $\sqrt{m - k^2}$. Note that if l exists, we always have $k \le l$.

Now for each pair (k, l) found this way:

- If $k = 0$, $N(m)$ is increased by 4, because the eligible integer pairs whose squares sum to m are $(0, \pm k)$ and $(\pm k, 0)$;

- Else if $k = l$, $N(m)$ is increased by 4. The elibible integer pairs are $(\pm k, \pm k)$.

- Else, $N(m)$ is increased by 8. The eligible integer pairs are $(\pm k, \pm l)$ and $(\pm l, \pm k)$.

Table 1 shows the values of $N(m)$ of a square lattice for m from 1 to 25.

Table 1: The values of $N(m)$ for the square lattice.

m	$N(m)$	m	$N(m)$	m	$N(m)$
1	4	11	0	21	0
2	4	12	0	22	0
3	0	13	8	23	0
4	4	14	0	24	0
5	8	15	0	25	12
6	0	16	4		
7	0	17	8		
8	4	18	4		
9	4	19	0		
10	8	20	8		

It can be shown that $\Theta_{\mathbb{Z}^2}(z) = (\theta_3(z))^2 - 1$, where $\theta_3(z) = 1 + 2\sum_{m=1}^{\infty} q^{m^2}$, $q = \mathrm{e}^{\pi i z}$.[2]

Convergence criterion

To compute the theta series practically, we also need a "convergence criterion" to decide at which term we can safely stop the summation without losing too much accuracy. Therefore, we examine the magnitude of the terms. Writing $z = x + iy$, where x and y are real and imaginary parts of z, the mth term of $\Theta_\Lambda(z)$ is

$$N(m)\mathrm{e}^{-\pi y m}\mathrm{e}^{i\pi x m} \tag{2}$$

So the norm of the mth term is $N(m)\mathrm{e}^{-\pi y m}$. When $y > 0$, $\mathrm{e}^{-\pi y m}$ decays much faster than the growth of $N(m)$, so to a first approximation, we can regard the magnitudes of the terms to be controlled by $\mathrm{e}^{-\pi y m}$ alone, *i.e.* we ignore $N(m)$ when considering magnitude.

Therefore, to find a reasonable stoping term t, we let $\epsilon > 0$ be a very small number and solve for t such that the "residue" magnitude is less than ϵ.

$$\sum_{m=t}^{\infty} \mathrm{e}^{-\pi y m} \leq \epsilon \tag{3}$$

Whence

$$t \geq \frac{\ln(\epsilon(1-\mathrm{e}^{-\pi y}))}{-\pi y} \tag{4}$$

Taking $t_{\epsilon,y}$ to be the smallest integer that satisfies (4). The theta series can be evaluated as

$$\Theta_{\mathbb{Z}^2}(z) = \sum_{m=1}^{t_{\epsilon,y}} N(m)\mathrm{e}^{\pi i z m} \tag{5}$$

In our program, we set $\epsilon = 10^{-6}$.

Results and discussion

Fig. 1 and 2 show the real and imaginary parts of $\Theta_{\mathbb{Z}^2}(z)$. The plot range is $-3 \leq \mathrm{Re}(z) \leq 3$, $0.05 \leq \mathrm{Im}(z) \leq 0.7$.

Both the real and the imaginary parts of the theta series are periodic in $\mathrm{Re}(z)$, with period 2. For fixed $\mathrm{Im}(z)$, the real part is an even function of $\mathrm{Re}(z)$, with the mirrors at integral values. The imaginary part is an odd function of $\mathrm{Re}(z)$. The inversion centers are integral values of $\mathrm{Re}(z)$.

For fixed $\mathrm{Re}(z)$, the series eventually decreases exponentially with $\mathrm{Im}(z)$.

Also note that the larger $\mathrm{Im}(z)$ is, the simpler is the shape of $\Theta_{\mathbb{Z}^2}(z)$ viewed as a function of $\mathrm{Re}(z)$. When $\mathrm{Im}(z)$ is very large, the real and imaginary parts are essentially cosine and sine curves. As $\mathrm{Im}(z)$ approaches 0, the fluctuation of $\Theta_{\mathbb{Z}^2}(z)$ becomes increasingly complex, resembling a Weierstrass (continuous but nowhere differentiable) function.

When $\mathrm{Re}(z)$ is an integer, $\Theta_{\mathbb{Z}^2}(z)$ is real. It behaves differently for even and odd $\mathrm{Re}(z)$. Fig. 3 plots $\Theta_{\mathbb{Z}^2}(z)$ as a function of $\mathrm{Im}(z)$ for even and odd $\mathrm{Re}(z)$, respectively.

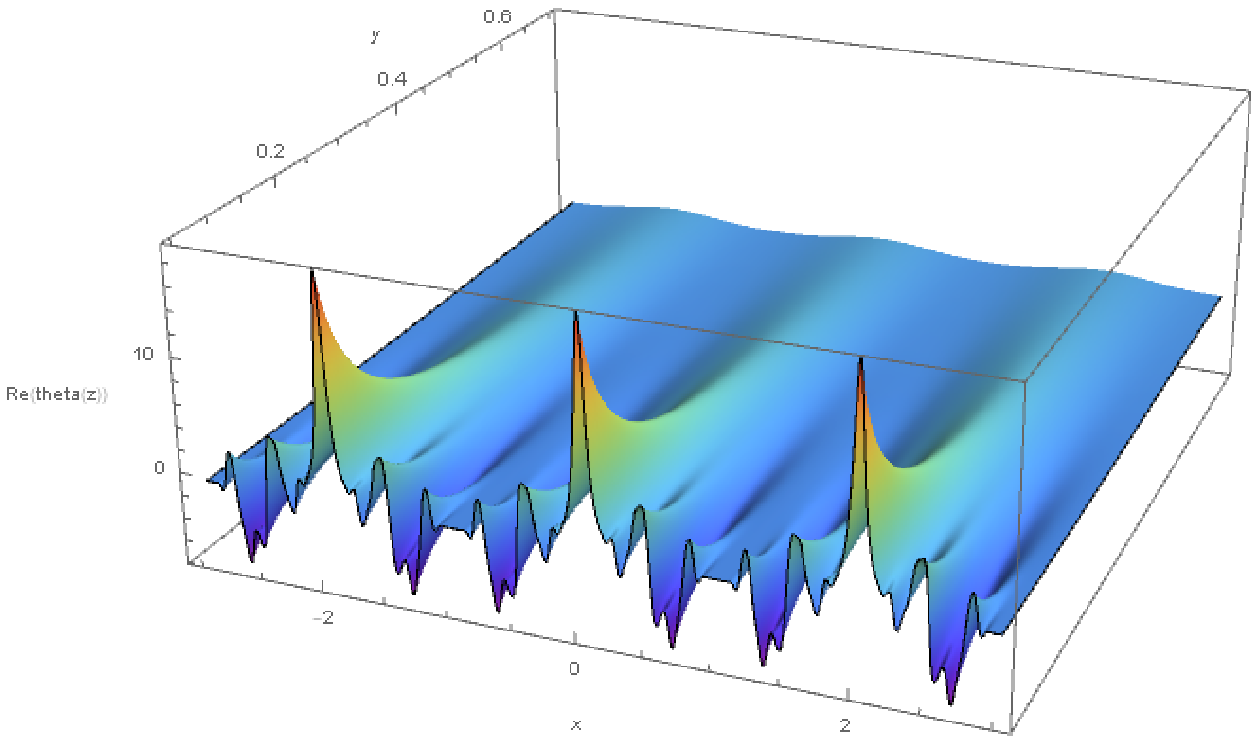

Figure 1: The real part of $\Theta_{\mathbb{Z}^2}(z)$.

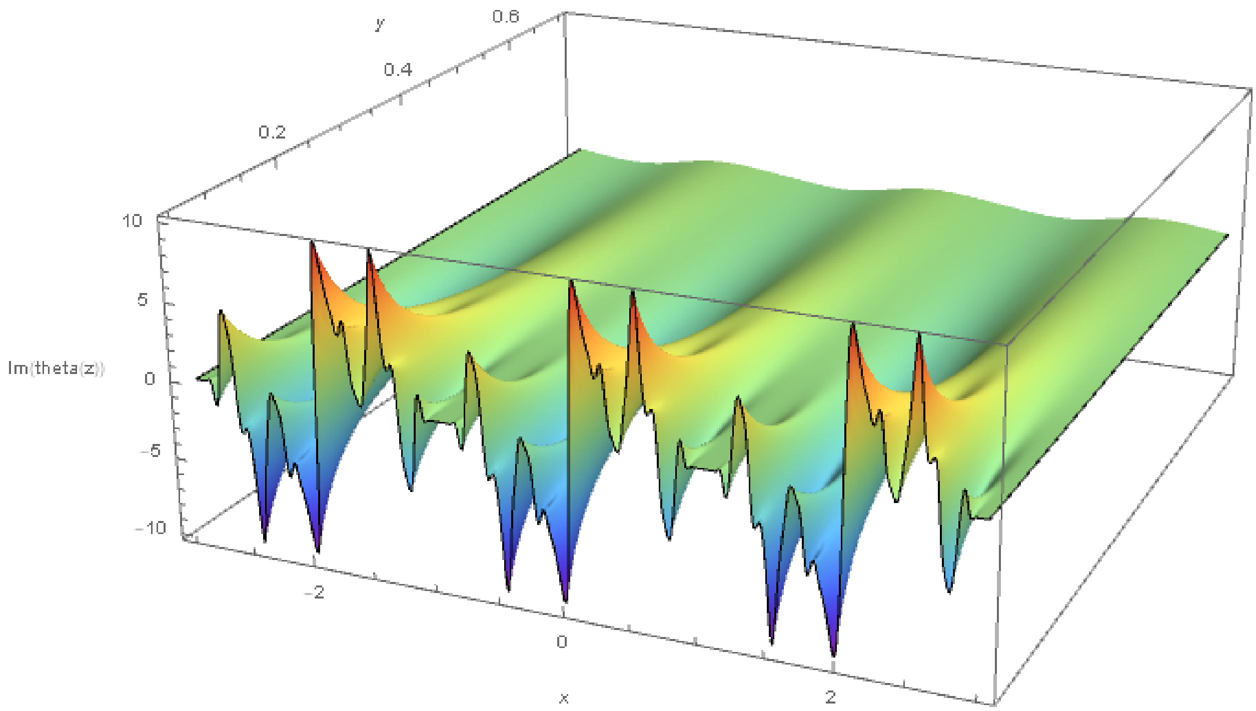

Figure 2: The imaginary part of $\Theta_{\mathbb{Z}^2}(z)$.

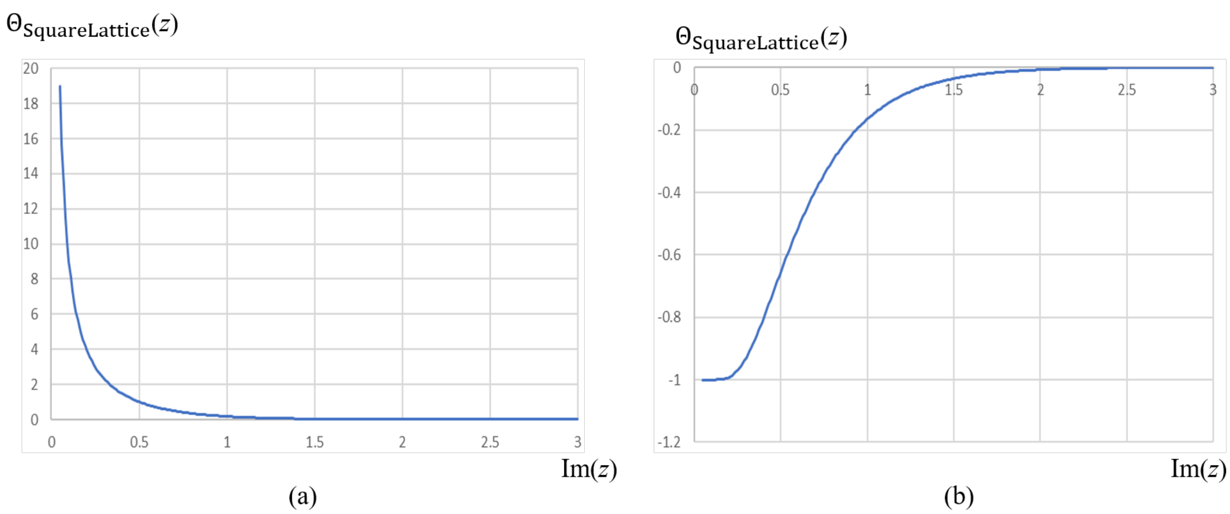

Figure 3: $\Theta_{\mathbb{Z}^2}(z)$ for (a) any even $\mathrm{Re}(z)$ and (b) any odd $\mathrm{Re}(z)$

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Other 2D lattices

For 2D lattices other than the square lattice, only $N(m)$ need to be treated differently.

For example, in the triangular lattice, the basis vectors are $\binom{1}{0}$ and $\begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}$. A lattice point can be expressed by the vector

$$\vec{v} = k \binom{1}{0} + l \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \; k, l \in \mathbb{Z} \tag{6}$$

Therefore, $|\vec{v}|^2 = k^2 + kl + l^2$. $N(m)$ is the number of integer pairs (k, l) such that $k^2 + kl + l^2 = m$, which can be obtained by any simple counting algorithm. The $N(m)$ values for the triangular lattice is given in Table 2.

Table 2: The values of $N(m)$ for the triangular lattice.

m	$N(m)$	m	$N(m)$	m	$N(m)$
1	6	11	0	21	12
2	0	12	6	22	0
3	6	13	12	23	0
4	6	14	0	24	0
5	0	15	0	25	6
6	0	16	6		
7	12	17	0		
8	0	18	0		
9	6	19	12		
10	0	20	0		

In general, there is a quadratic form $\alpha_1 k^2 + \alpha_2 kl + \alpha_3 l^2$ for each 2D primary lattice, where $\alpha_i \in \mathbb{R}$.[2] The treatments are all similar.

Conclusions

We have genearated the theta series for $\mathbb{Z}^2$ using Eqn. (1). Other primary 2D lattices can be similarly generated from their quadratic forms.

Appendices

The codes and output files for $\Theta_{\mathbb{Z}^2}(z)$ are uploaded at `https://github.com/Studio-Darboux-Carbonnier/LatticeSum`

References

(1) Nijboer, B. R.; De Wette, F. W. On the calculation of lattice sums. *Physica* **1957**,

(2) Conway, J. H.; Sloane, N. J. A. *Sphere packings, lattices and groups*; Springer Science & Business Media, 2013; Vol. 290.

(3) Zachary, C. E.; Torquato, S. Hyperuniformity in point patterns and two-phase random heterogeneous media. *Journal of Statistical Mechanics: Theory and Experiment* **2009**, *2009*, P12015.