

Multi-headed lattices and Green functions

Lin Jiu

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Qipin Chen, Amazon



Shane Chern

Journal of Physics A: Mathematical and Theoretical <onbehalfof@manuscriptcentral.com>

18:06 (45分钟前)



发送至 qipinche、chenxiaohang92、我 ▾

Dear Dr Jiu,

Re: "Multi-headed lattices and Green functions"

Manuscript reference: JPhysA-121035.R1

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We will now perform some final checks to ensure that we have everything we need to publish your Paper. These checks enable us to publish your Paper as quickly and efficiently as possible.

Lattice in \mathbb{Z}^N

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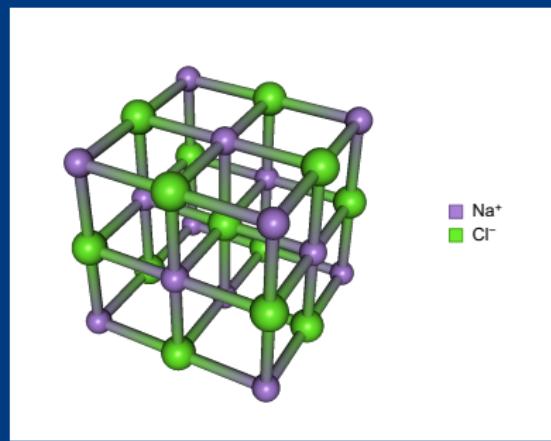
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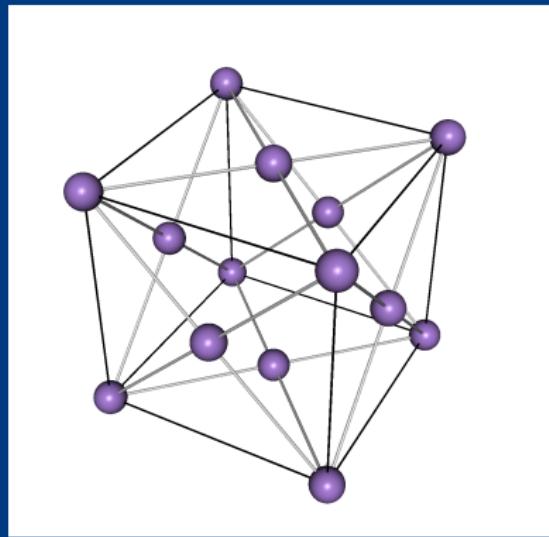
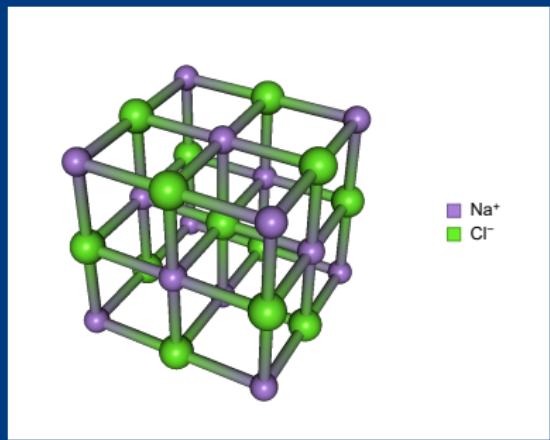
Bravais lattices

An arrangement of points in the three-dimensional space such that when viewed from each point the lattice appears exactly the same; from a mathematical perspective, it is a \mathbb{Z} -module generated by three linearly independent vectors in \mathbb{R}^3 .

NaCl



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Examples in \mathbb{Z}^3 : cubic lattices

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$$\text{simple: } \mathcal{L}_{V_{1,3}}$$

$$\text{face-centered: } \mathcal{L}_{V_{2,3}}$$

$$\text{body-centered: } \mathcal{L}_{V_{3,3}}$$

$$\mathcal{L}_{\mathcal{V}_{M,N}}$$

The M -headed lattice in dimension N :

$$\mathcal{V}_{M,N} := \{(v_1, \dots, v_N) \in \{-1, 0, 1\}^N : |v_1| + \dots + |v_N| = M\}.$$

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$$(v_1, v_2, v_3) \in \{-1, 0, 1\}^3 : |v_1| + |v_2| + |v_3| = 2.$$

Main Results

Table 1: M -Headed lattice in dimension N

N	M	Differential Equation		Pólya Number
		Order	Degree	
1	1	1	2	1
2	1	2	2	1
2	2	2	2	1
3	1	3	4	$1 - 2^4(\sqrt{3} + 1)\pi^3\Gamma(\frac{1}{24})^{-2}\Gamma(\frac{11}{24})^{-2}$ (≈ 0.34054)
3	2	3	3	$1 - 2^{\frac{14}{3}}3^{-2}\pi^4\Gamma(\frac{1}{3})^{-6}$ (≈ 0.25632)
3	3	3	2	$1 - 2^2\pi^3\Gamma(\frac{1}{4})^{-4}$ (≈ 0.28223)
4	1	4	4	≈ 0.19313
4	2	4	7	≈ 0.09571
4	3			
4	4	4	2	≈ 0.10605
5	1	5	6	≈ 0.13517
5	2	6	13	≈ 0.04657
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5	1	5	6	≈ 0.13517
5	2	6	13	≈ 0.04657
5	3	19	7	
5	3	14	110	≈ 0.01581
5	3	69	16	
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Definition

We say a chain \mathfrak{w} of sites:

$$\mathfrak{w} : 0 = \mathbf{s}_0 \rightarrow \mathbf{s}_1 \rightarrow \mathbf{s}_2 \rightarrow \cdots$$

is a *walk* if there is a bond from \mathbf{s}_j to \mathbf{s}_{j+1} for every $j \geq 0$, and each move from \mathbf{s}_j to \mathbf{s}_{j+1} is called a *step*.

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$P_{\mathcal{L}_{\mathcal{V}}}(\mathbf{s}, n)$:= the probability that a random walk ends at \mathbf{s} after n steps

Green Function

Definition

The Green function of the lattice \mathcal{L}_V is the generating function of $P_{\mathcal{L}_V}(\mathbf{s}, n)$:

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The *structure function*¹ is defined by, for $\theta := (\theta_1, \dots, \theta_N)$,

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Fact

$$P_{\mathcal{L}_V}(\mathbf{s}, z) = \frac{1}{(2\pi)^N} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{e^{-i \mathbf{s} \cdot \boldsymbol{\theta}} d\theta_1 \cdots d\theta_N}{1 - z \lambda_{\mathcal{L}_V}(\boldsymbol{\theta})}.$$

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main object— $r_{M,N}(n)$ and $\tilde{r}_{M,N}(n)$

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$r_{M,N}(n)$ and $\tilde{r}_{M,N}(n)$ (continued)

►

$$P_{M,N}(0, z) = P_{\mathcal{L}_V}(0, z) = \frac{1}{(2\pi)^N} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{d\theta_1 \cdots d\theta_N}{1 - \frac{z}{\binom{N}{M}} \sigma_M(\cos \theta_1, \dots, \cos \theta_N)}$$

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$$\tilde{R}_{M,N}(0, z) := \sum_{n \geq 0} r_{M,N}(2n) z^n \quad \tilde{r}_{M,N}(n) := r_{M,N}(2n).$$

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Proposition (Q. Chen, S. Chern, and LJ)

We have $r_{M,N}(2n+1) = 0$ for all $n \geq 0$ if M is odd or $M = N$.

Table 1: M -Headed lattice in dimension N [†]Entries with a gray background are newly computed in this work.

N	M	Differential Equation		Pólya Number
		Order	Degree	
1	1	1	2	1
2	1	2	2	1
2	2	2	2	1
3	1	3	4	$1 - 2^4(\sqrt{3} + 1)\pi^3\Gamma(\frac{1}{24})^{-2}\Gamma(\frac{11}{24})^{-2}$ (≈ 0.34054)
3	2	3	3	$1 - 2^{\frac{13}{2}}3^{-3}\pi^4\Gamma(\frac{1}{3})^{-6}$ (≈ 0.25632)
3	3	3	2	$1 - 2^2\pi^3\Gamma(\frac{1}{4})^{-4}$ (≈ 0.28223)
4	1	4	4	≈ 0.19313
4	2	4	7	≈ 0.09571
		11	5	
4	3	8	32	≈ 0.04332
		24	8	
4	4	4	2	≈ 0.10605
5	1	5	6	≈ 0.13517
5	2	6	13	≈ 0.04657
		19	7	
5	3	14	110	≈ 0.01581
		69	16	
5	4	9	24	≈ 0.01560
		33	6	
5	5	5	2	≈ 0.04473

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$$R_{3,4}(\mathbf{0}, z) = \frac{1}{\pi^4} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 (\star\star\star) \, dx_1 \, dx_2 \, dx_3 \, dx_4,$$

where the integrand $(\star\star\star)$ is

$$\frac{1}{(1 - 8z(x_1x_2x_3 + x_2x_3x_4 + x_3x_4x_1 + x_4x_1x_2))\sqrt{1 - x_1^2}\sqrt{1 - x_2^2}\sqrt{1 - x_3^2}\sqrt{1 - x_4^2}},$$

After around *one hour* of computation, we arrive at the following result.

Theorem 4.2. *The function $\tilde{R}_{3,4}(0, z)$ satisfies a differential equation of order 8 and degree 16. The differential equation is of the form*

$$\begin{aligned} & (1344z + \dots + 151026323282253922352374256330569782279536640z^{16}) \\ & + (18816z + \dots + 1366788225704397997288987019791656529629806592z^{16})\vartheta \\ & + (102144z + \dots + 53031215350304773123787860965203504943225818z^{16})\vartheta^2 \\ & + (212352z + \dots + 115337688798812453697631404177745706747281408z^{16})\vartheta^3 \\ & + (-42 + \dots + 15391679930285039325517386362534096505705332736z^{16})\vartheta^4 \\ & + (357 + \dots + 12917784851408785491873078058141402044309700608z^{16})\vartheta^5 \\ & + (-1113 + \dots + 6663616997264781396236424132096584504800444416z^{16})\vartheta^6 \\ & + (1512 + \dots + 1933136938012580206110390481031293213178068992z^{16})\vartheta^7 \\ & + (-756 + \dots + 2416421172516062575673798810128911651647258624z^{16})\vartheta^8. \end{aligned}$$

Accordingly, $\tilde{r}_{3,4}(n)$ satisfies a recurrence of order 16.

Meanwhile, if we directly apply creative telescoping to the summation

$$\tilde{r}_{3,4}(n) = \sum_{\substack{k_1, k_2, k_3, k_4 \geq 0 \\ k_1 + k_2 + k_3 + k_4 = n}} \binom{2n}{2k_1, 2k_2, 2k_3, 2k_4} \binom{2(n-k_1)}{n-k_1} \binom{2(n-k_2)}{n-k_2} \binom{2(n-k_3)}{n-k_3} \binom{2(n-k_4)}{n-k_4},$$

we get the following recurrence in **ONLY ten minutes!** This fact to some extent indicates that our summation expression is superior in a computational sense.

Theorem 4.3. *The sequence $\tilde{r}_{3,4}(n)$ satisfies a recurrence of order 4. The recurrence is of the form*

$$\begin{aligned} 0 &= (221086792032258663383040 + \dots + 198833002070411360n^{20})\tilde{r}_{3,4}(n) \\ &- (123596648884357621088256 + \dots + 135920997945424800n^{20})\tilde{r}_{3,4}(n+1) \\ &+ (2413729498666800513024 + \dots + 74521417678480n^{20})\tilde{r}_{3,4}(n+2) \\ &- (9569617440812835840 + \dots + 1074030451200n^{20})\tilde{r}_{3,4}(n+3) \\ &+ (9051531325562880 + \dots + 462944160n^{20})\tilde{r}_{3,4}(n+4). \end{aligned}$$

Accordingly, $\tilde{R}_{3,4}(\mathbf{0}, z)$ satisfies a differential equation of order 24 and degree 4.

Holonomic (D-finite)

Definition

A formal power series $F = F(z)$ over a field \mathbb{K} is called *D-finite/holonomic* if there are polynomials $v_0(z), \dots, v_K(z) \in \mathbb{K}[z]$ with $v_K(z)$ not identical to zero such that

$$(v_0(z) + v_1(z)D + \cdots + v_K(z)D^K)(F) = 0, \quad (1)$$

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Fact

Let $F(z) = \sum_{n=0}^{\infty} f(n)z^n$, then (1) shows $f(n)$ is P-finite/holonomic:

$$h_0(n)f(n) + h_1(n)f(n-1) + \dots + h_L(n)f(n-L) = 0,$$

for polynomials $h_0(n), \dots, h_L(n)$ with $h_0(n)$ and $h_L(n)$ not identical to zero.

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Hermite polynomial $H_n(x)$:

$$H_{n+2}(x) - 2xH_{n+1}(x) + (2 + 2n)H_n(x) = 0$$

$x_j = \cos \theta_j$ and $\vartheta = \vartheta_z := z(d/dz)$

$$R_{\mathbf{3},\mathbf{4}}(\mathbf{0},z) = \frac{1}{\pi^4} \int_{[-1,1]^4} \frac{dx_1 dx_2 dx_3 dx_4}{(1 - 8z(x_1 x_2 x_3 + x_2 x_3 x_4 + x_3 x_4 x_1 + x_4 x_1 x_2)) \sqrt{1-x_1^2} \sqrt{1-x_2^2} \sqrt{1-x_3^2} \sqrt{1-x_4^2}}$$

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Accordingly, $\tilde{R}_{3,4}(0, z)$ satisfies a differential equation of order 24 and degree 4.

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Corollary (Q. Chen, S. Chern, and LJ)

The Pólya number is approximately $P_{3,4}(0) \approx 0.04332$.

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Fact (For the second method, it takes only 10 mins)

$$R_{4,5}(0, z)$$

Remark

Using the integral

$$R_{4,5}(0, z) = \frac{1}{\pi^5} \int_{[-1,1]^5} (\ast\ast\ast\ast) dx_1 dx_2 dx_3 dx_4 dx_5$$

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The code for the integral expression had not yet finished running after even around ONE WEEK!

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Theorem (Q. Chen, S. Chern, and L.J.)

For $n \geq 0$,

$$r_{N-1,N}(2n) = \sum_{\substack{k_1, \dots, k_N \geq 0 \\ k_1 + \dots + k_N = n}} \binom{2n}{2k_1, \dots, 2k_N} \binom{2(n - k_1)}{n - k_1} \cdots \binom{2(n - k_N)}{n - k_N}.$$

Also, if N is even, $r_{N-1,N}(2n+1) = 0$; and if N is odd,

$$r_{N-1,N}(2n+1) = \sum_{\substack{k_1, \dots, k_N \geq 0 \\ k_1 + \dots + k_N = n + \frac{1-N}{2}}} \binom{2n+1}{2k_1 + 1, \dots, 2k_N + 1} \binom{2(n - k_1)}{n - k_1} \cdots \binom{2(n - k_N)}{n - k_N}.$$

Theorem

The function $R_{4,5}(0, z)$ satisfies a differential equation of order 9 and degree 24:

$$\begin{aligned} & (333047697408z + \dots + 3587135914162316664577589182300422144000000000000z^{24}) \\ & + (47239200 + \dots + 8746714696058467589996180287043036774400000000000z^{24})\vartheta \\ & + (291308400 + \dots + 9453516646138192392531605664037066506240000000000z^{24})\vartheta^2 \\ & + (740080800 + \dots + 5943864920522147046229253977370938834944000000000z^{24})\vartheta^3 \\ & + (1027452600 + \dots + 2395763624685018201440807167653926928384000000000z^{24})\vartheta^4 \\ & + (861131250 + \dots + 641926999294401201636284114667753701376000000000z^{24})\vartheta^5 \\ & + (449264475 + \dots + 114331247240822245206661000977438474240000000000z^{24})\vartheta^6 \\ & + (143193825 + \dots + 13051386184451845257422171891507920896000000000z^{24})\vartheta^7 \\ & + (25587900 + \dots + 866423326586435904331316912053026816000000000z^{24})\vartheta^8 \\ & + (1968300 + \dots + 25483039017248114833274026825089024000000000z^{24})\vartheta^9. \end{aligned}$$

Accordingly, $r_{4,5}(n)$ satisfies a recurrence of order 24.

Theorem

The sequence $r_{4,5}(n)$ satisfies a recurrence of order 6:

$$\begin{aligned}0 &= (2364822061925891270067722649600000 + \dots + 312808771118086225920n^{27})r_{4,5}(n) \\&\quad + (880540948213763261498004602880000 + \dots + 22881382331785936896n^{27})r_{4,5}(n+1) \\&\quad - (664078540666702251488371015680000 + \dots + 5976795675008958464n^{27})r_{4,5}(n+2) \\&\quad + (36337840931616555318702833664000 + \dots + 159149910074064896n^{27})r_{4,5}(n+3) \\&\quad + (1737772868400007324872130560000 + \dots + 3900964176134144n^{27})r_{4,5}(n+4) \\&\quad - (36446102109669030849285120000 + \dots + 51561082388480n^{27})r_{4,5}(n+5) \\&\quad - (154404486709237819219968000 + \dots + 138110042112n^{27})r_{4,5}(n+6).\end{aligned}$$

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Corollary

As $n \rightarrow \infty$, $r_{4,5}(n) \sim C_{4,5} \cdot 80^n n^{-\frac{5}{2}}$, where the constant $C_{4,5} \approx 0.0353$.

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The Pólya number is approximately $P_{4,5}(0) \approx 0.01560$.

$$R_{3,5}(0, z)$$

Fact

When calculating the $R_{3,5}(0, z)$, we crushed my desktop in Kunshan 2-3 times

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Hi Lin,

your observation is correct: I have not implemented any procedures to automatically parallelize the computations in HolonomicFunctions.

What can be done (and what I did in the past), but it is a bit cumbersome, is to parallelize the computation of FindCreativeTelescoping by using evaluation-interpolation, and chinese remaindering. For this purpose, the option Mode -> Modular can be used. This way you can let the different primes and evaluation points be computed in parallel, but you have to put together the results "manually". A necessary condition is that the computation is feasible for special values and modulo prime. This you can see when you follow the verbose output (Printlevel = 5).

Let me know in case you need further information.

Best wishes,
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$$\{\tilde{r}_{3,5}(n)\}_{n=0}^{54} = \{1, 80, 71280, \dots,$$

$$\underbrace{20198893220533155882232776 \dots 330349744141730893312000}_{200 \text{ digits!}} \Bigg)$$

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Problem

Let $N \geq 1$ be fixed. As sequences in M , are $\text{ord}(M, N)$ and $\text{deg}(M, N)$ unimodal? If so, do the peak positions take place around a half of N ?