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# Angular Lattice Sums and the Riemann Hypothesis

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# Outline

- Double sums: background
- Angular lattice sums- definitions, functional equation, evaluation
- Definition of  $\Delta_4$  and properties
- Two key theorems: Riemann hypothesis, distribution function for zeros on the critical line
- Gaps between zeros
- Future directions

# Background to Double Sums

- The basic reference: M L Glasser and I J Zucker, Lattice sums, *Theoretical chemistry advances and perspectives*, vol. 5, 67-139, 1980
- The lowest order sum:

$$C(0, 1; s) = \sum'_{p_1, p_2} \frac{1}{(p_1^2 + p_2^2)^s} = 4\zeta(s)L_{-4}(s)$$

The sum runs over all integers excluding the point at the origin in the square lattice. The analytic result is due to Lorenz (1871) and Hardy (1920), where

$$L_{-4}(s) = \sum_{p=0}^{\infty} \frac{1}{(4p+1)^s} - \sum_{p=0}^{\infty} \frac{1}{(4p+3)^s}$$

Both these are Dirichlet L functions, and by the Generalized Riemann Hypothesis have all their non-trivial zeros on the critical line

$$\Re(s) = \Re(\sigma + it) = \frac{1}{2}$$

## Epstein Zeta Functions

- Inspired by Hardy's result, a number of authors in the 1920's and 30's considered properties of zeros of double sums of the Epstein zeta type

$$Z(a, b, c; s) = \sum'_{p_1, p_2} \frac{1}{(ap_1^2 + 2bp_1p_2 + cp_2^2)^s}$$

Here the determinant of the quadratic form is taken to be negative. Potter and Titchmarsh (1935) and Kober (1936) showed that  $Z(a, b, c; s)$  has an infinite number of zeros on the critical line. Potter and Titchmarsh (1935) also exhibited numerically two zeros of  $Z(1, 0, 5; s)$  not lying on the critical line. Davenport and Heilbronn (1936) proved that, if the class number of the determinant of the quadratic form is even, or is odd and different from 1, then  $Z(a, b, c; s)$  has an infinite number of zeros lying off the critical line, in addition to those lying on it.

# Angular Lattice Sums

- We introduce two sets of lattice sums, depending on both the length of the vector from the origin to a point in the square lattice, and the angle between the vector and the Ox axis:

$$\mathcal{C}(n, m; s) = \sum'_{p_1, p_2} \frac{\cos^n(m\theta_{p_1, p_2})}{(p_1^2 + p_2^2)^s}, \quad \mathcal{S}(n, m; s) = \sum'_{p_1, p_2} \frac{\sin^n(m\theta_{p_1, p_2})}{(p_1^2 + p_2^2)^s}$$

Obvious properties of these sums include:

$$\mathcal{C}(0, 1; s) = \mathcal{C}(1, 0; s),$$

$$\mathcal{C}(1, m; s) = 0 \text{ unless } m \text{ is divisible by } 4$$

$$\mathcal{S}(n, m; s) = 0 \text{ if } n \text{ is odd}$$

$$\mathcal{C}(2, m; s) + \mathcal{S}(2, m; s) = \mathcal{C}(0, 1; s)$$

$$\mathcal{C}(2, 2m; s) - \mathcal{S}(2, 2m; s) = \mathcal{C}(1, 4m; s)$$

$$\mathcal{C}(2, 2m + 1; s) = \mathcal{S}(2, 2m + 1; s) = \frac{1}{2}\mathcal{C}(0, 1; s)$$

# Angular Lattice Sums-Evaluation

- We evaluate lattice sums of the form just introduced by combining the sums  $\mathcal{C}(0, 1; s)$  and  $\mathcal{C}(2n, 1; s)$

$$\sum_{(p_1, p_2)}' \frac{p_1^{2n}}{(p_1^2 + p_2^2)^{s+n}} = \mathcal{C}(2n, 1; s) = \frac{2\sqrt{\pi}\Gamma(s+n-1/2)\zeta(2s-1)}{\Gamma(s+n)}$$

$$+ \frac{8\pi^s}{\Gamma(s+n)} \sum_{p_1=1}^{\infty} \sum_{p_2=1}^{\infty} \left(\frac{p_2}{p_1}\right)^{s-1/2} p_1^n p_2^n \pi^n K_{s+n-1/2}(2\pi p_1 p_2).$$

This expression is valid for  $n$  non-zero, and the Macdonald function makes the double sum exponentially convergent. In practice, we need to take a summation region large enough so the argument of the Macdonald function exceeds the magnitude of its order. The expression is derived by taking the Mellin transform of the left-hand side, and using the Poisson summation formula to transform the sum over  $p_2$ , with the axial term being evaluated explicitly. The use of Hobson's integral gives the final form of the result.

# Angular Lattice Sums-Functional Equation

- McPhedran et al (2004) derived the following functional equation

$$G_{4m}(s) = \mathcal{C}(1, 4m; s) \frac{\Gamma(s+2m)}{\pi^s} = G_{4m}(1-s)$$

This expression is also valid for  $m$  zero, where it gives the functional equation for  $4\zeta(s)L_{-4}(s)$

The  $m$  dependence in the functional equation is represented in two related functions, the first of which is a ratio of two polynomials with zeros all on the real axis:

$$\mathcal{F}_{2m}(s) = \frac{\Gamma(1-s+2m)\Gamma(s)}{\Gamma(1-s)\Gamma(s+2m)} = \exp(2i\phi_{2m}(s)),$$

If  $|s| \gg 4m^2$ ,

$$\mathcal{F}_{2m}(s) \simeq 1 - \frac{4m^2}{s-1/2} + \frac{8m^4}{(s-1/2)^2}, \quad \phi_{2m}(s) \simeq \frac{2m^2i}{s-1/2} + \frac{im^2(8m^2-1)}{6(s-1/2)^3}.$$

## Distribution of Zeros-Numerical Data

- Numerical investigations suggest that the  $\mathcal{C}(1, 4m; s)$  all obey the Riemann hypothesis
- Surprisingly, all seem to have the same number density of zeros on the critical line
- This number density is the same as that of  $\mathcal{C}(0, 1; s)$

$$N_{\zeta}\left(\frac{1}{2}, t\right) = \frac{t}{2\pi} \log(t) - \frac{t}{2\pi} (1 + \log(2\pi)) + O(\log t)$$

$$N_{-4}\left(\frac{1}{2}, t\right) = \frac{t}{2\pi} \log(t) - \frac{t}{2\pi} (1 + \log(\pi/2)) + O(\log t)$$

$$N_{\mathcal{C}0,1}\left(\frac{1}{2}, t\right) = \frac{t}{\pi} \log(t) - \frac{t}{\pi} (1 + \log(\pi)) + O(\log t)$$

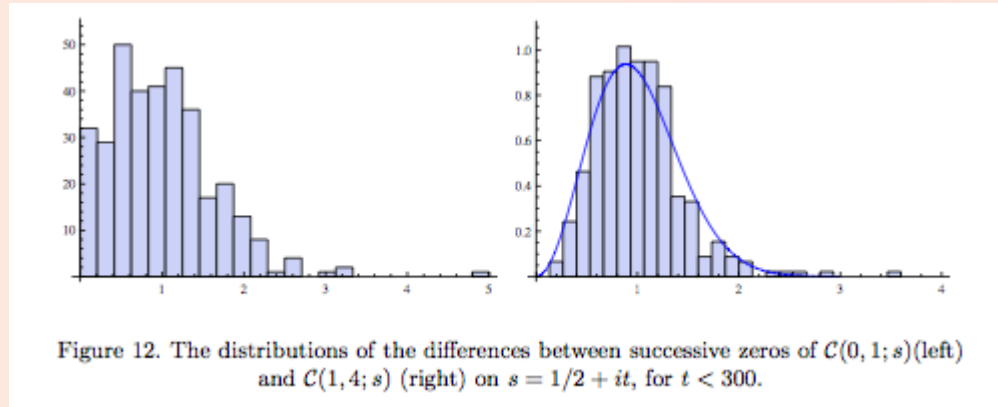
$$N_{\mathcal{C}1,4}\left(\frac{1}{2}, t\right) = N_{\mathcal{C}0,1}\left(\frac{1}{2}, t\right) = \frac{t}{\pi} \log(t) - \frac{t}{\pi} (1 + \log(\pi)) + O(\log t)$$



# Distribution of Zeros-Numerical Data 2

$t$	$n_{\zeta}$	$n_{-4}$	$n_{c14}$	$n_{\zeta} + n_{-4} + n_{c14}$	$n_{c18}$	$n_{c112}$
0-10	0	1	2	3	2	3
10-20	1	4	5	10	5	5
20-30	2	5	6	13	7	7
30-40	3	4	8	15	8	8
40-50	4	6	8	18	8	8
50-60	3	5	9	17	9	9
60-70	4	6	9	19	10	10
70-80	4	6	11	21	10	10
80-90	4	7	11	22	11	10
90-100	4	6	10	20	10	12
280-290	6	8	15	29	15	14
290-300	6	9	14	29	13	15
0-300	137	203	341	681	341	343
estimates	137	203	340	680		

# Distribution of Zeros-Numerical Data 2



For the Gaussian Unitary Ensemble (GUE) if the separation between zeros is normalized to have a mean of one, the distribution function for the separation takes the form:

$$P(S) = \frac{9S^2}{\pi^2} \exp\left(\frac{-4S^2}{\pi}\right)$$

Bogomolny and Lebouef (1994) comment that the left distribution is that of two uncorrelated GUE sets. However, it is clear that the right distribution is in accord with the GUE.

# The Analytic Function $\Delta_4$

- Connections between zeros of lattice sums can be established using quotient forms:

$$\Delta_4(2, 2m; s) = \frac{\mathcal{C}(1, 4m; s)}{\mathcal{C}(0, 1; s)}$$

**Theorem 7.1.** *The analytic function  $\Delta_4(2, 2m; s)$  obeys the functional equation*

$$\Delta_4(2, 2m; s) = \Delta_4(2, 2m; 1 - s) \mathcal{F}_{2m}(s). \quad (7.2)$$

*It has first order poles at  $s = -(2m - 1), -(2m - 2), \dots, -1$  and a first order zero at  $s = 0$ . Its only possible essential singularity is at infinity. On the critical line, it lies in either the first or third quadrants, with its argument being given by*

$$\arg[\Delta_4(2, 2m; 1/2 + it)] = \phi_{2m,c}(t) - \left[ \begin{array}{c} 0 \\ \pi \end{array} \right]. \quad (7.3)$$

*As  $\sigma \rightarrow \infty$  for any  $t$ , the argument of  $\Delta_4$  tends to zero exponentially, while as  $\sigma \rightarrow -\infty$  for any  $t$ , the argument of  $\Delta_4$  tends to zero algebraically.*

# The Analytic Function $\Delta_4$

- A key role is played by lines of constant phase coming from  $\sigma = \infty$

**Theorem 7.2.** *The only lines of constant phase of the  $\Delta_4(2, 2m; s)$  which can attain  $\sigma = \infty$  are equally spaced, and have interspersed lines of constant modulus. All such lines of constant phase either reach the critical line in the asymptotic region of  $t$  at a pole or a zero of  $\Delta_4(2, 2m; s)$ , or curve up and asymptote to each other at infinity.*

*Proof.* From (7.6), we have

$$\Delta_4(2, 4m - 2; \sigma + it) = 1 - \frac{e^{-it \log 2}}{2^{\sigma-1}} + O\left(\frac{1}{4^{\sigma+it}}\right), \quad (7.12)$$

and so the leading order estimate gives the lines of phase zero for  $\Delta_4(2, 4m-2; \sigma+it)$  as occurring at  $t = n\pi/\log 2$ , for  $n = 0, 1, 2, \dots$ . Halfway between these lines of phase zero are the lines on which the leading order estimate gives  $\partial\Delta_4(2, 4m - 2; \sigma + it)/\partial t = 0$ : these are lines of constant modulus, and in fact correspond to  $|\Delta_4(2, 4m - 2; \sigma + it)| = 1$ , for  $\sigma \rightarrow \infty$ . The same argument applies to  $\Delta_4(2, 4m; \sigma + it)$ , with  $\log 5$  replacing  $\log 2$  in the estimate for asymptotic placement of lines of phase zero and amplitude unity.

# The Analytic Function $\Delta_4$ 3

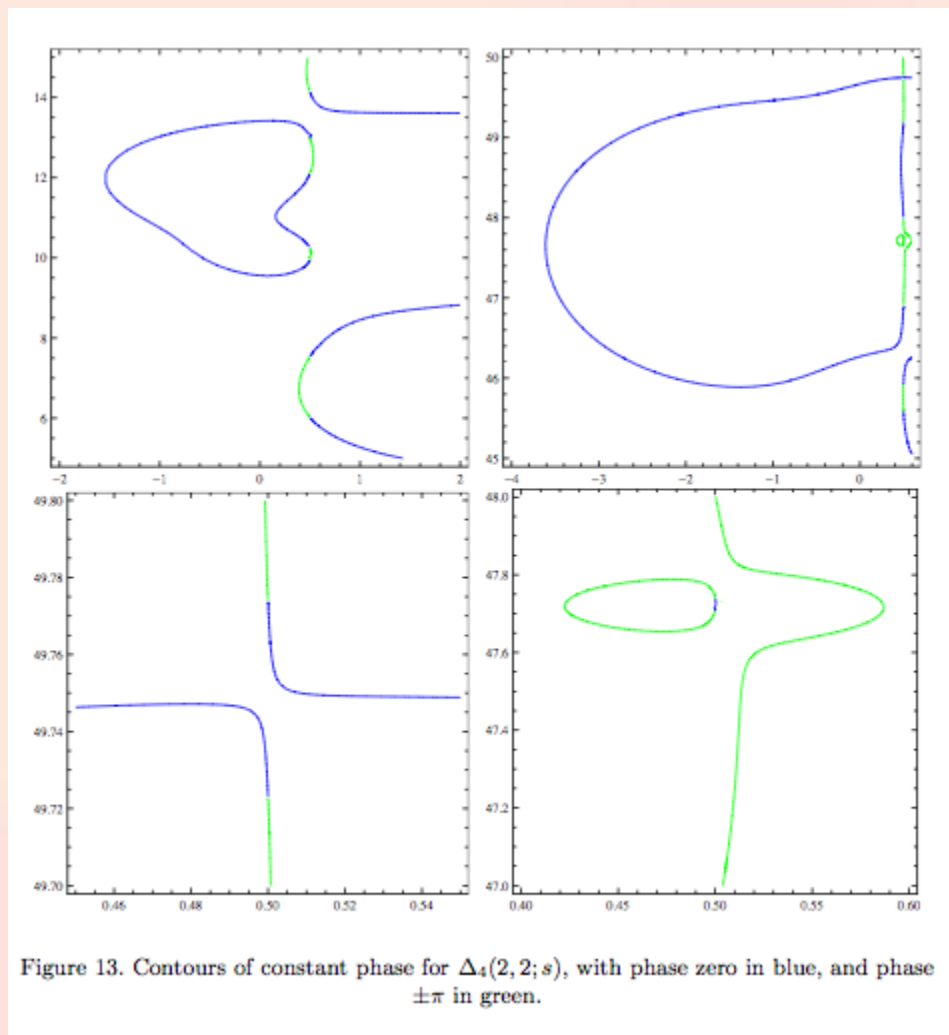
**Theorem 7.3.** *Suppose  $\mathcal{C}(0, 1; s)$  obeys the Riemann hypothesis. Then  $\mathcal{C}(1, 4m; s)$  obeys the Riemann hypothesis for any positive integer  $m$ . Conversely, if  $\mathcal{C}(1, 4m; s)$  obeys the Riemann hypothesis for some  $m$ , then  $\mathcal{C}(0, 1; s)$  obeys the Riemann hypothesis.*

*Proof.* Consider lines  $L_1$  and  $L_2$  in  $t > 0$  along which the phase of  $\Delta_4(2, 2m; s)$  for a given  $m$  is zero. Join these lines with two lines to the right of the critical line along which  $\sigma$  is constant. Then the change of argument of  $\Delta_4(2, 2m; s)$  around the closed contour  $C$  so formed is zero, so by the Argument Principle the number of poles inside the contour equals the number of zeros. Each pole is formed by a zero of  $\mathcal{C}(0, 1; s)$ , so if there are no such zeros within  $C$  there can be no zeros of  $\mathcal{C}(1, 4m; s)$  within  $C$ . We can repeat this procedure for all  $m$ .

Conversely, each zero of  $\Delta_4(2, 2m; s)$  is formed by a zero of  $\mathcal{C}(1, 4m; s)$ , so if there are no such zeros for some  $m$ , then there can be no poles, and hence no zeros of  $\mathcal{C}(0, 1; s)$ . These arguments prove the theorem in the region to the right of the critical line lying between lines of zero phase of  $\Delta_4(2, 2m; s)$ , with the result to the left of the critical line then guaranteed by the functional equation (7.2).

To complete the proof we need to show that any point in the region  $\sigma > 1/2$ ,  $t > 0$  is enclosed between lines of phase zero of  $\Delta_4(2, 2m; s)$  coming from  $\sigma = \infty$ . We note that  $t = 0$  is one such line, and that for any  $\sigma > 0$  the infinite number of such constant phase lines cannot cluster into a finite interval of  $t$ , since that would indicate an essential singularity of  $\Delta_4(2, 2m; s)$  for that  $\sigma$ .  $\square$

# The Analytic Function $\Delta_4$



# The Analytic Function $\Delta_4$ 5

**Theorem 7.5.** *Assuming the Riemann hypothesis applies to  $\mathcal{C}(1, 4m; s)$  or  $\mathcal{C}(0, 1; s)$ , then given any two lines of phase zero of  $\Delta_4(2, 2m; s)$  running from  $\sigma = \infty$  and*

*intersecting the critical line, the number of zeros and poles of  $\Delta_4(2, 2m; s)$  counted according to multiplicity and lying properly between the lines must be the same.*

*Proof.* We consider a contour composed of the two lines of phase zero, the segment between them on the critical line and a segment between them in the region  $\sigma \gg 1$ . The total phase change around this contour is strictly zero, since the region  $\sigma \gg 1$  has the phase of  $\Delta_4(2, 2m; s)$  constrained:  $-\pi \ll \arg[\Delta_4(2, 2m; s)] \ll \pi$ . More particularly, if  $P_u = (1/2, t_u)$  lies at the upper end of the segment on the critical line, and  $P_l = (1/2, t_l)$  at the lower end, the total phase change between a point approaching  $P_u$  on the contour from the right and a point leaving  $P_l$  going right is zero. This phase change is made up of contributions from the changes of phase at the zero or pole  $P_u$ , from the zero or pole  $P_l$ , from the  $N_z$  zeros and  $N_p$  poles on the critical line between  $P_u$  and  $P_l$ , and from the phase change between the zeros and poles. In this list, the first change is  $\phi_{2m,c}(t_u)$ , the phase on the critical line just below  $P_u$ . (We could also have a phase  $\phi_{2m,c}(t_u) - \pi$ , but it will be easily seen that in this alternative case the argument which follows will arrive at exactly the same conclusion.) The second change is  $-\phi_{2m,c}(t_l)$ , where  $\phi_{2m,c}(t_l)$  is the phase just above  $t_l$ . Giving zero  $n$  a multiplicity  $z_n$ , and pole  $n$  a multiplicity  $p_n$ , the phase change at the former is  $-\pi z_n$  and the latter  $\pi p_n$ . The phase change between zeros and poles is  $\phi_{2m,c}(t_l) - \phi_{2m,c}(t_u)$ . Hence, the phase constraint is

$$\phi_{2m,c}(t_u) - \phi_{2m,c}(t_l) - \pi \left[ \sum_{n=1}^{N_z} z_n - \sum_{n=1}^{N_p} p_n \right] + \phi_{2m,c}(t_l) - \phi_{2m,c}(t_u) = 0, \quad (7.13)$$

leading to

$$\sum_{n=1}^{N_z} z_n = \sum_{n=1}^{N_p} p_n, \quad (7.14)$$

as asserted.  $\square$



# The Analytic Function $\Delta_4$ 5

**Theorem 7.5.** *Assuming the Riemann hypothesis applies to  $\mathcal{C}(1, 4m; s)$  or  $\mathcal{C}(0, 1; s)$ , then given any two lines of phase zero of  $\Delta_4(2, 2m; s)$  running from  $\sigma = \infty$  and*

*intersecting the critical line, the number of zeros and poles of  $\Delta_4(2, 2m; s)$  counted according to multiplicity and lying properly between the lines must be the same.*

*Proof.* We consider a contour composed of the two lines of phase zero, the segment between them on the critical line and a segment between them in the region  $\sigma \gg 1$ . The total phase change around this contour is strictly zero, since the region  $\sigma \gg 1$  has the phase of  $\Delta_4(2, 2m; s)$  constrained:  $-\pi \ll \arg[\Delta_4(2, 2m; s)] \ll \pi$ . More particularly, if  $P_u = (1/2, t_u)$  lies at the upper end of the segment on the critical line, and  $P_l = (1/2, t_l)$  at the lower end, the total phase change between a point approaching  $P_u$  on the contour from the right and a point leaving  $P_l$  going right is zero. This phase change is made up of contributions from the changes of phase at the zero or pole  $P_u$ , from the zero or pole  $P_l$ , from the  $N_z$  zeros and  $N_p$  poles on the critical line between  $P_u$  and  $P_l$ , and from the phase change between the zeros and poles. In this list, the first change is  $\phi_{2m,c}(t_u)$ , the phase on the critical line just below  $P_u$ . (We could also have a phase  $\phi_{2m,c}(t_u) - \pi$ , but it will be easily seen that in this alternative case the argument which follows will arrive at exactly the same conclusion.) The second change is  $-\phi_{2m,c}(t_l)$ , where  $\phi_{2m,c}(t_l)$  is the phase just above  $t_l$ . Giving zero  $n$  a multiplicity  $z_n$ , and pole  $n$  a multiplicity  $p_n$ , the phase change at the former is  $-\pi z_n$  and the latter  $\pi p_n$ . The phase change between zeros and poles is  $\phi_{2m,c}(t_l) - \phi_{2m,c}(t_u)$ . Hence, the phase constraint is

$$\phi_{2m,c}(t_u) - \phi_{2m,c}(t_l) - \pi \left[ \sum_{n=1}^{N_z} z_n - \sum_{n=1}^{N_p} p_n \right] + \phi_{2m,c}(t_l) - \phi_{2m,c}(t_u) = 0, \quad (7.13)$$

leading to

$$\sum_{n=1}^{N_z} z_n = \sum_{n=1}^{N_p} p_n, \quad (7.14)$$

as asserted.  $\square$



# The Analytic Function $\Delta_4$ 6

**Corollary 7.6.** *If all zeros and poles on the critical line have multiplicity one, the numbers of zeros and poles on the critical line between any pair of lines of phase zero of  $\Delta_4(2, 2m; s)$  coming from  $\sigma = \infty$  are the same. The distribution functions for zeros  $N_{C_{1,4}}(\frac{1}{2}, t)$  and  $N_{C_{0,1}}(\frac{1}{2}, t)$  of (6.7) then must agree in all terms which go to infinity with  $t$ .*

*Proof.* The first assertion is a simple consequence of Theorem 7.5. The second follows from Theorem 7.2 and Theorem 7.5: the number of zeros and poles between successive zero lines coming from  $\sigma = \infty$  match for all such pairs of lines, and there are only a finite number of exceptional poles and zeros which may disturb the equality between numbers of zeros and poles. If lines of phase zero curve up and asymptote to the point at infinity, we apply Theorem 7.5 to the leftmost of these and the last line of phase zero cutting the critical line.  $\square$

## Future Work?

- Better numerics- the square lattice (e.g. more sums, bigger range of  $t$ , better statistics on gaps between zeros etc)
- Numerics and analytics on other lattice sums in 2D
- Lattice sums in higher dimensions
- The Riemann hypothesis itself? Is it more easily tackled in 2D than 1D?
- The results presented here should encourage other workers to enter this field.

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## **The Riemann Hypothesis for Angular Lattice Sums**

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