

**Numerical Studies of the Gauss  
Lattice Problem**

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# Numerical Studies of the Gauss Lattice Problem

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## 1. INTRODUCTION

The number of lattice points,  $N(R)$ , that lie in the closed circle of radius  $R$  about the origin is related to the distribution of the eigenvalues of the Laplacian in various cases. The magnitude of the deviation of this number from the area of that circle,

$$d(R) \equiv N(R) - \pi R^2, \quad (1)$$

is an open question in number theory. Indeed, Gauss [5] seems to have first raised this question in 1800, and he showed that

$$|d(R)| \leq K R^\theta \quad (2)$$

for  $\theta = 1$ . The least value of  $\theta$  for which this is true is not known, and that is the basic Gauss lattice problem, which is one of the leading open questions in number theory.

The spectral problems relate to the eigenvalues of the reduced wave equation:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \lambda \phi = 0 . \quad (3)$$

Solutions are

$$\phi(x, y) = A \exp i(px + qy) \quad (4a)$$

provided that

$$\lambda = p^2 + q^2 . \quad (4b)$$

Of course a domain,  $\Omega$ , and boundary conditions on  $\partial\Omega$  must be specified. For a square of side  $L$  with periodic conditions, say,

$$\phi(0, y) = \phi(L, y) \quad , \quad \phi(x, 0) = \phi(x, L) \quad (5)$$

it follows that  $p$  and  $q$  must be

$$p = \frac{2\pi}{L}m \quad , \quad q = \frac{2\pi}{L}n \quad ; \quad m, n = 0, \pm 1, \pm 2, \dots . \quad (6)$$

The number of linearly independent such eigenmodes that can exist with eigenvalues  $\lambda \leq \lambda_{\max}$  is just the number of lattice points  $(m, n)$  satisfying

$$m^2 + n^2 \leq R^2 \equiv \left(\frac{L}{2\pi}\right)^2 \lambda_{\max} ; \quad (7)$$

that is  $N(R)$  as defined above. If in place of the periodicity (5) we impose Dirichlet conditions

$$\phi(0, y) = \phi(L, y) = 0 \quad , \quad \phi(x, 0) = \phi(x, L) = 0 ,$$

then  $p$  and  $q$  must be, for independent eigenmodes,

$$p = \frac{\pi}{L}m \quad , \quad q = \frac{\pi}{L}n \quad ; \quad m, n = 1, 2, \dots . \quad (8)$$

The number of such eigenmodes that exist for  $\lambda \leq \lambda_{\max}$  is given by

$$N_Q(R) = \frac{1}{4}\{N(R) - 4[R] - 1\} , \quad (9)$$

where we have used  $[z] \equiv (\text{largest integer} \leq z)$ . The relation (9) results from the fact that only lattice points in the open positive quadrant are to be included.

The relation between  $N(R)$  and  $N_Q(R)$  seems to have caused some confusion in an early reference to the quantum aspects of the counting problem [2,3]. If we replaced  $\Omega$  by a rectangle rather than a square, the circle would be replaced by an ellipse. In three dimensions, if the square is replaced by a cube, the circle is replaced by a sphere.

In quantum systems the eigenvalues are the energy levels of the system and the distribution of these levels and their variation are of interest. The erratic variation of  $d(R)$  with  $R$  suggests the notion of quantum chaos (see Figure 1).

The lattice problem has been studied in great detail by mathematicians and physicists. Over the years many upper bounds, say  $\hat{\theta} > \theta$ , have been obtained. A list of these bounds and their discoverers is contained in Table I.

TABLE I

Date	Investigators	$\hat{\theta}$	$\sigma$
1800	Gauss [5]	1	
1906	Sierpinski [17]	$\frac{2}{3} = 0.66\overline{6}$	
1915	Hardy [7]	$\frac{1}{2} + \epsilon$ (conjectured), $\theta > \frac{1}{2}$ proven	
1928	Nieland [16]	$\frac{27}{41} = 0.6585365$	328
1929	Littlewood & Walfisz [14]	$\frac{37}{56} = 0.6607142$	448
1935	Titchmarsh [18]	$\frac{15}{23} = 0.6521739$	184
1942	Hua [11]	$\frac{13}{20} = 0.650\overline{0}$	160
1962	Yin [19]	$\frac{24}{37} = 0.648648$	148
1985	Kolesnik [13]	$\frac{278}{429} = 0.6480186$	143
1988	Iwaniec & Mozzochi [10]	$\frac{7}{11} + \epsilon = 0.6363\overline{63} + \epsilon$	88
1993	Huxley [9]	$\frac{46}{73} = 0.6301369$	73

The strange fractions in this table all have the form  $\hat{\theta} = \frac{2}{3}(1 - \frac{4}{\sigma})$  for some integer  $\sigma$  which is also listed. Huxley [9] makes the observation that the methods being employed to get the more recent results cannot be expected to yield  $\sigma < 64$  and thus will give at best  $\hat{\theta} = \frac{5}{8} = 0.625$ . The current least value due to Huxley is true not only for the circle but for any smooth convex closed curve (for which  $R$  is the “magnification” factor of the “unit” curve).

## 2. NUMERICAL APPROACH

Since all the rigorous bounds are relatively far from the ideal  $\frac{1}{2} + \epsilon$  conjectured by Hardy, it is perhaps of some interest to obtain numerical evidence of the behavior of  $d(R)$ . This has been done [4,15,12,1] but with no suggested improvements. These previous attempts sampled  $d(R)$  at various sets of uniformly spaced values  $\{R_j\}$ . But as  $d(R)$  is not a well-behaved function of  $R$ , such samplings do not yield any useful information. Indeed  $N(R)$  is a piecewise constant function of  $R$ , continuous from above, with jump discontinuities at those values of  $R$  for which  $R^2$  is the sum of the squares of two integers. Thus we can uniquely determine  $N(R)$  in  $R \leq R_{\max}$  by simply tabulating the values  $(R_k, N(R_k))$ , where the  $R_k$  are the **consecutive** values,  $k = 1, 2, 3, \dots$ , at which  $N(R)$  jumps. Obviously, if a lattice point lies on the circle with radius  $R_k$ , then  $R_k^2$  must be an integer and thus  $R_{k+1}^2 \geq R_k^2 + 1$ . So, although the spacing between consecutive jumps in  $N(R)$  may decrease as  $R$  grows, it is bounded below by:

$$\begin{aligned} \delta_k = R_{k+1} - R_k &\geq \sqrt{R_k^2 + 1} - R_k, \\ &\geq R_k \left[ \sqrt{1 + \frac{1}{R_k^2}} - 1 \right]. \end{aligned} \quad (10)$$

Also, if  $R_k^2 = p^2 + q^2$  for some integers  $p$  and  $q$ , then at least one of these integers must be greater than  $\frac{1}{2}R_k$ . Thus the spacing between jumps in  $N(R)$  cannot be greater than is implied by

$$R_{k+1}^2 \leq R_k^2 + \sqrt{2}R_k + 1,$$

and hence

$$\delta_k \leq R_k \left[ \sqrt{1 + \frac{1}{R_k^2} + \frac{\sqrt{2}}{R_k}} - 1 \right].$$

From (10) and the above we get that:

$$\frac{1}{2R_k} + \mathcal{O}\left(\frac{1}{R_k^3}\right) \leq \delta_k \leq \frac{1}{\sqrt{2}} + \mathcal{O}\left(\frac{1}{R_k}\right). \quad (11)$$

The conceptually simplest way to tabulate the piecewise constant function  $N(R)$  for  $0 \leq R \leq R_{\max}$  (an integer) is to generate the numbers  $R_{pq}^2 = p^2 + q^2$  for all integers  $p, q = 0, \pm 1, \dots, \pm R_{\max}$ . Then sort the resulting list into ascending order and count the number of entries up to each jump in the list. Recording the cumulative number of entries and the value of  $R_{pq}^2$  immediately **after** the jump yields the coordinates  $(R_k^2, N(R_k))$  of the vertices of  $N(R)$

versus  $R^2$  at the  $k^{\text{th}}$  jump. Obviously  $N(R_k)$  versus  $R_k$  can be recorded if required. One must remember not to tabulate beyond the value  $R_{\max}^2$ , as not all such contributions need come from lattice points in the square  $[-R_{\max}, R_{\max}]^2$ . The last jump recorded we denote by the index  $k_{\max}$ .

From the values of  $N(R_k)$  we compute  $d(R_k)$ , being sure to use as many significant digits in  $\pi$  as necessary, and then we determine the convex hull of the set:

$$\{P_k\}_1^{k_{\max}} \equiv \{\log R_k, \log |d(R_k)|\}_1^{k_{\max}}. \quad (12)$$

To accomplish this we first replace the set  $\{P_k\}$  by the set  $\{\hat{P}_j\}$  containing the cumulative maxima of  $\log |d(R_k)|$ . That is, we eliminate those consecutive  $P_k$  for which  $\log |d(R_k)| \leq \log |d(R_j)|$  for  $k \geq j + 1$ . The remaining set  $\{\hat{P}_j\}$  is such that both  $\{\log \hat{R}_j\}$  and  $\{\log |d(\hat{R}_j)|\}$  are monotone increasing. We relabel the indices so that  $j$  runs through consecutive integers. The piecewise linear function of  $\log R$ , say  $\hat{P}(\log R)$ , which joins adjacent points of  $\{\hat{P}_j\}_1^{j_{\max}}$  is strictly increasing but not necessarily convex. Starting at  $j = 2$ , we eliminate the point  $\hat{P}_j$  if  $\frac{\Delta \log |d(R_j)|}{\Delta \log R_j} \leq \frac{\Delta \log |d(R_{j+1})|}{\Delta \log R_{j+1}}$ , then reduce all indices  $i \geq j$  by one and continue the elimination procedure starting now from the larger of 2 and  $j - 1$ . The remaining set of points  $\{\hat{\hat{P}}_i\}_1^{i_{\max}}$  has a convex piecewise linear interpolant,  $\hat{\hat{P}}(\log R)$ ; this is the **convex hull** of the original set  $\{P_k\}_1^{k_{\max}}$ . The slope of the **final segment** of this convex hull is the best estimate of the least upper bound on  $\theta$  that we can get from our original set of data  $\{P_k\}_1^{k_{\max}}$ .

If subsequent calculations extend the range of data to larger values of  $R_{\max}$  we need simply find the convex hull of the new data, adjoin it to the current data and then determine the hull of the enlarged set.

### 3. COUNTING PROCEDURES

Two of the previous attempts to compute  $d(R)$  contain serious errors. In [15] the square root is fit by a table in order to speed up the calculations. But the table contains an error and thus the results for  $R > 3000$  are incorrect. This error was reported in [12]. The most recent work, by Bleher, Cheng, Dyson and Lebowitz [1] containing Tables 1a of  $\min\{\frac{d(r)}{r} | r < R\}$  and 1b of  $\max\{\frac{d(r)}{r} | r < R\}$  cannot be correct. Simply note that  $\frac{d(1)}{1} = 1 - \pi = -2.1415928 \dots$ . However, all the entries in Table 1a for  $R^2 \leq 3025$  have entries larger than  $d(1)$ . Upon comparing carefully their results with those of the present work, we have found that they have computed  $\frac{d(r)}{2\pi r}$  rather than  $\frac{d(r)}{r}$ . Thus all their entries must be multiplied by the factor  $\sqrt{2\pi} = 2.506628 \dots$  and then we obtain essentially exact agreement. Private communication with one of the

authors has confirmed the error. Fortunately, it does not invalidate their main results.

It was suggested in [12] that estimates out to  $R = 10^8$  would be required to get numerical evidence to support  $\theta < 0.6$ , an improvement on the current best proven bound. If we attempt to tabulate  $N(R)$  it would require  $N(R) \approx 3 \times 10^{16}$  lattice points or  $2 \times 10^{17}$  bytes of storage. The INTEL Touchstone-DELTA has 568 nodes with 16 Mb/node for a total of  $9 \times 10^9$  bytes. Thus with  $10^8$  DELTA machines we could store the data. But time estimates are equally prohibitive.

Thus our previous estimate had better be far off if numerical evidence is to be helpful. Indeed, our tabulation results seem to show that significant improvements can be obtained with much more modest estimates, say  $R \approx 10^5$ . In other words, sampling procedures do not shed any light on correct results but complete tabulation as suggested in [12] seems to do so.

To tabulate all values of  $p^2 + q^2$  out to  $R^2 = 10^{10}$  is not too difficult. But we wish to do it in a way that allows future improvements when the machines and/or the cycles are available.

Our tabulation procedure uses independent nodes on a parallel computer as follows. We choose a value  $R_{\max}$  up to which we will tabulate  $N(R)$  and special values of  $d(R)$ . If our machine has  $P$  processors or nodes we divide the disk  $r \leq R_{\max}$  into concentric rings  $R_j \leq r < R_{j+1}$  such that the rings have approximately equal areas, *i.e.*, with  $R_0 = 0$ :

$$\pi(R_{j+1}^2 - R_j^2) = \pi \frac{R_{\max}^2}{P} \quad ; \quad j = 0, 1, \dots, P-1.$$

We associate processor  $P_k$  with the  $k^{\text{th}}$  ring having **inner radius**  $R_k$  and outer radius  $R_{k+1}$ . Then initially, for  $0 \leq k \leq P-1$ , processor  $P_k$  computes  $N(R_k)$  by the fast algorithm devised in [12]. Next processor  $P_k$  computes and sorts by magnitude the set  $\{R_{ij}^2 - R_k^2 : R_k^2 \leq R_{ij}^2 \equiv i^2 + j^2 < R_{k+1}^2\}$ . In doing this we use the obvious fast procedures

$$R_{i,j\pm 1}^2 = R_{i,j}^2 \pm 2j + 1,$$

noting that a multiplication by 2 in binary is just a shift so that  $R_{i,j\pm 1}^2$  is formed from  $R_{i,j}^2$  by means of one shift and two adds — *i.e.*, no multiplications need be employed if floating point arithmetic is avoided during this counting stage. The same is true in forming  $R_{i\pm 1,j}^2$ . We use the sets  $\{R_{ij}^2 - R_k^2\}$  rather than  $\{R_{ij}^2\}$  so that fewer significant digits need be stored.

From the sorted sets each processor,  $P_k$ , computes the deviation increments  $\delta d(R) = [N(R) - N(R_k)] - \pi[R^2 - R_k^2]$  for  $R_k \leq R < R_{k+1}$ . Then the

deviation envelopes for  $d(R) = d(R_k) + \delta d(R)$  are determined and the convex hull of  $\log |d(R)|$  versus  $\log R$  is obtained. For the enumeration carried out to  $R_{\max} = 55,848$ , we get that

$$\hat{\theta} \leq 0.575 . \quad (13)$$

This suggested bound is significantly better than the best rigorous bound  $\hat{\theta} = 0.6301369$  due to Huxley. Of course, it is possible to justify a bound obtained from the convex hull process if we could get sufficiently sharp bounds on the magnitude of the jumps in  $N(R)$  versus the distance between maximal jumps. Then it could be possible to verify that the true convex hull up to a given  $R_{\max}$  had been obtained. Of course, the jump in  $N(R)$  is just the number of ways in which  $R^2$  can be written as the sum of two (integer) squares — another well-worked problem in number theory.

Graphs of some of our results show in Figure 1 the jumps in  $d(R)$  versus  $R^2$ . In Figure 2 we show the cumulative maximum positive and negative deviation bounds by plotting  $|d(R)|$  versus  $R^2$  on a log-log scale. It is stated in [1] that the negative deviations grow faster than the positive ones and this phenomenon shows clearly in our figure and in Fig. 1 of [1]. Finally, in Figure 3 we plot  $\frac{|d(R)|}{R^{\frac{1}{2}}(\log R)^{\frac{1}{4}}}$  versus  $R$ . Hardy showed [7] that

$$d(R) = \Omega\left(R^{\frac{1}{2}}(\log R)^{\frac{1}{4}}\right) . \quad (14)$$

This implies that for some constant,  $K$ , the values  $|d(R)|$  exceed  $K R^{\frac{1}{2}}(\log R)^{\frac{1}{4}}$  for infinitely many values of  $R$  as  $R \rightarrow \infty$ . With, say,  $K = 5$  we see that our tabulations do not even hint at this  $\Omega$ -result.

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