Richard Crandall and the Madelung constant for salt

John Zucker, Kings College London

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Abstract. A salt crystal is made up of alternate positive and negative electric charges based on a simple cubic lattice. The electrostatic energy of interaction of this array of charges was first calculated approximately by Madelung in 1918 [1]. Essentially it required the evaluation of the very slowly conditionally convergent triple sum

$$\alpha = \sum{}' \frac{(-1)^{(m+n+p)}}{(m^2+n^2+p^2)^{1/2}}.$$

This was the prototype for the evaluation of arrays of electric charges arranged on other crystal structures, all referred to as Madelung constants. However, any reference to *the* Madelung constant always implies the first example, α. No closed form for α has ever been found but Richard Crandall initiated novel attempts to provide better approximations to α with well-known constants of analysis and these are reviewed here.

Mathematician-physicist-inventor Richard Crandall

It is with great sadness that the present authors announce the passing of their dear colleague Richard Crandall, who died Thursday December 20, 2012, after a brief bout with acute leukaemia—the week before his 65th birthday on December 29.

Crandall had a long and colorful career. He was a physicist by training, studying with Richard Feynman as an undergrad at the California Institute of Technology, and receiving his Ph.D. in physics at MIT, under the tutelage of Victor Weisskopf, the Austrian-American physicist who discovered what is now known as the Lamb Shift and who was one of the most influential post-war physicists. Richard often commented that he thought digitally in the fashion of an electrical engineer.

Crandall was for many years at Reed College in Portland, Oregon, where he directed the Center for Advanced Computation. At the same time, he also worked for Next Computers (as Chief Scientist), and subsequently for Apple Computers (as Distinguished Scientist), where he was the head of Apple's Advanced Computation Group.

Crandall's research spanned both the theoretical and practical realms: prime numbers, cryptography, data compression, signal processing, fractals, epidemiology, and, of considerable interest to the present authors, experimental mathematics. He held several patents. He produced many algorithms that are incorporated into Apple's products, including the iPod and the iPhone. The library of fast Fourier transforms that was produced by his Advanced Computation Group at Apple was described by a colleague of ours as "miraculously" fast. He worked on image processing techniques for Pixar for 13 years, the last two to remove artifacts that reportedly could only be seen on Steve Jobs' personal projector or to meet Jobs' exacting personal requirements that raindrops should look like they did on celluloid (Richards tool was too natural for modern film goers).

Indeed, Crandall was a close colleague of Steve Jobs for many years. Crandall was preparing to write a biography of Jobs, which biography sadly will now not be written.

How we did not meet

Unfortunately I, John Zucker, never had the pleasure of meeting Richard in person. We established e-mail connection over our joint interest in the Madelung constant. It happened this way. In 1987 Richard produced two papers on α both of which I was asked to referee. They were of course both very good and were accepted. However, in one paper I communicated (as a referee anonymously) a proof of a conjecture he had made, and in the other, the result of a sum he had not known. From this he guessed very quickly who the anonymous reviewer was and we got into contact.

Ever since α first appeared it has been subjected to much analysis such as (a) finding ways to evaluate it rapidly, or (b) to see whether it might be expressed in terms of other constants of analysis. It was clear from his paper with Delord [2] that the problem of evaluating α to many decimal places was easily solved by Richard as he gave a value to some 50dp. It is given here to 24dp for future reference.

$$\alpha = -1.747\ 564\ 594\ 633\ 182\ 190\ 636\ 212\ldots \tag{1.1}$$

Let me point out immediately that for all practical purposes such as evaluating the lattice energy of salt the first four figures would be enough to compare with any experimental value. But just as one only requires π to only 35 digits to find the radius of the universe to the accuracy of the radius of a hydrogen atom, this doesn't stop mathematicians calculating it to 10 trillion digits. So in the paper with Buhler [3], (b) was tackled.

Richard and Madelung

Richard's conception was to find an *exact* expression for α made up of a part which could be evaluated in terms of well-known constants of analysis plus an exponentially fast converging residual sum.

Two of these sums which arise here are

$$S_+\left(m,n,p;\frac{\pi r}{t}\right) := S_+\left(\frac{\pi r}{t}\right) := \sum \frac{1}{r}\frac{(-1)^{m+n+p}}{\exp\frac{\pi r}{t}+1},$$

$$S_-\left(m,n,p;\frac{\pi r}{t}\right) := S_-\left(\frac{\pi r}{t}\right) := \sum \frac{1}{r}\frac{(-1)^{m+n+p}}{\exp\frac{\pi r}{t}-1}.$$

Here $r := \sqrt{m^2+n^2+p^2}$ and wherever $\sum$ appears it will denote summation over all indices from $-\infty$ to ∞. Note that

$$S_+\left(\frac{\pi r}{t}\right) + S_-\left(\frac{\pi r}{t}\right) = -2S_-\left(\frac{2\pi r}{t}\right). \tag{1.2}$$

Richard found the following *exact* expression for α.

$$\alpha_C(t) = 4tC(t) - \frac{\pi}{2t} + 2S_+\left(\frac{\pi r}{t}\right). \tag{1.3}$$

where

$$C(t) := \frac{t}{\pi}\sum{}' \frac{(-1)^m}{m^2+4t^2(n^2+p^2+q^2)} = \frac{1}{2\pi}\sum{}' \frac{(-1)^{m+n+p}}{m^2+n^2+p^2+4t^2(q+1/2)^2},$$

$\sum'$ implies summation over all indices from -∞ to ∞ excluding the case when all the indices are simultaneously zero.

The residual term $2S_+\left(\frac{\pi r}{t}\right)$ contributes very little to the value of α and the smaller t is the less it contributes. So if $C(t)$ could be evaluated it would provide an approximation to α. Now $C(t)$ involves finding a *four*-dimensional sum. Now lattice sums are often evaluated using properties of theta functions and because there are many more θ-function identities available in four than in three dimensions, they are more often easily evaluated than three dimensional sums. This indeed proved to be the case and the following evaluations were provided in [3]:

$$C(1) = -\frac{1}{8} + \frac{3\log 2}{4\pi}, \qquad C\left(\frac{1}{2}\right) = \frac{1}{\sqrt{2}}, \qquad C\left(\frac{1}{4}\right) = \frac{\sqrt{2\sqrt{2}-2}}{\pi}\beta\left(\frac{1}{8}\right),$$

where $\beta(x)$ is the *central* beta function defined by

$$\beta(p) := B(p,p) = \frac{\Gamma^2(p)}{\Gamma(2p)}.$$

So for $t = 1/4$

$$\alpha_C(1/4) = C(1/4) - 2\pi + 2S_{+3}\left(\frac{1}{4}\right) = \frac{\sqrt{2\sqrt{2}-2}}{\pi}\beta\left(\frac{1}{8}\right) - 2\pi + 2S_{+3}\left(\frac{1}{4}\right), \tag{1.4}$$

and we have

$$\frac{\sqrt{2\sqrt{2}-2}}{\pi}\beta\left(\frac{1}{8}\right) - 2\pi = -1.747523,$$

with the residual series $2S_+(4\pi r)$. Comparing this with (1.1) gives agreement to 4dp, good enough for any practical application. A full account of Richard's struggle with α is given in his masterly presentation in [4].

Tyagi's work

This probably inspired another investigator, Sandeep Tyagi, to another attack on α. In this work he naturally came into contact with Richard who communicated his work to myself. It encouraged me to find a value for $C(t)$ with $t < 1/4$, namely

$$C\left(\frac{1}{\sqrt{24}}\right) = \frac{\sqrt{3\sqrt{2}-6\sqrt{3}+6\sqrt{6}}}{2\pi}\beta\left(\frac{1}{8}\right).$$

So using this in (1.3) one has

$$\frac{\sqrt{3\sqrt{2}-6\sqrt{3}+6\sqrt{6}}}{2\pi}\beta\left(\frac{1}{8}\right) - \frac{\sqrt{6}}{\pi} = -1.7475621$$

with residual $2S_+(\sqrt{24}\pi r)$. This gives agreement to 5dp with(1.1). However, this is trivial compared with what Sandeep had achieved in [5]. Sandeep found another *exact* expression for α similar in structure to (1.3) but different. It was

$$\alpha_T(t) = T(t) - \frac{\pi}{6t} - S_-\left(\frac{\pi r}{t}\right). \tag{1.5}$$

where

$$T(t) := \frac{2t}{\pi}\sum\frac{(-1)^{(m+n+p)}}{m^2+n^2+p^2+4t^2q^2}$$

Sandeep was able to evaluate $T(t)$ for some values of t thus

$$T\left(\frac{1}{2}\right) = -\frac{1}{2} - \frac{\log 2}{\pi}, \qquad T\left(\frac{1}{4}\right) = -\frac{1}{4} - \frac{\log 2}{2\pi} + \frac{1}{\sqrt{2}}$$

Thus for $t = 1/4$

$$\alpha_T(1/4) = -\frac{1}{4} - \frac{\log 2}{2\pi} + \frac{1}{\sqrt{2}} - \frac{2\pi}{3} - 2S_-(4\pi r), \tag{1.6}$$

Very shrewdly he then took the average of (1.4) and (1.6) to obtain

$$\alpha_{CT} = -\frac{1}{8} + \frac{1}{2\sqrt{2}} - \frac{4\pi}{3} - \frac{\log 2}{4\pi} + \frac{\sqrt{2\sqrt{2}-2}}{2\pi}\beta\left(\frac{1}{8}\right) - 2S_-(8\pi r). \tag{1.7}$$

It is seen that the residual sum is even smaller.

(This result might have been found directly from a relation discovered later between $C(t)$ and $T(t)$. This is

$$4tC(t) + T(t) = 2T(t/2), \quad \text{hence} \quad 2T(1/8) = T(1/4) + C(1/4)$$

which gives (1.7) immediately.)

When we evaluate the constants in (1.7) we obtain -1.747 564 594 7 in which the error in α is just 1 in the tenth decimal place. A remarkable agreement!

Further refinement

As a kind of tribute to Richard I suggested to Sandeep we might try to improve on this. One way of doing this would be to find $C(1/8)$ but we were not able to do this. However, we could look at evaluating certain terms of $2S_{-}(8\pi r)$. Thus Sandeep considered finding this when m=n=0,n=p=0 and p=m=0. We then get three contributions all the same and finish with

$$2S_{-}(1,0,0;8\pi r) = -12\sum_{p=1}^{\infty}\frac{(-1)^p}{p(e^{8\pi p}-1)}. \tag{1.8}$$

Now using the result in [6]

$$\sum_{p=1}^{\infty}\frac{(-1)^p}{p(e^{2\pi pc}-1)} = -\frac{\pi c}{12} - \frac{1}{12}\log\frac{4}{kk'} \tag{1.9}$$

where k and k' are the values of the modulus and complimentary modulus of the complete elliptic integrals K and K' of the first kind which are found when $K'/K = c$. Here $c = 4$ and (1.8) can be evaluated to give

$$2S_{-}(1,0,0;8\pi r) = 4\pi + \frac{9}{2}\log(\sqrt{2}-1) - 6\log(2^{1/4}+1) - \frac{45}{8}\log 2. \tag{1.10}$$

When this is added to the constants of (1.7) we obtain -1.747 564 594 633 175 which agrees with α given by (1.1) to 1 in the fourteenth decimal place.

Thus encouraged, the next set in $2S_{-}(8\pi r)$ was evaluated. There are three terms of the form $(m=0, n=p), (n=0, m=p)$ and $(p=0, m=n)$ leading to

$$2S_{-}(1,1,0;8\sqrt{2}\pi r) = -\frac{24}{\sqrt{2}}\sum_{p=1}^{\infty}\frac{1}{p(e^{8\sqrt{2}\pi p}+1)}. \tag{1.11}$$

To evaluate this we require a result in [6]:

$$\sum_{p=1}^{\infty}\frac{1}{p(e^{2\pi pc}+1)} = -\frac{\pi c}{12} - \frac{1}{6}\log\frac{2K^3kk'}{\pi^3}, \tag{1.12}$$

with $c = 4\sqrt{2}$ in (1.11). The evaluation of (1.11) is somewhat involved but the result is

$$2S_{-}(1,1,0;8\sqrt{2}\pi r) = 8\pi + 2\sqrt{2}\log\frac{4(1-b)^2\sqrt{2b(1+b^2)}}{(1+b)^4} + 6\sqrt{2}\log\frac{2^{\frac{3}{4}}(1+b)^2\beta\left(\frac{1}{8}\right)}{64\pi}, \tag{1.13}$$

where $b := (2\sqrt{2}-2)^{\frac{1}{4}}$. Adding this contribution to (1.7) and (1.10) gives -1.747 564 594 633 182 191 7 and the disagreement with α occurs only in the eighteenth decimal place.

Finally let us add the contribution of $2S_{-}(8\pi r)$ when $m = n = p$. In this case

$$2S_{-}(1,1,1;8\sqrt{3}\pi r) = -\frac{16}{\sqrt{3}}\sum_{p=1}^{\infty}\frac{(-1)^p}{p(e^{8\sqrt{3}\pi p}-1)}. \tag{1.14}$$

and here $c = 4\sqrt{3}$ and $2S_{-}(1,1,1)$ may be evaluated to give

$$2S_{-}(1,1,1;8\sqrt{3}\pi r) = \frac{16}{3}\pi + \frac{4}{9}\sqrt{3}\log\frac{(1-d)^4}{32(1+d)^2\sqrt{2d(1+d^2)}}. \qquad (1.15)$$

where $d := \sqrt{(\sqrt{3}+1)/\sqrt{8}}$. When this is added to the constants of (1,7), (1.10) and (1.13) we obtain -1.747 564 594 633 182 190 636 22 where the agreement with α is now up to 22 decimal places. It is clear how further terms may be evaluated.

Conclusion

The Madelung constant was only a tiny part of Richard's many faceted interests. Far more important was his contribution to computational number theory amongst many other accomplishments. The brute force approach used here of evaluating terms of the residue sums to add more constants of analysis to the value of α would, I am sure, not have won the approval of Richard. He would have preferred a more subtle approach on the lines of Sandeep's derivation of (1.7). Still I think he would have been amused by the results given here.

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