Calculating $\zeta(2m)$ with Quantum Mechanics

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03/06/17

1 Background[1]

The Riemann zeta function is a map defined (for Re $s > 1$) by

$$\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s}$$

The zeta function has all sorts of applications in complex analysis and number theory, and surrounds some of the deepest open questions in those fields. Euler's first claim to fame was in 1734, when he solved the *Basel* problem—the task of evaluating this function at $s = 2$; he showed it was equal to $\frac{\pi^2}{6}$. This was before Riemann's work, so the question was not phrased in quite that way.

Euler eventually extended his method to calculate these values at even integers all the way up to $s = 26$, though he did not have a closed form. (A closed form for even positive integers is now known; the values at the odd positive integers remain an open problem.) We apply an example in quantum mechanics to give a method for calculating these values.

In classical mechanics, a particle has definite position and momentum at all times; its motion is governed by the differential equation $F = ma$. In principle, if one knows to infinite precision all the positions and momenta of the various particles in consideration and can exactly solve their $F = ma$ equations, one knows the state of the system for all time.

The story in quantum mechanics is not altogether different. The particle is described by a $\mathbb{C}$-valued wave function $\Psi(x, t)$. The evolution of its state is still governed by a differential equation, the (time-dependent) **Schrödinger equation:**

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi$$

[1] A more thorough introduction to quantum mechanics around the level seen here can be found in Griffiths' *Introduction to Quantum Mechanics*.

Here V is analogous to a classical potential; a higher potential means it's harder for a particle to get to a specific place. $\hbar$ is just a constant. The probability of finding the particle inside the interval $[a, b]$ is

$$\int_a^b |\Psi(x,t)|^2 \, \mathrm{d}x$$

with a normality condition imposed by ordinary probability:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, \mathrm{d}x = 1$$

This is sort of a boring equation; really, we're just insisting that our Ψ be L^2. Enforcing that the integral be 1 is just bookkeeping with constants and units (observe that wave functions in one dimension now have units of $L^{-1/2}$).

For moderately good reasons we often don't care about the time evolution of the wave function, so we write $\Psi(x, 0) = \psi(x)$ and mainly work with ψ. For extra confusion, it's typical to also call ψ "the wave function".

Unfortunately, solving PDEs of mixed degree in multiple variables seems kind of hard. It would be much simpler if we assumed that $\Psi(x,t)$ factored as $\psi(x)g(t)$. Then[2]

$$i\hbar\psi \frac{\mathrm{d}g}{\mathrm{d}t} = -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2\psi^2}{\mathrm{d}x^2} g + V\psi g$$

Now we can do a trick:

$$i\hbar \frac{\frac{\mathrm{d}g}{\mathrm{d}t}}{g} = \frac{-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2\psi^2}{\mathrm{d}x^2}}{\psi} + V$$

What does dividing through by ψg accomplish? Well, the LHS is purely a function of time, and the RHS is purely a function of space, so they must both be constant. There aren't that many letters of the alphabet, so let's call that constant E.[3] The LHS gives us the fairly uninteresting fact that the time-dependent part looks like

$$g(t) = e^{-iEt/\hbar}$$

and the time-independent piece satisfies the **time-independent Schrödinger equation:**

$$-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi$$

This is also traditionally called "the Schrödinger equation". Both equations can be thought of as eigenvalue equations for the operator applied to ψ on the left, conventionally called $\hat{H}$ (for Hamilton).

[2]This seems kind of extreme, but bear with me.

[3]Maybe we'll get lucky and it'll be the particle's energy, right? Who knows?

Wave functions lead to all sorts of weird and counter-intuitive results, some of which you may be familiar with. For instance, suppose we have two orthogonal[4] wave functions ψ_1, ψ_2 where $\psi_1(x, 0) = i$ for $0 < x < \frac{1}{2}$ and $\psi_2(x, 0) = -i$ for $0 < x < \frac{1}{2}$. In each of these wave functions there's a probability of

$$|\pm i|^2 \left(\frac{1}{2} - 0\right) = \frac{1}{2}$$

Of finding the particle within $[0, \frac{1}{2}]$. And yet if we take the quantum superposition[5]

$$\psi(x) := \frac{1}{\sqrt{2}} (\psi_1(x) + \psi_2(x))$$

Then the probability of finding a particle with wave function ψ within this interval is 0, not 1! This sort of effect gets called as "quantum interference". We humans like to focus on the probability density $|\psi|^2$, but it actually tells us very little about what happens when we mix wave functions together, because the probabilities aren't the things that add up. This occasionally causes confusion.

1.1 Phast Physics Phacts!

Physicists are lucky; their functions are always pretty nice.

Fact. Any $\Psi(x, t)$ satisfying the time-dependent equation satisfies the following:

- $\Psi(x, 0)$ is a linear combination of $\psi(x)$ that satisfy the time-independent equation;
- ...and $\Psi(x, t)$ is "the same" linear combination of $\psi(x)e^{-iEt/\hbar}$.
- ψ is continuous always, and $\frac{d\psi}{dx}$ is continuous away from points where V jumps from being finite to infinite (or vice versa).

It's correct to think about $\psi(x)e^{-iEt/\hbar}$ being the basis of solutions to the (time-independent) Schrödinger equation, and you can determine the coefficients thereof by doing it for $\Psi(x, 0)$, where the time-dependencies all go away. We've carefully avoided writing down any linear combinations because the basis might be countable vs. uncountable (discrete vs. continuous), and we don't want commit to writing either a sum or an integral prematurely.

[4]Wait, what's the inner product? It's $\langle \psi_1, \psi_2 \rangle = \int_{-\infty}^{\infty} \overline{\psi_1}\psi_2 \, dx$, as you might have guessed.

[5]Read this as "linear combination"; you can check for yourself that ψ is properly normalized.

2 The Infinite Square Well

Also called the particle in a box, this has the potential function

$$V(x) = \begin{cases} 0, & 0 \leq x \leq a \\ \infty, & \text{otherwise} \end{cases}$$

Note that in regions where $V(x)$ is infinite, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \infty\psi = E\psi$$

The RHS is finite (since ψ is supposed to be $\mathbb{C}$-valued), so to have things make sense we need $\psi = 0$ to make everything be 0.[6] Inside the well, the equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi$$

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2mE}{\hbar^2}\psi$$

Which we recognize as having solutions

$$\psi(x) = \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right), \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right)$$

But the boundary conditions (remember that ψ is continuous) force $\psi(0) = 0$, so the cosines are out, and we have (to enforce $\psi(a) = 0$)

$$\frac{\sqrt{2mE}}{\hbar}a = n\pi, n \in \mathbb{Z}^+$$

So we can rewrite our solutions as

$$\psi(x) = \sin\frac{n\pi x}{a}, n \in \mathbb{Z}^+$$

We still have to normalize, of course:

$$\int_0^a \sin^2\frac{n\pi x}{a}\ \mathrm{d}x = \ ?$$

Here's the physicist's argument for such things; clearly

$$\int_0^a \left(\sin^2\frac{n\pi x}{a} + \cos^2\frac{n\pi x}{a}\right)\ \mathrm{d}x = \int_0^a 1\ \mathrm{d}x = a$$

[6] This is an awfully cavalier treatment of multiplying 0 and ∞. Putting on the physicist hat tends to make one cavalier about such things.

And $\sin^2, \cos^2$ are just $\frac{\pi}{2}$-phase-shifted versions of each other. Since we're integrating over an integer number of periods they should contribute equally, and we get

$$\int_0^a \sin^2 \frac{n\pi x}{a} \, \mathrm{d}x = \frac{a}{2}$$

$$\int_0^a \left(\sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \right)^2 \, \mathrm{d}x = 1$$

Denote this function by $\psi_n(x)$. The ψ_n form an orthonormal set of functions (you can check normality yourself); Fourier analysis tells us that they span the space of functions on $[0, a]$, so they form a basis.

Finally we've arrived at the punchline. Write

$$c_n := \int_0^a f(x) \left(\sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \right) \, \mathrm{d}x$$

This is just us dotting f with our (orthonormal) basis vectors, so we can write

$$f(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

and so

$$\int_0^a f(x)^2 = \sum_{n=1}^{\infty} \int_0^a c_n^2 \left(\frac{2}{a} \sin^2 \frac{n\pi x}{a} \right) \, \mathrm{d}x$$

Suppose we had a function (WLOG real-valued; do you see why?) satisfying $c_n = \frac{1}{n^m}$; then, like magic, this would reduce to

$$\int_0^a f(x)^2 \, \mathrm{d}x = \sum_{n=1}^{\infty} \frac{1}{n^{2m}} = \zeta(2m)$$

Our job is just to find some f's that do this, and hope that we know how to integrate their squares.

3 The Legwork

As it turns out, polynomials do the job. Let's write our basis polynomials as $\dfrac{x^m}{a^m\sqrt{2a}}$. Why bother to do half the bookkeeping of normalization (i.e. units) here, but not the other half? And what's with the $\sqrt{2}$? The second question will be answered soon. The basis here isn't orthogonal under the inner product, and since we'll be taking linear combinations of these polynomials later, we'll have to normalize later regardless; there's no point doing so now. But we need to standardize the units for each wave function so that we can take $\mathbb{R}$-linear combinations later, so it doesn't hurt to get them right.

Let $u = \frac{n\pi x}{a}$, so $\mathrm{d}u = \frac{n\pi}{a}\,\mathrm{d}x$. Write $y := \frac{1}{n\pi}$. Then

$$\int_0^a \frac{x^m}{a^m\sqrt{2a}}\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\,\mathrm{d}x = \frac{1}{a^{m+1}}\left(\frac{a}{n\pi}\right)^{m+1}\int_0^{n\pi} u^m \sin u\,\mathrm{d}u = y^{m+1}\int_0^{n\pi} u^m\sin u\,\mathrm{d}u$$

We can now evaluate the integral at the end via integration by parts:

D	I
u^m	$\sin u$
mu^{m-1}	$-\cos u$
$m^{\underline{2}}u^{m-2}$	$-\sin u$
$m^{\underline{3}}u^{m-3}$	$\cos u$
$\vdots$	$\sin u$
$m!u$	$\vdots$
$m!$	$?'$
0	$?$

By $m^{\underline{k}}$ we mean the kth *falling power* (also known as the *falling factorial*),

$$m^{\underline{k}} := m(m-1)\cdots(m-k+1)$$

This a good friend of combinatorialists. The ? in the table is $\pm\sin$ or $\pm\cos$, the function depending on the parity of m and its sign depending on the parity of $\left\lfloor \frac{m}{2} \right\rfloor$.

We can do some nice pruning of this integral: since we're evaluating it over a whole number of periods, all of the sin terms will drop out, which also takes care of some sign-flipping issues. For the other terms, observe that for $k \geq 0$,

$$\left(m^{\underline{k}}u^{m-k}\cos u\right)\Big|_0^{n\pi} = m^{\underline{k}}\left((-1)^n y^{k-m} - \delta_{k,0}\right)$$

Since $0^k = 0$ when $k \neq 0$ but $0^0 = 1$ (a convention we forced on ourselves when we rewrote $m!$ as $m!u^0$). If m is odd, then we don't get a $k = 0$ term (0 is paired up with a sin). This means the Kronecker delta will only show up when m is even. Putting this all together gives

$$y^{m+1}\int_0^{n\pi} u^m \sin u\,\mathrm{d}u = \begin{cases} (-1)^{n+1}\displaystyle\sum_{\substack{k<m\\ k\text{ even}}}(-1)^{k/2}m^{\underline{k}}y^{k+1} + (1-(-1)^n)(-1)^{m/2}m!y^{m+1}, & m \equiv 0 \pmod 2\\ (-1)^{n+1}\displaystyle\sum_{\substack{k<m\\ k\text{ even}}}(-1)^{k/2}m^{\underline{k}}y^{k+1}, & m \equiv 1 \pmod 2\end{cases}$$

The first few examples are

$$
\begin{aligned}
m = 1 &: \frac{x^1}{a^1\sqrt{2a}} \mapsto p_1(y) := (-1)^{n+1}y \\
m = 2 &: \frac{x^2}{a^2\sqrt{2a}} \mapsto p_2(y) := (-1)^{n+1}y - 2(1-(-1)^n)y^3 \\
m = 3 &: \frac{x^3}{a^3\sqrt{2a}} \mapsto p_3(y) := (-1)^{n+1}y - 6(-1)^{n+1}y^3 \\
m = 4 &: \frac{x^4}{a^4\sqrt{2a}} \mapsto p_4(y) := (-1)^{n+1}y - 12(-1)^{n+1}y^3 + 24(1-(-1)^n)y^5 \\
m = 5 &: \frac{x^5}{a^5\sqrt{2a}} \mapsto p_5(y) := (-1)^{n+1}y - 20(-1)^{n+1}y^3 + 120(-1)^{n+1}y^5
\end{aligned}
$$

One could of course choose to write the signs differently; writing $-(-1)^{n+1}$ might seem silly compared to $(-1)^n$. However, writing only one of $(-1)^{n+1}$ and $(-1)^n$ is less likely to lead to sign mistakes when working with these polynomials, and we choose to write $(-1)^{n+1}$ so that the signs are alternating and start positive.

Let's flex our muscles with a few examples.

Example ($\zeta(2)$)**.** Here we just need p_1. We can write

$$
\begin{aligned}
\zeta(2) &= \sum_{n=1}^{\infty} \frac{1}{n^2} \\
&= \pi^2 \sum_{n=1}^{\infty} \left(\frac{(-1)^{n+1}}{n\pi} \right)^2 \\
&= \pi^2 \sum_{n=1}^{\infty} p_1(y)^2 \\
&= \pi^2 \int_0^a \left(\frac{x}{a\sqrt{2a}} \right)^2 \, \mathrm{d}x \\
&= \pi^2 \int_0^a \frac{x^2}{2a^3} \, \mathrm{d}x \\
&= \pi^2 \left(\frac{1}{6}\frac{x^3}{a^3} \right) \Big|_0^a \\
&= \frac{\pi^2}{6}
\end{aligned}
$$

This confirms Euler's famous result.

Example ($\zeta(6)$)**.** Eyeballing what we wrote above, we see that

$$p_3(y) - p_1(y) = -6(-1)^{n+1}y^3$$

Therefore

$$\begin{aligned}
\zeta(6) &= \sum_{n=1}^{\infty} \frac{1}{n^6} \\
&= \frac{\pi^6}{36} \sum_{n=1}^{\infty} \left(\frac{-6(-1)^{n+1}}{n^3\pi^3} \right)^2 \\
&= \frac{\pi^6}{36} \sum_{n=1}^{\infty} (p_3(y) - p_1(y))^2 \\
&= \frac{\pi^6}{36} \int_0^a \left(\frac{x^3}{a^3\sqrt{2a}} - \frac{x}{a\sqrt{2a}} \right)^2 \,\mathrm{d}x \\
&= \frac{\pi^6}{72} \int_0^a \left(\frac{x^6}{a^7} + \frac{x^2}{a^3} - 2\frac{x^4}{a^5} \right) \,\mathrm{d}x \\
&= \frac{\pi^6}{72} \left(\frac{1}{7} + \frac{1}{3} - \frac{2}{5} \right) \\
&= \frac{\pi^6}{72} \frac{8}{105} \\
&= \frac{\pi^6}{945}
\end{aligned}$$

Let's push ourselves now!

Example ($\zeta(10)$)**.** We need only p_1, p_3, and p_5; the fact that our basis is triangular in y^k is very helpful here. We can see that

$$p_5(y) - \frac{10}{3}p_3(y) + \frac{7}{3}p_1(y) = 120(-1)^{n+1}y^5$$

So

$$\begin{aligned}
\zeta(10) &= \sum_{n=1}^{\infty} \frac{1}{n^{10}} \\
&= \frac{\pi^{10}}{14400} \sum_{n=1}^{\infty} \left(p_5(y) - \frac{10}{3}p_3(y) + \frac{7}{3}p_1(y) \right)^2 \\
&= \frac{\pi^{10}}{28800} \int_0^a \left(\frac{x^5}{a^5\sqrt{a}} - \frac{10}{3}\frac{x^3}{a^3\sqrt{a}} + \frac{7}{3}\frac{x}{a\sqrt{a}} \right)^2 \,\mathrm{d}x
\end{aligned}$$

As all schoolchildren know, this integral evaluates to $\frac{640}{2079}$, so

$$\zeta(10) = \frac{\pi^{10}}{28800}\frac{640}{2079} = \frac{\pi^{10}}{45(2079)} = \frac{\pi^{10}}{93555}$$

Aren't we jumping the gun? We promised $\zeta(2m)$ for all integers m, but so far we've skipped from 2 to 6 to 10. What about the multiples of 4? This method isn't going to work; something like its dual is what we need.

Example ($\zeta(4)$)**.** Observe that squaring the $m = 3$ polynomial gives

$$\left((-1)^{n+1}y - 6(-1)^{n+1}y^3\right)^2 = y^2 - 12y^4 + 36y^6$$

So we can calculate $\zeta(4)$, provided we know $\zeta(2)$ and $\zeta(6)$ (which, fortunately, we do). Now

$$\int_0^a \left(\frac{x^3}{a^3\sqrt{2a}}\right)^2 \,\mathrm{d}x = \int_0^a \frac{x^6}{2a^7} = \frac{1}{14}$$

Instead of having the norm-calculating half of our work be hard and the ζ half being easy, the situation is reversed!

We can also write

$$\begin{aligned}
\int_0^a \left(\frac{x^3}{a^3\sqrt{2a}}\right)^2 \,\mathrm{d}x &= \sum_{n=1}^{\infty} \left((-1)^{n+1}y - 6(-1)^{n+1}y^3\right)^2 \\
&= \sum_{n=1}^{\infty} \left((-1)^{n+1}y - 6(-1)^{n+1}y^3\right)^2 \\
&= \sum_{n=1}^{\infty} \frac{1}{n^2\pi^2} - 12\sum_{n=1}^{\infty} \frac{1}{n^4\pi^4} + 36\sum_{n=1}^{\infty} \frac{1}{n^6\pi^6} \\
&= \frac{1}{\pi^2}\zeta(2) - \frac{12}{\pi^4}\sum_{n=1}^{\infty}\frac{1}{n^4} + \frac{36}{\pi^6}\zeta(6) \\
&= \frac{1}{6} - \frac{12}{\pi^4}\zeta(4) + \frac{4}{105}
\end{aligned}$$

Putting this together,

$$\begin{aligned}
\frac{1}{14} &= \frac{1}{6} + \frac{4}{105} - \frac{12}{\pi^4}\zeta(4) \\
\frac{15 - 35 - 8}{210} &= -\frac{12}{\pi^4}\zeta(4) \\
\zeta(4) &= \frac{\pi^4}{12}\frac{28}{210} = \frac{\pi^4}{90}
\end{aligned}$$

Why not use the even values of m—does the $(1 - (-1)^n)$ factor make them worthless? No, but it makes things messier. Here's one example for completeness.

Example ($\zeta(6)$, alternate method)**.** Observe that

$$\frac{x^2}{a^2\sqrt{2a}} - \frac{x}{a\sqrt{2a}} \mapsto -2(1-(-1)^n)y^3$$

So

$$\int_0^a \left(\frac{x^2}{a^2\sqrt{2a}} - \frac{x}{a\sqrt{2a}}\right)^2 \mathrm{d}x = \frac{1}{2}\int_0^a \left(\frac{x^4}{a^5} + \frac{x^2}{a^3} - 2\frac{x^3}{a^4}\right) \mathrm{d}x = \frac{1}{2}\left(\frac{1}{5} + \frac{1}{3} - 2\frac{1}{4}\right) = \frac{1}{60}$$

On the other hand,

$$\int_0^a \left(\frac{x^2}{a^2\sqrt{2a}} - \frac{x}{a\sqrt{2a}}\right)^2 \mathrm{d}x = \sum_{n=1}^{\infty}\left(\frac{-2(1-(-1)^n)}{n^3\pi^3}\right)^2 = \frac{16}{\pi^6}\sum_{n \text{ odd}}\frac{1}{n^6}$$

This isn't the zeta function at all! $1-(-1)^n$ gives 2 on all the odd n's and kills the even ones. Fortunately, there's a fix; observe that[7]

$$\begin{aligned}
\left(1-2^{-6}\right)\zeta(6) &= \left(1-\frac{1}{2^6}\right)\left(1+\frac{1}{2^6}+\frac{1}{3^6}+\frac{1}{4^6}+\cdots\right)\\
&= \left(1+\frac{1}{2^6}+\frac{1}{3^6}+\frac{1}{4^6}+\cdots\right) - \left(\frac{1}{2^6}+\frac{1}{4^6}+\frac{1}{6^6}+\cdots\right)\\
&= \sum_{n \text{ odd}}\frac{1}{n^6}
\end{aligned}$$

Putting this all together,

$$\frac{1}{60} = \frac{16}{\pi^6}\frac{63}{64}\zeta(6)$$

$$\zeta(6) = \frac{4\pi^6}{63}\frac{1}{60} = \frac{\pi^6}{63(15)} = \frac{\pi^6}{945}$$

which confirms the earlier result.

It's clear what the algorithm for computing $\zeta(2m)$ is now. First, calculate all the p_i for $i = 1, 3, 5, \cdots$, stopping at m or $m+1$ (whichever one is odd). If m is odd we can calculate $\zeta(2m)$ directly via a certain linear combination of these polynomials, which translates into a (nasty) definite, proper integral. If m is even, we first have to calculate $\zeta(2\ell)$ for all $\ell < m$, then calculate $\zeta(2m)$ indirectly via the final calculated p_i, which has some nasty ζ stuff involved but corresponds to an easy integral. Like Euler himself, we could now sit down and calculate the values all the way up to $\zeta(26)$. (Any reader with too much free time is welcome to attempt this.)

[7] Some readers might prefer to do this derivation in reverse by means of a geometric series.

4 The Quest for the Closed Form

In principle the problem is solved once reduced to computing some integrals of polynomials, though it would be nice to derive the closed form in terms of the Bernoulli numbers. I will see about expanding on this when I have some free time.