A Simple Rederivation of Onsager’s Solution of the 2D Ising Model Using Experimental Mathematics

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In this case study, we illustrate the great potential of experimental mathematics and symbolic computation by rederiving, ab initio, Onsager’s celebrated solution of the two-dimensional Ising model in zero magnetic field. Onsager’s derivation is extremely complicated, as are all the subsequent proofs. Unlike Onsager’s, our derivation is not rigorous, yet it is absolutely certain (and would be even if Onsager had not already derived it), and should have been acceptable to physicists who do not share mathematicians’ fanatical (and often misplaced) insistence on rigor.

Two Warm-Up Exercises

DEFINITION 1. For an \( n_1 \times n_2 \) matrix \( M = (m_{ij}) \) and positive real numbers \( x \) and \( y \),

\[
\text{weight}(M) (x, y) := x^{\frac{1}{2}} \left( \sum_{i,j} m_{ij} m_{i+1,j} m_{ij} m_{i,j+1} \right) \cdot y^{\sum_{i,j} m_{ij}}.
\]

(We make the convention that if \( i \) is \( n_1 \), then \( i + 1 = 1 \), and if \( j \) is \( n_2 \), then \( j + 1 = 1 \).)

DEFINITION 2. Let \( \mathcal{M}(n_1, n_2) \) be the set of \( n_1 \times n_2 \) matrices whose entries are either 1 or \(-1\) (of course, there are \( 2^{n_1 n_2} \) such matrices). The Laurent polynomial \( P_{n_1,n_2}(x,y) \) is defined as follows:

\[
P_{n_1,n_2}(x,y) := \sum_{M \in \mathcal{M}(n_1, n_2)} \text{weight}(M) (x, y).
\]

DEFINITION 3. For \( x, y \) positive real numbers,

\[
f(x,y) := \lim_{n \to \infty} \frac{\log P_{n_1,n_2}(x,y)}{n^2}.
\]

EXERCISE 1. Find an explicit closed-form expression for \( f(x, y) \).

DEFINITION 4. For an \( n_1 \times n_2 \times n_3 \) three-dimensional array \( M = (m_{i,j,k}) \) and a positive real number \( x \),

\[
\text{weight}'(M)(x) := x^{\frac{1}{2}} \left( \sum_{i,j,k} m_{i,j,k} m_{i+1,j,k} m_{i,j+1,k} m_{i,j,k+1} \right).
\]
\textbf{Definition 5.} Let $\mathcal{M}(n_1, n_2, n_3)$ be the set of $n_1 \times n_2 \times n_3$ three-dimensional arrays whose entries are either 1 or $-1$ (of course, there are $2^{n_1 n_2 n_3}$ such arrays). Define the Laurent polynomial in $x$ by

$$Q_{n_1, n_2, n_3}(x) := \sum_{M \in \mathcal{M}(n_1, n_2, n_3)} \text{weight}'(M)(x).$$

\textbf{Definition 6.} For $x$ a positive real number,

$$g(x) := \lim_{n \to \infty} \frac{\log Q_{n, n, n}(x)}{n^3}.$$  

\textbf{Exercise 2.} Find an explicit closed-form expression for $g(x)$.

We hope, dear readers, that you will spend some time trying to solve these two exercises, but please do not spend too much time! While we know that the limits exist \cite{8}, evaluating them explicitly has been an open problem for almost eighty years, and in spite of many attempts by the best minds in mathematical physics, both “exercises” are still wide open.

Exercise 1 is called “solving the two-dimensional Ising model with magnetic field,” while Exercise 2 is called “solving the three-dimensional Ising model in zero magnetic field.” Let us quote Ken Wilson, who was awarded the Physics Nobel Prize in 1982 for seminal (nonrigorous!) work on questions related to these two “exercises.”

When I entered graduate school I had carried out the instructions given to me by my father [notable chemist E. Bright Wilson, who coauthored, with Linus Pauling, the classic Introduction to Quantum Mechanics] and had knocked on both Murray Gell-Mann’s and Feynman’s doors and asked them what they were currently doing. Murray wrote down the instructions given to me by my father [no-tential physical viewpoint, it would have been considered “only” a conjecture it had been done before Onsager’s rigorous derivation. But this conjecture would have been so plausible that it would have been wholeheartedly accepted by the theoretical physics community.

\textbf{What Is an “Explicit” Answer?}  
From now on, we will write $f(x)$ instead of $f(x, 1)$, and $P_{n_1, n_2, n_3}(x)$ instead of $P_{n_1, n_2}(x)$. Onsager’s elegant solution involves an infinite series, which entails taking a limit. The definition of the function $f(x)$ also involves taking a limit (namely of $\frac{\log(P_{n, n}(x))}{n}$ as $n \to \infty$). Why is the former limit better than the latter?

Indeed, the notion of “explicit,” or “closed form,” is vague and cultural. In ancient Greece, a geometric construction was acceptable only if it used straightedge and compass. In algebra, for a long time, a solution was acceptable only if it could be expressed in terms of the four elementary operations and root extractions. In enumerative combinatorics, a solution was (and sometimes still is) considered to be in closed form only if it is a product and/or quotient of factorials. And there are many other examples.

In a famous position paper \cite{7}, Herb Wilf tackled this problem in combinatorics. He was inspired to write it when he was asked to referee a paper containing a “formula” for a certain quantity. It turned out that computing the quantity via the formula took much longer than using the definition. Inspired by the—at the time—new paradigm of “computational complexity,” he suggested that an “answer” is an efficient algorithm to compute the quantity in question.

How would we compute $f(x)$, using the definition, for a specific “numeric” $x$? We can, in principle, compute the sequence of Laurent polynomials $P_{n,n}(x)$ directly, for, say, $n \leq 30$, get the first finite sequence of numbers $\{\log(P_{n,n}(x))/n^3\}_{n=1}^{30}$, see whether they get closer and closer, and estimate the limit. Alas, computing $P_{n,n}(x)$ by brute force involves adding up $2^n$ terms, each of which takes $O(n^3)$ operations to compute. This is hopeless! Also, to be fully rigorous, one has to be able to find a priori bounds for the error, and for each $\epsilon$ find (rigorously) an $n$, such that $|f(x) - \log(P_{n, n}(x))/n^3| < \epsilon$ for $n \geq n_\epsilon$. This is truly hopeless.

On the other hand, using elementary calculus, Onsager’s solution enables us to compute $f(x)$ very fast, to any desired accuracy.

Onsager’s Explicit Formula for the Zero-Field 2D Ising Model. Let

$$G(z) := \frac{1}{4} \sum_{r=1}^{\infty} \left( \frac{2r}{r} \right)^{\frac{2r}{r}} \frac{x^{2r}}{r}.$$

Then

$$f(x, 1) = \ln(x + x^{-1}) + G \left( \frac{x - x^{-1}}{x + x^{-1}} \right).$$

Onsager’s proof \cite{5}, and all subsequent proofs, are very complicated. We will soon show how this formula could have been naturally derived, way back in 1941, if they had had the software and hardware that we have today (and even, probably, thirty years ago).
$G(z)$, and hence of $f(x)$. It is impossible to extract this information directly from the definition.

This motivation may be interesting, but it is irrelevant to us. All we want is to answer Exercise 1 in the special case $y = 1$, with as little effort as possible and making full use of the computer. We require only elementary calculus and very elementary matrix algebra. We don’t even use eigenvalues!

**Recommended Reading**

Even though it is irrelevant to our story, for those readers who wish to know the context and background, we strongly recommend Barry Cipra’s very lucid and very engaging introduction to the Ising model [1]. We also recommend the excellent books [6] and [9].

**Symbol-Crunching**

Of course, it would be nice to find an expression for $f(x)$ in terms of the symbol $x$. Computing $P_{n,n}(x)$ for any specific $n$ is a finite (albeit huge) computation, involving summing $2^n$ monomials, so we can’t go very far. But let’s assume that we live in an ideal world, or that quantum computing has become a reality. Then computing $P_{n,n}(x)$, and in particular $P_{n,1}(x)$, being finite, is always possible. The first, very natural, step, already proposed in 1941, was motivated by the combinatorial argument (see below and [6, Chapter 6, eq. (1.9)], where we replace $x^2$ by $x$), is to write

$$P_{n,1}(x) = \frac{(x + 2 + x^{-1})^{n/2}}{Z_{n,1}(w)},$$

where $w = \frac{e^x - 1}{e^x + 1}$. It follows from a simple combinatorial argument that $Z_{n,1}(w)$ is a polynomial in $w$, of degree $n_1n_2$.

Taking logarithms and dividing by $n_1n_2$, we get

$$\frac{\log P_{n,1}(x)}{n_1n_2} = -2 \log 2 + \log \left(\frac{1}{2} + \frac{1}{2} x^{-1}ight) + \frac{\log Z_{n,1}(w)}{n_1n_2}.$$

Using the fact (do it!) that $x^{-1} + 2 + x = \frac{4}{1 - e^{-2x}}$, we get that

$$f(x) = \log 2 - \log(1 - w^2) + \lim_{n \to \infty} \frac{\log Z_{n,1}(w)}{n^2},$$

where $w = \frac{e^x - 1}{e^x + 1}$.

So from now on, all we need is to find

$$F(w) := \lim_{n \to \infty} \frac{\log Z_{n,1}(w)}{n^2}.$$

It turns out (and it follows from elementary considerations) that the sequence $\frac{1}{n^2} \log Z_{n,1}(w)$ converges in the sense of formal power series. More precisely, for every positive integer $r$, the coefficient of $w^r$ in $F(w)$ (our object of desire) coincides with that of $\frac{1}{n^2} \log Z_{n,1}(w)$ as soon as $n > r$. So a natural experimental mathematics approach would be to try to find as many Taylor coefficients of $F(w)$ as our computer allows and look for a pattern that would enable us to conjecture a closed-form expression for the Taylor coefficients of $F(w)$, thereby determining $F(w)$ and hence $f(x)$.

In an ideal world, with an indefinitely large computer, this very naive approach would have succeeded. Alas, as it turned out, we would have needed to compute $P_{n,n}(x)$ for $n = 96$, and since $2^{96}$ is such a big number, this very naive brute-force approach is doomed to failure in our tiny universe.

**Using Transfer Matrices**

A much more efficient approach to computing the Laurent polynomials $P_{n,n}(x)$ (and hence the polynomials $Z_{n,1}(w)$) was suggested in the seminal paper of Kramers and Wannier [3]. That was also Onsager’s starting point. It is easy to see (see [6, p. 118]) that for each $n_1$, there are easily computed $2^{n_1} \times 2^{n_1}$ matrices, let’s call them $A_{n_1}(x)$, such that

$$P_{n,1}(x) = \text{trace} A_{n_1}(x)_{n_1}.$$

With today’s computers, it is possible to compute these for $n_1 \leq 12$ and as large an $n_2$ as desired. But once again, one can (still) not go very far.

In 1941, B. L. van der Waerden suggested an ingenious (very elementary) combinatorial approach, described beautifully in Barry Cipra’s article [1] (see also [6, Chapter 6] and [9] for nice accounts). He observed that the coefficients of $w$ in the polynomial $Z_{n,1}(w)$ have a nice combinatorial interpretation. Putting $N = n_1n_2$, it turned out (and is easy to see; see [6]) that for every positive integer $r$, the coefficient of $w^r$ in $Z_{n,1}(w)$, let’s call it $p_r$, is the number of “lattice polygons” with $r$ edges that can lie in an $n_1 \times n_2$ “toroidal rectangle,” i.e., the set $\{0, 1, \ldots, n_1\} \times \{0, 1, \ldots, n_2\}$ with 0 identified with $n_1$ and $n_2$ respectively. A lattice polygon is a collection of edges such that every participating vertex has an even number (0, 2, or 4) of neighbors. It follows in particular that $p_r$ is zero if $r$ is odd.

It also follows from elementary combinatorial considerations that for $n_1, n_2 > r$, the coefficient $p_r$ is a certain polynomial in $N$ [6, p. 150, eq. (1.17)], and hence may be written $p_r(N)$, and we can write

$$p_r(N) = Na_r^{(1)} + N^2 a_r^{(2)} + \cdots + N^m a_r^{(m)}.$$

Now it also follows from elementary considerations, already known in 1941, that once you take the log, divide by $N = n_1n_2$, and take the limit, only the coefficients of $N$ in these “Ising polynomials” survive, and that

$$F(w) = \lim_{n \to \infty} \frac{\log Z_{n,n}(w)}{n^2} = \sum_{r=1}^{\infty} a_r^{(r)} w^r.$$

It remains to compute as many Ising polynomials $p_r(N)$ as our computers will allow us, extract the coefficients $a_r^{(r)}$ of $N$, and hope to detect a pattern that will enable us to conjecture the general coefficient of $F(w)$, and hence know $f(x)$.

**How to Compute the Combinatorial Ising Polynomials**

The first thing that comes to mind, and works well for small $r$, is to actually look for the kind of lattice polygons that can show up; but as $r$ gets larger, this gets out of hand. Rather than do the intricate combinatorics, we use the fact that

$$P_{n,1}(x) = \text{trace} A_{n_1}(x)_{n_1},$$

from which we can compute
$Z_{n_1,n_2}(w)$ for $n_1 \leq 12$ (say) and $n_2$ as large as desired. For each individual coefficient of $w^r$ ($r$ even), we output it for sufficiently many specific $n_1$ and $n_2$, and then using undetermined coefficients or interpolation, we fit them into a polynomial (whose degree we know beforehand). In fact, it is possible to get $p_{2r}(N)$ by looking at $n_1 = r - 2$, $n_2 > r$, by excluding obvious polygons that belong to the $(r - 2) \times n_2$ toroidal rectangle but are impossible for a larger rectangle.

**The Ising Polynomials**

Using this very naive approach (using only matrix multiplication and then taking the trace), our beloved computers came up with the following first 10 Ising polynomials (we were able to find quite a few more, but as we will soon see, the first ten polynomials suffice):

\[
\begin{align*}
p_2(N) &= 0, & p_4(N) &= N, & p_6(N) &= 2N, \\
p_8(N) &= \frac{1}{2}N(9 + N), & p_{10}(N) &= 2N(6 + N), \\
p_{12}(N) &= \frac{1}{6}N(7 + N)(32 + N), \\
p_{14}(N) &= N(130 + 21N + N^2), \\
p_{16}(N) &= \frac{1}{24}N(11766 + 1715N + 102N^2 + N^3), \\
p_{18}(N) &= \frac{1}{3}N(5876 + 776N + 49N^2 + N^3), \\
p_{20}(N) &= \frac{1}{120}N(980904 + 118830N + 7415N^2 + 210N^3 + N^4).
\end{align*}
\]

Extracting the coefficients of $N$, we get

\[
z = \frac{a_{0,0} + a_{1,0}(x + x^*) + a_{0,1}xx^* + a_{2,0}(x + x^*)^2 + a_{1,1}(x + x^*)xx^* + a_{0,2}(xx^*)^2}{b_{0,0} + b_{1,0}(x + x^*) + b_{0,1}xx^* + b_{2,0}(x + x^*)^2 + b_{1,1}(x + x^*)xx^* + b_{2,2}(xx^*)^2},
\]

where $a_{ij}$ and $b_{ij}$ are undetermined coefficients, we get a system of polynomial equations that can be easily solved using Gröbner bases. This gets translated into an equation relating $z$ and $w$ by eliminating $x$, using the fact that $x = \frac{1+wz}{w}$. The (computer-generated) result is an equation of the form

\[
(\cdots + (\cdots)w + (\cdots)w^5 + (\cdots)w^3 + (\cdots)w^4 + (\cdots)z + (\cdots)wz + (\cdots)w^2z + (\cdots)w^3z + (\cdots)w^4z = 0,
\]

where the dots stand for certain linear combinations of the undetermined coefficients, which we suppress here because of their size. In order to ensure that the solution for $w$ of this equation is a series in $z$ with odd exponents only, it suffices to force the coefficients of all terms $w^{i+j}$ with $i+j$ even to equal zero. This gives a linear system whose solution brings the equation down to

\[
(w - 1)(w + 1)(a_{0,0} + a_{0,1} + a_{2,0}) + (1 + w^2)z(b_{0,0} - b_{1,0} + b_{2,0}) = 0.
\]

**Duality Saves the Day**

Way back in 1941, in the seminal paper that we have already mentioned, Kramers and Wannier discovered the duality relation (see [1] for a lucid explanation)

\[
f\left(\frac{x+1}{x-1}\right) = f(x) - \log\left(\frac{x - x^{-1}}{2}\right).
\]

Letting

\[
x^* = \frac{x + 1}{x - 1},
\]

the duality relation can be written as

\[
f(x^*) = f(x) - \log\left(\frac{x - x^{-1}}{2}\right),
\]

or in a more symmetric form,

\[
f(x) - \log(x + x^{-1}) = f(x^*) - \log(x^* + (x^*)^{-1}).
\]

It follows that a more natural, and hopefully more user-friendly, function to consider is

\[
\tilde{f}(x) := f(x) - \log(x + x^{-1}),
\]

and we have that $\tilde{f}(x)$ is unchanged under the involution $x \leftrightarrow x^*$:

\[
\tilde{f}(x^*) = \tilde{f}(x).
\]

It is natural to change from the variable $w$ to one that is invariant under the interchange $x \leftrightarrow x^*$. There are many possibilities. Obviously, in order to ensure the invariance, we can set $z = R(x, x^*)$ for any symmetric rational function $R$. We only need to ensure that when $w$ is expressed as a series in $z$, this series has positive order, so that we are allowed to substitute it into $R(w)$. Since $R(w)$ has only even exponents, we may also prefer that the series $w = u(z)$ have only odd exponents in $z$, so that the substitution does not introduce odd exponents into $R(w)$.

If we try a generic template (ansatz) for a symmetric rational function with numerator and denominator of degree at most two,
This suggests the choice

\[ z = \frac{cw(1 - w^2)}{(1 + w^2)^2} \]

or

\[ w = \frac{z}{c} + \frac{3z^5}{c^5} + \frac{22z^5}{c^7} + \frac{211z^7}{c^9} + \frac{2306z^9}{c^{11}} + \cdots, \]

for some nonzero constant \( c \). The value of \( c \) is not important. We take \( c = 2 \).

Let \( f(x) \), in terms of \( w \), be written \( \tilde{F}(w) \). Then (since \( x + x^{-1} = \frac{2(1 + w^2)}{1 + w^2} \), note that \( x = \frac{1 + w}{1 - w} \))

\[
\tilde{F}(w) := f(x) - \log(x + x^{-1})
\]

\[ = - \log(1 - w^2) + F(w) + \log 2 - \log \left( \frac{2(1 + w^2)}{1 - w^2} \right) \]

\[ = - \log(1 + w^2) + \sum_{i=0}^{\infty} a_i^{(1)} w^i, \]

giving

\[
\tilde{F}(w) = -w^2 + \frac{3}{2} w^4 + \frac{5}{3} w^6 + \frac{19}{4} w^8 + \frac{59}{5} w^{10} + \frac{75}{2} w^{12} + \frac{909}{7} w^{14} + \frac{3923}{8} w^{16} + \frac{17627}{9} w^{18} + \frac{81743}{10} w^{20} + O(w^{22}).
\]

Changing the variable to \( z \), and renaming \( \tilde{F}(w) \) to \( G(z) \), we get

\[ G(z) = \frac{1}{4} z^2 - \frac{9}{32} z^4 - \frac{25}{48} z^6 + \frac{1225}{1024} z^8 - \frac{3969}{1280} z^{10} - \frac{17787}{2048} z^{12} - \frac{18401}{7168} z^{14} - \frac{41409225}{524288} z^{16} - \frac{147744025}{589824} z^{18} \]

\[ = \frac{2621440}{262144}. \]

The first ten terms of the sequence of coefficients, let’s call them \( \{b_{2r}\}_{r=1}^{10} \),

\[
\begin{align*}
  &1, 9, 25, 1225, 3969, 17787, 184041, 41409225, 147744025, 524288, 589824, \ldots,
\end{align*}
\]

factorize nicely, which indicates that the series might be hypergeometric, i.e., the ratio of consecutive terms is a rational function of \( r \). This is good news, since the famous sine and cosine functions and many other functions that come up in physics (e.g., the Hermite and Legendre polynomials, which are so important in quantum mechanics) and elsewhere are hypergeometric.

By setting up an ansatz

\[ \frac{b_{2r+2}}{b_{2r}} = \frac{a_0 + a_1 x + a_2 x^2 + a_3 x^3}{b_0 + b_1 x + b_2 x^2 + b_3 x^3}, \]

plugging in the known values for \( 1 \leq r \leq 9 \), and simplifying, we get a system of nine linear equations in the seven unknowns \( a_0, a_1, a_2, a_3, b_0, b_1, b_2 \). If you take a random such system, it is most likely unsolvable. If the computer finds a solution, it is great news. What is true for the first nine values is probably true forever.

This means that the sequence of ratios \( b_{2r+2}/b_{2r} \) probably matches a rational function in \( r \). Given the ratios \( \{b_{2r+2}/b_{2r}\}_{r=1}^{9} \), the computer immediately established that

\[ \frac{b_{2r+2}}{b_{2r}} = \frac{r(2r + 1)^2}{(r + 1)^3}, \]

for \( 1 \leq r \leq 9 \), and if true for all \( r \), this would imply the closed-form expression for the coefficients

\[ b_{2r} = -\left(\frac{2}{r}\right)^2. \]

Since we can nowadays easily extend the sequence \( b_{2r} \) up to (at least) sixteen terms, we did so, and this “guess” indeed continued to hold, which makes it virtually certain that the guess is correct. Combining everything, we derived, ab initio, by pure guessing (and very elementary and natural reasoning), Onsager’s formidable formula.

**What’s Next?**

Now that we have rediscovered Onsager’s explicit formula for \( f(x) = f(x, 1) \), a natural next step toward the general case \( f(x, y) \) is to determine an explicit expression for \( m(x) = \frac{\partial f(x, y)}{\partial y} \), i.e., the next term in the Taylor series expansion of \( f(x, y) \) with respect to \( y \) at \( y = 1 \). Physicists call this the “spontaneous magnetization.”

Using transfer matrices, as before, it is easy to compute the first few terms of \( m(x) \) as a series in \( x \) (or \( w \), or \( z \)), and we don’t even need a computer to guess an explicit expression for them: they all are zero. But that’s just a part of the story.

Onsager observed that \( m(x) \) is zero only for \( x < 1 + \sqrt{2} \), while for \( x \geq 1 + \sqrt{2} \), it is equal to

\[
\left( \frac{(x^2 + 1)^2(x^2 - 2x - 1)(x^2 + 2x - 1)}{(x - 1)(x + 1)^2} \right)^{1/8}.
\]

According to Thompson [6, p. 135], this expression “was first derived by Onsager in the middle of the 1940s, but in true Onsager fashion he has not to this day published his derivation.”

We don’t know how he found this expression, but here is one way one could have searched for it, using experimental mathematics. For specific numbers \( x, y \), we can compute numerical approximations of \( f(x, y) \) using the original definition (Definition 3 above). For example, taking \( f(x, y) \approx \log P_{x,n}(x, y) / n! \) with \( n \approx 20 \) gives several correct digits at a reasonable computational cost. From the numerical estimates of \( f(x, y) \) for various points \( x, y \), we can obtain numerical estimates for \( m(x) \) and \( m'(x) \), for various points \( x \).

The idea is to fit a differential equation against this numeric data. Suppose we suspect a differential equation of the form

\[
(a_0 + a_1 x + \cdots + a_{10} x^{10}) m(x) + (b_0 + b_1 x + \cdots + b_{10} x^{10}) m'(x) = 0,
\]

\[ \frac{\partial^2 m}{\partial x^2} = \frac{m(x)}{x + 1}. \]

\[ m(x) = 0, \]

\[ m'(x) = 0. \]
with unknown integer coefficients $a_i$, $b_i$ to be determined. So for a specific point $x$, the task is to find a so-called integer relation of the real numbers $m(x), \ldots, x^{10}m(x), m'(x), \ldots, x^{10}m'(x)$. There are well-known algorithms for finding such relations [2, 4].

In order to recover the relation from the values at a single point $x$, we would need to compute these values to a rather high precision, which is not an easy thing to do. We can get along with less precision using several evaluation points and searching for a simultaneous integer relation of the numbers $m(x), \ldots, x^{10}m(x), m'(x), \ldots, x^{10}m'(x)$, for several $x$. It turns out that by using enough evaluation points, we need only about six decimal digits of accuracy of $m(x)$ and $m'(x)$ for each of these points in order to establish a convincing guess. Unfortunately, this is still a bit more than what we were able to obtain by a direct computation via transfer matrices.

Supporting Software
For Maple and C programs, as well as output files, please visit the web page http://sites.math.rutgers.edu/~zeilberg/mamarim/mamarimhtml/onsager.html.

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