The Farey Fraction Spin Chain

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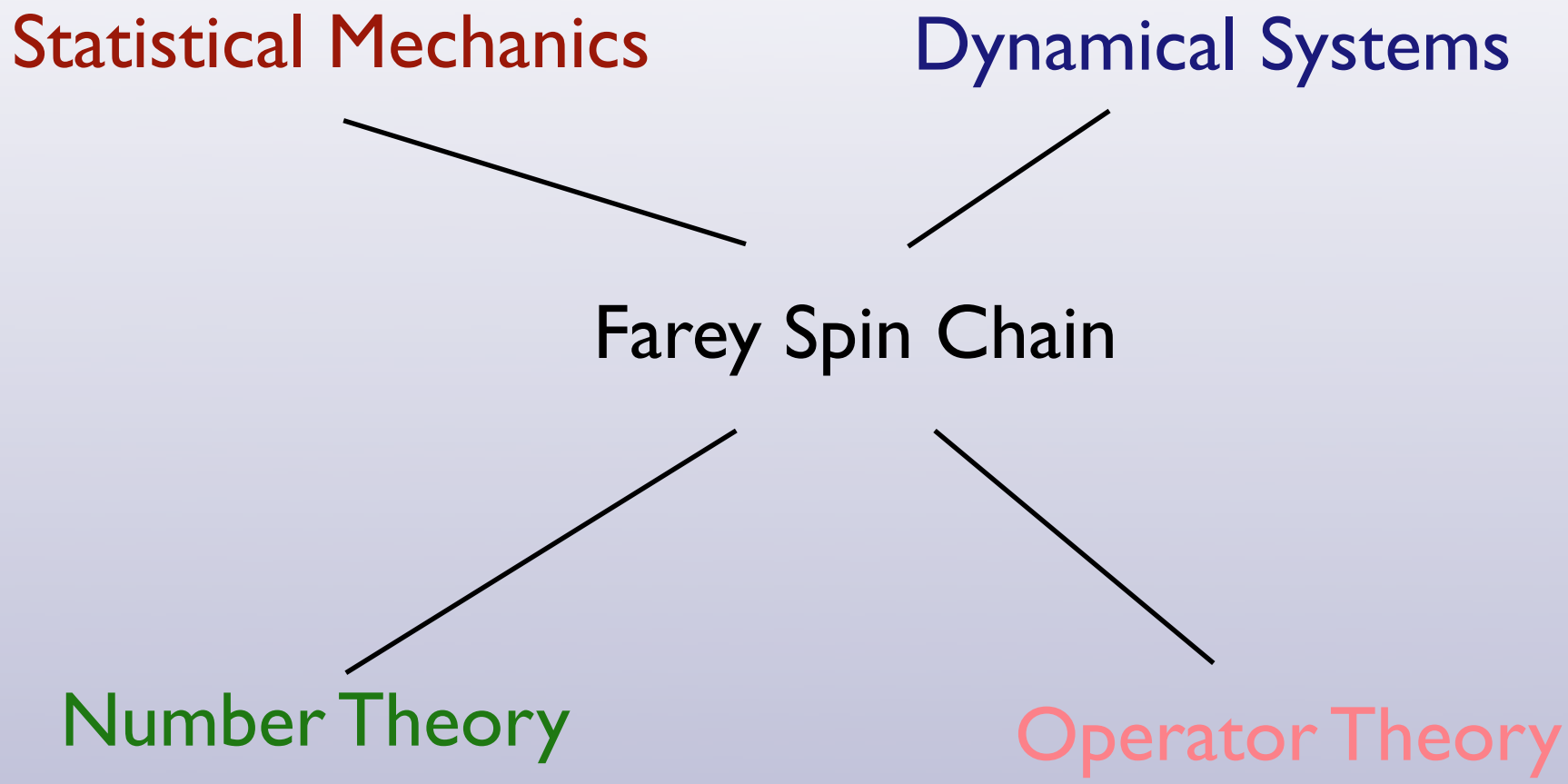
Materials Theory


Statistical Mechanics
Dynamical Systems
Farey Spin Chain
Number Theory
Operator Theory

From a physicist's point of view:

Number theorist := someone who is willing to spend an infinite amount of time on an impossible problem.

- Farey fractions
- mini–course in statistical mechanics
- “trace” model
- generalized Knauf model
- critical Farey tree partition function
- summary

Farey Fractions:

The Farey fractions (modified Farey sequence) may be defined by addition:

									level
$\frac{0}{1}$								$\frac{1}{1}$	1
$\frac{0}{1}$				$\frac{1}{2}$				$\frac{1}{1}$	2
$\frac{0}{1}$		$\frac{1}{3}$		$\frac{1}{2}$		$\frac{2}{3}$		$\frac{1}{1}$	3
$\frac{0}{1}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{2}{5}$	$\frac{1}{2}$	$\frac{3}{5}$	$\frac{2}{3}$	$\frac{3}{4}$	$\frac{1}{1}$	4

At each level, we keep the fractions previously generated (the "old" fractions) and generate "new" ones. If

$$\frac{a}{c} \text{ and } \frac{b}{d}$$

are neighboring fractions at level k, then a "new" fraction

$$\frac{a+b}{c+d}$$

appears between them at level $k+1$. In this way, all rationals in [0,1] are generated as $k \to \infty$.

Alternatively, one can generate the Farey fractions using products of the matrices

$$A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

Each such product of k matrices is denoted

$$M_k = \underbrace{AAB \ldots BAA}_{k} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

$$\frac{a}{c} \qquad \frac{b}{d}$$

When the product begins with A, one has

$$\frac{b}{d} < \frac{a}{c}$$

with a/c the neighbor of b/d at level k, and all $2^{k-1}+1$ fractions are generated.

Of course, there is a more charming way to generate them....

Which may explain the name...

Mini–course in Statistical Mechanics:

The Farey fraction spin chains are a set of physical models built on Farey fractions. (Originally studied by Cvitanovic, Fiegenbaum, and others as models of intermittency; later by Knauf and co-workers.) To get an idea of their physical interest, we introduce a few stat mech quantities.

Consider the following simple model of a magnet: a chain composed of k molecules ("spins"), each of which can point either up ↑ or down ↓. The *magnetization* = (number of up spins - the number of downs) / k. In order to account for thermal effects, we must perform a certain weighted average over all possible arrangements (configurations or states) of ups and downs, then let the length k of the chain (the number of spins) go to ∞.

With k spins there are 2^k configurations (states).

$$\underbrace{\uparrow\uparrow\downarrow\ldots\uparrow\downarrow\downarrow}_{k}$$

The probability of a given *configuration* (the "Boltzmann factor") depends on its energy E and the temperature T:

$$p = \frac{e^{-E/T}}{Z}$$

where the *partition function* Z_k is just the normalizing factor:

$$Z_k = \sum_{configs} e^{-E/T}.$$

Note that the probability of a configuration (state) decreases with its energy. Thus the state of lowest energy (the "ground state") has the largest probability. This is generally ordered (magnetized) and dominates at low temperatures, as we will see.

The *partition function* Z_k plays another role as well. Its logarithm gives the *free energy f*, the function that determines the thermodynamic behavior of the system. Explicitly,

$$f = -T \lim_{k \to \infty} \frac{\ln Z_k}{k}.$$

Of course, for arbitrary choices of energy E, it is not obvious that f will exist. If it does exist, its singularities (as a function of T) determine the phase transitions of the model. Their nature determines the type ("order") of phase transition. In our case there is a phase transition between a magnetized (ordered) state and unmagnetized (disordered) state.

To specify our model, we must list the configurations and assign an energy to each one. For us, a configuration is just one of the 2^k products of k matrices A and B. Each $A = \uparrow$, spin up, while $B = \downarrow$, spin down. Thus the configuration with all As has all spins up

$$\underbrace{\uparrow\uparrow\uparrow\ldots\uparrow\uparrow}_{k} = A^k = \begin{pmatrix} 1 & 0 \\ k & 1 \end{pmatrix}$$

Here the chain is completely magnetized.

The Trace Model:

There are various ways to define the energy that are of interest. Most of them use the product of the *k* matrices mentioned

$$M_k = \underbrace{AAB\ldots BAA}_{k} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

Note that det(*A*) = det(*B*) = 1, so *ad* - *bc* = 1, and all matrix entries are non-negative. For the Trace Model, the energy of a given configuration is

$$E_i = \ln[Tr(M_i)] = \ln(a+d),$$

so the partition function is simply

$$Z_k(T) = \sum_{i=1}^{2^k} \frac{1}{Tr(M_i)^{1/T}}$$

The ground state is all spins up (or down)

$$\underbrace{\uparrow\uparrow\uparrow\ldots\uparrow\uparrow}_{k} = A^k = \begin{pmatrix} 1 & 0 \\ k & 1 \end{pmatrix}$$

with energy

$$E_{k,0} = ln[Tr(A^k)] = ln2.$$

Turning over one or more spins gives an "excited state", with energy that grows with chain length at least like

ln(k). The maximum excited state energy grows like k for the "antiferromagnetic" state

$$\underbrace{\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\ldots\uparrow\downarrow}_{k}$$

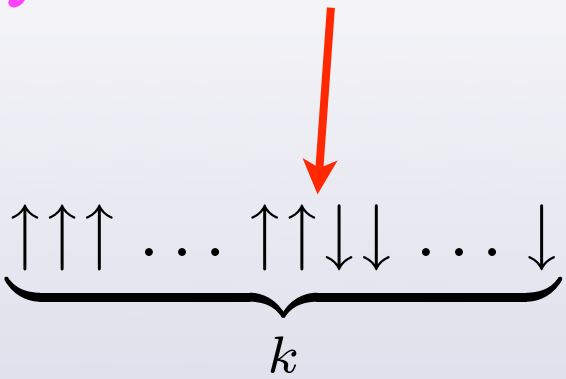
Now there are only two ground states, but exponentially many excited states (2^k-2). Additionally, the free energy is known to exist, and there is a single phase transition at temperature $T_c = 1/2$. For $k \rightarrow \infty$, the ground states dominate at low temperatures. However, for $T > T_c$, the system goes into a disordered (thermodynamic) state, i.e. it undergoes a phase transition.

It is unusual to find a phase transition at finite T in a one–dimensional system. Generally such systems are always ordered or always disordered. The transition here is also interesting because it is "second–order" (the first derivative of f is continuous at T_c).

The following (quite heuristic) argument explains why one–dimensional systems usually don't have a phase transition.

Assume an ordered state at low temperature. Suppose the energy of a defect is ε. Then the entropy of a defect is

$$\Delta s = \log k,$$



where k is the number of spins. Hence the free energy change due to the extra defect is

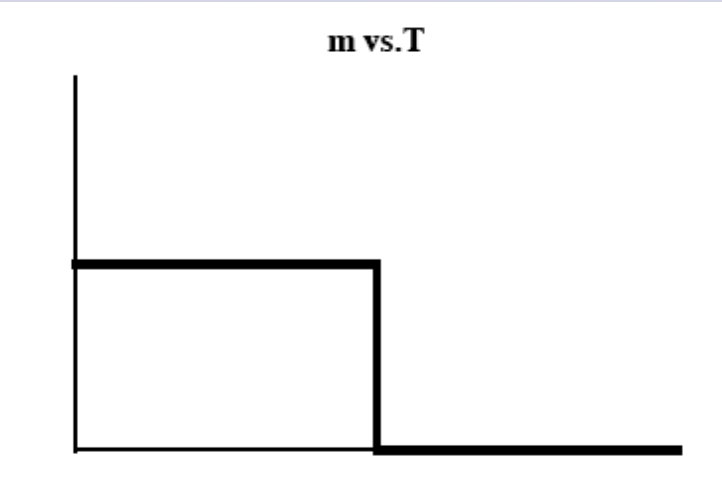
$$\Delta f = \epsilon - T \log k,$$

which will always be < 0 (favored) for k large enough, unless

i.) ε = ∞ (when the system is always ordered) or

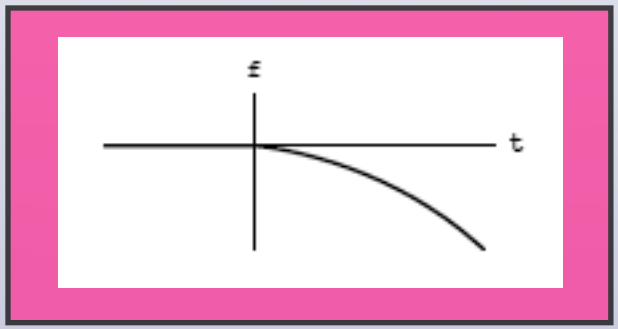
ii.) the interactions are long–ranged (the case here–note the energy of a defect in the KSC is logarithmic in k).

The magnetization (for an ∞ chain) goes from saturated ($m = 1$) to paramagnetic ($m = 0$) at the transition, which occurs at $T_c = 1/2$. The low–temperature state is completely ordered, with no thermal effects at all (this is also unusual).



The free energy f vanishes for $T < T_c$, and is negative for $T > T_c$. Just above the transition it has the form (Fiala, PK, and Özlük, 2003)

$$f \sim \frac{T - T_c}{\ln(T - T_c)}$$



(we'll explain how this is known shortly). This functional form means that the transition is (barely) second–order.

Summary:

$$M_k = \underbrace{AAB\ldots BAA}_{k} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

$$E_i = \ln(a+d)$$

$$Z_k(T) = \sum_{i=1}^{2^k} \frac{1}{(a+d)^{1/T}} \left(= \sum_n \frac{\Phi_k(n)}{n^{1/T}} \right)$$

$$f = -T \lim_{k\to\infty} \frac{\ln Z_k}{k}.$$

$$f \sim \frac{T - T_c}{\ln(T - T_c)} \qquad (T_c = 1/2)$$

The trace model has inspired some work in number theory. Define first

$$\Phi_k(n) = |\{M_k | Tr(M_k) = n\}|$$

i.e., the number of configurations in a chain of length *k* with energy ln(*n*) ("density of states"). (As mentioned, using Φ_k, Z_k becomes a Dirichlet series.) However, Φ_k turns out to be difficult to handle. If one lets

$$\Phi(n) = \sum_{k=1}^{\infty} \Phi_k(n)$$

and defines a summed "density of states"

$$\Psi(N) = \sum_{n=2}^{N} \Phi(n)$$

Kallies, Özlük, Peter and Snyder (2001) and Boca (2005) have shown, using results for reduced quadratic irrationalities, that as $N \to \infty$ the summed density of states

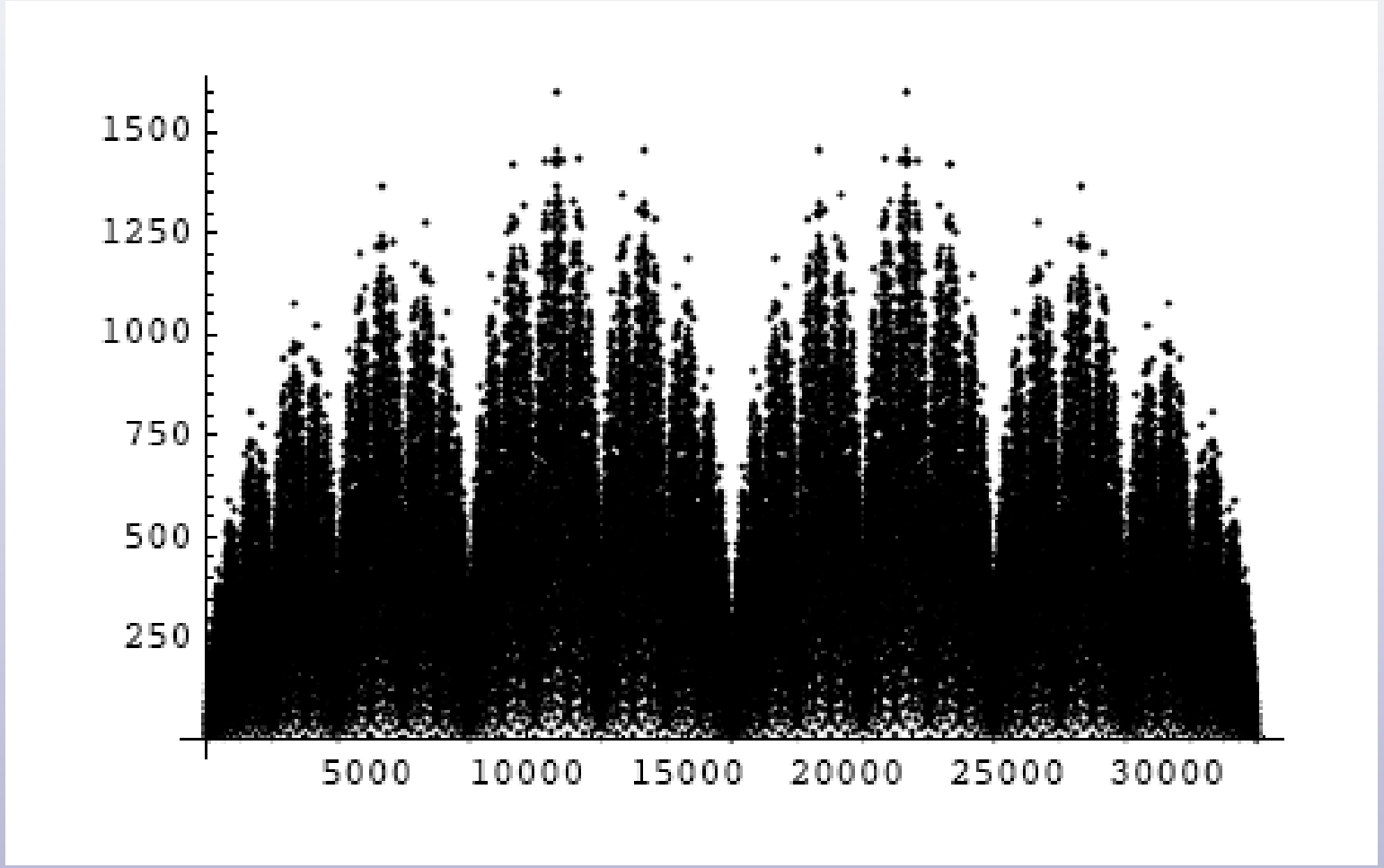
$$\Psi(n) = \frac{6}{\pi^2} n^2 \log(n) + c\, n^2 + O(n^{\frac{9}{5}+\epsilon}).$$

Additionally, M. Peter (2001) proved that for the density of states itself

$$\lim_{N \to \infty} \frac{\Phi(N)}{NlnN}$$

does not even exist! (it's a distribution). Generically, the reason is that there is fractal behavior in this model (the Farey chain was originally studied as a model of intermittency in chaos)...

For instance, here are the Farey denominators at level $k = 16$:



Generalized Knauf model:

Next we consider the generalized Knauf model (thanks Don Zagier!), in which the energy is defined via $E_i = ln(cx+d)$, with a parameter $x \geq 0$ – recall that the configuration matrix is given by

$$M_k = \underbrace{AAB \ldots BAA}_{k} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

The resulting partition function is

$$Z_k(x, \beta) = \sum_{i=1}^{2^k} \frac{1}{(cx+d)^\beta}$$

(with $\beta = 1/T$)

The free energy, however, is exactly the same as in the trace model. So why bother?

1) Because we can see very clearly the connection with dynamical systems, and

2) certain correlation functions (expectation values) can be exactly calculated.

First, to generate M_{k+1} multiply M_k by A or B; i.e. $M_{k+1} = \{M_k A\ ,\ M_k B\}$. From this a functional recursion relation follows immediately:

$$Z_{k+1}(x,\beta) = \frac{1}{(x+1)^{\beta}} Z_k\left(\frac{x}{x+1},\beta\right) + Z_k(x+1,\beta)$$

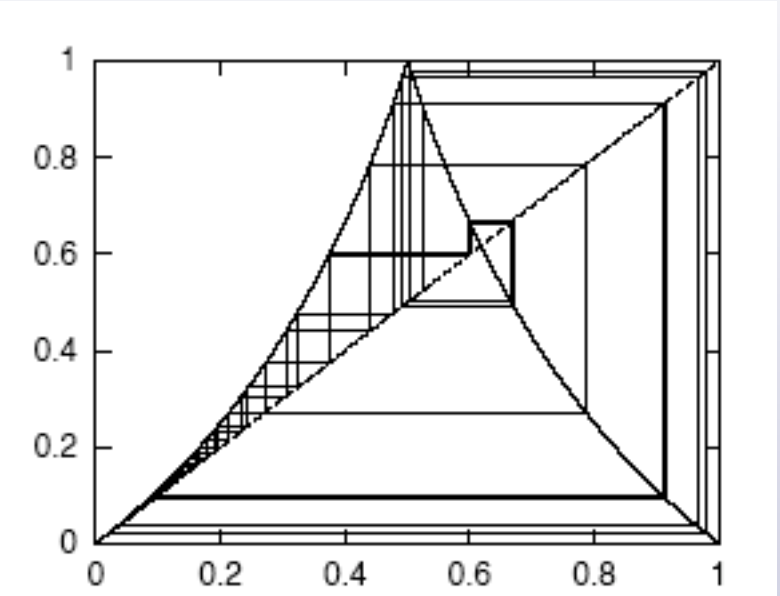
Note that if we set $x = 0$, only $Z_k(0,\beta)$ and $Z_k(1,\beta)$ appear.

This closure is very useful.

(Note that our recursion relation is closely related to the "Lewis three–term equation" which has been extensively studied in the theory of the Selberg ζ–function.)

Next, consider the Farey map on [0,1]

$$f(x) = \begin{cases} \frac{x}{1-x}, & x \le 1/2 \\ \frac{1-x}{x}, & 1/2 < x \end{cases}$$



The associated transfer operator is

$$\mathcal{L}\varphi(x) = \sum_{f(y)=x} |f'(y)|^{-\beta} \varphi(y)$$

$$= \frac{1}{(1+x)^{2\beta}} \varphi\left(\frac{x}{1+x}\right) + \frac{1}{(1+x)^{2\beta}} \varphi\left(\frac{1}{1+x}\right)$$

What is the connection with the Farey fractions? The inverse maps ("presentation functions") are

$$F_0 = \frac{x}{1+x}, \; F_1 = \frac{1}{1+x}.$$

Acting on *1/2*, these generate the "new" Farey fractions (the "Farey tree"). E.g. $F_0(1/2)=1/3$, $F_1(1/2)=2/3$;

$F_0 F_0(1/2)=1/4$, $F_1 F_0(1/2)=3/4$, etc.

At each level k the 2^{k-2} new fractions are generated by composition of F_0 and F_1.

Using the "evenness" property

$$Z_k(x,\beta) = \frac{1}{x^\beta} Z_k(\frac{1}{x},\beta)$$

it follows that the transfer operator is the same as the rhs of the functional recursion for $Z_k(x,\beta)$. One finds easily that

$$Z_k(x,\beta) = \frac{1}{2}\mathcal{L}^{k+1}1(x)$$

which implies that the spectrum of the transfer operator determines the partition function and free energy. Prellberg (2003) has determined the spectrum. His result for the leading eigenvalue λ then gives the form of the free energy near the transition quoted above:

$$f \sim \frac{T - T_c}{\ln(T - T_c)}$$

The expectation value of a quantity Q in statistical mechanics is the weighted sum over configurations given by

$$< Q >= \sum_i \frac{Q_i e^{-E_i/T}}{Z},$$

where Q_i is the value of Q in the i^{th} configuration, and E_i is the energy of the i^{th} configuration. When Q involves quantities at more than one location (e.g. on the spin chain), this is called a "correlation function".

Now for some correlation (expectation value) results. The following are for the $x = 0$ case, which is the "canonical" partition function studied by Knauf and co–workers. In this case there is an up–spin (matrix A) at the beginning of the chain, so at low temperatures all spins are up (for $k \rightarrow \infty$).

Our results are in terms of the leading eigenvalue λ

$$\lambda = e^{-\beta f}$$

of the transfer operator $\mathcal{L}$. Using the functional recursion and spin flip behavior (the "evenness" mentioned is invariance under spin flip) we find, above the transition,
(Fiala and PK, 2004)

$$\langle \underbrace{\ldots}_{\infty} \uparrow \underbrace{\ldots}_{n} \rangle = \frac{1}{2}(1 + \frac{2-\lambda}{\lambda^{n+1}}),$$

The rhs is always > *1/2*, due to the initial up–spin.

On the other hand

$$\langle \underbrace{\ldots}_{\infty} \uparrow \underbrace{\ldots}_{n} \downarrow \rangle = \frac{\lambda - 1}{2\lambda} = \langle \underbrace{\ldots}_{\infty} \downarrow \underbrace{\ldots}_{n} \downarrow \rangle$$

So the down–spin on the rh edge cancels the effect of the initial up spin, making the function independent of *n* and of the direction of the spin at distance *n*.

This would seem to be a curious edge effect, but we also find...

$$\langle \underbrace{\cdots}_{\infty} \uparrow \underbrace{\cdots}_{n} \downarrow \underbrace{\uparrow \cdots \uparrow \cdots \uparrow}_{r-1} \rangle = \frac{\lambda - 1}{2\lambda^r} = \langle \underbrace{\cdots}_{\infty} \downarrow \underbrace{\cdots}_{n} \downarrow \underbrace{\uparrow \cdots \uparrow \cdots \uparrow}_{r-1} \rangle .$$

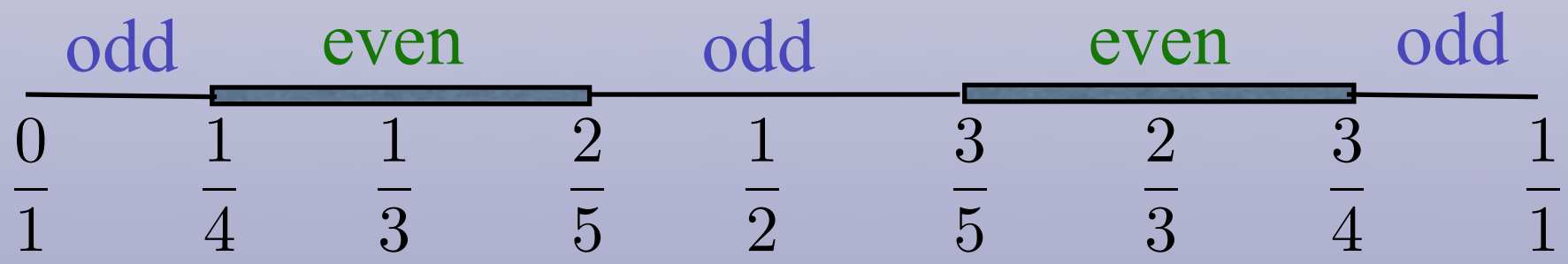
This exhibits the same effects, which is unexpected.

The spins on the rh edge are a cluster, which removes the spin asymmetry from the spin at distance *n*. What is striking is that this occurs regardless of the cluster size *r*, and for any temperature above the transition. In the next talk, Thomas Prellberg will demonstrate that such clusters provide a mechanism for the phase transition.

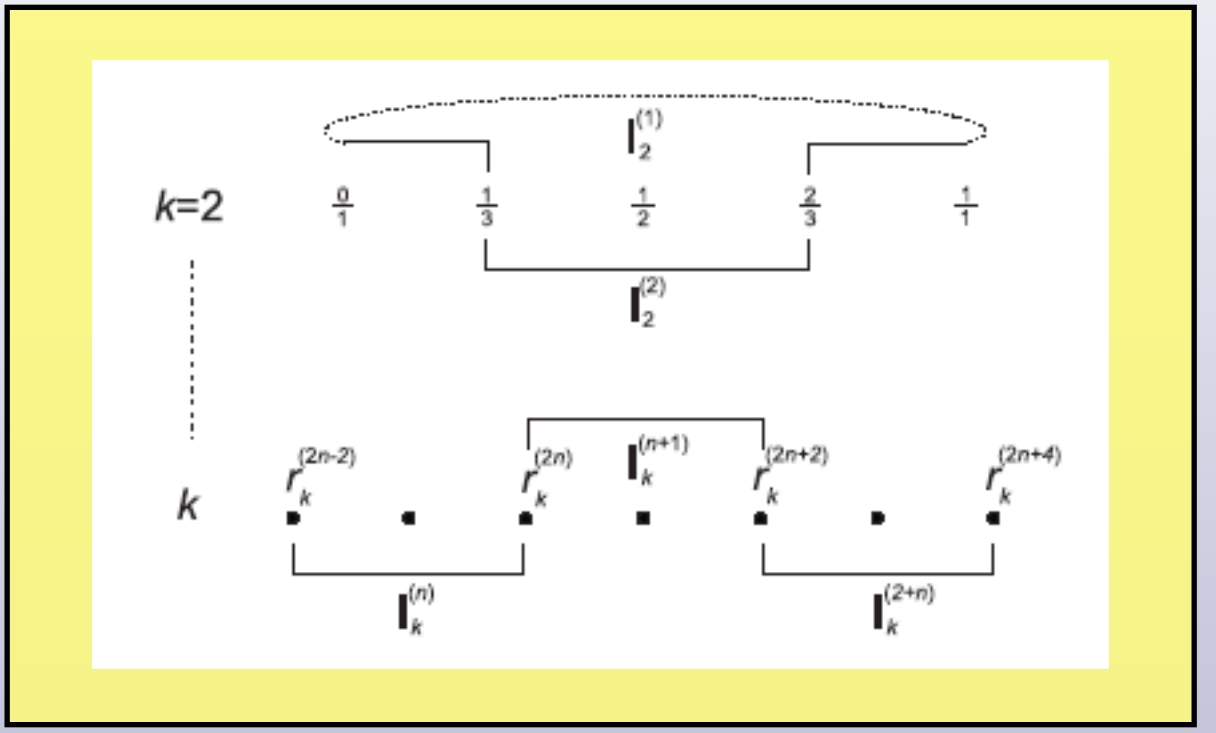
Critical Farey tree partition function:

The Farey tree partition function was originally studied by Feigenbaum et al as a model of multifractals. It has the same free energy f as the other Farey models. At the critical point, it reduces to the sum over alternate differences between new Farey fractions (at each level). These differences are called "even" intervals. The complementary set are the "odd" intervals.

For instance, at level $k = 4$



At an arbitrary level, there are many even and odd intervals



One can show (Fiala and PK, 2005) that

$$\frac{2}{k+1} + \frac{2}{3}\sum_{j=1}^{k-2} I_{k-j}^{(e)} \frac{2j+3}{(j+1)(j+2)} \leq I_k^{(o)} \leq 1.$$

Here $I_k^{(o)}$ is the sum of odd intervals at level k, and $I_k^{(e)}$ the sum of even intervals (which is the same as the Farey tree partition function). Thus, if there were an $\varepsilon > 0$ such that $I_k^{(e)} > \varepsilon$ for all k, the lhs would diverge. Hence

$$\liminf_{k\to\infty} I_k^{(e)} = 0.$$

Numerically, it is clear that the limit is zero.
This is apparently a new and unexpected property of the Farey fractions.

Summary:

We considered the Farey Fraction Spin Chain, one-dimensional statistical mechanical models built on the Farey fractions (modified Farey sequence).

1) Dynamical systems connection proves, rigorously, a (barely) second-order phase transition.

2) Certain correlation functions are calculated exactly.

3) The partition function at the critical point suggests a subtle, apparently new, property of the Farey fractions.

4) Rigorous results by number theorists for the "density of states"; a close connection to the Lewis three-term equation.

Here are some references:

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