

The Farey Fraction Spin Chain

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Supported by NSF-DMR
Materials Theory

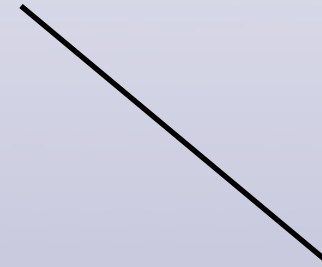
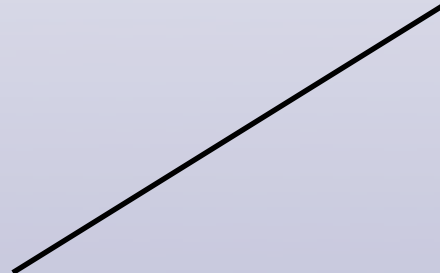
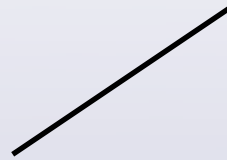
Statistical Mechanics

Dynamical Systems

Farey Spin Chain

Number Theory

Operator Theory



“Mathematicians and physicists:
It’s like Mars and Venus...”

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
- cluster approximation

- including a magnetic field
- renormalization group analysis
- cluster approximation analysis
- critical Farey tree partition function
- summary

Farey Fractions:

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

											<u>level</u>
$\frac{0}{1}$										$\frac{1}{1}$	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 $k \rightarrow \infty$.

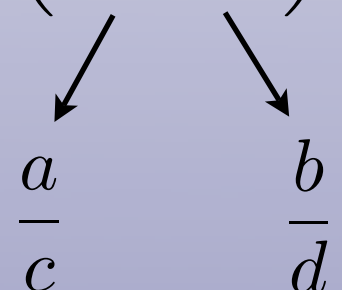
Alternatively, one can generate the Farey fractions using products of the matrices

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

and

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

Each such product of k matrices is denoted

$$M_k = \underbrace{AAB \dots BAA}_k = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$


The diagram shows two arrows originating from the matrix. One arrow points from the element c in the bottom-left position to the fraction $\frac{a}{c}$. The other arrow points from the element d in the bottom-right position to the fraction $\frac{b}{d}$.

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 more charming way to generate them....



Which explains
the name...

Mini-course in Statistical Mechanics:

The **Farey fraction spin chains** are a set of physical models built on the Farey fractions. To get an idea of their physical interest, we need to introduce a few quantities from statistical mechanics.

Consider the following simple model of a magnet: a chain composed of k molecules (“spins”), each of which can point either up \uparrow or down \downarrow . 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).

$$\underbrace{\uparrow\uparrow\downarrow \dots \uparrow\downarrow\downarrow}_k$$

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:

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

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,

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

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. Both their location and nature are of interest, especially the latter, as we will see. In our case there is a phase transition between a **magnetized** (ordered) state and **unmagnetized** (disordered) state.

In order 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 A s has all spins up

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

Here the chain is **completely magnetized**.

The Trace Model:

There are various ways to **define the energy** that are of physical interest. One can use the product of the k matrices mentioned

$$M_k = \underbrace{AAB \dots BAA}_k = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

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

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

so the **partition function** is simply

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

The **ground state** is all spins up (or down)

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

with energy

$$E_{k,0} = \ln[\text{Tr}(A^k)] = \ln 2.$$

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

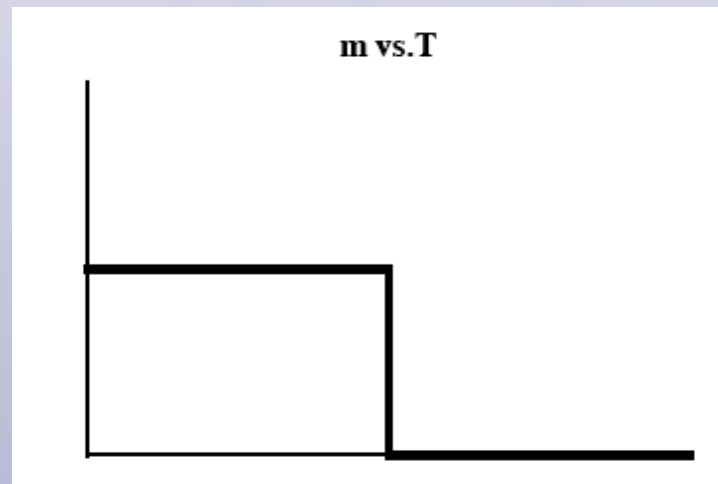
$\ln(k)$. The **maximum excited state energy** grows like k
for the “antiferromagnetic” state

$$\underbrace{\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow \dots \uparrow\downarrow}_k$$

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.

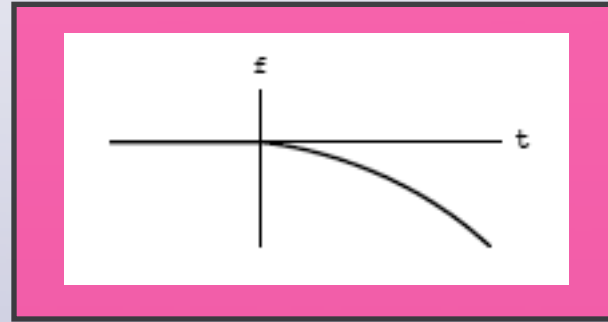
It is **unusual** to find a phase transition at finite T in a one-dimensional system. Generally such systems are always ordered or always disordered. The transition here is also interesting because it is “**second-order**” (the first derivative of f is continuous at T_c).

The **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:

$$M_k = \underbrace{AAB \dots BAA}_k = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

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

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

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

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

The trace model has inspired some work in **number theory**.

Define first

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

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 $N \rightarrow \infty$ the **summed** density of states

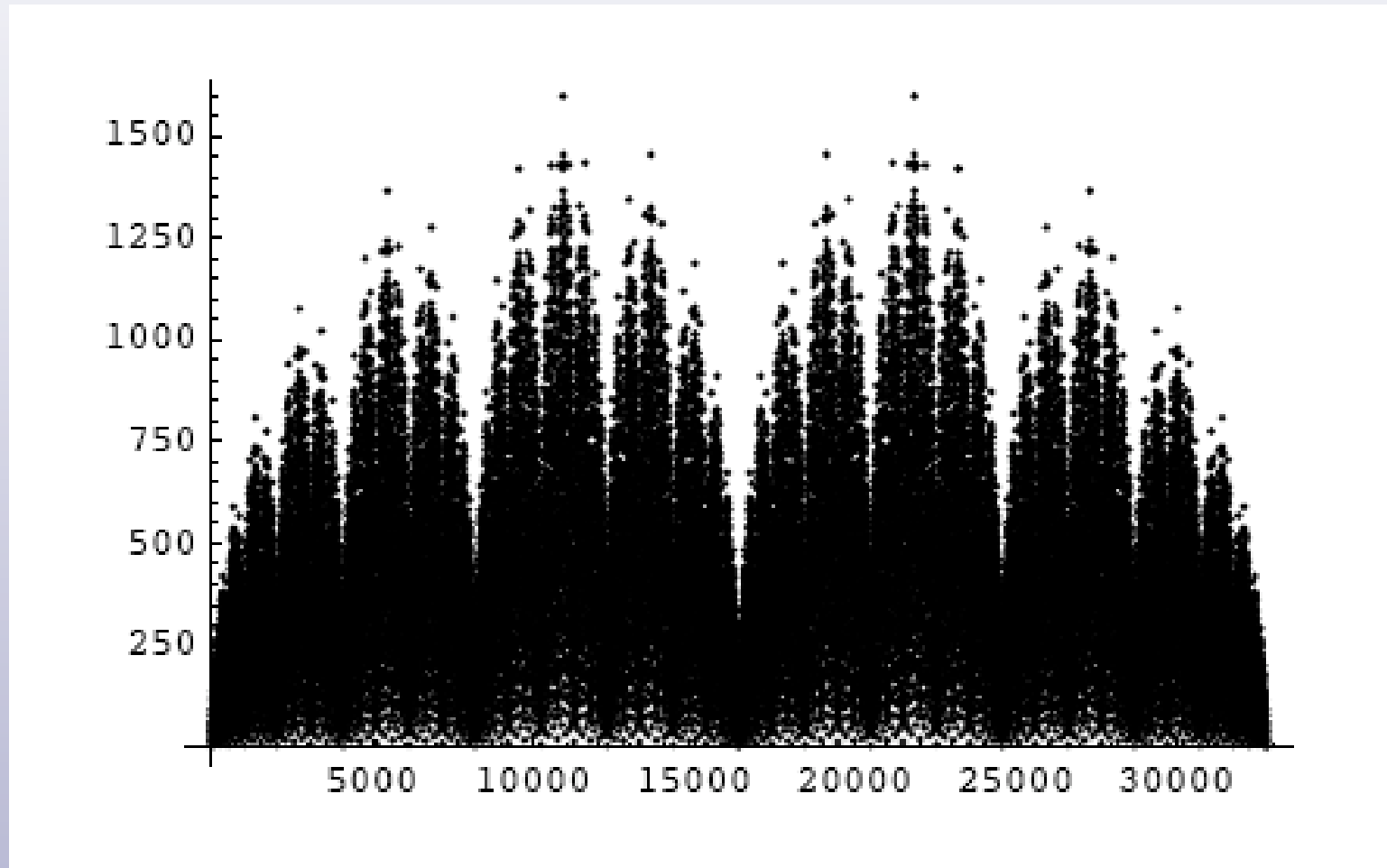
$$\Psi(N) = \frac{6}{\pi^2} N^2 \ln(N) + cN^2 + O(N^{\frac{9}{5} + \epsilon}).$$

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

$$\lim_{N \rightarrow \infty} \frac{\Phi(N)}{N \ln N}$$

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

$$M_k = \underbrace{AAB \dots BAA}_k = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

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.

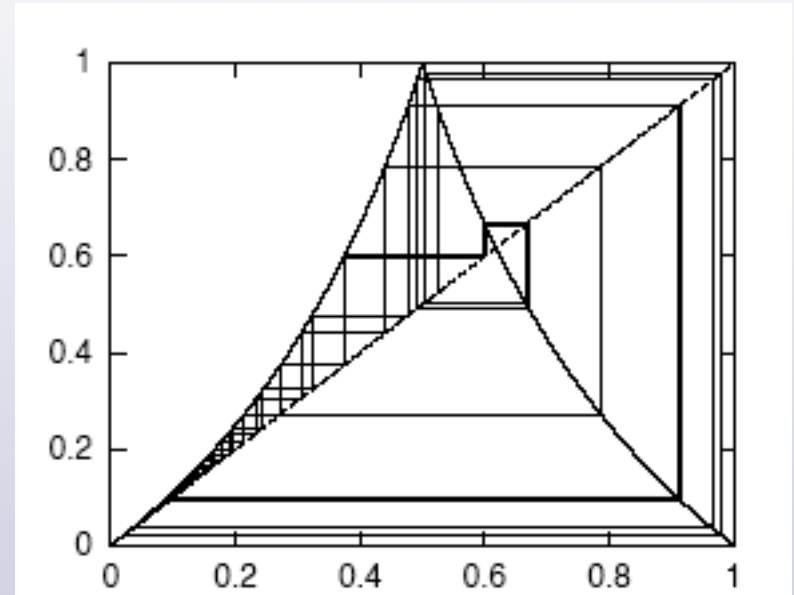
This closure is very useful.

(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 $[0,1]$

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

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

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

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

$$F_0 F_0(1/2)=1/4, \quad F_1 F_0(1/2)=3/4, \text{ etc.}$$

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

Using the “**evenness**” property

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

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

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

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)

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

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

On the other hand

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

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...

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

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. We will see that such clusters provide a **mechanism** for the phase transition.

Cluster approximation:

The **dynamical system connection** suggests (via linearization of the return map) a **cluster approximation** (Prellberg, Fiala and PK 2005).

Introduce the matrix S

$$S = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Now consider each **configuration** as a **series of clusters** of up and down spins. Using S one finds, for example

$$\underbrace{\uparrow\uparrow \dots \uparrow}_m \underbrace{\downarrow\downarrow \dots \downarrow}_n = (A^m S)(S B^n) = \begin{pmatrix} 0 & 1 \\ 1 & m \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & n \end{pmatrix}$$

then assume a **non–interacting** cluster form for the energy

$$\text{Tr}[(A^m S)(SB^n)] \approx \text{Tr}[(A^m S)]\text{Tr}[(SB^n)]$$

so that the energy becomes **additive**,

$$E_i \approx \ln(m) + \ln(n).$$

Applying this to an **arbitrary** excited state makes the energy of each configuration a sum and leads to the **grand partition function**

$$G(z, \beta) := \sum_{k=1}^{\infty} z^k Z_k(\beta) = 2^{-\beta+1} \frac{z}{1-z} + \frac{z \partial_z \Lambda^2(z, \beta)}{1 - \Lambda^2(z, \beta)}.$$

ground states

excited states

For our spin chain the **cluster generating function**

$$\Lambda(z, \beta) = \sum_{n=1}^{\infty} \frac{z^n}{(n(n+1))^{\beta/2}}.$$

The free energy (and phase boundary) are given in terms of the singularities of G . One has $\beta f(\beta) = \ln z_c(\beta)$, where z_c is the smallest singularity of G for real z . This can arise from the first term, due to the ordered states, or the second term, due to the clusters. A change-over from one to the other gives rise to a phase transition.

Asymptotic analysis reproduces the rigorous results

$$T_c = 1/2 \text{ and}$$

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

The significance of the cluster approximation for the Farey fractions has not been explored...

(The cluster approximation results in a model closely related to the “necklace” models of Fisher and Felderhof.)

Including a magnetic field:

There is **no Hamiltonian per se** in this model. However the interactions are **many-body, long-range**, and **ferromagnetic**. Hence it is natural to introduce a magnetic field with ferromagnetic coupling

$$E_k = \ln[\text{Tr}(M_k)] - h(N_{\uparrow} - N_{\downarrow})$$

where N_{\uparrow} is the number of up spins (A matrices) and N_{\downarrow} the number of down spins (B matrices) in a given configuration. This new coupling term should be **relevant** (in the scaling sense).

Assuming Ising-like behavior with a **marginal field** (thanks M.E. Fisher!), one can perform an RG analysis (Fiala and PK 2004). Due to the marginal field, this is a bit more complicated than normally, but the results are completely **consistent** with our rigorous results and there are **no apparent violations** of scaling theory.

(One finds RG eigenvalues are $y_t = d = y_h$.)

Since this model has long-range interactions, RG is a bit suspect. So it is interesting to apply the **cluster approximation** to this extended model. One finds (Prellberg, Fiala and PK 2005) a **grand partition function** $G(z, \beta, h) = G^\uparrow(z, \beta, h) + G^\uparrow(z, \beta, -h)$

$$G^\uparrow(z, \beta, h) \approx 2^{-\beta} \frac{ze^{-\beta h}}{1 - ze^{-\beta h}} + \frac{ze^{-\beta h} \partial_1 \Lambda(ze^{-\beta h}, \beta) \Lambda(ze^{\beta h}, \beta)}{1 - \Lambda(ze^{-\beta h}, \beta) \Lambda(ze^{\beta h}, \beta)}$$

With the same **cluster generating function** Λ as before. Asymptotic analysis gives results **similar** to what one finds with RG

The main **RG and cluster** results are:

1) for the free energy at $h = 0$ and T near T_c (with $t = T - T_c$)

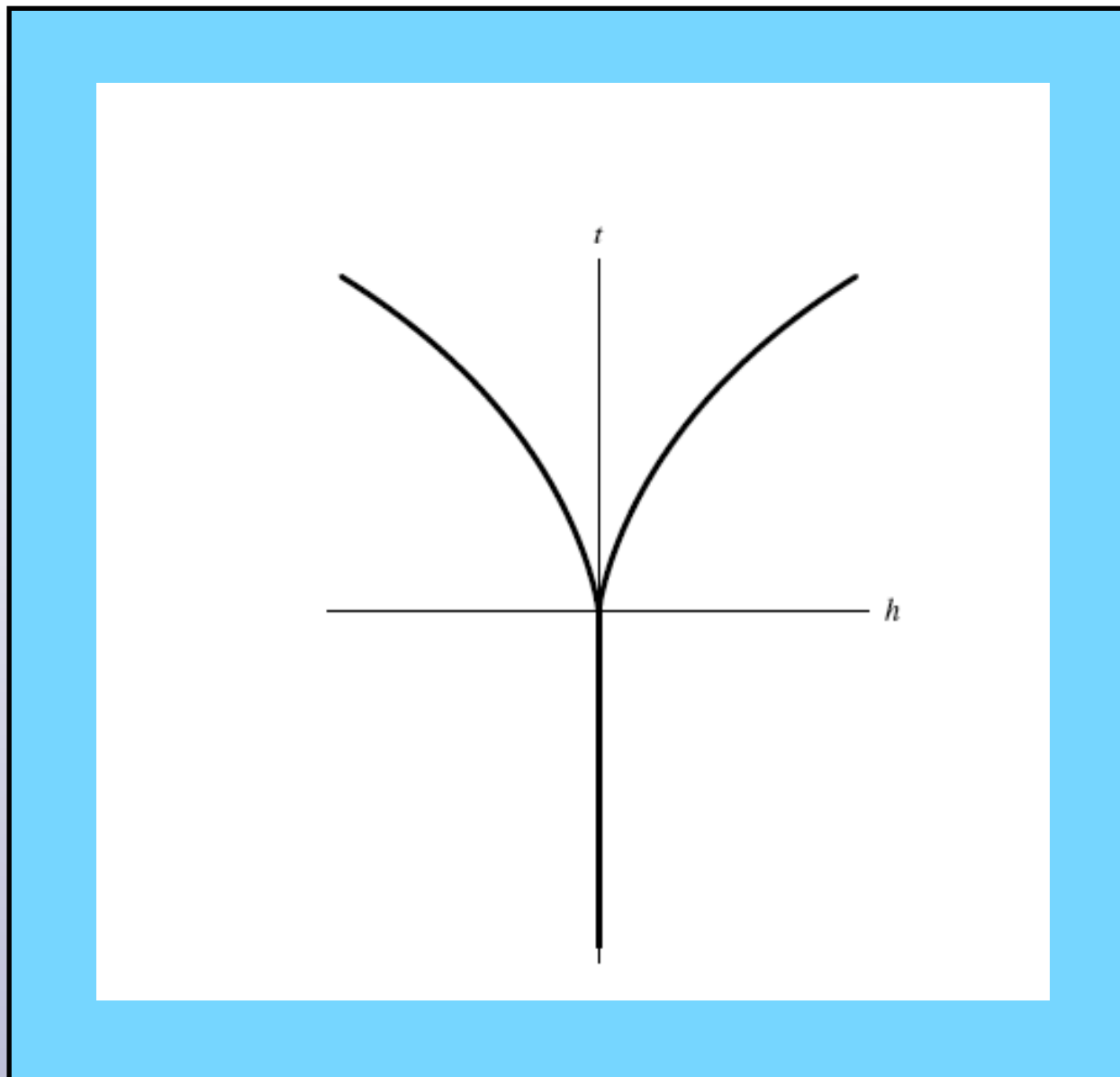
$$f \sim \frac{C}{\beta_c} \frac{t}{\log t}.$$

The constant C differs in the two cases, but the **temperature dependence agrees** with the rigorous result.

2) for the **phase boundary**:

$$h_c \sim -\frac{C}{\beta_c} \frac{t}{\log t}.$$

(With again, different constants in the two cases.) The phase diagram is



all transitions are first-order **except** $h = 0 = t$.

3) For the **free energy** at small h , near the second-order point, via cluster analysis

$$f \sim \frac{C}{\beta_c} \frac{t}{\log t} - \frac{\beta_c}{2C} \frac{h^2}{t}$$

$$(h \ll t / \log t)$$

and from RG

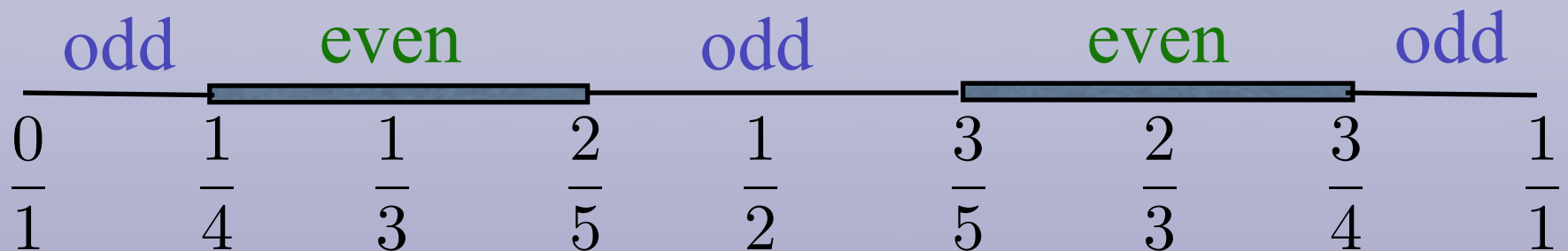
$$f \sim a \frac{t}{\log t} + b \frac{h^2 \log t}{t}$$

Here the magnetic field term has a **different t -dependence** in the two cases. Which (if either) is correct is unclear. It does not seem to be possible to alter the RG analysis to make the two agree without changing the $h = 0$ term.

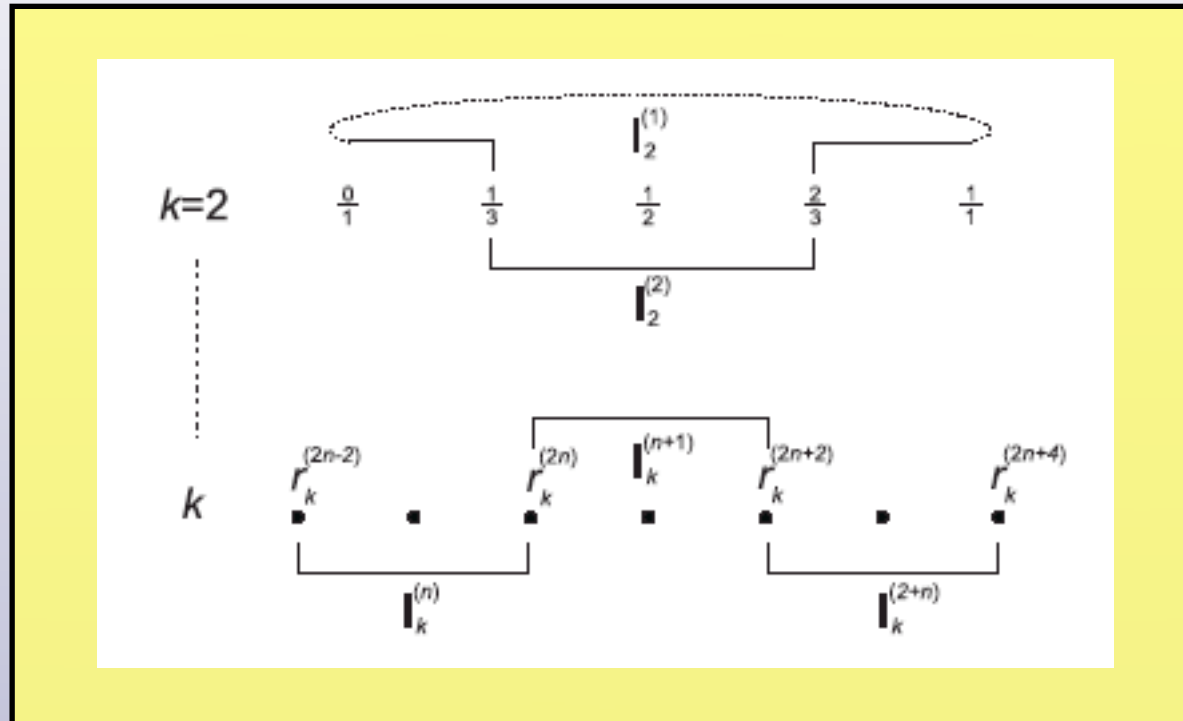
Critical Farey tree partition function:

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

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

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

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

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 phase diagram, including an external magnetic field, found via renormalization group and also a (dynamical system inspired) cluster approximation. Results almost consistent.
- 4) The partition function at the critical point suggests a subtle, apparently new, property of the Farey fractions.
- 5) 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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