Statistical mechanics of long-range interacting systems: Lecture 3

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ICTS Bangalore School on Statistical Physics XIII, 18 july-20 july 2022

July 20, 2022

Plan

- The min-max method: long+short range XY model
- Large deviations: Cramèr's theorem
- Three-states Potts model
- Modified XY model
- Free electron laser
- Mean-field ϕ^4 model

Tutorial

- Law of large numbers and central limit theorem
- Coin tossing
- Solution of the HMF model in the canonical and microcanonical ensemble.

The min-max method

Let us assume that the canonical partition sum can be written in the following form

$$Z(\beta, N) = \int dx \exp(-NU(\beta, x))$$

with U a differentiable function of β and x, a dummy variable. Then $\phi(\beta) = \beta f(\beta) = \inf_x U(\beta, x)$. Let us introduce the Legendre-Fenchel transform of U $s(\varepsilon, x) = \inf_\beta(\beta\varepsilon - U(\beta, x))$. Then, one can prove that

$$s(\varepsilon) = \sup_x(s(\varepsilon, x)) = \sup_x \inf_\beta(\beta\varepsilon - U(\beta, x))$$

Inverting the inf with the sup, one gets the concave envelope of $s(\varepsilon)$

$$s^*(\varepsilon) = \inf_\beta \sup_x(\beta\varepsilon - U(\beta, x))$$

On the other hand the Legendre-Fenchel transform of both s and s^* is ϕ. We use $\sup\inf \leq \inf\sup$.

Long and short-range XY model

$$H = -K\sum_{i=1}^{N}\cos\left(\theta_{i+1}-\theta_i\right) + \frac{J}{2N}\sum_{i,j=1}^{N}[1-\cos(\theta_i-\theta_j)]$$

$$Z \sim \int zdz \prod_{i=1}^{N} d\theta_i \exp\left(-\frac{N\beta}{2}z^2 + \beta z\sum_{i=1}^{N}\cos\theta_i + \beta K\sum_{i=1}^{N}\cos\left(\theta_{i+1}-\theta_i\right)\right)$$

The integral over the θ_i can be performed using the transfer operator method
$\mathcal{T}\psi(\theta) = \int d\alpha \exp(\beta z(\cos\theta + \cos\alpha)/2 + \beta K\cos(\theta-\alpha)\psi(\alpha)$.

$$Z = \int zdz \exp\left(-\frac{N\beta}{2}z^2 + N\ln\lambda(\beta z, \beta K)\right)$$

where $\lambda(\beta z, \beta K)$ is the maximal eigenvalue of the transfer operator. Entropy is then obtained using the min-max method.

$$s(\varepsilon) = \sup_z \inf_\beta \left[\beta\varepsilon - \beta\frac{(1+z^2)}{2} + \ln\lambda(\beta z, K\beta) + \frac{1}{2}\ln\frac{2\pi}{\beta}\right]$$

Cramèr's theorem

Let $\mathbf{X} \in R^d$ be a random variable with given PDF and $\mathbf{X}_i, i = 1, \ldots, N$, a sample of $\mathbf{X}$.
Let $\mathbf{M}_N = \frac{1}{N} \sum_i \mathbf{X}_i$ be sample mean
Which is the PDF of the sample mean? (Cramèr)
Compute the generating function

$$\Psi(\lambda) =< \exp(\lambda \cdot \mathbf{X}) >,$$

with $\lambda \in R^d$ and the average $< \cdot >$ performed on the PDF of $\mathbf{X}$ If $\Psi(\lambda) < \infty$ and differentiable, then

$$P(\mathbf{M}_N = \mathbf{x}) \sim \exp(-NI(\mathbf{x}))$$

where the rate function $I(\mathbf{x})$ is given by the Legendre-Fenchel transform of $\ln(\Psi(\lambda))$

$$I(\mathbf{x}) = \sup_{\lambda \in R^d} (\lambda \cdot \mathbf{x} - \ln(\Psi(\lambda)))$$

Entropy and free energy

Step 1 Express the Hamiltonian in terms of global variables γ

$$H_N(\omega_N) = \widetilde{H}_N\left(\gamma(\omega_N)\right) + R_N(\omega_N)$$

(ω_N a phase-space configuration) leading to
$h(\gamma) = lim_{N\to\infty} \widetilde{H}_N\left(\gamma(\omega_N)\right)/N$.

Step 2 Compute the entropy functional in terms of the global variables using, e.g., Cramèr's theorem

$$s(\gamma) = \lim_{N\to\infty} \frac{1}{N} \ln \Omega_N(\gamma)$$

with $\Omega_N(\gamma)$ the number of microscopic configurations with fixed γ.

Step 3 Solve the microcanonical and canonical variational problems

$$s(\varepsilon) = \sup_{\gamma}\left(s(\gamma) \mid h(\gamma) = \varepsilon\right) \ ,$$

$$\beta f(\beta) = \inf_{\gamma}\left(\beta h(\gamma) - s(\gamma)\right)$$

Potts model-I

$$H_N^{Potts} = -\frac{J}{2N}\sum_{i,j=1}^{N} \delta_{S_i,S_j} \quad .$$

$S_i = a, b, c$

Step 1

$$\widetilde{H}_N^{Potts} = -\frac{JN}{2}(n_a^2 + n_b^2 + n_c^2)$$

Step 2

$$\gamma = \left(\frac{1}{N}\sum_i \delta_{S_i,a}, \frac{1}{N}\sum_i \delta_{S_i,b}, \frac{1}{N}\sum_i \delta_{S_i,c} \right) \quad .$$

Local random variables

$$\mathbf{X}_k = (\delta_{S_k,a}, \delta_{S_k,b}, \delta_{S_k,c})$$

Potts model-II

Generating function

$$\Psi(\lambda_a, \lambda_b, \lambda_c) = \frac{1}{3} \sum_{S=a,b,c} \left(e^{\lambda_a \delta_{S,a} + \lambda_b \delta_{S,b} + \lambda_c \delta_{S,c}} \right) = \frac{1}{3} \left(e^{\lambda_a} + e^{\lambda_b} + e^{\lambda_c} \right)$$

Rate function

$$I(\gamma) = \sup_{\lambda_a, \lambda_b, \lambda_c} \left(\lambda_a n_a + \lambda_b n_b + \lambda_c n_c - \ln \Psi(\lambda_a, \lambda_b, \lambda_c) \right) \quad .$$

Exact solution $\lambda_\ell = \ln n_\ell$, with $\ell = a, b, c$

$$I(\gamma) = n_a \ln n_a + n_b \ln n_b + (1 - n_a - n_b) \ln(1 - n_a - n_b) + \ln 3$$

Entropy

$$s(\gamma) = -I(\gamma) + \ln \mathcal{N}$$

where the normalization factor is $\mathcal{N} = 3$

Potts model-III

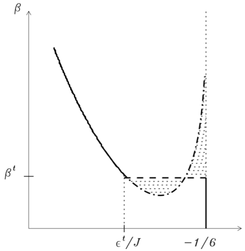
Step 3

Microcanonical entropy

$$s(\varepsilon) = \sup_{n_a,n_b} \Big(-n_a \ln n_a - n_b \ln n_b - (1-n_a-n_b)\ln(1-n_a-n_b) \;\Big|\; -\frac{J}{2}\left(n_a^2+n_b^2+(1-n_a-n_b)^2\right) = \epsilon \Big)$$

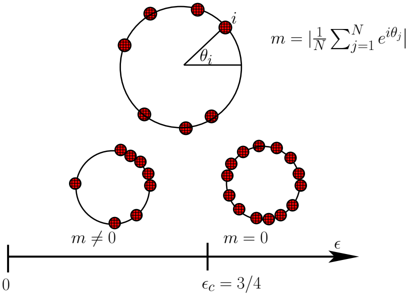
Canonical free energy

$$\beta f(\beta) = \inf_{n_a,n_b,n_c} \Big(n_a \ln n_a + n_b \ln n_b + n_c \ln n_c - \frac{\beta J}{2}\left(n_a^2+n_b^2+n_c^2\right) \Big)$$



Generalized XY model

$$H_{XY} = \sum_{i=1}^{N} \frac{p_i^2}{2} - \frac{J}{2N}(\sum_{i=1}^{N} \vec{s}_i)^2 - \frac{K}{4N^3}\left[(\sum_{i=1}^{N} \vec{s}_i)^2\right]^2 , \quad \vec{s}_i = (\cos\theta_i, \sin\theta_i)$$



Entropy of XY model

Step 1 Global variables

$$\gamma = (m_x, m_y, \mathcal{E}_K) \text{ with } \mathcal{E}_K = \lim_{N\to\infty} \sum_i p_i^2/N$$

$$h(\gamma) = \frac{1}{2}\left(\mathcal{E}_K - Jm^2 - Km^4/2\right)$$

Step 2

$$\mathbf{X} = \left(\cos\theta, \sin\theta, p^2\right) \text{ Local random variable}$$

$$\Psi(\lambda) \simeq I_0(\sqrt{\lambda_x^2 + \lambda_y^2})/\sqrt{-\lambda_K} \text{ where } \lambda = (\lambda_x, \lambda_y, \lambda_K)$$

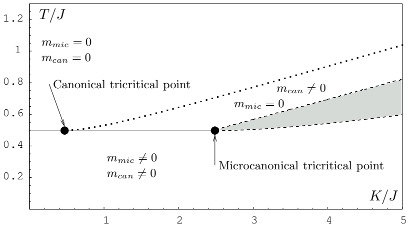
$$I(\gamma) = -s(\gamma) = \sup_\lambda(\lambda_K \mathcal{E}_K + \lambda_x m_x + \lambda_y m_y +$$

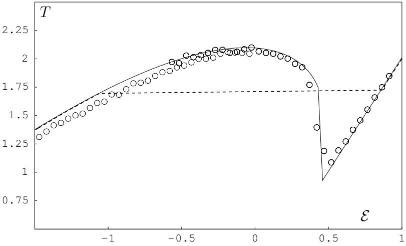
$$+ \ln(-\lambda_K)/2 - \ln(I_0(\sqrt{\lambda_x^2 + \lambda_y^2})))$$

Step 3 Entropy

$$s(\varepsilon) = \sup_\gamma\{s(\gamma) \mid \mathcal{E}_K = 2\varepsilon + Jm^2 + Km^4/2)\}$$

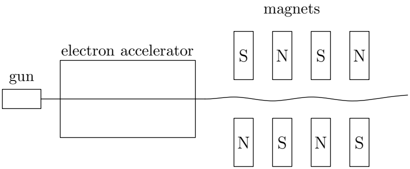
Phase diagram and caloric curves





- At $K/J = 0$ (HMF model), second order phase transition at $T/J = 0.5$. Ensembles are equivalent.
- For $K/J < 1/2$ ensembles are inequivalent. Negative specific heat for $1/2 < K \leq 5/2$; Temperature jumps for $K > 5/2$.
- Right figure shows the caloric curve for $K/J = 10$. The points are results of a molecular dynamics simulation with $N = 100$

Free Electron Laser



Colson-Bonifacio model

$$
\begin{aligned}
\frac{d\theta_j}{dz} &= p_j \\
\frac{dp_j}{dz} &= -\mathbf{A}e^{i\theta_j} - \mathbf{A}^* e^{-i\theta_j} \\
\frac{d\mathbf{A}}{dz} &= i\delta\mathbf{A} + \frac{1}{N}\sum_j e^{-i\theta_j}
\end{aligned}
$$

Microcanonical solution

Hamiltonian

$$H_N = \sum_{j=1}^{N} \frac{p_j^2}{2} - N\delta A^2 + 2A \sum_{j=1}^{N} \sin(\theta_j - \varphi)$$

where $A = \sqrt{\mathbf{A}\mathbf{A}^*}$.

Entropy

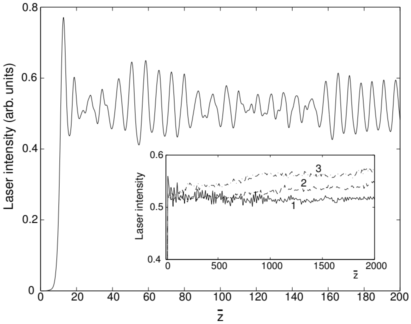
$$s(\varepsilon, \sigma, \delta) = \sup_{A,m} \left[\frac{1}{2} \ln \left[2\left(\varepsilon - \frac{\sigma^2}{2} \right) + 4Am + 2(\delta - \sigma)A^2 - A^4 \right] + s_{conf}(m) \right.$$

where $m = \sqrt{m_x^2 + m_y^2}$, $m_x = \sum_i \cos\theta_i / N$, $m_y = \sum_i \sin\theta_i / N$, σ is the total average momentum $\sum_i p_i / N + A^2$ and

$$s_{conf}(m) = -\sup_{\lambda} \left[\lambda m - \ln I_0(\lambda) \right]$$

Ensembles are equivalent for this model. There is a second order phase transition at $\varepsilon = -1/(2\delta)$, $\delta < 0$.

Time relaxation of the laser intensity



$N = 5000$ (curve 1), $N = 400$ (curve 2), $N = 100$ (curve 3)
On a first stage the system converges to a quasi-stationary state. Later it relaxes to equilibrium on a time $O(N)$. The quasi-stationary state is a Vlasov equilibrium, sufficiently well described by Lynden-Bell's distributions.

Mean-field ϕ^4 model

$$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2} - \frac{1}{4} q_i^2 + \frac{1}{4} q_i^4 \right) - \frac{1}{4N} \sum_{i,j=1}^{N} q_i q_j .$$

Global variables

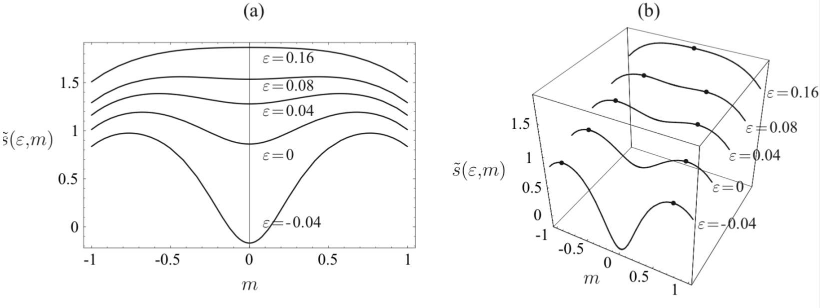
$$u = \frac{1}{N} \sum_{i=1}^{N} p_i^2 \quad , \quad z = \frac{1}{4N} \sum_{i=1}^{N} (q_i^4 - q_i^2) \quad , \quad m = \frac{1}{N} \sum_{i=1}^{N} q_i$$

$$\ln \Psi(\lambda_u, \lambda_z, \lambda_m) = -\frac{\ln \lambda_u}{2} + \ln \int dq \exp(-\lambda_m q - \lambda_z (q^4 - q^2)) + \text{const}$$

$$s(u, z, m) = \inf_{\lambda_u, \lambda_z, \lambda_m} (\lambda_u u + \lambda_z z + \lambda_m m - \ln \Psi)$$

$$s(\varepsilon, m) = \sup_{u,z} (s(u, z, m) | \varepsilon = \frac{u}{2} + z - \frac{m^2}{4})$$

Entropy of the mean-field ϕ^4 model



Negative susceptibility

Thermodynamics first law for magnetic systems $TdS = dE - hdM$.
In the microcanonical ensemble

$$h(\varepsilon, m) = -\frac{\partial s}{\partial m} \Big/ \frac{\partial s}{\partial \varepsilon} = -\frac{1}{\beta(\varepsilon, m)} \frac{\partial s}{\partial m}.$$

In the canonical ensemble

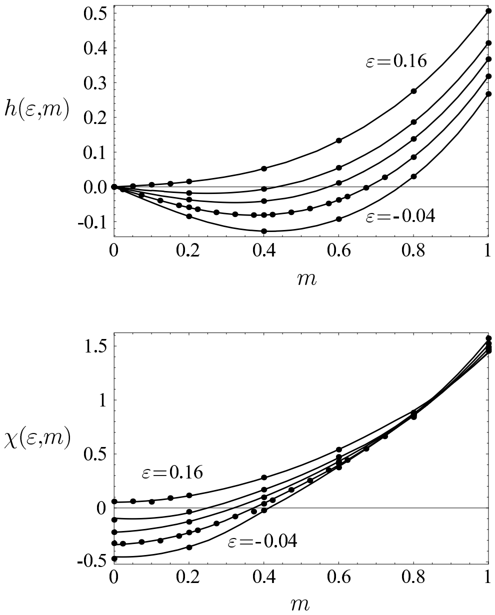
$$f(\beta, h) = \inf_{\varepsilon, m} \left[\varepsilon - hm - \frac{1}{\beta} s(\varepsilon, m) \right].$$

which gives $\partial s / \partial m = -hm$, $\partial s / \partial \varepsilon = \beta$, in agreement with the microcanonical expressions for h and β.

$$\chi = \frac{\partial m}{\partial h} = \beta \frac{s_{\varepsilon\varepsilon}}{s_{\varepsilon m}^2 - s_{\varepsilon\varepsilon} s_{mm}}$$

In the canonical ensemble $s_{\varepsilon\varepsilon} > 0$ and the denominator is positive as a consequence of stationarity, hence $\chi > 0$. In the microcanonical ensemble $s_{mm} < 0$ and, at free energy saddles, $s_{\varepsilon\varepsilon} < 0$, hence susceptibility can be negative.

Comparison with numerics



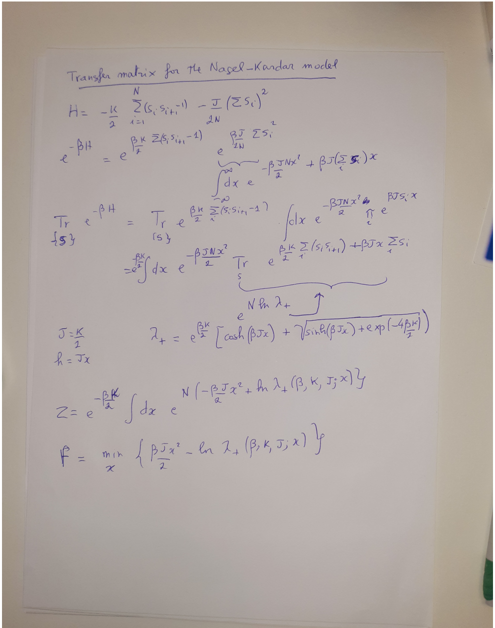
Conclusions

- Large deviations are a powerful tool to derive microcanonical entropies.
- Examples: Potts model, generalized XY model, Colson-Bonifacio model of the free electron laser, ϕ^4 theory

Tutorial

- Transfer matrix for Kardar-Nagel
- Law of large numbers and central limit theorem
- Coin tossing
- Solution of the HMF model in the canonical and microcanonical ensemble.

Transfer matrix for Kardar-Nagel



Law of large numbers

Consider a sample of N independent, identically distributed (i.i.d.) random variables

$$x_1, x_2, \ldots, x_N$$

with PDF $f(x)$ and expectation μ: $< x >= \int f(x) x dx = \mu$
Then, the sample mean

$$X_N = \frac{1}{N} \sum_{i=1}^{N} x_i$$

converges to μ almost surely

$$\text{Prob}\left\{ \lim_{N \to \infty} X_N = \mu \right\} = 1$$

Central limit theorem

Consider a function $g(x)$ of the random variable x and the sample mean

$$G_N = \frac{1}{N}\sum_{i=1}^{N} g(x_i)$$

Define

$$t_N = \frac{G_N - < g(x) >}{\sqrt{\text{var}\left\{G_N\right\}}} = \frac{\sqrt{N}(G_N - < g(x) >)}{\sqrt{\text{var}\{g(x)\}}}$$

Then ($\sigma^2 = \text{var}\{g\}$)

$$\lim_{N\to\infty} \text{Prob}\{a < t_N < b\} = \int_a^b \frac{\exp[-t^2/2]}{\sqrt{2\pi}} dt$$

$$f(G_N) = \frac{1}{\sqrt{2\pi(\sigma^2/N)}} \exp\left[\frac{N(G_N - < g >)^2}{2\sigma^2}\right]$$

Coin tossing and large deviations

$$X_k = \pm 1 \quad , \quad S_N = \frac{1}{N}\sum_{k=1}^{N} X_k$$

$$P(S_N = x) = \frac{N!}{N_+! N_-! 2^N} = \frac{N!}{\left(\frac{(1+x)N}{2}\right)! \; \left(\frac{(1-x)N}{2}\right)! \; 2^N}$$

Using the Stirling's formula in the large N limit

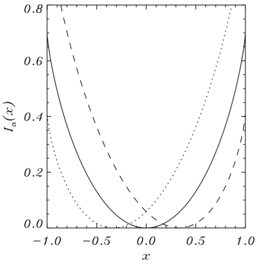
$$\ln P(x) \sim -N\left(\frac{(1+x)}{2}\ln(1+x) + \frac{(1-x)}{2}\ln(1-x)\right) \quad \sim -NI(x)$$

The *rate function* $I(x)$ has a single minimum in $x = 0$, the most probable value and is in this case symmetric around the minimum. S_N fulfills a *large deviation principle*, characterized by the rate function $I(x)$.

The coin toss experiment can be thought as a microscopic realization of a chain of N non-interacting Ising spins. $I(x)$ corresponds to the opposite of the Boltzmann entropy of a macrostate characterized by a fraction x of up-spins.

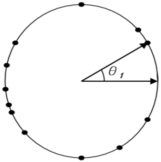
Unbiased/Biased coin tossing using Cramèr

- **Unbiased:** $d\mu = [\delta(X-1) + \delta(X+1]dX/2$; $\Psi(\lambda) = \langle \exp(\lambda X) \rangle = \cosh\lambda$; $I(x) = \sup_\lambda (\lambda \cdot x - \ln\cosh\lambda)$, whose critical point is $\lambda = \operatorname{arcth} x$.
- **Biased:** $d\mu = [(1-\alpha)\delta(X-1) + \alpha\delta(X+1]dX$, with $\alpha \in [0,1]$ and $\alpha = 1/2$ corresponding to the unbiased case; $\Psi_\alpha(\lambda) = \exp(\lambda) - 2\alpha \sinh\lambda$. $I_\alpha(\lambda)$ is plotted in the figure for $\alpha = 1/3, 1/2, 2/3$. This model corresponds to an ensemble of non-interacting Ising spins whose probability to take the upper value is different from the one for the down value.



HMF model

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^{N} (1 - \cos(\theta_i - \theta_j))$$



Magnetization $\mathbf{M} = \lim_{N\to\infty} \left(\frac{\sum_{i=1}^{N} \cos\theta_i}{N}, \frac{\sum_{i=1}^{N} \sin\theta_i}{N} \right) = (M_x, M_y)$

Energy $U = \lim_{N\to\infty} \frac{H}{N}$

Solution of the HMF model in the canonical ensemble-I

Configurational partition function

$$Z_{conf}(\beta, N) \propto \int d\theta_1 \dots d\theta_N \exp\left\{ \frac{\beta}{2N} \left[\left(\sum_{i=1}^{N} \cos\theta_i \right)^2 + \left(\sum_{i=1}^{N} \sin\theta_i \right)^2 \right] \right.$$

Using the Hubbard-Stratonovich transformation

$$Z_{conf}(\beta, N) \propto \int dx_1 dx_2 \exp\left\{ N \left[-\frac{\beta(x_1^2 + x_2^2)}{2} + \ln I_0(\beta(x_1^2 + x_2^2)^{\frac{1}{2}}) \right] \right\}$$

where I_0 is the modified Bessel function of zero order

$$I_0(z) = \int_0^{2\pi} d\theta \exp\left(z_1 \cos\theta + z_2 \sin\theta\right) = \int_0^{2\pi} d\theta \exp\left(z \cos\theta\right)$$

Solution of the HMF model in the canonical ensemble-II

Going to polar coordinates

$$Z_{conf}(\beta, N) \propto \int_0^\infty dx \exp\left\{N\left[-\frac{\beta x^2}{2} + \ln I_0(\beta x)\right]\right\}$$

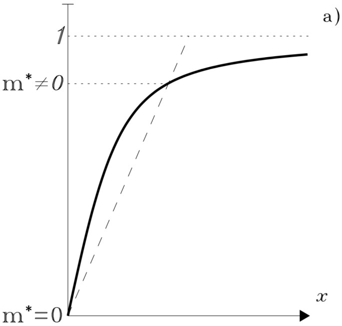
In the thermodynamic limit $N \to \infty$, collecting also the contribution of kinetic energy

$$\phi(\beta) = \beta f(\beta) = \frac{\beta}{2} - \frac{1}{2}\ln 2\pi + \frac{1}{2}\ln\beta + \inf_{x\geq 0}\left[\frac{\beta x^2}{2} - \ln I_0(\beta x)\right]$$

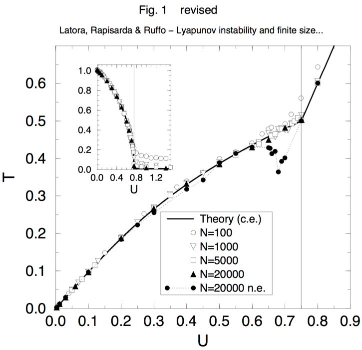
The infimum is solved for

$$x = \frac{I_1(\beta x)}{I_0(\beta x)}$$

Solution of the HMF model in the canonical ensemble: the consistency equation



Equilibrium phase transition



$$U_c = 3/4 = 0.75,\ T = (\partial S/\partial U)^{-1} = \lim_{N\to\infty} \sum_i p_i^2/N$$

Solution of the HMF model in the microcanonical ensemble-I

Using the min-max method, the microcanonical entropy is given by

$$s(\varepsilon) = \sup_x \left\{ \inf_{\beta \geq 0} \left[\beta\varepsilon - \tilde{\phi}(\beta, x) \right] \right\}$$

with $\tilde{\phi}(\beta, x)$ given above before the infimum.
The stationary points are the same in the two ensembles.

$$\frac{\partial \tilde{\phi}}{\partial \beta} = \frac{1}{2} + \frac{1}{2\beta} + \frac{1}{2}x^2 - x\frac{I_1(\beta x)}{I_0(\beta x)} = \varepsilon$$

$$\frac{\partial \tilde{\phi}}{\partial x} = \beta x - \beta\frac{I_1(\beta x)}{I_0(\beta x)} = 0$$

This system of equations can be solved in β to give a consistency equation in x.

Solution of the HMF model in the microcanonical ensemble-II

$$B(x) = \frac{x}{2\varepsilon - 1 + x^2}$$

where $B = [I_1/I_0]^{-1}$. There is a unique solution $x = 0$ of this consistency equation above the second order phase transition energy $\varepsilon = 3/4$. Ensembles are equivalent and give the same entropy

$$s(\varepsilon) = \text{const} + \frac{1}{2}\ln\left(\frac{xI_0^2[xB(x)]}{2B(x)}\right) - xB(x)$$

The microcanonical inverse temperature $\beta = \partial s/\partial\varepsilon$ at the critical point is $\beta_c = 2$.
One can also check the canonical $\tilde{\phi}_{xx} > 0$ and microcanonical $\tilde{\phi}_{\beta\beta}$ stability conditions.