Three dimensional Ising system with spin 1.

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$$\beta H = -K\sum_{i=1}^{N}\sigma_i\sigma_{i+1}$$

where B is an external magnetic field,

$$K = \frac{J}{k_B T} = \beta J\ ,$$

We use the periodic boundary condition

$$\sigma_1 = \sigma_{N+1}\ .$$

The partition function,

$$Z = \sum_{\sigma_1=\pm 0,1}\ \sum_{\sigma_2=0,\pm 1}\ \sum_{\sigma_3=0,\pm 1}\cdots\sum_{\sigma_{N-1}=0,\pm 1}\ \sum_{\sigma_N=0,\pm 1}\exp(-\beta H)\ .$$

The part related the sites i and i+1 in the Boltzmann factor

$$T(\sigma_i,\sigma_{i+1}) = \langle\sigma_i|\hat{T}|\sigma_{i+1}\rangle = \exp(K\sigma_i\sigma_{i+1})\ .$$

The martix T is expressed by the 3x3 matrix as

$$\hat{T} = \begin{pmatrix} \langle 1|\hat{T}|1\rangle & \langle 1|\hat{T}|0\rangle & \langle 1|\hat{T}|-1\rangle \\ \langle 0|\hat{T}|1\rangle & \langle 0|\hat{T}|0\rangle & \langle 0|\hat{T}|-1\rangle \\ \langle -1|\hat{T}|1\rangle & \langle -1|\hat{T}|0\rangle & \langle -1|\hat{T}|-1\rangle \end{pmatrix}$$

$$= \begin{pmatrix} e^{K} & 1 & e^{-K} \\ 1 & 1 & 1 \\ e^{-K} & 1 & e^{K} \end{pmatrix}$$

$$= \begin{pmatrix} x & 1 & 1/x \\ 1 & 1 & 1 \\ 1/x & 1 & x \end{pmatrix}$$

with $x = e^{K}$

We solve the eigenvalue problem using the Mathematica.

The eigenvalues:

$$\lambda_1 = \frac{x^2 - 1}{x} = 2\sinh(K)$$

$$\lambda_2 = \frac{1 + x + x^2 + \sqrt{1 - 2x + 11x^2 - 2x^3 + x^4}}{2x}$$
$$= \frac{1}{2} + \cosh(K) + \frac{1}{2}\sqrt{(2\cosh K - 1)^2 + 8}$$

$$\lambda_3 = \frac{1 + x + x^2 - \sqrt{1 - 2x + 11x^2 - 2x^3 + x^4}}{2x}$$
$$= \frac{1}{2} + \cosh(K) - \frac{1}{2}\sqrt{(2\cosh K - 1)^2 + 8}$$

The corresponding eigenkets:

$$|\lambda_1\rangle = \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix}, \qquad |\lambda_2\rangle = \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix}, \qquad |\lambda_3\rangle = \begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix}$$

and the unitary matrix given by

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}$$

$$\hat{U}^{+}\hat{T}\hat{U} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

We note that

$$\lambda_2 > \lambda_1 > \lambda_3 \qquad \text{for } x > 1.$$

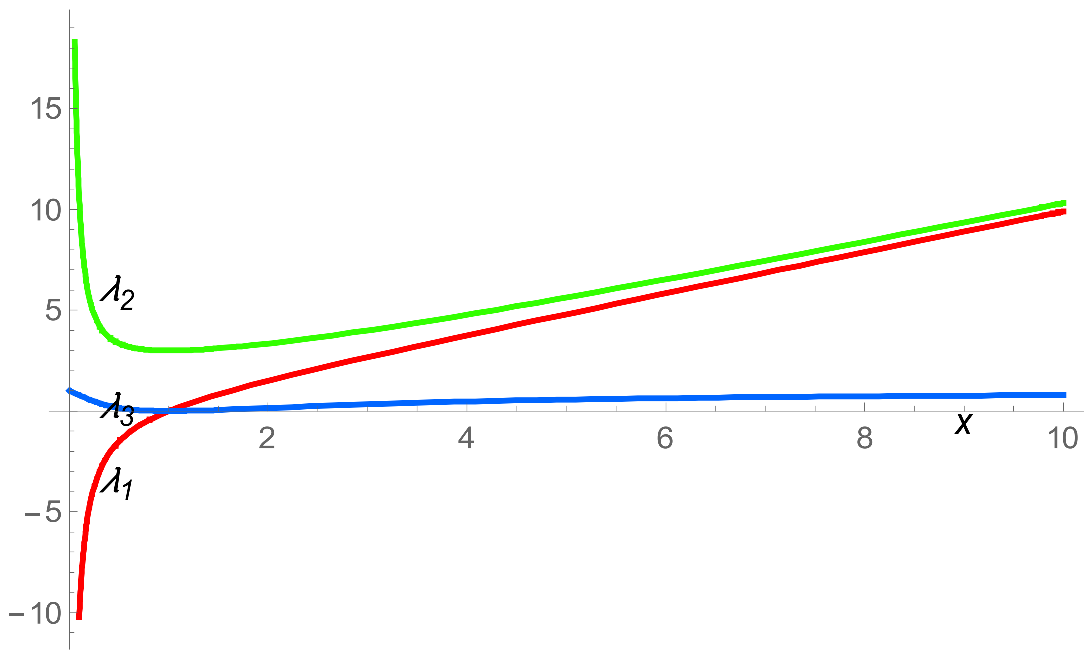


Fig. Plot of λ_1, λ_1, and λ_1 as a function of x, with $x = e^K$. As $T \to 0$, $x \to \infty$.

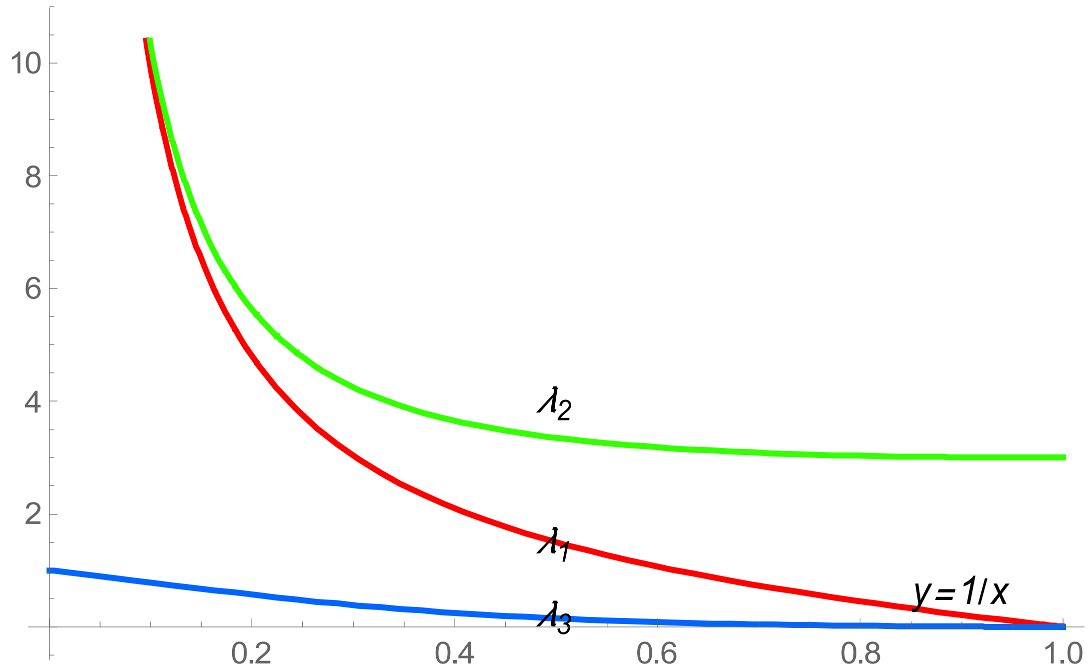


Fig. Plot of λ_1, λ_1, and λ_1 as a function of x, with $y = 1/x = e^{-K}$. As $T \to 0$, $y \to 0$

Using this notation, Z can be rewritten as

$$\begin{aligned}
Z &= \sum_{\sigma_1=0,\pm1}\sum_{\sigma_2=0.\pm1}\sum_{\sigma_3=0,\pm1}\cdots\sum_{\sigma_{N-1}=0,\pm1}\sum_{\sigma_N=0,\pm1} T(\sigma_1,\sigma_2)T(\sigma_2,\sigma_3)T(\sigma_3,\sigma_4)\cdots T(\sigma_{N-1},\sigma_N)T(\sigma_N,\sigma_1) \\
&= \sum_{\sigma_1=0,\pm1}\sum_{\sigma_2=0,\pm1}\sum_{\sigma_3=0,\pm1}\cdots\sum_{\sigma_{N-1}=0,\pm1}\sum_{\sigma_N=0,\pm1} \langle\sigma_1|\hat{T}|\sigma_2\rangle\langle\sigma_2|\hat{T}|\sigma_3\rangle\langle\sigma_3|\hat{T}|\sigma_4\rangle\cdots\langle\sigma_{N-1}|\hat{T}|\sigma_N\rangle\langle\sigma_N|\hat{T}|\sigma_1\rangle
\end{aligned}$$

Here we use the closure relation (quantum mechanics)

$$\sum_{\sigma_2=0,\pm1}|\sigma_2\rangle\langle\sigma_2| = \hat{1}.$$

Then we get

$$\sum_{\sigma_2=\pm1}\langle\sigma_1|\hat{T}|\sigma_2\rangle\langle\sigma_2|\hat{T}|\sigma_3\rangle = \langle\sigma_1|\hat{T}^2|\sigma_3\rangle$$

The partition function can be expressed by a simple form

$$Z = \sum_{\sigma_1=\pm1} \langle \sigma_1 | \hat{T}^N | \sigma_1 \rangle = Tr[\hat{T}^N]$$

We now calculate the partition function. The matrix T can be expressed using the Pauli matrix

$$\begin{aligned} Z &= Tr[\hat{T}^N] \\ &= Tr[(\hat{U}^+\hat{T}\hat{U})(\hat{U}^+\hat{T}\hat{U})\cdots(\hat{U}^+\hat{T}\hat{U})] \\ &= Tr[(\hat{U}^+\hat{T}\hat{U})^N] \\ &= \lambda_1{}^N + \lambda_2{}^N + \lambda_3{}^N \end{aligned}$$

In the limit of $N \to \infty$

$\lambda_2{}^N >> \lambda_1{}^N$ and $\lambda_2{}^N >> \lambda_3{}^N$ for $x > 1$.

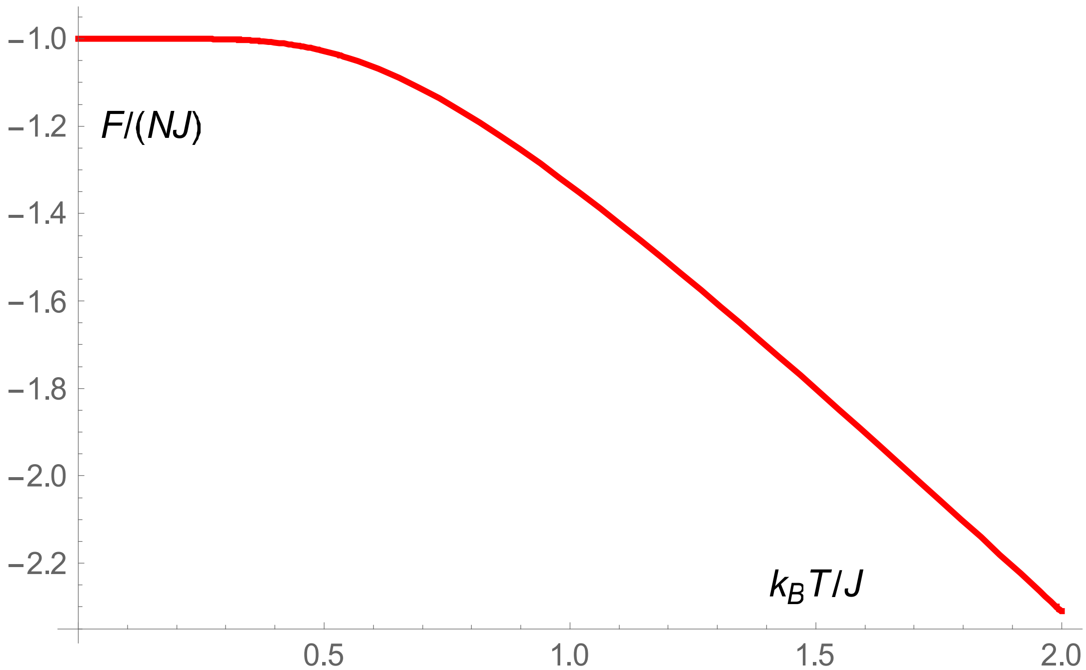
<u>The free energy per spin is</u>

$$\frac{F}{N} = f = -\frac{k_B T}{N} \ln Z = -\frac{k_B T}{N} \ln(\lambda_1{}^N + \lambda_2{}^N + \lambda_3{}^N).$$

or

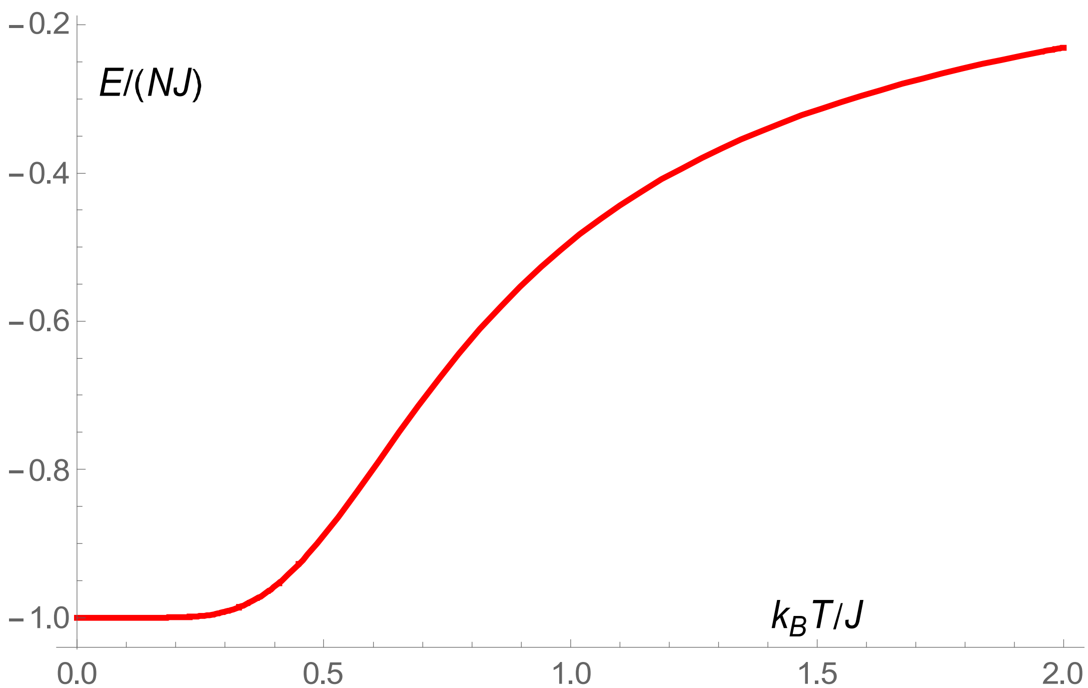
$$\begin{aligned} f &\approx -\frac{k_B T}{N} \ln(\lambda_2{}^N) \\ &= -k_B T \ln(\lambda_2) \\ &= -k_B T \ln(\frac{1}{2} + \cosh(K) + \frac{1}{2}\sqrt{(2\cosh K - 1)^2 + 8}] \end{aligned}$$

When $K \to 0$, $f = -k_B T \ln 3$. This corresponds to a state of complete randomness in a system with 3^N microstates.



The energy per spin is

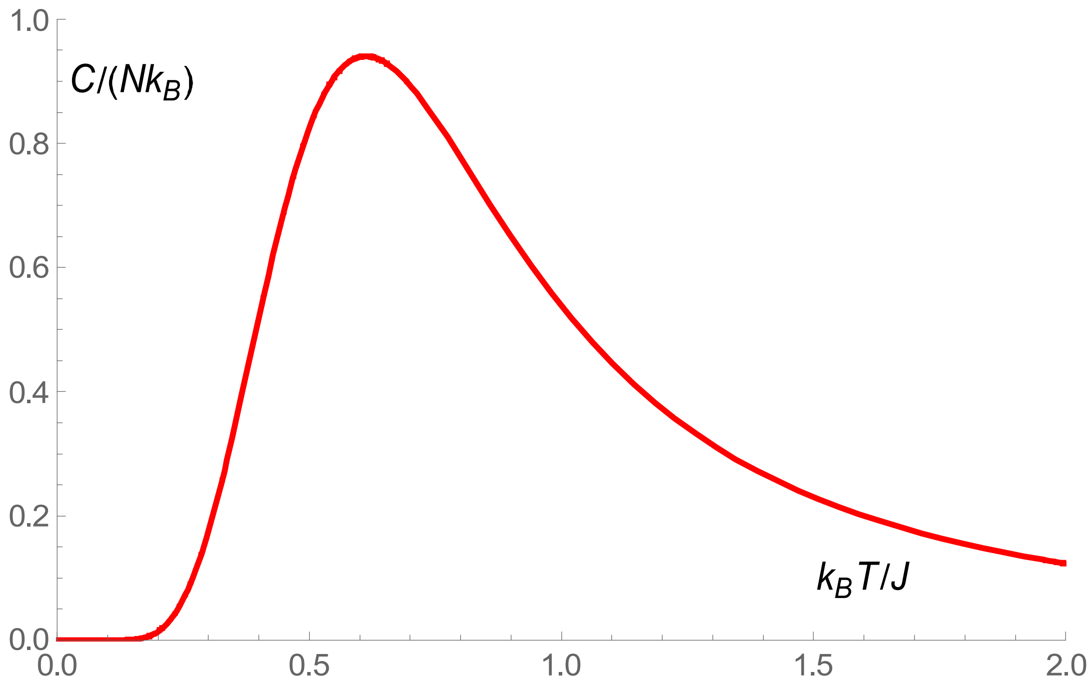
$$\frac{E}{N} = -\frac{1}{N}\frac{\partial}{\partial\beta}\ln Z = \frac{\partial}{\partial\beta}(\beta f) = -k_B T^2 \frac{\partial}{\partial T}(\beta f)\,.$$



The heat capacity per spin

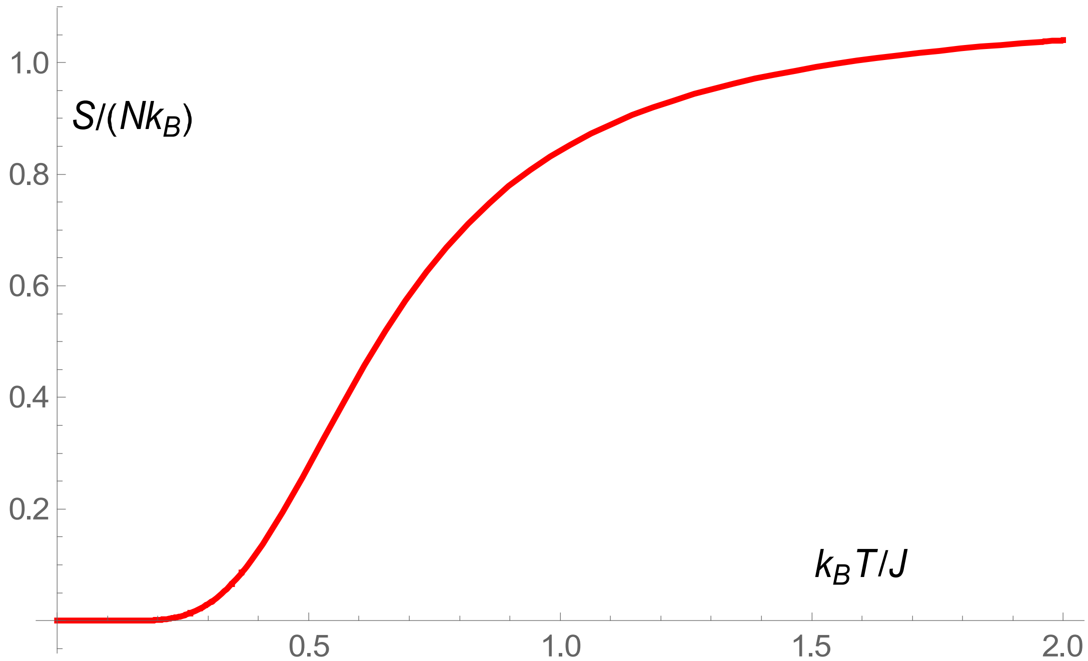
$$\frac{C}{N} = \frac{d}{dT}(\frac{E}{N})$$

The heat capacity shows a maximum (= 0.94055) at $\frac{k_B T}{J} = 0.612063$.



The entropy per spin

$$\frac{S}{N} = \frac{1}{T}(\frac{E}{N} - \frac{F}{N})$$



with eigenvalues

$$\begin{pmatrix}\lambda_1\\ \lambda_2\end{pmatrix} = \frac{1}{2}\left[(1+2\cosh K) \pm \{8+(2\cosh K-1)^2\}^{1/2}\right], \ \lambda_3 = 2\sinh K.$$

Since λ_1 is the largest eigenvalue of $\mathbf{P}$,

$$\frac{1}{N}\ln Q \approx \ln\lambda_1 = \ln\left\{\frac{1}{2}\left[(1+2\cosh K)+\{8+(2\cosh K-1)^2\}^{1/2}\right]\right\},$$

which leads to the quoted expression for the free energy A.

In the limit $T \to 0$, $K \to \infty$, with the result that $\cosh K \approx \frac{1}{2}e^K$ and hence $A \approx -NJ$; this corresponds to a state of perfect order in the system, with $U = -NJ$ and $S = 0$. On the other hand, when $T \to \infty, \cosh K \to 1$ and hence $A \to -NkT\ln 3$; this corresponds to a state of complete randomness in a system with 3^N microstates.