

A nontrivial example that can  
be solved exactly

---

## The Ising chain



## Ising model in 1D

### Ising model in 1D

Partition function

Transfer matrix

Partition function

Free energy

Eigenvalues

Free energy solution

Mean-field theory

- In one dimension, we can solve the Ising model exactly.
- We can use this solution to gain insight into the limitations of the mean-field approximation.



# Ising model in 1D

## Ising model in 1D

Partition function

Transfer matrix

Partition function

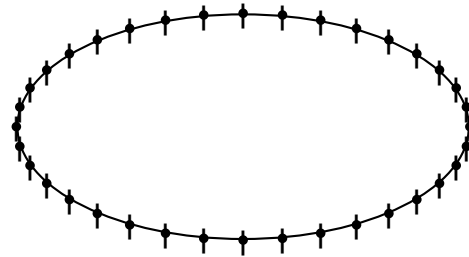
Free energy

Eigenvalues

Free energy solution

Mean-field theory

- In one dimension, we can solve the Ising model exactly.
- We can use this solution to gain insight into the limitations of the mean-field approximation.
- For simplicity, we consider  $N$  spins equally spaced on a ring:





# Ising model in 1D

## Ising model in 1D

Partition function

Transfer matrix

Partition function

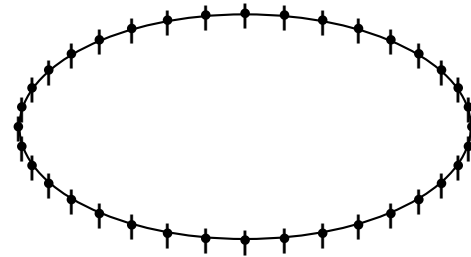
Free energy

Eigenvalues

Free energy solution

Mean-field theory

- In one dimension, we can solve the Ising model exactly.
- We can use this solution to gain insight into the limitations of the mean-field approximation.
- For simplicity, we consider  $N$  spins equally spaced on a ring:



- The spins then satisfy the periodic boundary conditions

$$\sigma_i = \sigma_{i+N},$$

and the energies of the nearest-neighbor Ising Hamiltonian are

$$E_\sigma = -J \sum_{i=1}^N \sigma_i \sigma_{i+1} - h \sum_{i=1}^N \sigma_i.$$



# Partition function

Ising model in 1D

Partition function

Transfer matrix

Partition function

Free energy

Eigenvalues

Free energy solution

Mean-field theory

- The second term can be rewritten so that it has the same symmetry as the first term:

$$E_\sigma = -J \sum_{i=1}^N \sigma_i \sigma_{i+1} - \frac{h}{2} \sum_{i=1}^N (\sigma_i + \sigma_{i+1}).$$

# Partition function

Ising model in 1D

Partition function

Transfer matrix

Partition function

Free energy

Eigenvalues

Free energy solution

Mean-field theory

- The second term can be rewritten so that it has the same symmetry as the first term:

$$E_{\sigma} = -J \sum_{i=1}^N \sigma_i \sigma_{i+1} - \frac{h}{2} \sum_{i=1}^N (\sigma_i + \sigma_{i+1}).$$

- The partition function of the Ising chain is then

$$\begin{aligned} Z_C &= \sum_{\sigma} \exp(-\beta E_{\sigma}) \\ &= \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \exp \left\{ \beta \sum_{i=1}^N \left[ J \sigma_i \sigma_{i+1} + \frac{h}{2} (\sigma_i + \sigma_{i+1}) \right] \right\} \\ &= \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \prod_{i=1}^N \exp \left\{ \beta \left[ J \sigma_i \sigma_{i+1} + \frac{h}{2} (\sigma_i + \sigma_{i+1}) \right] \right\}. \end{aligned}$$



## Transfer matrix

Ising model in 1D

Partition function

Transfer matrix

Partition function

Free energy

Eigenvalues

Free energy solution

Mean-field theory

- Let us now define a  $2 \times 2$  matrix  $P$  with matrix elements

$$P_{\sigma_i \sigma_j} = \langle \sigma_i | P | \sigma_j \rangle = \exp \left\{ \beta \left[ J \sigma_i \sigma_j + \frac{h}{2} (\sigma_i + \sigma_j) \right] \right\}.$$



# Transfer matrix

- Ising model in 1D
- Partition function
- Transfer matrix**
- Partition function
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- Let us now define a  $2 \times 2$  matrix  $P$  with matrix elements

$$P_{\sigma_i \sigma_j} = \langle \sigma_i | P | \sigma_j \rangle = \exp \left\{ \beta \left[ J \sigma_i \sigma_j + \frac{h}{2} (\sigma_i + \sigma_j) \right] \right\}.$$

- In particular, we have

$$\begin{aligned} \langle + | P | + \rangle &= \exp[\beta(J + h)], & \langle - | P | - \rangle &= \exp[\beta(J - h)], \\ \langle + | P | - \rangle &= \langle - | P | + \rangle = \exp(-\beta J), \end{aligned}$$

hence

$$P = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}.$$

# Transfer matrix

- Ising model in 1D
- Partition function
- Transfer matrix**
- Partition function
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- Let us now define a  $2 \times 2$  matrix  $P$  with matrix elements

$$P_{\sigma_i \sigma_j} = \langle \sigma_i | P | \sigma_j \rangle = \exp \left\{ \beta \left[ J \sigma_i \sigma_j + \frac{h}{2} (\sigma_i + \sigma_j) \right] \right\}.$$

- In particular, we have

$$\begin{aligned} \langle + | P | + \rangle &= \exp[\beta(J + h)], & \langle - | P | - \rangle &= \exp[\beta(J - h)], \\ \langle + | P | - \rangle &= \langle - | P | + \rangle = \exp(-\beta J), \end{aligned}$$

hence

$$P = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}.$$

- In terms of this matrix, the partition function is

$$\begin{aligned} Z_C &= \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \prod_{i=1}^N \langle \sigma_i | P | \sigma_{i+1} \rangle \\ &= \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \langle \sigma_1 | P | \sigma_2 \rangle \langle \sigma_2 | P | \sigma_3 \rangle \cdots \langle \sigma_N | P | \sigma_{N+1} \rangle. \end{aligned}$$



# Partition function

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function**
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- But since  $\sigma_{N+1} = \sigma_1$ , this is just

$$\begin{aligned} Z_C &= \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \langle \sigma_1 | P | \sigma_2 \rangle \langle \sigma_2 | P | \sigma_3 \rangle \cdots \langle \sigma_N | P | \sigma_1 \rangle \\ &= \sum_{\sigma_1=\pm 1} \langle \sigma_1 | P^N | \sigma_1 \rangle, \end{aligned}$$

or

$$Z_C = \text{tr}(P^N).$$



# Partition function

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function**
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- But since  $\sigma_{N+1} = \sigma_1$ , this is just

$$\begin{aligned} Z_C &= \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \langle \sigma_1 | P | \sigma_2 \rangle \langle \sigma_2 | P | \sigma_3 \rangle \cdots \langle \sigma_N | P | \sigma_1 \rangle \\ &= \sum_{\sigma_1=\pm 1} \langle \sigma_1 | P^N | \sigma_1 \rangle, \end{aligned}$$

or

$$Z_C = \text{tr}(P^N).$$

- The trace is easiest to evaluate in a basis where  $P$  is diagonal.



# Partition function

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function**
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- But since  $\sigma_{N+1} = \sigma_1$ , this is just

$$\begin{aligned} Z_C &= \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \langle \sigma_1 | P | \sigma_2 \rangle \langle \sigma_2 | P | \sigma_3 \rangle \cdots \langle \sigma_N | P | \sigma_1 \rangle \\ &= \sum_{\sigma_1=\pm 1} \langle \sigma_1 | P^N | \sigma_1 \rangle, \end{aligned}$$

or

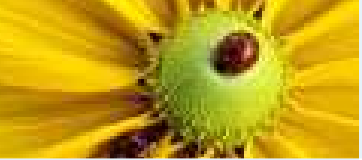
$$Z_C = \text{tr}(P^N).$$

- The trace is easiest to evaluate in a basis where  $P$  is diagonal.
- Let  $\lambda_1$  and  $\lambda_2$  be the eigenvalues of  $P$ ; i.e., the solutions to

$$\det(P - \lambda I) = 0.$$

- In a basis of its own eigenvectors,  $P$  has the form

$$P = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \Rightarrow P^N = \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix}.$$



## Free energy

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- The trace of  $P^N$  is then just

$$\text{tr}(P^N) = \lambda_1^N + \lambda_2^N.$$

# Free energy



- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy**
- Eigenvalues
- Free energy solution
- Mean-field theory

- The trace of  $P^N$  is then just

$$\text{tr}(P^N) = \lambda_1^N + \lambda_2^N.$$

- Choosing  $\lambda_1$  to be the larger eigenvalue, we have

$$Z_C = \lambda_1^N [1 + (\lambda_2/\lambda_1)^N],$$

and the magnetic free energy is

$$\begin{aligned}\tilde{A} &= -k_B T \log Z_C \\ &= -Nk_B T \log \lambda_1 - k_B T \log [1 + (\lambda_2/\lambda_1)^N].\end{aligned}$$

# Free energy

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- The trace of  $P^N$  is then just

$$\text{tr}(P^N) = \lambda_1^N + \lambda_2^N.$$

- Choosing  $\lambda_1$  to be the larger eigenvalue, we have

$$Z_C = \lambda_1^N [1 + (\lambda_2/\lambda_1)^N],$$

and the magnetic free energy is

$$\begin{aligned}\tilde{A} &= -k_B T \log Z_C \\ &= -Nk_B T \log \lambda_1 - k_B T \log [1 + (\lambda_2/\lambda_1)^N].\end{aligned}$$

- Since  $\lambda_2 < \lambda_1$ , the second term vanishes in the thermodynamic limit  $N \rightarrow \infty$ , and we have simply<sup>1</sup>

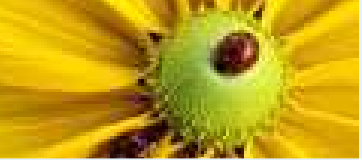
$$\tilde{A} = -Nk_B T \log \lambda_1.$$

- Hence, our last remaining problem is to find the eigenvalues of  $P$ .

---

<sup>1</sup>Exercise: Show that you get the same result for  $\tilde{A}$  even when  $\lambda_2 = \lambda_1$ .





# Eigenvalues

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy
- Eigenvalues**
- Free energy solution
- Mean-field theory

- To find the eigenvalues of  $P$ , we need to solve the secular equation

$$\det \begin{pmatrix} e^{\beta(J+h)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} - \lambda \end{pmatrix} = 0.$$



# Eigenvalues

Ising model in 1D

Partition function

Transfer matrix

Partition function

Free energy

Eigenvalues

Free energy solution

Mean-field theory

- To find the eigenvalues of  $P$ , we need to solve the secular equation

$$\det \begin{pmatrix} e^{\beta(J+h)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} - \lambda \end{pmatrix} = 0.$$

- The roots of the secular equation are

$$\lambda_1 = e^{\beta J} \left( \cosh \beta h + \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right),$$

$$\lambda_2 = e^{\beta J} \left( \cosh \beta h - \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right),$$

which satisfy  $\lambda_1 > \lambda_2$  as required.

# Eigenvalues

Ising model in 1D

Partition function

Transfer matrix

Partition function

Free energy

Eigenvalues

Free energy solution

Mean-field theory

- To find the eigenvalues of  $P$ , we need to solve the secular equation

$$\det \begin{pmatrix} e^{\beta(J+h)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} - \lambda \end{pmatrix} = 0.$$

- The roots of the secular equation are

$$\lambda_1 = e^{\beta J} \left( \cosh \beta h + \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right),$$

$$\lambda_2 = e^{\beta J} \left( \cosh \beta h - \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right),$$

which satisfy  $\lambda_1 > \lambda_2$  as required.

- In the special case  $h = 0$ , the solutions reduce to

$$\lambda_1 = 2 \cosh \beta J, \quad \lambda_2 = 2 \sinh \beta J.$$



## Free energy solution

Ising model in 1D  
Partition function  
Transfer matrix  
Partition function  
Free energy  
Eigenvalues  
Free energy solution  
Mean-field theory

- Hence, the free energy in the thermodynamic limit is

$$\tilde{A}(T, h) = -Nk_{\text{B}}T \log \left[ e^{\beta J} \left( \cosh \beta h + \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right) \right].$$



## Free energy solution

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy
- Eigenvalues
- Free energy solution**
- Mean-field theory

- Hence, the free energy in the thermodynamic limit is

$$\tilde{A}(T, h) = -Nk_{\text{B}}T \log \left[ e^{\beta J} \left( \cosh \beta h + \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right) \right].$$

- This closed-form solution is completely regular (except at  $T = 0$ ) and analytic in both  $T$  and  $h$ .



## Free energy solution

Ising model in 1D

Partition function

Transfer matrix

Partition function

Free energy

Eigenvalues

Free energy solution

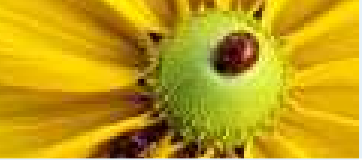
Mean-field theory

- Hence, the free energy in the thermodynamic limit is

$$\tilde{A}(T, h) = -Nk_{\text{B}}T \log \left[ e^{\beta J} \left( \cosh \beta h + \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right) \right].$$

- This closed-form solution is completely regular (except at  $T = 0$ ) and analytic in both  $T$  and  $h$ .
- There is consequently no non-analytic behavior (at finite  $T$ ) in any of the physically meaningful thermodynamic variables such as

$$M = - \left( \frac{\partial \tilde{A}}{\partial B} \right)_T, \quad \chi_T(B) = \frac{\mu_0}{V} \left( \frac{\partial M}{\partial B} \right)_T.$$



## Mean-field theory

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- However, our mean-field calculations predicted a second-order phase transition in  $M(T)$  at the nonzero temperature

$$T_c = qJ/k_B,$$

where  $q = 2$  in one dimension.



## Mean-field theory

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- However, our mean-field calculations predicted a second-order phase transition in  $M(T)$  at the nonzero temperature

$$T_c = qJ/k_B,$$

where  $q = 2$  in one dimension.

- We therefore conclude that the mean-field approximation is qualitatively incorrect for the 1D Ising model.





## Mean-field theory

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- However, our mean-field calculations predicted a second-order phase transition in  $M(T)$  at the nonzero temperature

$$T_c = qJ/k_B,$$

where  $q = 2$  in one dimension.

- We therefore conclude that the mean-field approximation is qualitatively incorrect for the 1D Ising model.
- This is perhaps not surprising, since we expected the relative importance of fluctuations to be greatest in 1D.
- Conclusion: Fluctuation effects can be very important, especially in reduced dimensions.



## Mean-field theory

- Ising model in 1D
- Partition function
- Transfer matrix
- Partition function
- Free energy
- Eigenvalues
- Free energy solution
- Mean-field theory

- However, our mean-field calculations predicted a second-order phase transition in  $M(T)$  at the nonzero temperature

$$T_c = qJ/k_B,$$

where  $q = 2$  in one dimension.

- We therefore conclude that the mean-field approximation is qualitatively incorrect for the 1D Ising model.
- This is perhaps not surprising, since we expected the relative importance of fluctuations to be greatest in 1D.
- Conclusion: Fluctuation effects can be very important, especially in reduced dimensions.
- Even in 3D, fluctuations change the magnetization near  $T_c$  in a nontrivial way, since although mean-field theory does correctly predict

$$m(T) \propto (T_c/T - 1)^\beta,$$

it predicts a critical exponent  $\beta = 1/2$ , which disagrees with the measured value  $\beta = 0.334$ .