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- ▶ Assume that each particle can take on two states (which we will call spin): “up” spins for which  $S_i = +1$  and “down” spins with  $S_i = -1$ .
- ▶ If these spins only interact with their nearest neighbours and are placed in an external field, we can write a simple Hamiltonian for the system as

$$\mathcal{H} = -\frac{J}{2} \sum_{i=1}^N \sum_j' S_i S_j - H \sum_{i=1}^N S_i,$$

- ▶  $J$  is the coupling between the spins
- ▶  $H$  is an external field.



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- ▶  $H > 0$ , second term is minimized when the spins point up
- ▶  $H < 0$ , second term is minimized when the spins point down

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$$M = \sum_{i=1}^N S_i, \quad (1)$$

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- ▶ Finite temperatures: is there a phase transition? Does it depend on dimension?

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For there to be a phase transition, there must be a discontinuity in a derivative (1st derivative, or 2nd derivative, etc) of  $F$ .

Clearly,  $F$  is perfectly analytic so there is *no phase transition in the one dimensional Ising model with  $H = 0$ .*

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where

$$I = \frac{1}{2\pi} \int_0^\pi d\phi \ln \left\{ \frac{1}{2} \left[ 1 + \left( 1 - \kappa^2 \sin^2 \phi \right)^{1/2} \right] \right\}, \quad (6)$$

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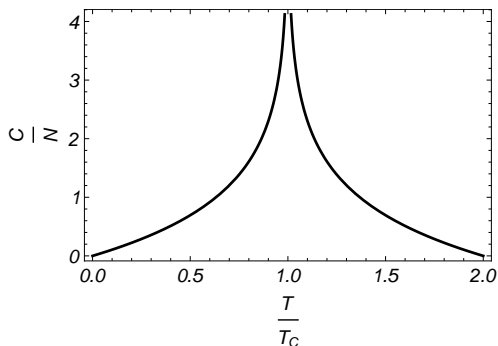
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- ▶ Second order phase transition with temperature  $T_C = 2.27J/k_B$
- ▶ Not analytically solved in 3d, but transition temperature found numerically to be  $T_C = 4.52J/k_B$

## Heat Capacity - 2d Zero field Ising Model

$$\frac{C}{N} = \frac{1}{N} \left( \frac{\partial \langle E \rangle}{\partial T} \right)_{H=0} \sim \frac{8k_B}{\pi} (\beta J)^2 \ln \left| \frac{1}{T - T_C} \right|. \quad (7)$$



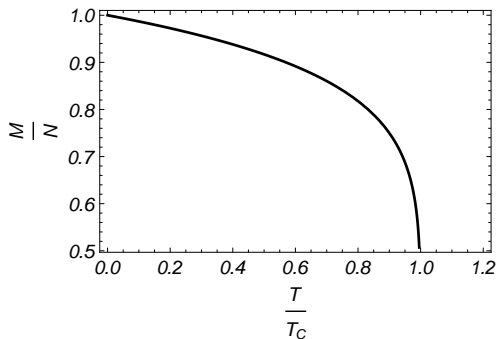


## Magnetization - 2d Zero field Ising Model

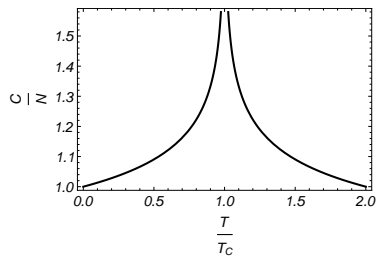
The magnetization for  $T < T_C$  is

$$\frac{M}{N} \propto (T_C - T)^\beta, \quad T < T_c \quad (8)$$

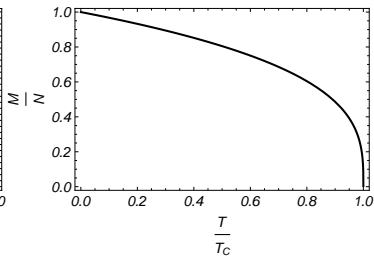
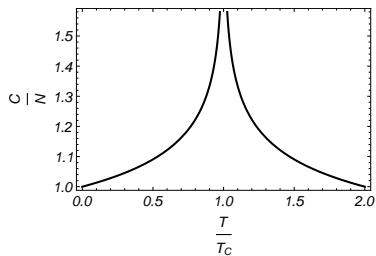
with  $\beta = 1/8$ .



## 3d Zero field Ising Model



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## Some Critical Exponents: 3d Ising model

Near the critical temperature the heat capacity has the form

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- ▶  $\alpha$  and  $\beta$  are referred to as *critical exponents*
- ▶ critical exponents typically used to characterize the phase transition.

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- ▶ Normalization (sum rule) requires that  $\sum_{\nu} P(\mu \rightarrow \nu) = 1$
- ▶ Need to define a Markov process such that it obeys the correct statistics - the states end up created according to e.g. the Boltzmann distribution

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- ▶ For transition probabilities satisfying this equation, the probability distribution  $p_{\mu}$  is an equilibrium of the dynamics of the Markov process.
- ▶ Unfortunately, satisfying this equation does not ensure that the probability distribution will go to  $p_{\mu}$  from any state of the system if we run the process for long enough

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- ▶ Remove possibility of spurious limit cycles by introducing **detailed balance condition**

$$p_\mu P(\mu \rightarrow \nu) = p_\nu P(\nu \rightarrow \mu) \quad (18)$$

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- Rewrite detailed balance condition

$$\frac{P(\mu \rightarrow \nu)}{P(\nu \rightarrow \mu)} = \frac{p_\nu}{p_\mu} = \text{desired distribution} \quad (19)$$

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- For the Ising model, the desired distribution is the Boltzmann distribution thus

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- ▶  $g(\mu \rightarrow \nu)$  is the **selection probability**: the probability that given an initial state  $\mu$ , we generate a new “trial” state  $\nu$
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- ▶ Applying this factorization:

$$\frac{P(\mu \rightarrow \nu)}{P(\nu \rightarrow \mu)} = \frac{g(\mu \rightarrow \nu)A(\mu \rightarrow \nu)}{g(\nu \rightarrow \mu)A(\nu \rightarrow \mu)} \quad (21)$$



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$$A(\mu \rightarrow \nu) = A_0 e^{-\frac{1}{2}\beta(E_\nu - E_\mu)} \quad (24)$$

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- ▶ Want to find the choice that maximizes the acceptance ratios (and thus makes the algorithm most efficient)

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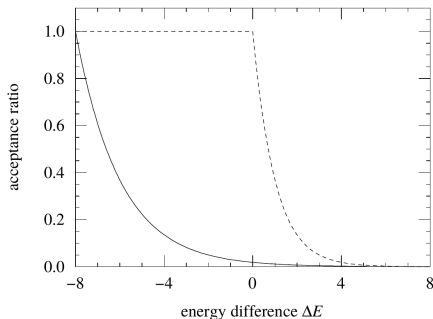
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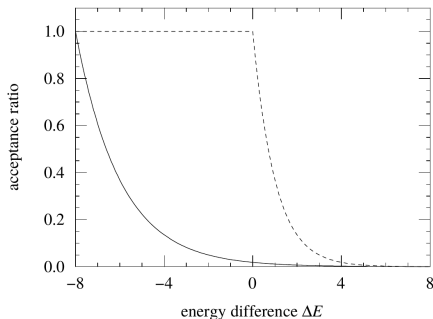
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Example: energy autocorrelation function:

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- ▶ See section 3.1.1. in the book on blackboard for some tricks associated with implementing this algorithm