Quantum Phase Transition in Transverse Ising Models

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Outline

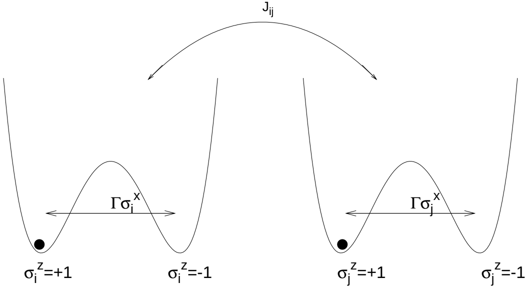
- Introduction
- Pseudo-spin representation
- Mean field theory for TIM
- BCS theory of superconductivity
- Renormalisation techniques for TIM
- Suzuki-Trotter formalism: classical correspondence
- Summary

Introduction

- Cooperative interactions between spin-like degrees of freedom can describe the order-disorder transition in many systems
- Transverse Ising Model (TIM) successfully describes a class of such systems
- A specific example being the ferro-electric ordering in Pottasium Dihydrogen Phosphate (KDP)
- TIM is essentially a quantum model; it incorporates zero temperature fluctuations
- TIM in d-dimension corresponds to Ising model in $(d+1)$ dimension.

Pseudo-spin picture

- In KDP, in each site the oxygen atom creates a double well and the proton resides in one of them



- In Pseudo-spin picture, the proton residing in left or right well can be represented by the states $|\uparrow>$ and $|\downarrow>$ respectively.
- Dipolar interactions between nearest neighbor sites form the cooperative (exchange-interaction) term.
- Proton being a quantum object, a tunneling term is required to study the system's behavior.

Pseudo-spin picture Contd.

- In formulating the tunneling term, note that

$$\sigma^x|\uparrow\rangle = |\downarrow\rangle \quad \text{and} \quad \sigma^x|\downarrow\rangle = |\uparrow\rangle,$$

- A transverse field will correctly represent the tunneling term
- Therefore, the Hamiltonian of the system can be written as

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x,$$

where, σ^α's $\rightarrow$ Pauli spin matrices,
J_{ij} $\rightarrow$ cooperative interactions and
Γ $\rightarrow$ tunneling integral, which depends on width and height of the barrier, particle mass etc.

Pseudo spin picture Contd.

- Spin 1/2 case: σ^z has two eigen values ± 1, which corresponds to a spin being parallel on anti-parallel with $z-$ axis.
- If we take

$$|\uparrow\rangle \Leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and

$$|\downarrow\rangle \Leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

then taking these two eigen-vectors as basis, the Pauli matrices have the following representation

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Mean Field Theory for TIM

$T = 0$

- One can make the non-commuting parts of the Hamiltonian commuting, by assuming

$$\sigma_i^z = |\vec{\sigma}| \cos\theta, \quad \text{and} \quad \sigma_i^x = |\vec{\sigma}| \sin\theta,$$

- The energy of the semi-classical system reduces to

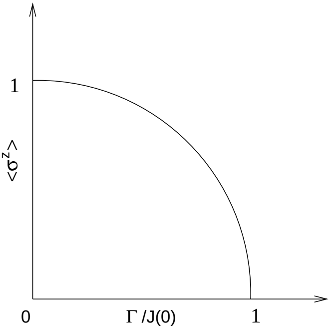
$$E = -\sigma\Gamma \sin\theta - \frac{1}{2}\sigma^2 J(0) \cos^2\theta,$$

$J(0) = J_i(0) = \sum_{(ij)} J_{ij}$, where j denotes the j-th nearest neighbor.

- Average values of the spin components are $\langle \sigma^x \rangle = \cos\theta$ and $\langle \sigma^z \rangle = \sin\theta$.

MFT for TIM

- Minimisation of the energy function gives $\sin\theta = \Gamma/J(0)$ or, $\cos\theta = 0$.
- Thus following cases may occur



- For $\Gamma = 0$, $\langle\sigma^x\rangle = 0$ and order parameter $\langle\sigma^z\rangle = 1$
- If $\Gamma < J(0)$, then both $\langle\sigma^x\rangle \neq 0$ and $\langle\sigma^z\rangle \neq 0$.
- When $\Gamma \leq J(0)$, then we must have $\cos\theta = 0$, implying $\langle\sigma^z\rangle = 0$ i.e., full disorder.
- So, even in the absence of thermal fluctuation, only quantum fluctuation can lead to an order-disorder phase transition of the system as Γ increases from 0 to $J(0)$.

- One can write the Hamiltonian as

$$\mathcal{H} = -\sum_i \vec{\mathbf{h}}_i.\vec{\sigma}_i.$$

where, $\vec{\mathbf{h}}_i = \Gamma\hat{x} + \left(\frac{1}{2}\sum_j J_{ij}\langle\sigma_j^z\rangle\right)\hat{z}$, and $\vec{\sigma}_i = \sigma_i^x\hat{x} + \sigma_i^z\hat{z}$,

- Under MF approximation one can replace $\vec{\mathbf{h}}_i$ by $\vec{\mathbf{h}} = \Gamma\hat{x} + \langle\sigma^z\rangle J(0)\hat{z}$.
- Implying $\vec{\sigma} = \tanh(\beta|\vec{\mathbf{h}}|).\frac{\vec{\mathbf{h}}}{|\vec{\mathbf{h}}|}$ and $|\vec{\mathbf{h}}| = \sqrt{\Gamma^2 + (J(0)\langle\sigma^z\rangle)^2}$.
- Therefore, $\langle\sigma^z\rangle = [\tanh(\beta|\vec{\mathbf{h}}|)]\left(\frac{J(0)\langle\sigma^z\rangle}{|\vec{\mathbf{h}}|}\right)$, and $\langle\sigma^x\rangle = [\tanh(\beta|\vec{\mathbf{h}}|)]\frac{\Gamma}{|\vec{\mathbf{h}}|}$.

MFT for TIM

$\Gamma = 0$

- Here, $\langle \sigma^z \rangle = \tanh\left(\frac{J(0)\langle \sigma^z \rangle}{k_B T}\right)$ and $\langle \sigma^x \rangle = 0$.
- Graphical solution gives $\langle \sigma^z \rangle \neq 0 \quad \text{for} \quad k_B T < J(0)$
  $\langle \sigma^z \rangle = 0 \quad \text{for} \quad k_B T > J(0)$.
- It shows that without quantum fluctuation, thermal fluctuation can drive the system to complete disorder beyond $T_c = J(0)$.

$k_B T = 0$

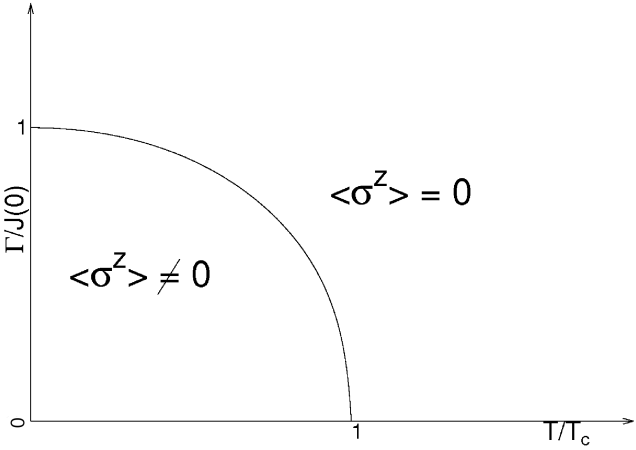
- Here, $\langle \sigma^z \rangle = \frac{J(0)\langle \sigma^z \rangle}{\sqrt{(\Gamma)^2 + (J(0)\langle \sigma^z \rangle)^2}}$
- Phase boundary: $\langle \sigma^z \rangle \rightarrow 0$ $1 = \frac{J(0)}{\Gamma_c} \Rightarrow \Gamma_c = J(0)$ as obtained earlier.

$k_B T$ finite

- Phase boundary: $\langle \sigma^z \rangle \rightarrow 0$.
  $\langle \sigma^z \rangle = \tanh\left(\frac{\Gamma_c}{k_B T}\right) \frac{J(0)\langle \sigma^z \rangle}{\Gamma}$ or, $\tanh\left(\frac{\Gamma_c}{k_B T}\right) = \frac{\Gamma_c}{J(0)}$.

MFT for TIM

The phase boundary is as follows



BCS theory of Superconductivity

- The cooperative Hamiltonian in the BCS theory of superconductivity has the following form
  $\mathcal{H} = \sum_k \epsilon_k^0 (c_k^\dagger c_k + c_{-k}^\dagger c_{-k}) - V \sum_{kk'} c_{k'}^\dagger c_{-k'}^\dagger c_{-k} c_k$
- In terms of the number operator $\hat{n}_k = c_k^\dagger c_k$, the above Hamiltonian reduces to $(\sum\limits_k \epsilon_k = 0)$

  $\mathcal{H} = -\sum_k \epsilon_k^0 (1 - \hat{n}_k - \hat{n}_{-k}) - V \sum_{kk'} c_{k'}^\dagger c_{-k'}^\dagger c_{-k} c_k.$
- Considering the low-lying spectra containing the pair of electrons in state $(k, -k)$, the relevant states are pair occupied (denoted by $|1_k 1_{-k}\rangle$) or pair unoccupied (denoted by $|0_k 0_{-k}\rangle$).
- Then
  $(1 - \hat{n}_k - \hat{n}_{-k})|1_k 1_{-k}\rangle = (1 - 1 - 1)|1_k 1_{-k}\rangle = -|1_k 1_{-k}\rangle$, and
  $(1 - \hat{n}_k - \hat{n}_{-k})|0_k 0_{-k}\rangle = (1 - 0 - 0)|0_k 0_{-k}\rangle = |0_k 0_{-k}\rangle$

BCS theory Contd.

- The correspondence to the pseudo-spin picture can be made by noting $|1_k 1_{-k}\rangle \Leftrightarrow |\downarrow\rangle_k$, $|0_k 0_{-k}\rangle \Leftrightarrow |\uparrow\rangle_k$, and$(1 - n_k - n_{-k}) \Leftrightarrow \sigma^z_k$.
- Since $c^\dagger_k c^\dagger_{-k} |\uparrow\rangle_k = |\downarrow\rangle_k, \quad c^\dagger_k c^\dagger_{-k} |\downarrow\rangle_k = 0$

& $\quad c_{-k} c_k |\downarrow\rangle_k = |\uparrow\rangle_k, \quad c_{-k} c_k |\uparrow\rangle_k = 0$, and:

$$\sigma^- = \sigma^x - i\sigma^y = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}; \qquad \sigma^+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}.$$

One can identify

$$c^\dagger_k c^\dagger_{-k} = \tfrac{1}{2}\sigma^-_k, \quad c_{-k} c_k = \tfrac{1}{2}\sigma^\dagger_k.$$

BCS theory Contd.

- With the above identifications, the Hamiltonian can be written as $\mathcal{H} = -\sum_k \epsilon_k^0 \sigma_k^z - \frac{1}{4} V \sum_{kk'} \sigma_{k'}^- \sigma_k^+$.
- Further, the term $\sum_{kk'} (\sigma_{k'}^x \sigma_k^y - \sigma_{k'}^y \sigma_k^x)$ vanishes due to symmetric summing done over k and k'.
- Hence the pseudo-spin BCS Hamiltonian reads $\mathcal{H} = -\sum_k \epsilon_k^0 \sigma_k^z - \frac{1}{4} V \sum_{kk'} (\sigma_{k'}^x \sigma_k^x + \sigma_{k'}^y \sigma_k^y)$.
- As before, the Hamiltonian can be written as $\mathcal{H} = -\sum_k \vec{\mathbf{h}}_k . \vec{\sigma}_k$, with $\vec{\mathbf{h}}_k = \epsilon_k^0 \hat{z} + \frac{1}{4} V \sum_{k'} (\langle \sigma_{k'}^x \rangle \hat{x} + \langle \sigma_{k'}^y \rangle \hat{y})$
- Using $\langle \sigma_k^x \rangle = \langle \sigma_k^y \rangle$, $\quad \vec{\mathbf{h}}_k = \epsilon_k^0 \hat{z} + \frac{1}{2} V \sum_{k'} \langle \sigma_{k'}^x \rangle \hat{x}$
- If

$$\tan \theta_k = \frac{h_k^x}{h_k^z} = \frac{\frac{1}{2} V \sum_{k'} \langle \sigma_{k'}^x \rangle}{\epsilon_k^0} \equiv \frac{\Delta}{\epsilon_k^0}$$

then $\sin \theta_k = \frac{\Delta}{\sqrt{\Delta^2 + \epsilon_k^{0\,2}}}$ and $\cos \theta_k = \frac{\epsilon_k^0}{\sqrt{\Delta^2 + \epsilon_k^{0\,2}}}$.

BCS theory: Excitation spectra at $T = 0$

- $\Delta = \frac{1}{2} V \sum_{k'} \langle \sigma^x_{k'} \rangle = \frac{1}{2} V \sum_{k'} \sin\theta_{k'} = \frac{1}{2} \sum_{k'} \frac{\Delta}{\sqrt{\Delta^2 + \epsilon_k^{0\,2}}}$.
- With ρ_F as the density of states near the Fermi level, the above equation gives

$$1 = \frac{1}{2} V \rho_F \int_{-\omega_D}^{\omega_D} \frac{d\epsilon}{\sqrt{\Delta^2 + \epsilon^2}} = V \rho_F \sinh^{-1}(\omega_D/\Delta).$$

  here ω_D is Debye frequency.
- Thus $\Delta = \Delta(T = 0) = \frac{\omega_D}{\sinh(1/V\rho_F)} \cong 2\omega_D e^{-1/V\rho_F}$,

(if $\rho_F V << 1$)

- at first approximation, the excitation spectrum is obtained as the energy ϵ_k to reverse a pseudo- spin in the field $\tilde{\mathbf{h}}_k$, i.e., $\epsilon_k = 2|\tilde{\mathbf{h}}_k| = 2\left(\epsilon_k^{0\,2} + \Delta^2\right)^{1/2}$. Minimum excitation energy is 2Δ, i.e. Δ gives the energy gap in the excitation spectrum.

BCS theory: Estimating transition temperature

- For $T = 0$, $\langle \sigma_k^z \rangle = \tanh\left(\beta|\vec{\mathbf{h}}_k|\right)$.
- Hence, $\tan\theta_k = \frac{h_k^x}{h_k^z} = \frac{V}{2\epsilon_k^0}\sum_k \langle \sigma_{k'}^z \rangle$

$=\left(\frac{V}{2\epsilon_k^0}\right)\sum_{k'}\tanh\left(\beta|\vec{\mathbf{h}}_{k'}|\right)\sin\theta_{k'} \equiv \frac{\Delta(T)}{\epsilon_k}$.

- The superconducting transition is characterised by vanishing of the gap Δ. Hence, as $T \to T_c$, $\Delta \to 0$.
- Hence: $1 = \frac{V}{2}\sum_{k'}\frac{1}{\epsilon_{k'}^0}\tanh\left(\frac{\epsilon_{k'}^0}{T_c}\right)$. or,

  $\frac{2}{V\rho_F} = \int_{-\omega_D}^{\omega_D}\frac{d\epsilon}{\epsilon}\tanh\left(\frac{\epsilon}{2T_c}\right) = 2\int_0^{\omega_D/2T_c}\frac{\tanh x}{x}dx$.
- Solution: $T_c = 1.14\omega_D e^{-1/V\rho_F}$. $\Rightarrow 2\Delta(T=0) \simeq 3.5T_c$.
- This is consistent with experimental results for a number of materials (ex: Al, Pb, Cd).

Real space renormalization for Transverse Ising chain

- Real space block renormalization can be applied to transverse Ising chain.
- Consider the 1D Hamiltonian

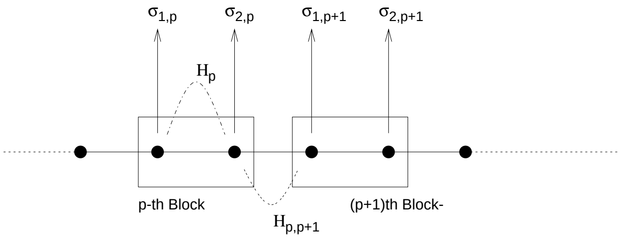
$$
\begin{aligned}
\mathcal{H} &= -\Gamma \sum_{i=1}^{N} \sigma_i^z - J \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x \\
&= \mathcal{H}_B + \mathcal{H}_{IB} \quad \text{(say)}.
\end{aligned}
$$

Here

$$
\mathcal{H}_B = \sum_{p=1}^{N/b} \mathcal{H}_p \quad ; \qquad \mathcal{H}_p = -\sum_{i=1}^{b} \Gamma \sigma_{i,p}^z - \sum_{i-1}^{b-1} J \sigma_{i,p}^x \sigma_{i+1,p}^x
$$

and $\mathcal{H}_{IB} = \sum_{p=1}^{N/(b-1)} \mathcal{H}_{p,p+1} \quad ; \qquad \mathcal{H}_{p,p+1} = -J \sigma_{b,p}^x \sigma_{1,p+1}^x.$

- The above rearrangement of the Hamiltonian recasts the picture of N spins with nearest-neighbour interaction into one in which there are $N/(b-1)$ blocks, each consisting of b number of spins.
- Consider $b = 2$:



The 4 eigen states of $\mathcal{H}_p$ can be expressed as the linear combinations of the eigen states of $\sigma^z_{1,p} \otimes \sigma^z_{2,p}$; namely, $|\uparrow\uparrow\rangle, \quad |\downarrow\downarrow\rangle, \quad |\uparrow\downarrow\rangle, \quad \text{and} \quad |\downarrow\uparrow\rangle.$

RSRG Contd.

- The (orthonormal) eigen states of $\mathcal{H}_p$ are:

$$
\begin{aligned}
|0\rangle &= \frac{1}{\sqrt{1+a^2}}(|\uparrow\uparrow\rangle + a|\downarrow\downarrow\rangle) \\
|1\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\
|2\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \\
|3\rangle &= \frac{1}{\sqrt{1+a^2}}(a|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle).
\end{aligned}
$$

- Check: $\mathcal{H}_P|0\rangle = -(2\Gamma + Ja)\frac{1}{\sqrt{1+a^2}}\left[|\uparrow\uparrow\rangle + \left(-\frac{2\Gamma - J/a}{2\Gamma + Ja}\right) a|\downarrow\downarrow\rangle\right]$
$\Rightarrow \frac{2\Gamma - J/a}{2\Gamma + Ja} = -1 \Rightarrow a = \frac{\sqrt{4\Gamma^2 + J^2} - 2\Gamma}{J}$.

RSRG Contd.

- $$\begin{aligned} \mathcal{H}_p|0\rangle &= E_0|0\rangle, \quad E_0 = -\sqrt{4\Gamma^2 + J^2} \\ \mathcal{H}_p|1\rangle &= E_1|1\rangle, \quad E_1 = -J \\ \mathcal{H}_p|2\rangle &= E_2|2\rangle, \quad E_2 = +J \\ \mathcal{H}_p|3\rangle &= E_3|3\rangle, \quad E_3 = +\sqrt{4\Gamma^2 + J^2}. \end{aligned}$$
- We take $|0\rangle$ and $|1\rangle$ as the renormalized eigen states of the renormalized spins σ' where $\langle 0|\sigma'^x|1\rangle = \frac{1+a}{\sqrt{2(1+a^2)}}$, giving $J' = J\frac{(1+a)^2}{2(1+a^2)}$.
- Since $E_1 - E_0 = 2\Gamma'$ (was 2Γ for unrenormalized state) $\Gamma' = \frac{J}{2}[\sqrt{4\lambda^2+1}+1]$
- The fixed points of the recurrence relations are $\lambda^\star = 0$

$\lambda^\star \to \infty \quad$ and $\quad \lambda^\star \simeq 1.277$ with $\lambda = \frac{\Gamma}{J}$

RSRG Contd.

- If correlation length $\xi \sim (\lambda - \lambda_c)^{-\nu}$, then in the renormalized system $\xi' \sim (\lambda' - \lambda_c)^{-\nu}$.
- $\xi'/\xi = b = \left(\frac{\lambda' - \lambda_c}{\lambda - \lambda_c}\right)^{-\nu} \Rightarrow \left.\frac{d\lambda'}{d\lambda}\right|_{\lambda=\lambda_c\equiv\lambda^\star} = b^{-1/\nu} \Rightarrow \nu \approx 1.47$ (compare with 2d exact result $\nu = 1$).
- Similarly, $z \approx 0.55$ (compare with $z = 1$ in 2d) and $s = \nu z \approx 0.81$ (compare with $s = 1$ for 2d).
- Results improve rapidly for larger b values.

- Suzuki-Trotter formalism is essentially a method to transform a d-dimensional quantum Hamiltonian into a $(d+1)$-dimensional effective classical Hamiltonian giving the same canonical partition function.
- Consider the Hamiltonian

$$\begin{aligned}\mathcal{H} &= -\Gamma \sum_{i=1}^{N} \sigma_i^x - \sum_{(i,j)} J_{ij}\sigma_i^z \sigma_j^z \\ &\equiv \mathcal{H}_0 + \mathcal{V}\end{aligned}$$

- Trotter formula:
  $\exp(A_1 + A_2) = \lim_{M\to\infty} [\exp A_1/M \exp A_2/M]^M$, even when $[A_1, A_2] \neq 0 \Rightarrow$
  Partition function $Z = Tre^{-\beta\mathcal{H}} =$

$\lim_{M\to\infty} Tr \prod_{k=1}^{M} \langle \sigma_{1,k} \ldots \sigma_{N,k} | \exp\left(\frac{-\beta\mathcal{H}_0}{M}\right) \exp\left(\frac{-\beta\mathcal{V}}{M}\right) | \sigma_{1,k} \ldots \sigma_{N,k} \rangle$.

Suzuki-Trotter Contd.

- Now $\prod_{k=1}^{M} \langle \sigma_{1,k} \ldots \sigma_{N,k} | \exp\left(\frac{\beta}{M} \sum_{i,j} \sigma_i^z \sigma_j^z \right) | \sigma_{1,k+1} \ldots \sigma_{N,k+1} \rangle =$ $\exp\left[\sum_{i,j=1}^{N} \sum_{k=1}^{M} \frac{\beta J_{ij}}{M} \sigma_{i,k} \sigma_{j,k} \right]$
- Also,

$$\prod_{k=1}^{M} \langle \sigma_{1,k} \ldots \sigma_{N,k} | \exp\left[\frac{\beta \Gamma}{M} \sum_i \sigma_i^x \right] | \sigma_{1,k+1} \ldots \sigma_{N,k+1} \rangle$$

$$= \left(\frac{1}{2} \sinh\left[\frac{2\beta\Gamma}{M} \right] \right)^{\frac{NM}{2}} \exp\left[\frac{1}{2} \ln \coth\left(\frac{\beta\Gamma}{M} \right) \sum_{i=1}^{N} \sum_{k=1}^{M} \sigma_{i,k} \sigma_{i,k+1} \right].$$

since: $e^{a\sigma^x} = e^{-i(ia\sigma^x)} = \cos(ia\sigma^x) - i\sin(ia\sigma^x) =$ $\cosh(a) + \sigma^x \sinh(a)$, $\Rightarrow$ $\langle \sigma | e^{a\sigma^x} | \sigma' \rangle = \left[\frac{1}{2} \sinh(2a) \right]^{1/2} \exp\left[(\sigma\sigma'/2) \ln \coth(a) \right]$,

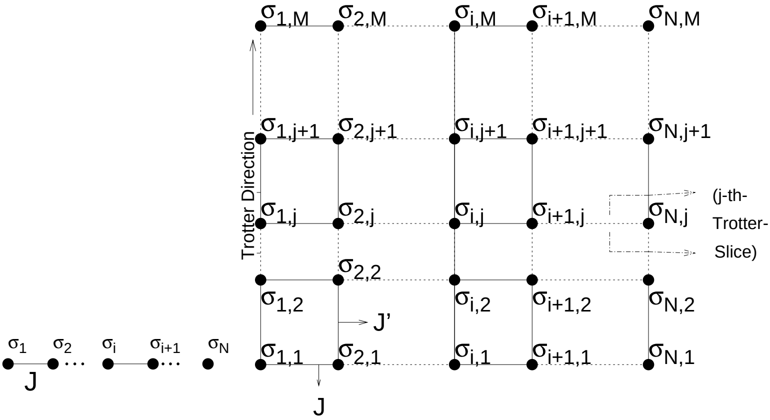
- since $\langle\uparrow|e^{a\sigma^x}|\uparrow\rangle = \langle\downarrow|e^{a\sigma^x}|\downarrow\rangle = \cosh(a) = \left[\frac{1}{2}\sinh(2a).\coth(a)\right]^{1/2}$ and $\langle\uparrow|e^{a\sigma^x}|\downarrow\rangle = \langle\downarrow|e^{a\sigma^x}|\uparrow\rangle = \sinh(a) = \left[\frac{1}{2}\sinh(2a)/\coth(a)\right]^{1/2}$.
- Thus the partition function reads

$$Z = C^{\frac{NM}{2}} Tr_\sigma(-\beta\mathcal{H}_{eff}[\sigma]) \quad ; \quad C = \frac{1}{2}\sinh\frac{2\beta\Gamma}{M}$$

- Where the effective classical Hamiltonian is

$$\mathcal{H}_{eff}(\sigma) = \sum_{(i,j)}^{N}\sum_{k=1}^{M}\left[-\frac{J_{ij}}{M}\sigma_{ik}\sigma_{jk} - \frac{\delta_{ij}}{2\beta}\ln\coth\left(\frac{\beta\Gamma}{M}\right)\sigma_{ik}\sigma_{ik+1}\right].$$

- The Hamiltonian $\mathcal{H}_{eff}$ is a classical one, since the variables $\sigma_{i,k}$'s involved are merely the eigen-values of σ^z, and hence there is no non-commuting part in $\mathcal{H}_{eff}$.
- M should be at the order of $\hbar\beta$ (we have taken $\hbar = 1$ in the calculation) for a meaningful comparison of the interaction in the Trotter direction with that in the original Hamiltonian.



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