The Quantum Monte Carlo Simulation of Transverse Field Ising Model

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Outline

1 Worm Algorithm

2 Numerical Results

Holstein-Primakoff Transformation

TFI:

$$\mathcal{H} = -t\sum_{\langle ij\rangle}\sigma_i^x\sigma_j^x - h\sum_i \sigma_i^z = K + U$$

Hopping and pairing terms:

$$K = K_1 + K_2 = -t\sum_{\langle ij\rangle}(\sigma_i^+\sigma_j^- + \text{h.c.}) - t\sum_{\langle ij\rangle}(\sigma_i^+\sigma_j^+ + \text{h.c.})$$

HP transformation: $b_i(b_i^\dagger) = \sigma_i^+(\sigma_i^-), n_i = b_i^\dagger b_i = (\sigma_i^z + 1)/2$

$$\Rightarrow \mathcal{H} = -t\sum_{\langle ij\rangle}(b_i^\dagger b_j + \text{h.c.}) - t\sum_{\langle ij\rangle}(b_i^\dagger b_j^\dagger + \text{h.c.}) - \mu\sum_i n_i$$

where $\mu = 2h$.

$\mathcal{Z}$ Configurations

$$\mathcal{Z} = \mathrm{Tr}\left(\mathrm{e}^{-\beta\mathcal{H}}\right) = \sum_{a_0} \langle \alpha_0 | \, \mathrm{e}^{-\beta\mathcal{H}} \, | \alpha_0 \rangle$$

$$= \lim_{\mathrm{d}\tau = \frac{\beta}{n}, n\to\infty} \sum_{\{\alpha_i\}} \langle \alpha_0 | \, \mathrm{e}^{-\mathcal{H}\mathrm{d}\tau} \, | \alpha_{n-1} \rangle \cdots \langle \alpha_i | \, \mathrm{e}^{-\mathcal{H}\mathrm{d}\tau} \, | \alpha_0 \rangle$$

$$= \sum_{\alpha_0} \sum_{\mathcal{N}}^{\infty} \int_0^\beta \int_{\tau_1}^\beta \cdots \int_{\tau_{\mathcal{N}-1}}^\beta \prod_{k=1}^{\mathcal{N}} \mathrm{d}\tau_k \, F(t,h)$$

$$F(t,h) = t^{\mathcal{N}_h + \mathcal{N}_p} \mathrm{e}^{-\int_0^\beta U(\tau)\,\mathrm{d}\tau}$$

$\mathcal{N}_h$ and $\mathcal{N}_p$: number of hopping and pairing kinks. $\mathcal{N}_h + \mathcal{N}_p = \mathcal{N}$.

$\mathcal{Z}$ configuration: several loops of spin-up (and kinks) in the $(d+1)$D space-time.
Statistical weight of a $\mathcal{Z}$ configuration:

$$W_{\mathcal{Z}}(t,h) = \prod_{k=1}^{\mathcal{N}} \mathrm{d}\tau \, F(t,h)$$

$\mathcal{G}$ Configurations

$$\mathcal{G}(\boldsymbol{x}_I, \tau_I; \boldsymbol{x}_M, \tau_M) = \mathrm{Tr}\left[T_\tau\left(\sigma_I^x(\tau_I)\sigma_M^x(\tau_M)\mathrm{e}^{-\beta\mathcal{H}}\right)\right]$$

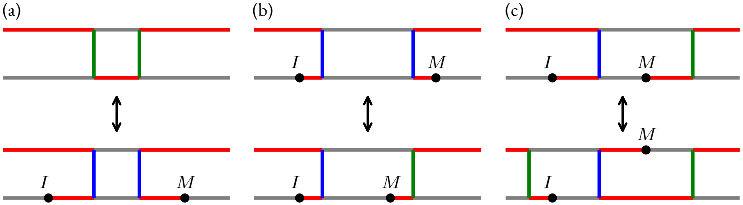
$\mathcal{G}$ configuration: $\mathcal{Z}$ configuration + an open path of spin-up with two ending points "Ira" (I) and "Masha" (M).

Statistical weight of a $\mathcal{G}$ configuration:

$$W_{\mathcal{G}} = \frac{\mathrm{d}\tau_I \mathrm{d}\tau_M}{\omega_G} \prod_{k=1}^{\mathcal{N}} \mathrm{d}\tau_k \, F(t, h)$$

- Key idea: move the defect M of the open path to produce different $\mathcal{G}$ and $\mathcal{Z}$ configurations for sampling. (Like a worm wriggling!)

Updates



(a) Create/annihilate defects I and M.

$$\frac{d\tau_I}{\beta N}\frac{d\tau_M}{\tau_a}\cdot W_{\mathcal{Z}}\cdot\mathcal{P}_{\text{crea}}=\mathcal{A}_a\cdot W_{\mathcal{G}}\cdot\mathcal{P}_{\text{anni}}\Rightarrow\begin{cases}P_{\text{crea}}=\min\left[1,\mathcal{A}_a\tau_a\frac{\beta N}{\omega_G}\frac{F_{\text{new}}}{F_{\text{old}}}\right]\\ P_{\text{anni}}=\min\left[1,\frac{1}{\mathcal{A}_a\tau_a}\frac{\omega_G}{\beta N}\frac{F_{\text{new}}}{F_{\text{old}}}\right]\end{cases}$$

(b) Move imaginary time of defect M.

$$P_{\text{move}}=\min\left\{1,\frac{F_{\text{new}}}{F_{\text{old}}}\right\}$$

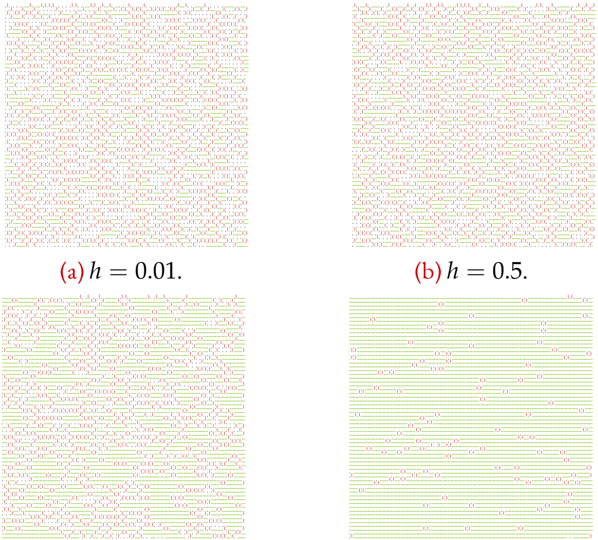
(c) Insert/delete a kink.

$$\mathcal{A}_c\cdot\frac{1}{z_d}\cdot\frac{d\tau}{\tau_c}\cdot W\cdot\mathcal{P}_{\text{inse}}=\mathcal{A}_c\cdot\frac{1}{z_d}\cdot\frac{1}{n_k}\cdot W_+\cdot\mathcal{P}_{\text{dele}}\Rightarrow\begin{cases}P_{\text{inse}}=\min\left[1,\frac{\tau_c}{n_k+1}\frac{F_{\text{new}}}{F_{\text{old}}}\right]\\ P_{\text{dele}}=\min\left[1,\frac{n_k}{\tau_c}\frac{F_{\text{new}}}{F_{\text{old}}}\right]\end{cases}$$

τ_a, τ_b, τ_c: ranges for choosing random time displacement.
A priori probabilities: $\mathcal{A}_a+\mathcal{A}_b+2\mathcal{A}_c=1$.

Outline

Visualization



(a) $h = 0.01$. (b) $h = 0.5$.

(c) $h = 1.0$. (d) $h = 1.5$.

Calculated quantities

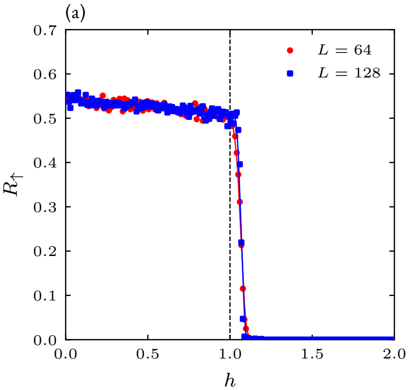
- Topological quantities: winding number $W^l \Rightarrow$ total winding number $W \Rightarrow$ wrapping probability R.
- Physical quantities: correlation functions.

$$\overline{\sigma_i^z} \equiv \frac{1}{L^2} \sum_{j,k} \sigma_{j,k}^z,$$

$$\overline{\sigma_i^z \sigma_{i+n}^z} \equiv \frac{1}{L^2} \sum_{j,k} \sigma_{j,k}^z \sigma_{j+n,k}^z,$$

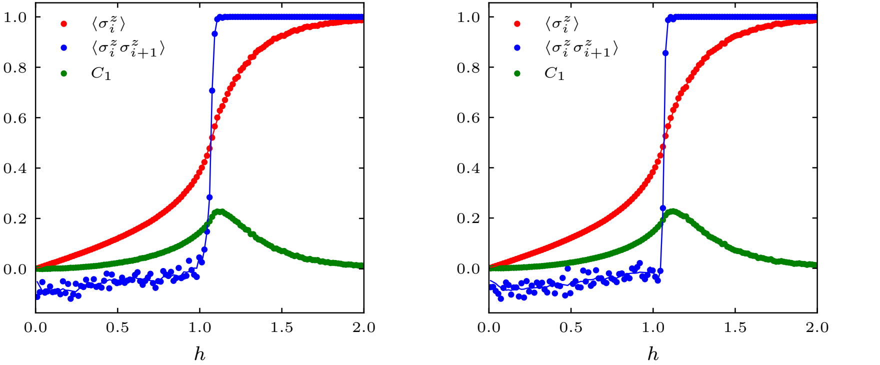
$$C_n \equiv \overline{\sigma_i^z \sigma_{i+n}^z} - \overline{\sigma_i^z}^2,$$

Wrapping Probabilities



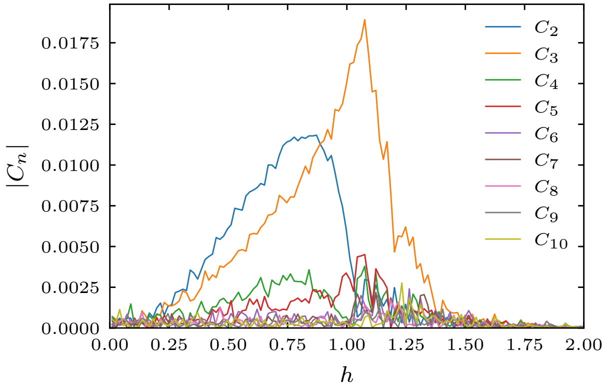
Wrapping probabilities $R_\uparrow$ and $R_\downarrow$ versus the transverse field h. (a) Spin-up. (b) Spin-down.

Correlation Functions



Expectation values of spin states $\overline{\sigma_i^z}$, product of NN spins $\overline{\sigma_i^z\sigma_{i+1}^z}$ and correlation function C_1 versus transverse field h. (a) $L = 64$. (b) $L = 128$.

Correlation Functions



Correlation functions $|C_n|$ versus the transverse field h.

Thank you for listening!