Review of theoretical free energy calculations for Transverse Field Ising Model

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In this paper, the major theoretical derivations and computations for calculating the free energy of the transverse field Ising model (TFIM) are presented[1]. The Hamiltonian for 1D TFIM with periodic boundary conditions (PBC) is defined as

$$H = -J\sum_{j=1}^{N} S_j^x S_{j+1}^x - g\sum_{j=1}^{N} S_j^z$$

Employing the Jordan-Wigner transformations

$$c_n = \exp\left(\pi i \sum_{j=1}^{n-1} S_j^+ S_j^-\right) S_n^- \quad c_n^\dagger = \exp\left(-\pi i \sum_{j=1}^{n-1} S_j^+ S_j^-\right) S_n^+$$

(with $S_j^\pm = S_j^x \pm i S_j^y$), one could convert the Hamiltonian to the following fermion form:

$$H = \frac{gN}{2} - g\sum_{i=1}^{N} c_i^\dagger c_i - \frac{J}{4}\sum_{i=1}^{N-1}\left(c_i^\dagger - c_i\right)\left(c_{i+1}^\dagger + c_{i+1}\right) + \frac{J}{4}\exp(i\pi N_f)\left(c_N^\dagger - c_N\right)\left(c_1^\dagger + c_1\right),$$

where $N_f = \sum_{j=1}^{N} c_j^\dagger c_j$ is the total fermion number ($c_j^\dagger c_j = S_j^z + \frac{1}{2}$). Casting the fermion Hamiltonian into a form similar to the BCS Hamiltonian of conventional superconductors, we obtain

$$H = \sum_{j=1}^{N}\left[-\frac{J}{4}\left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j\right) - g c_j^\dagger c_j + \frac{J}{4} c_j c_{j+1} + \frac{J}{4} c_{j+1}^\dagger c_j^\dagger\right] + \frac{gN}{2}$$

with the following boundary conditions

$$\begin{aligned} c_{N+1} &= c_1, \text{ for } N_f \equiv 1 (\bmod 2) \\ c_{N+1} &= -c_1 \text{ for } N_f \equiv 0 (\bmod 2). \end{aligned}$$

(note that PBC/anti-PBC (APBC) is imposed on the case with odd/even total fermion number, respectively). Introducing

$$c_n = \frac{1}{\sqrt{N}}\sum_k c_k e^{ikn}, c_n^\dagger = \frac{1}{\sqrt{N}}\sum_k c_k^\dagger e^{-ikn}$$

[1] The general results and arguments of this paper are based on the following article: He and Guo, *The boundary effects of transverse field Ising model*, https://arxiv.org/pdf/1707.02400.pdf, [cond-mat.stat-mech], 8 Jul 2017.

with k labeling the momentum, which takes the values of

$$k \in \Lambda_a, \Lambda_a = \left\{\pm\frac{\pi}{N}, \pm\frac{3\pi}{N}, \cdots, \pm\frac{(N-1)\pi}{N}\right\} \text{ for APBC}$$
$$k \in \Lambda_p, \Lambda_p = \left\{0, \pm\frac{2\pi}{N}, \pm\frac{4\pi}{N}, \cdots, \pm\frac{(N-2)\pi}{N}, \pi\right\} \text{ for PBC},$$

the Hamiltonian could be transformed to the momentum space (note that $N =$ number of sites and is **even** for ferromagnetic (FM) case. Also, it is essential to note that *both* PBC and APBC contributions should be considered for the fermion Hamiltonian calculations). Consequently, the two pieces of the Hamiltonian for PBC and APBC would become

$$H_a = \sum_{k\in\Lambda_a}\left[\xi_k c_k^\dagger c_k + \xi_k c_{-k}^\dagger c_{-k} + i\frac{J}{2}\sin k c_{-k}c_k - i\frac{J}{2}\sin k c_k^\dagger c_{-k}^\dagger\right] + \frac{gN}{2}$$
$$H_p = \sum_{k\in\Lambda_p}\left[\xi_k c_k^\dagger c_k + \xi_k c_{-k}^\dagger c_{-k} + i\frac{J}{2}\sin k c_{-k}c_k - i\frac{J}{2}\sin k c_k^\dagger c_{-k}^\dagger\right] + \frac{gN}{2} + \xi_0 c_0^\dagger c_0 + \xi_\pi c_\pi^\dagger c_\pi$$

with $\xi_k = -\frac{J}{2}\cos k - g$, $\Lambda'_a = \{k|k \in \Lambda_e, k > 0\}$, and $\Lambda'_p = \{k|k \in \Lambda_e, k > 0, k \neq \pi\}$. Diagonalization of the Hamiltonian is achieved by means of Bogoliubov transformation as follows:

$$\begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k^* & u_k \end{pmatrix}\begin{pmatrix} \eta_k \\ \eta_{-k}^\dagger \end{pmatrix}.$$

Choosing $u_k = \sqrt{E_k + \xi_k/2E_k}$ and $v_k = i\,\mathrm{sgn}\,k\sqrt{E_k - \xi_k/2E_k}$, we arrive at the following dispersion relationship

$$E_k = \sqrt{(J/2)^2 + g^2 + Jg\cos k}.$$

Therefore, the diagonalized form of the fermion Hamiltonian (for PBC and APBC) could be rewritten as

$$H_a = E_0 + \sum_{k\in\Lambda_a} E_k\left(\eta_k^\dagger\eta_k + \eta_{-k}^\dagger\eta_{-k}\right)$$
$$H_p = E_1 + \sum_{k\in\Lambda'_p} E_k\left(\eta_k^\dagger\eta_k + \eta_{-k}^\dagger\eta_{-k}\right) + \xi_0 c_0^\dagger c_0 + \xi_\pi c_\pi^\dagger c_\pi$$

where $E_0 = -\sum_{\mathrm{k}\in\Lambda'_a} E_k$ and $E_1 = g - \sum_{\mathrm{k}\in\Lambda'_p} E_k$, respectively. Therefore, the spectra of the fermion Hamiltonian could be computed as

$$E(\{n_k\}) = \sum_{k\in\Lambda_a}\left[-\frac{E_k}{2}(1-n_k) + \frac{E_k}{2}n_k\right], \quad \sum_k n_k \equiv \nu_a (\mathrm{mod}\ 2)$$
$$E(\{n_k\}) = \sum_{k\in\Lambda_p}\left[-\frac{E_k}{2}(1-n_k) + \frac{E_k}{2}n_k\right], \quad \sum_k n_k \equiv \nu_p (\mathrm{mod}\ 2)$$

where $n_k = 0$ or 1 (the occupation number of eigenmode η_k). For the FM case, one could find that

$$v_a = 0, v_p = \begin{cases} 0, & g < J/2 \\ 1, & g > J/2 \end{cases}$$

Employing the specified spectra of the Hamiltonian, it would be a straightforward procedure to derive expressions for different partition functions of PBC and APBC contributions of fermion Hamiltonian:

$$Z_{a1} = \prod_{k \in \Lambda_a} \left(e^{\frac{E_k}{2t}} + e^{-\frac{E_k}{2T}} \right), \quad Z_{p1} = \prod_{k \in \Lambda_p} \left(e^{\frac{E_k}{2T}} + e^{-\frac{E_k}{2T}} \right)$$
$$Z_{a2} = \prod_{k \in \Lambda_a} \left(e^{\frac{E_k}{2T}} - e^{-\frac{E_k}{2T}} \right), \quad Z_{p2} = \prod_{k \in \Lambda_p} \left(e^{\frac{E_k}{2T}} - e^{-\frac{E_k}{2T}} \right)$$

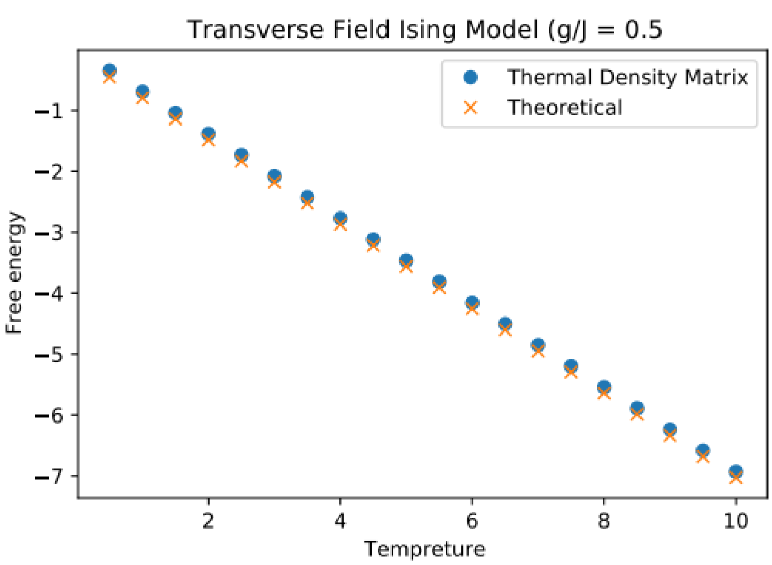
The total partition function for the FM case (using fermion number parity) could be then written as

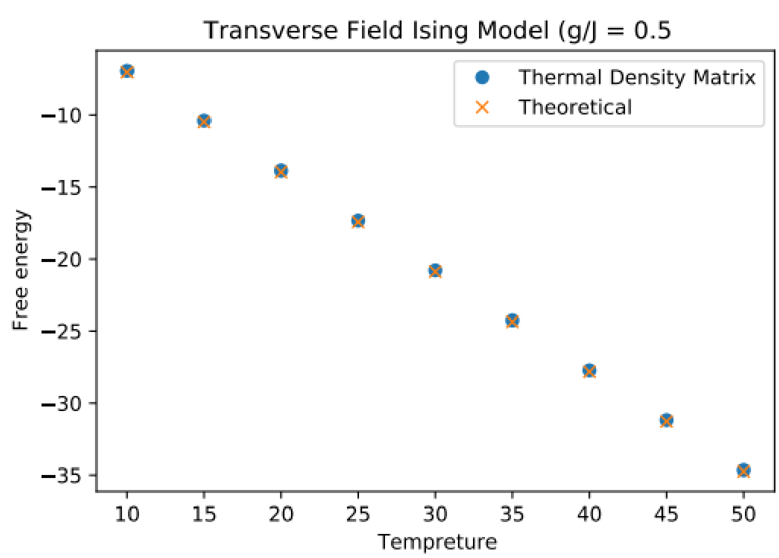
$$Z_{FM} = \frac{1}{2} \left[Z_{a1} + Z_{a2} + Z_{p1} - \mathrm{sgn}\left(h - \frac{J}{2} \right) Z_{p2} \right].$$

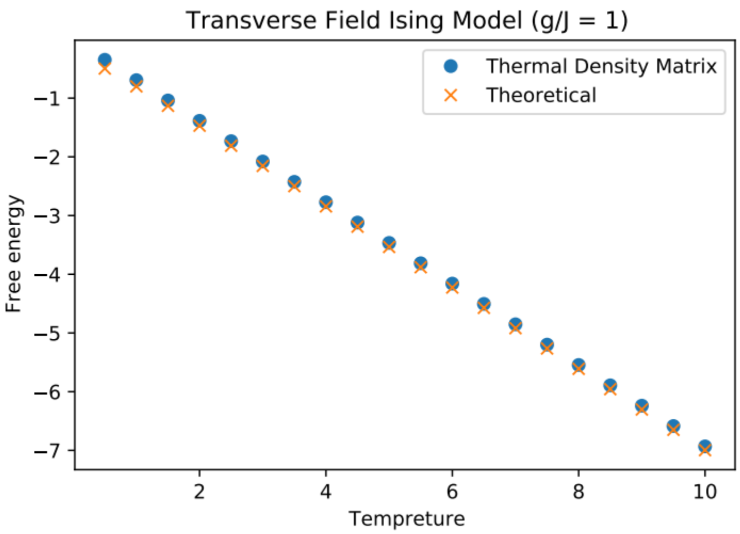
Finally, the free energy for the FM case is calculated using the total partition function of the system:

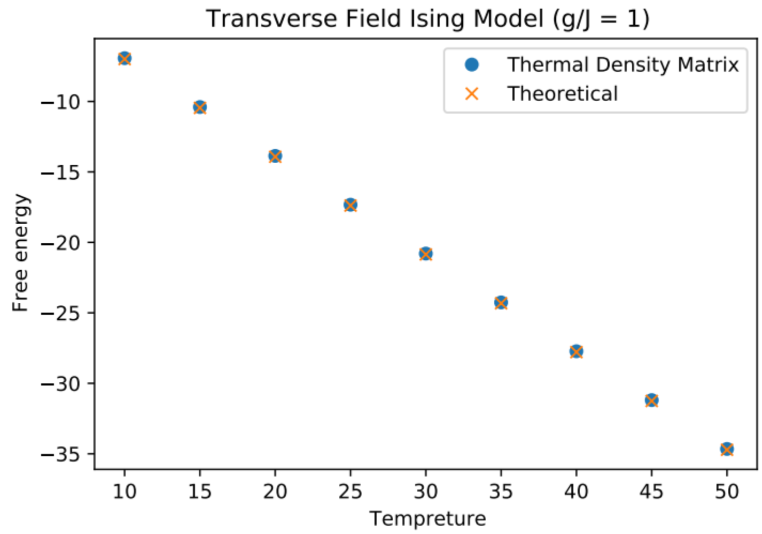
$$F_{FM} = -T \ln Z_{FM},$$

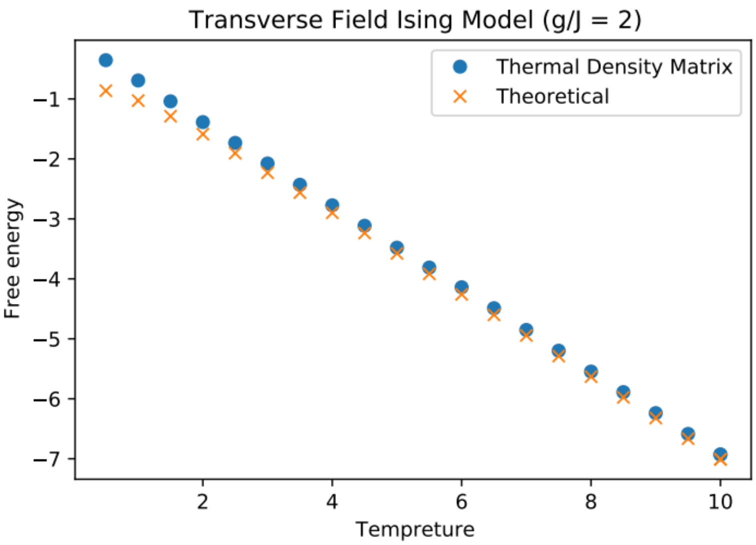
(with T is temperature). The following figures demonstrate the plots of free energy of TFIM as a function of temperature for the density matrix model compared to the theoretical results reported in this paper.

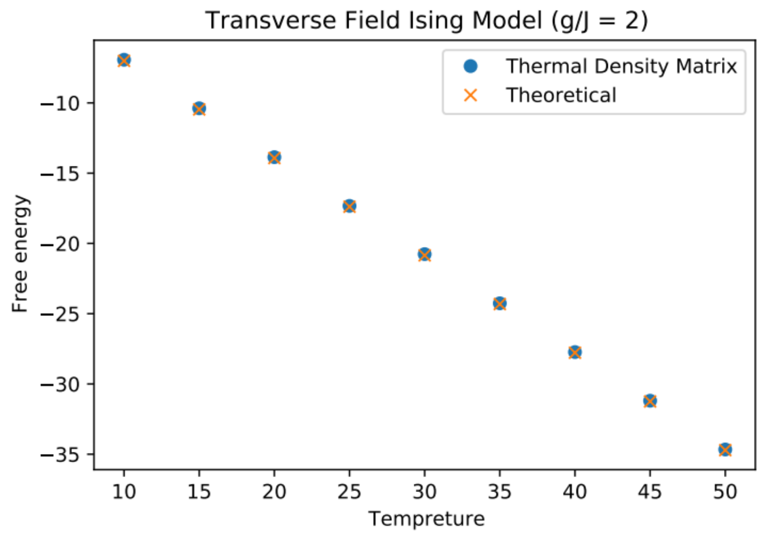





Transverse Field Ising Model (g/J = 1)
Thermal Density Matrix
Theoretical
Free energy
−1
−2
−3
−4
−5
−6
−7
2
4
6
8
10
Tempreture


Transverse Field Ising Model (g/J = 1)
Thermal Density Matrix
Theoretical
Free energy
−10
−15
−20
−25
−30
−35
10
15
20
25
30
35
40
45
50
Tempreture


Transverse Field Ising Model (g/J = 2)
Thermal Density Matrix
Theoretical
Free energy
−1
−2
−3
−4
−5
−6
−7
2
4
6
8
10
Tempreture


Transverse Field Ising Model (g/J = 2)
Thermal Density Matrix
Theoretical
Free energy
−10
−15
−20
−25
−30
−35
10
15
20
25
30
35
40
45
50
Tempreture