

Review of primary theoretical free energy calculations for ferromagnetic Transverse Field Ising Model

In this paper, a brief summary of theoretical results and computations for calculating the free energy of the ferromagnetic (FM) transverse field Ising model (TFIM) is presented¹. The Hamiltonian for 1D TFIM with periodic boundary conditions (PBC) is defined as

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

Applying the following Jordan-Wigner transformations

$$c_n = \exp\left(\pi i \sum_{j=1}^{n-1} S_j^+ S_j^-\right) S_n^-, \quad c_n^\dagger = \exp\left(-\pi i \sum_{j=1}^{n-1} S_j^+ S_j^-\right) S_n^+ \quad (2)$$

(with $S_j^\pm = S_j^x \pm iS_j^y$), one could immediately convert the Hamiltonian of Eq. (1) to the following *fermion form*:

$$H = \frac{gN}{2} - g \sum_{i=1}^N c_i^\dagger c_i - \frac{J}{4} \sum_{i=1}^{N-1} (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) + \frac{J}{4} \exp(i\pi N_f)(c_N^\dagger - c_N)(c_1^\dagger + c_1), \quad (3)$$

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

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

with the following boundary conditions

$$\begin{aligned} c_{N+1} &= c_1 \text{ for } N_f \equiv 1(\text{mod}2) \\ c_{N+1} &= -c_1 \text{ for } N_f \equiv 0(\text{mod}2). \end{aligned} \quad (5)$$

Notice that the PBC is imposed on the case with an *odd* fermion number, and anti-PBC (APBC) is imposed on the case with an *even* fermion number, respectively. The Hamiltonian of Eq. (4) could be transformed into the momentum space by introducing

¹ The arguments of this paper are based on Y. He and H. Guo *J. Stat. Mech.* (2017) 093101.

$$c_n = \frac{1}{\sqrt{N}} \sum_k c_k e^{ikn}, \quad c_n^\dagger = \frac{1}{\sqrt{N}} \sum_k c_k^\dagger e^{-ikn} \quad (6)$$

with k labeling the momentum that takes the following set of values

$$\begin{aligned} k \in \Lambda_a, \Lambda_a &= \left\{ \pm \frac{\pi}{N}, \pm \frac{3\pi}{N}, \dots, \pm \frac{(N-1)\pi}{N} \right\} \text{ for APBC} \\ k \in \Lambda_p, \Lambda_p &= \left\{ 0, \pm \frac{2\pi}{N}, \pm \frac{4\pi}{N}, \dots, \pm \frac{(N-2)\pi}{N}, \pi \right\} \text{ for PBC.} \end{aligned} \quad (7)$$

Notice that N is the number of sites in Eq. (7), which could be **even** for the FM case. It is also essential to note that *both* PBC and APBC contributions of Eq. (7) must be included for the fermion Hamiltonian calculations of FM models. Employing the transformations of Eq. (6), the Hamiltonian of Eq. (4) could be converted into the following PBC and APBC pieces:

$$H_a = \sum_{k \in \Lambda'_a} \left[\xi_k c_k^\dagger c_k + \xi_k c_{-k}^\dagger c_{-k} + i \frac{J}{2} \sin k c_{-k} c_k - i \frac{J}{2} \sin k c_k^\dagger c_{-k}^\dagger \right] + \frac{gN}{2}, \quad (8)$$

$$H_p = \sum_{k \in \Lambda'_p} \left[\xi_k c_k^\dagger c_k + \xi_k c_{-k}^\dagger c_{-k} + i \frac{J}{2} \sin k c_{-k} c_k - i \frac{J}{2} \sin k c_k^\dagger c_{-k}^\dagger \right] + \frac{gN}{2} + \xi_0 c_0^\dagger c_0 + \xi_\pi c_\pi^\dagger c_\pi \quad (9)$$

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

$$\begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k^* & u_k \end{pmatrix} \begin{pmatrix} \eta_k \\ \eta_{-k}^\dagger \end{pmatrix}. \quad (10)$$

Setting $u_k \equiv \sqrt{E_k + \xi_k / 2E_k}$ and $v_k \equiv i \operatorname{sgn} k \sqrt{E_k - \xi_k / 2E_k}$, we finally obtain the energy dispersion relationship:

$$E_k = \sqrt{(J/2)^2 + g^2 + Jg \cos k}. \quad (11)$$

Applying the transformations of Eq. (10) and using the dispersion relation of Eq. (11), the diagonalized form of the fermion Hamiltonian (of Eq. (8) and (9)) would become

$$H_a = E_0 + \sum_{k \in \Lambda'_a} E_k (\eta_k^\dagger \eta_k + \eta_{-k}^\dagger \eta_{-k}), \quad (12)$$

$$H_p = E_1 + \sum_{k \in \Lambda'_p} E_k (\eta_k^\dagger \eta_k + \eta_{-k}^\dagger \eta_{-k}) + \xi_0 c_0^\dagger c_0 + \xi_\pi c_\pi^\dagger c_\pi, \quad (13)$$

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

$$E(\{n_k\}) = \sum_{k \in \Lambda_a} \left[-\frac{E_k}{2}(1 - n_k) + \frac{E_k}{2}n_k \right] ; \quad \sum_k n_k \equiv v_a \pmod{2}, \quad (14)$$

$$E(\{n_k\}) = \sum_{k \in \Lambda_p} \left[-\frac{E_k}{2}(1 - n_k) + \frac{E_k}{2}n_k \right] ; \quad \sum_k n_k \equiv v_p \pmod{2}, \quad (15)$$

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

$$v_a = 0, v_p = \begin{cases} 0, & g < J/2 \\ 1, & g > J/2. \end{cases} \quad (16)$$

Employing Eq. (15), it would be a straightforward exercise to write the expressions for partition functions of PBC and APBC contributions of the TFIM fermion Hamiltonian sectors of Eq. (12) and (13):

$$Z_{a1} = \prod_{k \in \Lambda_a} \left(e^{\frac{E_k}{2T}} + e^{-\frac{E_k}{2T}} \right) ; \quad Z_{p1} = \prod_{k \in \Lambda_p} \left(e^{\frac{E_k}{2T}} + e^{-\frac{E_k}{2T}} \right), \quad (17)$$

$$Z_{a2} = \prod_{k \in \Lambda_a} \left(e^{\frac{E_k}{2T}} - e^{-\frac{E_k}{2T}} \right) ; \quad Z_{p2} = \prod_{k \in \Lambda_p} \left(e^{\frac{E_k}{2T}} - e^{-\frac{E_k}{2T}} \right). \quad (18)$$

Note that in Eq. (17) and (18), the subscript p refers to PBC, and the subscript a refers to APBC contributions of each piece of the Hamiltonian, respectively. Using Eq. (17) and (18), the total partition function of FM TFIM could be then written as

$$Z_{FM} = \frac{1}{2} \left[Z_{a1} + Z_{a2} + Z_{p1} - \text{sgn} \left(g - \frac{J}{2} \right) Z_{p2} \right]. \quad (19)$$

Finally, the free energy of the FM TFIM could be simply written using the total partition function of Eq. (19) as follows:

$$F_{FM} = -T \ln Z_{FM}, \quad (20)$$

with T denoting the temperature of the system.