Transverse Field Ising Model

M.Sc. (Physics) 3rd Semester Project Report

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1 Abstract

We present here techniques to exactly solve a 1D transverse quantum Ising chain where each site represents a 2D complex Hilbert space. One way to analytically solve this model is by mapping it to spinless fermions. Starting with Jordan Wigner transformation, we map the Ising model to spinless fermions, followed by a Bogoliubov transformation to subsequently map the system to free fermions. We make use of numerics to verify the analytical solution. More specifically, we numerically diagonalize the Ising Hamiltonian and analyze the energy spectrum with various plots. In future, we plan to study Quantum Phase transitions (QPT) and explore the solutions to the 1D transverse Ising model with each site being an N dimensional hilbert space.

2 Introduction

Named after the Physicist Ernst Ising, the Ising model a mathematical model of ferromagnetism used to understand phase transitions of a thermodynamic system. It is a mathematical model and can be mapped to a physical system by making appropriate transformations. The reason to study such a model is that it helps to grasp all sorts of behaviour relating to phase transitions (like symmetry breaking in low temperature region) and is one of the few exactly solvable models for which we can calculate thermodynamic quantities. The Hamiltonian of such a system is given by,

$$H(\sigma) = -\sum_{\langle i\ j \rangle} J_{ij}\sigma_i\sigma_j - \sum_j h_j\sigma_j, \tag{1}$$

It has an interaction term and a external field term. Our model of interest, the transverse Ising model, is a variation of the classical Ising model with the direction of external field being perpendicular to the direction of spins at each site. The Hamiltonian of the transverse Ising model therefore, is given by,

$$H(\sigma) = -\sum_{\langle i\ j \rangle} J_{ij}\sigma_i^x\sigma_j^x - \sum_j h_j\sigma_j^z, \tag{2}$$

where each site represents a 2D complex Hilbert space. As we will see later in the report, this model is a prototypical example of Quantum Phase transition (A phase transition driven by quantum fluctuations instead of thermal fluctuations). To investigate quantum mechanical properties of this model, canonical quantization of appropriate classical quantities has to be performed. The observables are replaced with operators and classical states are replaced with quantum states. We work in $T = 0$K region so theoretically, there is no contribution in phase transitions due to thermal fluctuations.

The aim of this project is to present techniques to exactly solve this Hamiltonian and obtain the energy spectrum. This is done by mapping the system to spinless fermions. The procedure to find solution to this model can be briefly broken down into 3 steps: Doing a Jordan Wigner(JW) transformation on the Hamiltonian, followed by a Fourier transform and a Bogoliubov transformation. The hamiltonian obtained after JW transformation presents terms which show coupling of fermions. The decoupling can be done in two steps. We apply a discrete Fourier transform. Then we apply a Bogoliubov transformation to obtain a diagonalized Hamiltonian and subsequently get the energy spectrum.

Phase transitions occuring at zero temperature are known as quantum phase transition (QPT). Unlike classical phase transitions, they are realised by varying a non thermal parameter (such as magnetic field) keeping the temperature at 0K. A system in equilibrium at T=0K is always in ground state and the phase transition is purely due to quantum fluctuations which is our area of interest.

We make use of numerics to investigate the ground state of the system. All the computations are done using Python. We show numerically that energy gap between ground and first excited states for $g < 1$ tends to zero in the thermodynamic limit (N$\to \infty$), and they become degenerate.

3 Jordan-Wigner transformation

The Transverse Field Ising Hamiltonian (TFIH) is given by,

$$H = -J\sum_i \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x - h\sum_i \hat{\sigma}_i^z, \tag{3}$$

where $h = Jg$

The Ising chain has N lattice sites with each site representing a 2-dimensional Hilbert space (spin 1/2 particle). Such a spin 1/2 system can be mapped to a system of spinless fermion with spin-up state of Ising associated with an unoccupied site and spin-down state of Ising associated with an occupied site.

The generators used in both of these systems are,

$$\tag{4}$$

Spin 1/2 Ising system

$$\hat{\sigma}_i^+ = \frac{1}{2}(\hat{\sigma}_i^x + i\hat{\sigma}_i^y), \quad \hat{\sigma}_i^- = \frac{1}{2}(\hat{\sigma}_i^x - i\hat{\sigma}_i^y), \quad \hat{\sigma}_i^z \tag{5}$$

Fermion system

$$c_i, \quad c_i^\dagger, \quad n = c_i^\dagger c_i \tag{6}$$

where c_i annhilates a fermion at site i and $c_i^\dagger$ creates a fermion. We can obtain a one-to-one mapping of operators between the two systems by mapping each of the generators of Hilbert space of Ising chain to the generators of Hilbert space of spinless fermions such that the commutation relations are still preserved. For a single site i, such a trasnformation is given by,

$$\hat{\sigma}_i^z = 1 - 2c_i^\dagger c_i \tag{7}$$

The operation of flipping the spin (up to down or down to up) is then equivalent to operation of creating/annhilating a fermion.

$$\hat{\sigma}_i^+ = c_i \quad \hat{\sigma}_i^- = c_i^\dagger \tag{8}$$

We see that under these transformations, the commutation relations of both the systems are preserved.

$$\{c_i^\dagger, c_i\} = \{\hat{\sigma}_i^+, \hat{\sigma}_i^-\} = 1 \tag{9}$$

and for

$$\begin{aligned} &[\hat{\sigma}_i^+, \hat{\sigma}_i^-] = 2i\hat{\sigma}_i^z \quad , \\ &[c_i, c_i^\dagger] = 2(1 - 2c_i^\dagger c_i) \end{aligned} \tag{10}$$

upto some factors.

This transformation fails to preserve the commutation relations when the full ising chain is taken into consideration (i.e, operators acting on different sites)

$$\{c_i^\dagger, c_j\} = 0 \neq \{\hat{\sigma}_i^+, \hat{\sigma}_j^-\} \tag{11}$$

and

$$[\hat{\sigma}_i^+, \hat{\sigma}_j^-] = 0 \neq [c_i, c_j^\dagger] \tag{12}$$

Following the intuition of Jordan and Wigner, we redefine our transformations as,

$$\begin{aligned} \hat{\sigma}_i^z &= (1 - 2c_i^\dagger c_i) \\ \hat{\sigma}_i^+ &= \prod_{j<i}(1 - 2c_j^\dagger c_j)c_i \\ &= \prod_{j<i}\hat{\sigma}_j^z c_i \end{aligned} \tag{13}$$

$$
\begin{aligned}
\hat{\sigma}_i^- &= \prod_{j<i}(1-2c_j^\dagger c_j)c_i^\dagger \\
&= \prod_{j<i}\hat{\sigma}_j^z c_i^\dagger
\end{aligned} \tag{14}
$$

That is, creating/annhilating of fermions at a site i is dependent on operators of all the sites less than i ($\prod_{j<i}(1-2c_j^\dagger c_j)$). Hence, JW transformations are highly non-local.

Analogously, using $\hat{\sigma}_j^z = (\hat{\sigma}_j^z)^{-1}$, we can write,

$$
c_i = (\prod_{j<i}\hat{\sigma}_j^z)\hat{\sigma}_i^+ \tag{15}
$$

$$
c_i^\dagger = (\prod_{j<i}\hat{\sigma}_j^z)\hat{\sigma}_i^- \tag{16}
$$

It can be verified that the equations (8),(9),(10) and (11) are satisfied for this new transformation. Also,

$$
\hat{\sigma}_i^x = \prod_{j<i}(1-2c_j^\dagger c_j)(c_i + c_i^\dagger) \tag{17}
$$

3.1 Transformation of hamiltonian

We now use the newly found transformed equations to express the TFIH in terms of fermionic operators a system of finite size N,

$$
H = -J(\sum_i \hat{\sigma}_i^x\hat{\sigma}_{i+1}^x + g\sum_i \hat{\sigma}_i^z) \tag{18}
$$

We use $h = Jg$ to simplify calculations. A spin system is always periodic. But the transformed fermionic system might be periodic or anti-periodic (or both). Hence, we separately treat the boundary ineraction term.

$$
H = -J(g\sum_i \hat{\sigma}_i^z + \sum_{i=1}^{N-1}\hat{\sigma}_i^x\hat{\sigma}_{i+1}^x + \hat{\sigma}_N^x\hat{\sigma}_1^x) \tag{19}
$$

Apply the JW transformation to this hamiltonian (39),

$$
\begin{aligned}
&= -JgN + 2Jgc_i^\dagger c_i - J\sum_{i=1}^{N-1}[(c_{i+1}c_i + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger)] \\
&+ \prod_{j=1}^{N}\hat{\sigma}_j^z(c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)
\end{aligned} \tag{20}
$$

This Hamiltonian describes spinless fermions hopping on a lattice.
<u>**Note**</u>: We can ignore the boundary term in the limit N$\rightarrow \infty$

We define,

$$\mu_N^x = \prod_{i=1}^{N} \hat{\sigma}_i^z \tag{21}$$

as the parity operator. We observe that the parity operator commutes with the hamiltonian,

$$[\mu_x^N, H] = 0 \tag{22}$$

The hamiltonian hence is split into two sectors with μ_N^x. The plus sign characterizes configurations with an even number of fermions and the minus sign with an odd number of fermions:

$$H = (\frac{1+\mu_N^x}{2})H^+ + (\frac{1-\mu_N^x}{2})H^- \tag{23}$$

Here, $H^{\pm}$ have the form of (20) with $\mu_N^x = \pm 1$. To satisfy the boundary terms, we have to apply appropriate boundary conditions to each sector.

For $\mu_N^x = +1$ (even no. of fermions) we have to impose **Anti-Periodic** boundary condition.

$$c_{i+N}^{(+)} = -c_i^{(+)} \tag{24}$$

For $\mu_N^x = -1$ (odd no. of fermions) we have to impose **Periodic** boundary condition.

$$c_{i+N}^{(-)} = c_i^{(-)} \tag{25}$$

With the definitions above, the hamiltonian can be written as,

$$H^{\pm} = -JgN - J\sum_{i=1}^{N}[(c_{i+1}^{(\pm)}c_i^{(\pm)} + c_{i+1}^{(\pm)\dagger}c_i^{(\pm)} + c_i^{(\pm)\dagger}c_{i+1}^{(\pm)} + c_i^{(\pm)\dagger}c_{i+1}^{(\pm)\dagger}) - 2Jgc_i^{(\pm)\dagger}c_i^{(\pm)}] \tag{26}$$

Therefore, the spin 1/2 system has been mapped to spinless fermions.

4 Fourier Transformation

The Hamiltonian above presents terms such as $c_i^\dagger c_{i+1}^\dagger$ which implies the fermions are coupled. To map this hamiltonian to hamiltonian of free fermions, we need to decouple the fermions (i.e eliminate $c_i^\dagger c_{i+1}^\dagger$ like terms).This we apply a discrete fourier transform.

We sum over integer modes on odd fermions sector and half-integer modes on even fermions sector,

$\underline{\mu_N^x = 1}$ (Odd fermion number)

$$q \in N + \frac{1}{2} = \frac{1}{2}, \frac{3}{2} ... N - \frac{1}{2} \tag{27}$$

$\underline{\mu_N^x = -1}$ (Even fermion number)

$$q \in N = 0, 1..., N - 1 \tag{28}$$

We define,

$$c_i^{\pm} = \frac{e^{\frac{\iota\pi}{4}}}{N} \sum_q e^{\frac{\iota 2\pi}{N} qi} c_q \tag{29}$$

$$c_q = e^{\frac{-\iota\pi}{4}} \sum_i^N e^{\frac{-\iota 2\pi}{N} qi} c_i^{\pm} \tag{30}$$

Using the above definitions, the hamiltonian we get, is given by,

$$H^{\pm} = \frac{1}{N} \sum_q 2[h - Jcos(\frac{2\pi}{N} q)] c_q^{\dagger} c_q + \frac{J}{N} \sum_q sin(\frac{2\pi}{N} q) \{c_q c_{-q} + c_{-q}^{\dagger} c_q^{\dagger}\} - JgN \tag{31}$$

This Hamiltonian can be written as a sum of 2x2 matrices,

$$H^{\pm} = \sum_k [c_k^{\dagger} \quad c_{-k}] \begin{bmatrix} h - Jcos(\frac{2\pi}{N} q) & -Jsin(\frac{2\pi}{N} q) \\ -Jsin(\frac{2\pi}{N} q) & Jcos(\frac{2\pi}{N} q) - h \end{bmatrix} \begin{bmatrix} c_k \\ c_{-k}^{\dagger} \end{bmatrix} \tag{32}$$

We can diagonalise this 2x2 matrix using Bogoliubov transformation.

5 Bogoliubov Transformation

We map this hamiltonian to a new set of fermionic operators χ_k via Bogoliubov transformation.

$$\begin{bmatrix} c_k \\ c_{-k}^{\dagger} \end{bmatrix} = \begin{bmatrix} cos\theta_k & sin\theta_k \\ -sin\theta_k & cos\theta_k \end{bmatrix} \begin{bmatrix} \chi_k \\ \chi_{-k}^{\dagger} \end{bmatrix} \tag{33}$$

which is just O(2) rotation in fourier space. Using this in (31) and demanding the off diagonal terms to be zero (matrix to be diagonal), we get

$$tan(2\theta_k) = \frac{sin(\frac{2\pi}{N}q)}{h/J - cos(\frac{2\pi}{N}q)} \tag{34}$$

Therefore, the final form of hamiltonian is,

$$H^{\pm} = \sum_q \epsilon(\frac{2\pi}{N}q)\{\chi_q^\dagger \chi_q - \frac{1}{2})\} \tag{35}$$

where

$$\epsilon(\alpha) = 2\sqrt{(J^2 + h^2 - 2Jh\cos(\alpha))} \tag{36}$$

$\epsilon(\alpha)$ here is the energy difference between an excited state and the ground state (for single particle excitations). Since this energy $\epsilon(\alpha)$ is never negative, the ground state would have no $_q$ fermions and hence $|0\rangle = 0$. That is, ground state of the Ising model in an arbitrary transverse field is equivalent to the vacuum state of free fermion.

The difference between ground state energy and first excited state energy (minimum excitation energy) is given by,

$$\epsilon(0) = 2|J - h| \tag{37}$$

or,

$$\epsilon(0) = 2J|1 - g| \qquad \forall J > 0 \tag{38}$$

At g=1, this gap vanishes. This point is the Quantum phase transition point. It represents a phase boundary between ordered and disordered phase.

6 Numerics

With the help of numerics, we try to verify the analytical solution for the energy spectrum. Since the Bogoliubov quasi particle hamiltonian is just transformation of TFIH, they have the same energy eigenvalues. We can calculate TFIH matrix (which is just tensor product of pauli matrices) and numerically calculate the eigenvalues ,further, verifying the analytical solution. The TFIH is diagonalized numerically (using an in built function called scipy.linalg.eigvals) and the ground, first and second excited state energies are calculated corresponding to different g values. This procedure is repeated for different system sizes N (number of lattice sites) as shown below.
Note:- The order of TFIH is 2^N and hence the calculations require heavy computation as N increases.

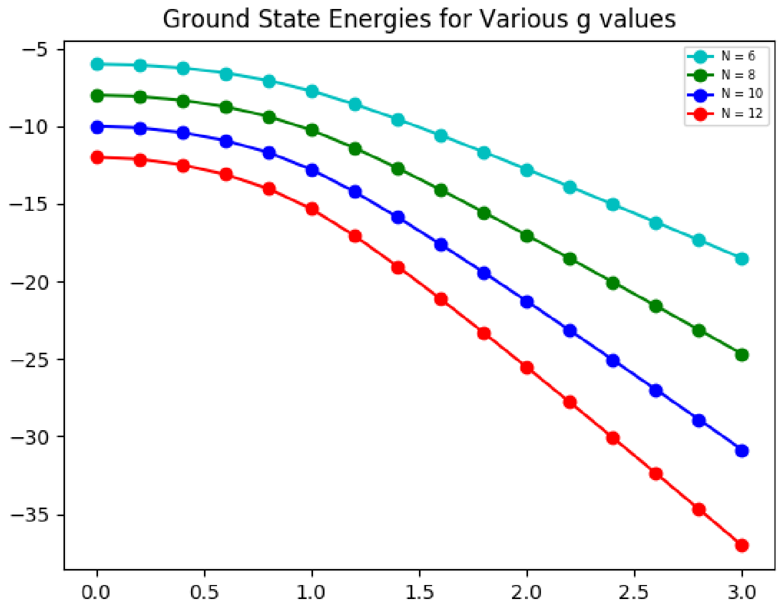

Figure 1: Ground state energies for different system sizes N

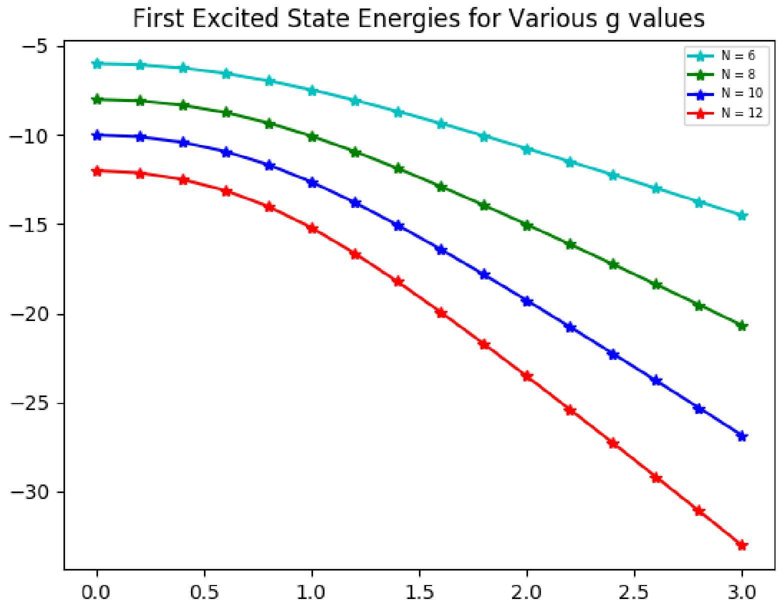

Figure 2: First excited state energies for different system sizes N

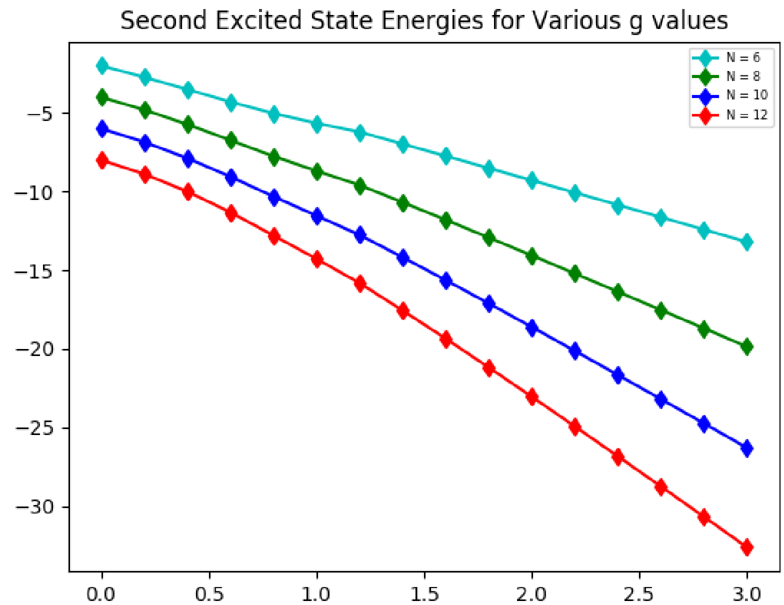

Figure 3: Second excited state energies for different system sizes N

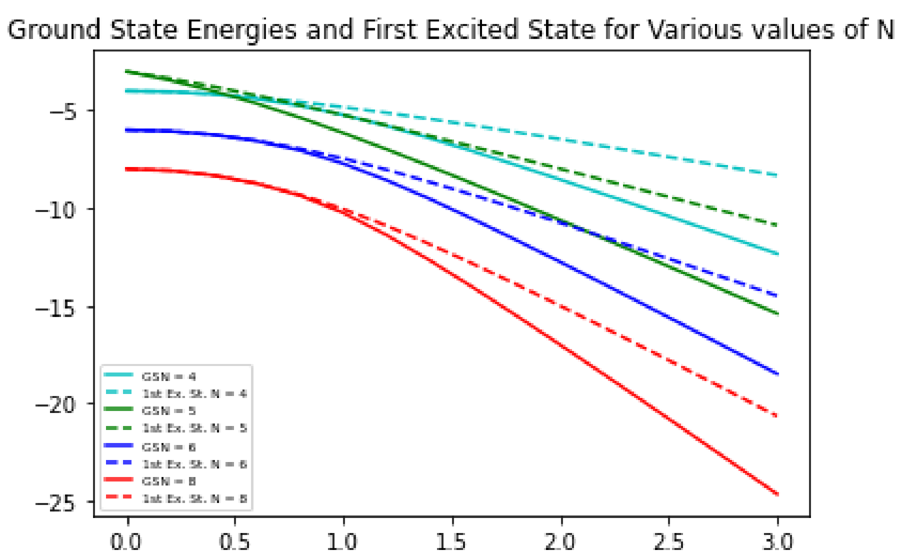

Figure 4: Ground and first excited state energies for different N. Note that for $|g| < 1$, the energy gap between the two curves reduces as N increases.

7 Discussions and conclusions

To solve the Transverse Field Ising Model we mapped the spin 1/2 system to a system of spinless fermions. The resulting hamiltonian contained coupled so the uncoupling of fermionic operators was done in two steps: applying a fourier transform (to exploit the translation symmetry) followed by a bogoliubov transformation to diagonalize the hamiltonian. The resulting hamiltonian represents a system of bogoliubov quasi particles. This solution is of great significance as it shows phase transition can also occur purely due to quantum fluctations.

Numerically, we see that the energy gap between the first and ground excited states tends to zero for $|g| < 1$ as N increases. This verifies that there is a phase transition occuring at g=1.

Appendix A Transverse Ising hamiltonian in terms of fermionic operators

$$H = -J(\sum_i \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + g \sum_i \hat{\sigma}_j^z)$$

$$= -J(g \sum_{i=1}^{N} \hat{\sigma}_i^z + \sum_{i=1}^{N-1} \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + \hat{\sigma}_N^x \hat{\sigma}_1^x)$$

$$= -J[\sum_{i=1}^{N} [g(1-2c_i^\dagger c_i)] + \sum_{i=1}^{N-1} [\prod_{j<i}(1-2c_j^\dagger c_j)(c_i + c_i^\dagger) \prod_{j<i+1}(1-2c_j^\dagger c_j)(c_{i+1} + c_{i+1}^\dagger)] + \hat{\sigma}_N^x \hat{\sigma}_1^x]$$

Now,

$$\boxed{\hat{\sigma}_N^x \hat{\sigma}_1^x = (\prod_{j=1}^{N-1} \hat{\sigma}_j^z (c_i + c_i^\dagger))(c_i + c_i^\dagger) = \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)}$$

Therefore,

$$= -J[\sum_{i}^{N} [g(1-2c_i^\dagger c_i)] + \sum_{i=1}^{N-1} [\prod_{j<i} \hat{\sigma}_j^z (c_i + c_i^\dagger) \prod_{j<i} \hat{\sigma}_j^z (c_{i+1} + c_{i+1}^\dagger - 2c_i^\dagger c_i c_{i+1} - 2c_i^\dagger c_i c_{i+1}^\dagger)]$$

$$+ \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)]$$

$$= -J[\sum_{i=1}^{N} [g(1-2c_i^\dagger c_i)] + \sum_{i=1}^{N-1} [\prod_{j<i} (\hat{\sigma}_j^z)^2 (c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger - 2c_i^\dagger c_i c_{i+1} - 2c_i^\dagger c_i c_{i+1}^\dagger)] +$$

$$+ \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)]$$

$$= -J[\sum_{i=1}^{N} [g(1-2c_i^\dagger c_i)] + \sum_{i=1}^{N-1} [\prod_{j<i} (\hat{\sigma}_j^z)^2 (c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger - 2c_i^\dagger c_i c_{i+1} - 2c_i^\dagger c_i c_{i+1}^\dagger)]$$

$$+ \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)]$$

$$= -J[\sum_{i=1}^{N} [g(1-2c_i^\dagger c_i)] + \sum_{i=1}^{N-1} [(c_i c_{i+1} + c_i c_{i+1}^\dagger - 2c_i c_i^\dagger c_i c_{i+1} - 2c_i c_i^\dagger c_i c_{i+1}^\dagger + c_i^\dagger c_{i+1}$$

$$+ c_i^\dagger c_{i+1}^\dagger - 2c_i^\dagger c_i^\dagger c_i c_{i+1} - 2c_i^\dagger c_i^\dagger c_i c_{i+1}^\dagger)] + \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)]$$

$$= -J[\sum_{i=1}^{N} [g(1-2c_i^\dagger c_i)] + \sum_{i=1}^{N-1} [(c_i c_{i+1} + c_i c_{i+1}^\dagger - 2(1-c_i^\dagger c_i) c_i c_{i+1} - 2(1-c_i^\dagger c_i) c_i c_{i+1}^\dagger +$$

$$c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger)] + \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)] \tag{39}$$

$$
\begin{aligned}
&= -J[(gN - 2g\sum_{i=1}^{N} c_i^\dagger c_i) + \sum_{i=1}^{N-1}[(c_i c_{i+1} + c_i c_{i+1}^\dagger - 2c_i c_{i+1} - 2c_i c_{i+1}^\dagger + c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger)] \\
&+ \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)] \\
&= -JgN + 2Jg\sum_{i=1}^{N} c_i^\dagger c_i - J\sum_{i=1}^{N-1}[(-c_i c_{i+1} - c_i c_{i+1}^\dagger + c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger)] \\
&+ \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)] \\
&= -JgN + 2Jg\sum_{i=1}^{N} c_i^\dagger c_i - J\sum_{i=1}^{N-1}[(c_{i+1} c_i + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger)] \\
&+ \prod_{j=1}^{N} \hat{\sigma}_j^z (c_N c_1 + c_N^\dagger c_1 + c_N c_1^\dagger + c_N^\dagger c_1^\dagger)]
\end{aligned}
\tag{40}
$$

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