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## Solving Transverse Field Ising Model

### References

- “Topological phases and quantum computation” by Alexei Kitaev and Chris Laumann
- Section 6.1 of “Quantum Information Meets Quantum Matter: From Quantum Entanglement to Topological Phases of Many-Body Systems” by Bei Zeng, Xie Chen, Duan-Lu Zhou, and Xiao-Gang Wen.
- An introduction to lattice gauge theory and spin systems by John B. Kogut

## Introduction to the Bogoliubov Transformation

The Bogoliubov transformation, named after Nikolai Bogoliubov, is a cornerstone in quantum physics for analyzing systems of interacting particles. It is crucial in studying quantum many-body systems, illuminating phenomena such as superfluidity and superconductivity. This transformation facilitates a change of basis in the space of particle states, merging particle creation and annihilation operators into a new, simplified representation.

### The Bogoliubov Transformation for Fermions

In fermionic systems, creation ( $c_k^\dagger$ ) and annihilation ( $c_k$ ) operators adhere to canonical anticommutation relations essential for maintaining fermionic statistics:

$$\{c_k, c_{k'}^\dagger\} = \delta_{kk'}, \quad \{c_k, c_{k'}\} = \{c_k^\dagger, c_{k'}^\dagger\} = 0.$$

The Bogoliubov transformation introduces quasiparticle operators ( $a_k$  and  $a_k^\dagger$ ) defined as:

$$a_k = u_k c_k - v_k c_{-k}^\dagger, \quad a_k^\dagger = u_k c_k^\dagger - v_k c_{-k},$$

where  $u_k$  and  $v_k$  are real coefficients<sup>1</sup> that must satisfy the normalization condition  $u_k^2 + v_k^2 = 1$  to preserve fermionic statistics. There is an extra condition between  $u_k$ ,  $v_k$ , and  $u_{-k}$ ,  $v_{-k}$ :

$$u_k v_{-k} = -u_{-k} v_k. \tag{1}$$

For example, one possible choice is

$$u_{-k} = u_k, \quad v_{-k} = -v_k. \tag{2}$$

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<sup>1</sup>In general,  $u_k$  and  $v_k$  can be chosen to be complex numbers. We assume they are real just for our convenience.

## Detailed Computation of Anticommutation Relations

### Anticommutation of $a_k$ and $a_k^\dagger$

$$\begin{aligned}
 \{a_k, a_{k'}^\dagger\} &= (u_k c_k - v_k c_{-k}^\dagger)(u_{k'} c_{k'}^\dagger - v_{k'} c_{-k'}) \\
 &\quad + (u_{k'} c_{k'}^\dagger - v_{k'} c_{-k'}) (u_k c_k - v_k c_{-k}^\dagger) \\
 &= u_k u_{k'} \{c_k, c_{k'}^\dagger\} + v_k v_{k'} \{c_{-k}^\dagger, c_{-k'}\} \\
 &= u_k^2 \delta_{kk'} + v_k^2 \delta_{kk'} \\
 &= (u_k^2 + v_k^2) \delta_{kk'} = \delta_{kk'},
 \end{aligned} \tag{3}$$

confirming that the transformation preserves the anticommutation relations for fermions.

### Anticommutation of $a_k$ and $a_{k'}$ , and $a_k^\dagger$ and $a_{k'}^\dagger$

Similar computations for  $\{a_k, a_{k'}\}$  and  $\{a_k^\dagger, a_{k'}^\dagger\}$  show that all terms cancel out due to the antisymmetric properties of fermionic operators, leading to:

$$\{a_k, a_{k'}\} = \{a_k^\dagger, a_{k'}^\dagger\} = 0,$$

thus maintaining the fermionic statistics post-transformation. You might worry about the relations between  $k$  and  $-k$ . For example,

$$\begin{aligned}
 \{a_k, a_{-k}\} &= \{u_k c_k - v_k c_{-k}^\dagger, u_{-k} c_{-k} - v_{-k} c_k^\dagger\} \\
 &= -u_k v_{-k} - v_k u_{-k} = 0,
 \end{aligned} \tag{4}$$

where the last equality comes from the extra condition Eq. (1) we imposed before.

## Application in Superconductivity

### The BCS Hamiltonian

The BCS Hamiltonian for a superconductor is expressed as:

$$H = \sum_{k>0} \epsilon_k (c_k^\dagger c_k + c_{-k}^\dagger c_{-k}) - \sum_{k>0} (\Delta_k c_k^\dagger c_{-k}^\dagger + \Delta_k^* c_{-k} c_k), \tag{5}$$

where  $\epsilon_k$  represents the kinetic energy of fermions relative to the Fermi level, and  $\Delta_k$  is the superconducting gap parameter, which will be specified later. Note that  $\Delta_k = -\Delta_{-k}$  automatically and we can assume  $\Delta_k$  is real without loss of generality (Think about why?).

Given the Bogoliubov transformations:

$$\begin{aligned}
 a_k &= u_k c_k - v_k c_{-k}^\dagger, \\
 a_k^\dagger &= u_k c_k^\dagger - v_k c_{-k}, \\
 a_{-k} &= u_k c_{-k} + v_k c_k^\dagger,
 \end{aligned}$$

$$a_{-k}^\dagger = u_k c_{-k}^\dagger + v_k c_k,$$

where we have chosen  $u_{-k} = u_k$  and  $v_{-k} = -v_k$ , the inverse transformations are:

$$\begin{aligned} c_k &= u_k a_k + v_k a_{-k}^\dagger, \\ c_k^\dagger &= u_k a_k^\dagger + v_k a_{-k}. \end{aligned}$$

These expressions allow us to rewrite the original fermion operators in terms of the new quasiparticle operators.

## Kinetic Energy Term

For the kinetic energy term,  $\epsilon_k(c_k^\dagger c_k + c_{-k}^\dagger c_{-k})$ , using the inverse transformation yields:

$$\begin{aligned} & \epsilon_k \left[ (u_k a_k^\dagger + v_k a_{-k})(u_k a_k + v_k a_{-k}^\dagger) + (u_k a_{-k}^\dagger - v_k a_k)(u_k a_{-k} - v_k a_k^\dagger) \right] \\ &= \epsilon_k \left[ (u_k^2 a_k^\dagger a_k + v_k^2 a_k a_k^\dagger) + 2u_k v_k a_k^\dagger a_{-k}^\dagger + 2u_k v_k a_{-k} a_k + (u_k^2 a_{-k}^\dagger a_{-k} + v_k^2 a_{-k} a_{-k}^\dagger) \right] \\ &= \epsilon_k \left[ (u_k^2 - v_k^2) a_k^\dagger a_k + 2u_k v_k a_k^\dagger a_{-k}^\dagger + 2u_k v_k a_{-k} a_k + (u_k^2 - v_k^2) a_{-k}^\dagger a_{-k} \right] + \text{constant} \end{aligned} \quad (6)$$

## Pairing Energy Term

For the pairing term,  $-\Delta_k c_k^\dagger c_{-k}^\dagger - \Delta_k c_{-k} c_k$ , using the inverse transformation yields:

$$\begin{aligned} & -\Delta_k (u_k a_k^\dagger + v_k a_{-k})(u_k a_{-k}^\dagger - v_k a_k) - \Delta_k (u_k a_{-k} - v_k a_k^\dagger)(u_k a_k + v_k a_{-k}^\dagger) \\ &= -\Delta_k \left[ -2u_k v_k a_k^\dagger a_k + 2u_k v_k a_{-k} a_{-k}^\dagger + (u_k^2 - v_k^2) a_{-k} a_k + (u_k^2 - v_k^2) a_k^\dagger a_{-k}^\dagger \right] \\ &= -\Delta_k \left[ -2u_k v_k a_k^\dagger a_k + 2u_k v_k a_{-k}^\dagger a_{-k} + (u_k^2 - v_k^2) a_{-k} a_k + (u_k^2 - v_k^2) a_k^\dagger a_{-k}^\dagger \right] + \text{constant} \end{aligned} \quad (7)$$

## Simplification and Diagonalization

This process involves collecting terms that contribute to the diagonal form of the Hamiltonian,  $E_k a_k^\dagger a_k$ , and identifying those that cancel out or contribute to the constant term. The total Hamiltonian is

$$\begin{aligned} H &= \sum_{k>0} \left[ \epsilon_k (u_k^2 - v_k^2) + 2\Delta_k u_k v_k \right] \left[ a_k^\dagger a_k + a_{-k}^\dagger a_{-k} \right] \\ &+ \sum_{k>0} \left[ 2\epsilon_k u_k v_k - \Delta_k (u_k^2 - v_k^2) \right] \left[ a_k^\dagger a_{-k}^\dagger + a_{-k} a_k \right] + \text{constant}. \end{aligned} \quad (8)$$

To diagonalize this Hamiltonian, we require:

$$2\epsilon_k u_k v_k - \Delta_k (u_k^2 - v_k^2) = 0. \quad (9)$$

## Expressions for $u_k$ and $v_k$

To diagonalize the Hamiltonian,  $u_k$  and  $v_k$  are expressed in terms of  $\epsilon_k$  and  $\Delta_k$  as follows:

$$u_k^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta_k^2}} \right), \quad (10)$$

$$v_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta_k^2}} \right), \quad (11)$$

After the transformation, the Hamiltonian becomes diagonal:

$$H = \sum_k E_k a_k^\dagger a_k + \text{constant}, \quad (12)$$

where  $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$  is the quasiparticle energy.

## 1d $p$ -wave superconductor

### What does “topological” mean?

We have discussed that one phase of the 1d  $p$ -wave superconductor is “topological.” But what exactly does topological mean here?

One way to see the topological nature of the phase is through the momentum-space formulation. In terms of the Fourier modes, the Hamiltonian

$$H = \sum_j -\mu c_j^\dagger c_j - t c_{j+1}^\dagger c_j - t c_j^\dagger c_{j+1} + \Delta c_{j+1}^\dagger c_j^\dagger + \Delta^* c_j c_{j+1} \quad (13)$$

becomes

$$H = \sum_k (-2t \cos k - \mu) c_k^\dagger c_k + \Delta e^{-ik} c_k^\dagger c_{-k}^\dagger + \Delta^* e^{ik} c_{-k} c_k \quad (14)$$

$$= \sum_k (-2t \cos k - \mu) c_k^\dagger c_k - i\Delta \sin k c_k^\dagger c_{-k}^\dagger + i\Delta^* \sin k c_{-k} c_k \quad (15)$$

$$= \frac{1}{2} \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \begin{pmatrix} -2t \cos k - \mu & -2i\Delta \sin k \\ 2i\Delta^* \sin k & 2t \cos k + \mu \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} + \text{const.} \quad (16)$$

Defining the momentum-dependent pairing function

$$\Delta_k := -2i\Delta \sin k, \quad (17)$$

we can write the matrix as

$$H_k = \begin{pmatrix} -2t \cos k - \mu & \Delta_k \\ \Delta_k^* & 2t \cos k + \mu \end{pmatrix} = (-2t \cos k - \mu) \sigma_z + \text{Re}(\Delta_k) \sigma_x - \text{Im}(\Delta_k) \sigma_y = \vec{d}_k \cdot \vec{\sigma}, \quad (18)$$

where the  $\sigma$ 's are the Pauli matrices,

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (19)$$

This matrix therefore effectively describes a spin-1/2 in a magnetic field pointing in the  $\vec{d}_k$  direction. The ground state of this spin points in the direction opposite to  $\vec{d}_k$  and has eigenvalue  $-|\vec{d}_k|$ .

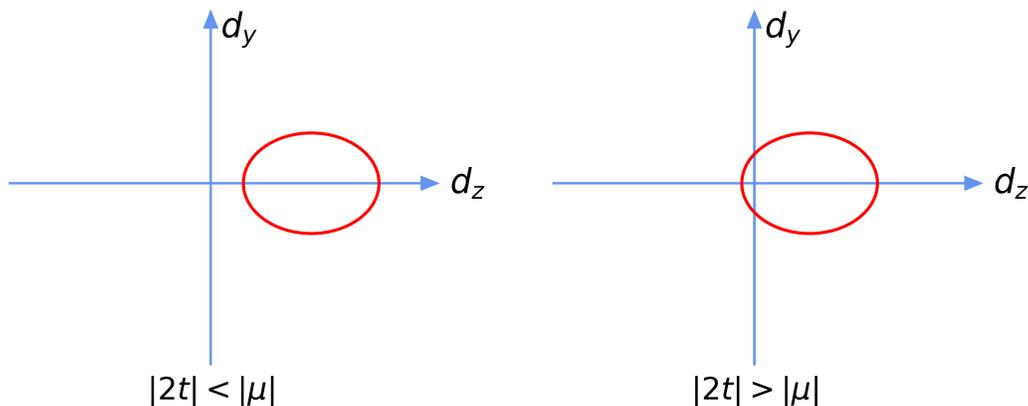
Depending on the parameters  $t$ ,  $\mu$ , and  $\Delta$ , the vector  $\vec{d}_k$  traces out trajectories with different topological properties as  $k$  varies over the Brillouin zone. Without loss of generality, we may choose a gauge in which  $\Delta$  is real. In that case,

$$\Delta_k = -2i\Delta \sin k, \quad (20)$$

so equivalently,

$$H_k = (-2t \cos k - \mu)\sigma_z + 2\Delta \sin k \sigma_y = \vec{d}_k \cdot \vec{\sigma}. \quad (21)$$

When  $|2t| < |\mu|$ , the  $\vec{d}_k$  vector traces out a closed curve that does not contain the origin. On the other hand, when  $|2t| > |\mu|$ , the  $\vec{d}_k$  vector traces out a closed curve that does contain the origin. These two cases correspond, respectively, to the trivial and topological phases. When  $|2t| = |\mu|$ , the  $\vec{d}_k$  vector passes through the origin, indicating the presence of gapless modes at the critical point.



This criterion for the topological phase is easy to apply, but it only works for a quadratic Hamiltonian. What if we add quartic or even higher-order terms to the Hamiltonian? How can we then determine whether a phase is topological?

Our previous discussion based on edge modes provides such an approach. It works for any local Hamiltonian. Given a Hamiltonian, we can solve for its ground state and check whether there is a two-fold degeneracy, namely two lowest-energy states whose energy difference is exponentially small in the system size. Moreover, we would like to verify that this degeneracy arises from edge states. A more precise way to say this is that the two nearly degenerate ground states differ only through the occupation of an edge mode, while local observables supported deep in the bulk have the same expectation values in the two states up to corrections that are exponentially small in the system size. In this sense, the two-fold degeneracy comes from the edge Majorana modes. This near-degeneracy is stable against local perturbations as long as the bulk gap remains open.

Hence, the edge state provides a concrete signature of the topological phase in a Majorana chain. In the topologically trivial phase of the Majorana chain, there is no edge state. More generally, a topologically trivial phase is one that can be adiabatically deformed into a product state without closing the bulk gap. For the Majorana chain, we can see this explicitly. In the topologically trivial phase, one can continuously deform the Hamiltonian to the point  $t = \Delta = 0$ , where the ground state is simply the vacuum state of all  $c$  modes and is therefore a product state. In the topologically nontrivial phase, this is no longer possible without closing the bulk gap. Indeed, one may instead deform the Hamiltonian to the special point  $\mu = 0$

and  $t = \Delta$ , where the correlation length vanishes and the Majorana zero modes are exactly localized at the two ends. Even at this special point, however, the ground state is still far from a trivial product state in terms of the physical  $c$  modes. Therefore, this phase is topologically nontrivial.

## Quantum phases of matter and transverse-field Ising model

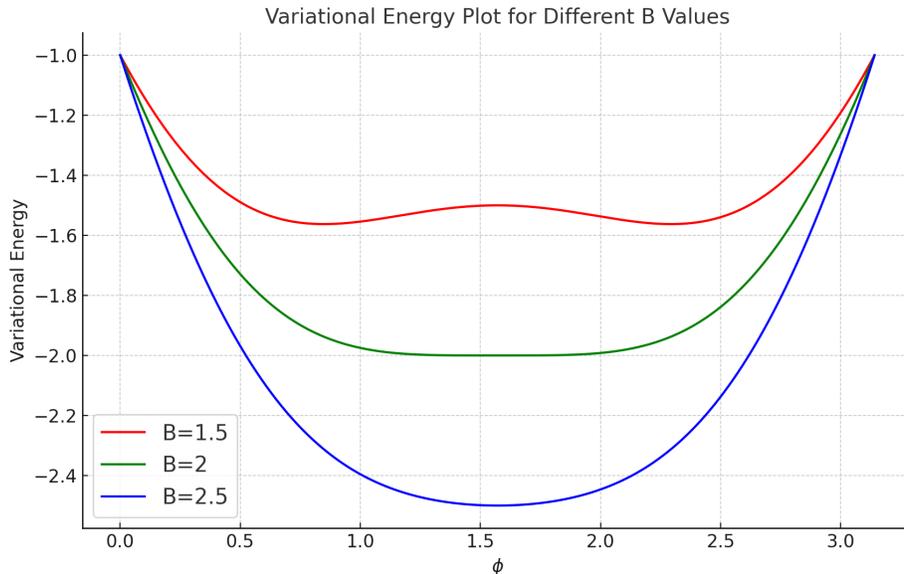


Figure 1: The variational energies  $\epsilon(\phi)$  for  $B = 1.5, 2, 2.5$ . (Note that Fig. 6.3 of “Quantum Information Meets Quantum Matter” by Bei Zeng, Xie Chen, Duan-Lu Zhou, and Xiao-Gang Wen has a typo.)

Quantum phases of matter are phases of matter at zero temperature. So, quantum phases correspond to the ground states of the quantum Hamiltonians that govern the systems. In this book, we mainly discuss those quantum phases of matter. Crystal, conductors, insulators, superfluids, and magnets can exist at zero temperature and are examples of quantum phases of matter.

Again, physicists used to believe that Landau symmetry breaking theory also describes all possible quantum phases of matter, and all possible (continuous) quantum phase transitions. (Quantum phase transitions, by definition, are zero-temperature phase transitions.) For example, the superfluid is described by a  $U(1)$  symmetry breaking.

The simplest example to demonstrate the Landau symmetry-breaking theory for quantum phases is the transverse-field Ising model on a 1-dimensional chain. The total Hilbert space of the transverse-field Ising model is formed by  $\frac{1}{2}$  spins (qubits) on each site. The Hamiltonian is given by

$$H_{\text{Ising}} = - \sum_i (Z_i Z_{i+1} + B X_i), \quad (22)$$

where  $X_i, Y_i, Z_i$  are the Pauli matrices acting on the  $i$ -th spin. The Hamiltonian has a spin-flip symmetry,  $\mathcal{T}$ , generated by  $\bigotimes_i X_i$ :  $[H, \bigotimes_i X_i] = 0$ .

One way to obtain the ground state of the transverse-field Ising model is to use the variational approach. To design the variational trial wave function, we note that when  $B = 0$  the ground states are two-

fold degenerate and are given by  $\bigotimes_i |\uparrow_i\rangle$  and  $\bigotimes_i |\downarrow_i\rangle$ . When  $B \gg 1$  the ground state is given by  $\bigotimes_i (|\uparrow_i\rangle + |\downarrow_i\rangle)/\sqrt{2}$ . Thus, we choose our trial wave function as

$$|\Psi_\phi\rangle = \bigotimes_i [\cos(\phi/2)|\uparrow_i\rangle + \sin(\phi/2)|\downarrow_i\rangle], \quad (23)$$

where  $\phi$  is the variational parameter. The average energy per site is given by

$$\varepsilon(\phi) = \frac{\langle \Psi_\phi | H | \Psi_\phi \rangle}{N_{\text{site}}} = - [\cos^2(\phi/2) - \sin^2(\phi/2)]^2 - 2B \cos(\phi/2) \sin(\phi/2). \quad (24)$$

We note that the spin-flip transformation  $\bigotimes_i X_i$  changes  $|\Psi_\phi\rangle \rightarrow |\Psi_{\pi-\phi}\rangle = \bigotimes_i X_i |\Psi_\phi\rangle$ . So  $\varepsilon(\phi)$  satisfies  $\varepsilon(\phi) = \varepsilon(\pi - \phi)$  due to the spin-flip symmetry.

In Fig. 1, we plot the variational energy  $\varepsilon(\phi)$  for  $B = 1.5, 2, 2.5$ . We see a symmetry-breaking transition at  $B = 2$ . For  $B > 2$ , the energy is minimized at  $\phi = \pi/2$  and the trial ground state does not break the spin-flip symmetry  $\phi \rightarrow \pi - \phi$ . For  $B < 2$ , the energy is minimized at two places  $\phi = \pi/2 \pm \Delta\phi$ , which give rise to two degenerate ground states  $|\Psi_{\pi-\Delta\phi}\rangle$  and  $|\Psi_{\pi+\Delta\phi}\rangle$ . Each of the ground states breaks the spin-flip symmetry.

However, this approach does not give the correct phase transition point. To derive the critical point exactly, we first notice a self-duality of this model under

$$\begin{aligned} Z_i Z_{i+1} &\rightarrow \tilde{X}_{i+\frac{1}{2}}, \\ X_i &\rightarrow \tilde{Z}_{i-\frac{1}{2}} \tilde{Z}_{i+\frac{1}{2}}. \end{aligned} \quad (25)$$

Up to some energy rescaling, the parameter  $B$  becomes  $B^{-1}$ , which will be discussed in more detail in the next section. Therefore, if we expect that there are two phases, the phase transition must happen at  $B^*$  such that

$$B^* = B^{*-1} \Rightarrow |B^*| = 1. \quad (26)$$

## Matching of the Phase Transition Points

It's noteworthy that a fermionic Hamiltonian, defined as

$$H_f = \sum_j -\mu c_j^\dagger c_j - t c_{j+1}^\dagger c_j - t c_j^\dagger c_{j+1} + \Delta c_{j+1}^\dagger c_j^\dagger + \Delta^* c_j c_{j+1}, \quad (27)$$

with parameters  $t = \Delta = 1$ , is equivalent to

$$H_b = - \sum_i (Z_i Z_{i+1} + \frac{\mu}{2} X_i). \quad (28)$$

This equivalence highlights that the phase transition point  $|\mu| = |2t|$  aligns perfectly with  $|B| = 1$ , offering a consistent framework for understanding quantum phase transitions within this model.

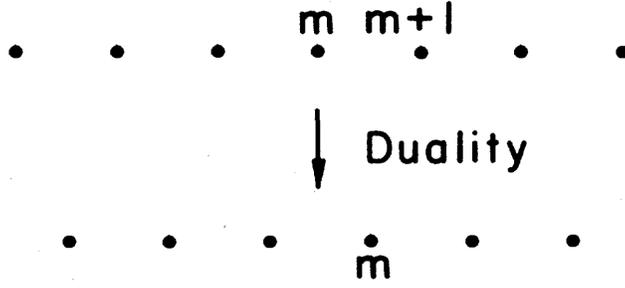


Figure 2: Dual transformation for a spatial lattice.

## Self-duality of the Ising model

Our first step towards developing a detailed understanding of the Ising model is to derive a mapping between its high- and low-temperature behaviors. As a by-product of this construction, we shall understand the special significance of the point  $B$ . This mapping is called a "duality" transformation (Kramers and Wannier, 1941).

Consider the one-dimensional quantum-mechanical formulation of the model

$$H = - \sum_j X_j - \lambda \sum_j Z_j Z_{j+1}. \quad (29)$$

The first element of the duality transformation associates a new ("dual") lattice with our original spatial lattice. Sites of the original lattice will be associated with links of the "dual" lattice and vice versa. The transformation is visualized in Fig. 2.

Operators are placed on the dual lattice, so a spin system complete with a Hamiltonian will be generated from the original system. Define the operators on the dual lattice

$$\begin{aligned} \tilde{X}_n &= Z_{n-1} Z_n, \\ \tilde{Z}_n &= \prod_{m < n} X_m. \end{aligned} \quad (30)$$

So,  $\tilde{X}_n$  senses whether the spins on adjacent sites are aligned or not.  $\tilde{Z}_n$  flips all the spins to the left of  $n$ . The dual operators have several important properties: (1) They satisfy the same Pauli spin algebra as  $X$  and  $Z$ . (2) The Hamiltonian can be rewritten simply using the dual spin operators. To check the first point, recall the algebra that defines the Pauli matrices. On a given site,

$$\begin{aligned} X_n Z_n &= -Z_n X_n, \\ X_n^2 &= Z_n^2 = 1, \end{aligned} \quad (31)$$

and on different sites, they commute,

$$[X_n, Z_m] = 0, \text{ etc., if } n \neq m. \quad (32)$$

One check that  $\tilde{X}_n$  and  $\tilde{Z}_m$  satisfy the same algebra by using Eq. (30) directly. For example, to check that

$$\tilde{X}_n \tilde{Z}_n = -\tilde{Z}_n \tilde{X}_n, \quad (33)$$

note that only one factor of  $X$  and  $Z$  are on the same site. Then, the first relation of Eq. (31) implies Eq. (33). One proves that

$$\tilde{X}_n \tilde{Z}_m = \tilde{Z}_m \tilde{X}_n, \quad n \neq m, \quad (34)$$

by observing that an even number of  $X$ 's and  $Z$ 's are interchanged when passing from one side of Eq. (4.22) to the other. An even number of interchanges always produces a positive sign.

The second point is verified as directly. Since

$$X_m = \tilde{Z}_{m+1}\tilde{Z}_m, \quad (35)$$

the Hamiltonian is

$$H = -\sum_n \tilde{Z}_n \tilde{Z}_{n+1} - \lambda \sum_n \tilde{X}_n = \lambda \left( -\sum_n \tilde{X}_n - \lambda^{-1} \sum_n \tilde{Z}_n \tilde{Z}_{n+1} \right), \quad (36)$$

which has the same form as the Hamiltonian written in terms of the  $X, Y, Z$ 's,

$$H(X, Y, Z; \lambda) = \lambda H(\tilde{X}, \tilde{Y}, \tilde{Z}; \lambda^{-1}). \quad (37)$$

But since the  $X, Y, Z$ 's and  $\tilde{X}, \tilde{Y}, \tilde{Z}$ 's have the same algebra, this is an expression of symmetry for the original model alone—it states that the high-temperature and low-temperature properties of the model map onto one another! It is called "self-duality." In particular, Eq. (37) implies that each eigenvalue of  $H$  satisfies the relation

$$E(\lambda) = \lambda E(\lambda^{-1}). \quad (38)$$

This has a very important implication. Consider the mass gap  $G(\lambda)$  of the Hamiltonian as a function of  $\lambda$ . Suppose it vanishes at some particular point. This would be a critical point of the theory because the correlation length would diverge there. But Eq. (38) states that if the gap vanishes at a certain  $\lambda$ , it must also vanish at  $\lambda^{-1}$ ! Therefore, if we assume that the critical point is unique, the self-duality of the model implies that it occurs at

$$\lambda_c = 1. \quad (39)$$

This result agrees with our earlier observations. In the next section, we shall compute the mass gap and find

$$G(\lambda) = 2|1 - \lambda|, \quad (40)$$

in agreement with these considerations.

Note that the self-duality of the model yields the critical point only if one *assumes* that the point is unique. This is a reasonable (and true) assumption for the simple Ising model, but it is not true for more intricate, self-dual theories (Elitzur et al., 1979).

## Strong Coupling Expansions for the Mass Gap

Determining the phase diagram and calculating critical indices for a statistical mechanics system can be approached through several methods:

1. Exact solution of the model.
2. Calculations using the renormalization group.
3. Perturbative expansions.

These methodologies are applied in Kogut’s review paper, which I strongly encourage students to read for a more thorough understanding. Initially, we will focus on the third method, exploring both strong and weak coupling expansions within the quantum Hamiltonian formulation of the Ising model. Through these analyses, we aim to compute the critical temperature  $\lambda$  and the mass gap critical index  $\nu$ . Given the model’s simplicity, we anticipate deriving exact values for all parameters. Understanding these expansion techniques is invaluable, as they are equally applicable to more complex theories where exact solutions and renormalization group methods are not readily accessible.

We begin with a calculation of the mass gap of the Hamiltonian,

$$H = \sum_n (1 - X_n) - \lambda \sum_n Z_n Z_{n+1}. \quad (41)$$

Consider the theory at high temperature, i.e.,  $\lambda$  very small. If we write

$$H = H_0 + \lambda V, \quad (42)$$

with

$$H_0 = \sum_n (1 - X_n), \quad (43)$$

$$V = - \sum_n Z_n Z_{n+1}, \quad (44)$$

then we are ready to do perturbation expansions in  $\lambda$ . First we must determine the  $\lambda = 0$  ground state. To minimize  $H_0$  we must choose the spins at every site such that

$$X_n |+\rangle = |+\rangle \quad (\text{for all } n). \quad (45)$$

It is convenient to refer to  $|+\rangle$  as having all spins “up.” This terminology is different from that used earlier in connection with Eq. (41). In that basis, the eigenstates of  $X$  are  $|+\rangle$  with eigenvalue  $+1$  and  $|-\rangle$  with eigenvalue  $-1$ . Then  $Z$  acts as a spin-flip operator within this basis. Therefore, we can describe the perturbation  $V$ , Eq. (44), as an operator that flips the spins on adjacent sites.

To calculate the mass gap, we must obtain the expansion for the ground-state energy and the first excited state. In the  $\lambda = 0$  limit, the first excited state above  $|+\rangle$  consists of just one flipped spin. This state is  $N$ -fold degenerate ( $N$  is the number of sites of the lattice) because the flipped spin could occur anywhere on the spatial lattice. However, this degeneracy is resolved by constructing states which have definite momentum. Consider the zero-momentum state

$$|\mathbf{1}\rangle = \frac{1}{\sqrt{N}} \sum_n Z_n |+\rangle, \quad (46)$$

whose energy is the mass gap. The notation  $|\mathbf{1}\rangle$  indicates that  $Z$  has flipped one spin down. The state equation (46) is properly normalized, i.e.,  $\langle \mathbf{1} | \mathbf{1} \rangle = 1$ .

We want to calculate the  $\lambda$  expansion for the mass gap to sufficiently high orders that we can sensibly discuss values of  $\lambda$  near unity where the phase transition is expected. So, we need the formulas of Raleigh–Schrödinger perturbation theory to high order. They are easily obtained from the elegant Wigner–Brillouin formulas (Baym, 1969).

## Time-Independent Perturbation Theory

Time-independent perturbation theory represents one of the two main branches of perturbation theory, distinguished from its counterpart, time-dependent perturbation theory, by the stationary nature of its

Hamiltonian; that is, the Hamiltonian lacks temporal dependence. This theoretical framework was elucidated by Erwin Schrödinger in a seminal 1926 paper, emerging shortly after his pioneering contributions to wave mechanics. Schrödinger's exposition acknowledged the foundational insights of Lord Rayleigh, who had previously explored the harmonic vibrations of strings under the influence of minor inhomogeneities. Consequently, this body of work is often recognized as the Rayleigh–Schrödinger perturbation theory.

The formalism commences with the unperturbed Hamiltonian  $H_0$ , presumed to be free from time-dependent influences. Characterized by distinct energy levels and eigenstates,  $H_0$  is described by the timeless Schrödinger equation:

$$H_0|n\rangle = \epsilon_n^{(0)}|n\rangle, \quad n = 1, 2, 3, \dots \quad (47)$$

We postulate discrete energy spectra for tractability. The superscript (0) signifies association with the unperturbed system, and we employ the bra-ket notation for state representation.

A perturbation is subsequently imposed on the Hamiltonian. Consider  $V$  as a Hamiltonian encapsulating a mild physical perturbation, such as potential energy induced by an external field, rendering  $V$  a Hermitian operator. The perturbation parameter  $\lambda$  is introduced as a dimensionless scalar that transitions smoothly from 0 (indicating no perturbation) to 1 (representing full perturbation). The perturbed Hamiltonian thus takes the form:

$$H = H_0 + \lambda V \quad (48)$$

Accordingly, the energy levels and eigenstates of the perturbed Hamiltonian continue to satisfy the time-independent Schrödinger equation,

$$(H_0 + \lambda V)|n'\rangle = \epsilon_n|n'\rangle. \quad (49)$$

Our aim is to articulate  $\epsilon_n$  and  $|n\rangle$  in reference to the energy levels and eigenstates of the original Hamiltonian. Assuming the perturbation's magnitude to be negligible, we can expand them into a Maclaurin series of  $\lambda$ ,

$$E_n = \epsilon_n^{(0)} + \lambda\epsilon_n^{(1)} + \lambda^2\epsilon_n^{(2)} + \dots \quad (50)$$

$$|n'\rangle = |n\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \dots \quad (51)$$

Integrating the power series expansion into the Schrödinger equation yields

$$(H_0 + \lambda V)(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \dots) = (\epsilon_n^{(0)} + \lambda\epsilon_n^{(1)} + \dots)(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \dots), \quad (52)$$

which facilitates the resolution of the energy expansion as

$$\epsilon_n^{(1)} = \langle n|V|n\rangle, \quad (53)$$

$$\epsilon_n^{(2)} = \langle n|VgV|n\rangle, \quad (54)$$

$$\epsilon_n^{(3)} = \langle n|VgVgV|n\rangle - \langle n|V|n\rangle\langle n|Vg^2V|n\rangle, \quad (55)$$

$$\epsilon_n^{(4)} = \langle n|VgVgVgV|n\rangle - \langle n|VgV|n\rangle\langle n|Vg^2V|n\rangle \quad (56)$$

$$+ \langle n|V|n\rangle\langle n|V|n\rangle\langle n|Vg^3V|n\rangle \quad (57)$$

$$- \langle n|V|n\rangle\langle n|VgVg^2V + Vg^2VgV|n\rangle, \quad (58)$$

where  $g$  denotes the resolvent (projected green function)

$$g = (1 - |n\rangle\langle n|)/(\epsilon_n^{(0)} - H^{(0)}). \quad (59)$$

It is easy to apply these formulas and determine the mass gap. It is helpful to represent the terms of the perturbation expansion pictorially. Let a single vertical line (Fig. 3) represent a flipped spin at a certain

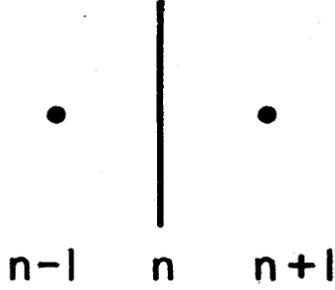


Figure 3: A flipped spin on site  $n$ .

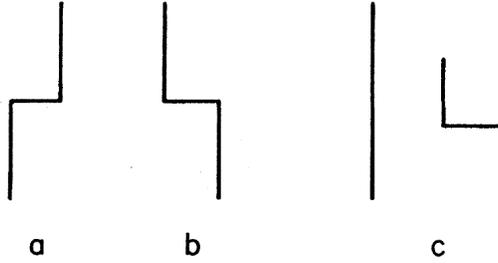


Figure 4: Two possible actions of the potential  $V$  on a state initially containing a flipped spin.

site. The potential  $V$  can act on the flipped spin and move it one lattice spacing to the left or right. Alternatively,  $V$  can act on the  $\lambda = 0$  vacuum and flip two nearest-neighbor spins over. These effects are shown in Fig. 4. These figures should be read vertically as a guide to Eq. (58). For example, Fig. 4 shows a contribution to  $\langle n|V|n\rangle$ : the flipped spin is initially on site  $n$ , then  $V$ , which is represented by a horizontal link, acts and flips that spin down while raising the nearest neighbor. The spin-up nearest neighbor is present in the final state. Another figure shows a spin configuration that contributes to the state  $V|n\rangle$ .

Let us compute the gap through  $\lambda^3$ . The zeroth-order energy is just  $\epsilon_0 = 2$ . This is so because when one spin is flipped, one term in  $H_0$  is increased by two units. The first-order coefficient  $\epsilon_1$  is  $-2$ . It is minus because of the minus sign in the expression for  $V$ , and the 2 records the presence of two graphs in Fig. 4a and Fig. 4b. To obtain this result mechanically, evaluate the matrix element

$$\langle \mathbf{1}|V|\mathbf{1}\rangle = -\frac{1}{N} \sum_{n,n'} \langle +|Z_n \sum_m (Z_m Z_{m+1}) Z_{n'}|+\rangle = -2. \quad (60)$$

There are two contributions:  $n = m$  and  $m + 1 = n'$  or  $n' = m$  and  $m + 1 = n$ . Since  $Z^2 = 1$ , each term gives a factor  $N$ , canceling the normalization  $N^{-1}$ . Other terms in the sums contribute nothing since, in those cases, the state  $Z_n Z_m Z_{m+1} Z_{n'}|+\rangle$  contains some flipped spins, so its projection onto  $|0\rangle$  vanishes.

Second-order graphs are shown in Fig. 5. In these cases, there is a sum over intermediate states. The energy denominators are  $(2 - 6)^{-1}$ , since 2 is the energy of the initial state and 6 is the energy of the intermediate state (three spin flips, each producing two units of energy). The intermediate state is labeled

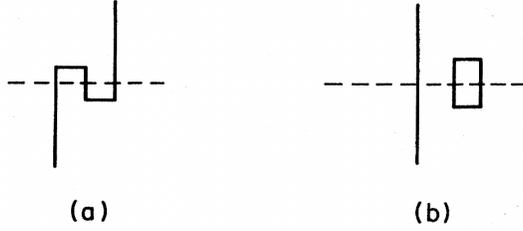


Figure 5: Second order contribution to the energy of  $|1\rangle$ . The dashed lines label intermediate states.

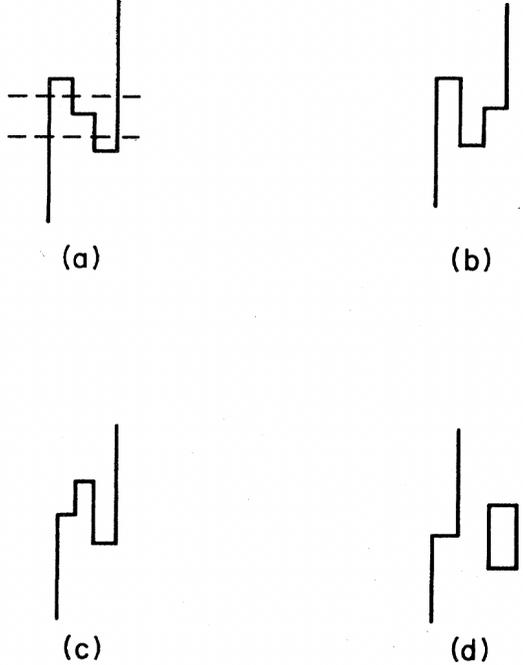


Figure 6: Third order contribution to the energy of  $|1\rangle$ . The dashed lines labeling intermediate states are shown only for the first graph.

by the dashed horizontal line in the figure. The second-order results organized by figure number are

$$\begin{aligned}
 \text{Fig. 5a} &= 2 \left( \frac{1}{2-6} \right) \lambda^2, \\
 \text{Fig. 5b} &= (N-2) \left( \frac{1}{2-6} \right) \lambda^2.
 \end{aligned}
 \tag{61}$$

The third-order contributions are obtained similarly. There are contributions from the  $\langle n|VgVgV|n\rangle$  piece of Eq. (58) shown in Fig. 6, as well as the  $-\langle n|V|n\rangle\langle n|Vg^2|V|n\rangle$  piece which is easily obtained from the

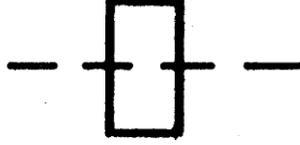


Figure 7: Second-order contribution to the vacuum energy. The dashed lines label intermediate states.

lower-order calculations. Collecting these results

$$\begin{aligned}
 \text{Fig. 6a} &= -2 \left( \frac{1}{4 \cdot 4} \right) \lambda^3, \\
 \text{Fig. 6b} &= -2 \left( \frac{1}{4 \cdot 4} \right) \lambda^3, \\
 \text{Fig. 6c} &= -2 \left( \frac{1}{4 \cdot 4} \right) \lambda^3, \\
 \text{Fig. 6d} &= -2(N-3) \left( \frac{1}{4 \cdot 4} \right) \lambda^3, \\
 -\langle n|V|n\rangle\langle n|Vg^2V|n\rangle &= -(-2\lambda) \left[ \frac{2}{16} + \frac{(N-2)}{16} \right] \lambda^2.
 \end{aligned} \tag{62}$$

To finally obtain the mass gap we must calculate the shift in the vacuum energy through this order in  $\lambda$  and take the difference of the two series. The zeroth-order energy is zero—the constant term  $\sum_n 1$  was added to the Hamiltonian to achieve this. The first-order correction is also zero, since  $V|0\rangle$  does not project onto  $|0\rangle$ . Second-order effects are shown in Fig. 7,

$$\text{Fig. 7} = -(N/4)\lambda^2. \tag{63}$$

Third-order effects vanish identically.

Collecting these results, we find the series for the gap

$$G(\lambda) = (2 - 2\lambda) + (0)\lambda^2 + (0)\lambda^3 + \dots, \tag{64}$$

where the second- and third-order coefficients have vanished identically! Higher-order calculations confirm the obvious suspicion—the series truncates after the first term. So, we find an *exact* result

$$G(\lambda) = 2(1 - \lambda), \tag{65}$$

for  $\lambda < 1$ . Note that  $G(\lambda)$  vanishes at  $\lambda_c = 1$ . This proves that the Ising model has just two phases separated by a continuous phase transition. We also learn from Eq. (65) that the critical exponent  $\nu$  is unity

$$\nu = 1, \tag{66}$$

which is another exact result. The fact that we have obtained the correct answer (see Table I) constitutes an example of universality—the singularities in the critical region of the model are independent of its detailed lattice structure.

Since the gap must satisfy the duality condition Eq. (38)

$$G(\lambda) = \lambda G(\lambda^{-1}), \tag{67}$$

the resulting equation (65), which was derived only for  $\lambda < 1$ , can be extended to all  $\lambda$ ,

$$G(\lambda) = 2|1 - \lambda|, \tag{68}$$

as was recorded earlier.