

Topological Qubit

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1 Introduction

Anyons only exist in 2D and follow different statistics than Bosons and Fermions. The exchange of particles of Bosons or Fermions will a phase factor of ± 1 , but

the exchange position of Anyons will have a phase factor of $e^{i\phi}$. It exists in 2D because of the topological property.

1.1 What are Majorana zero modes(MZM)

Majorana zero modes(MZM) are quasiparticle excitations in certain materials that are their own antiparticles. They are characterized by being zero-energy states, meaning they don't carry any energy, and are non-local, with their wavefunctions spread out over a region rather than being localized at a single point. These properties make them promising candidates for building robust, fault-tolerant quantum computers.

Non-Abelian Statistics:

MZMs exhibit non-Abelian statistics, meaning that when two or more MZMs are "braided" around each other, the quantum state of the system changes in a non-trivial way. This braiding operation can be used to perform quantum computations.

Topological Protection:

Because of their non-local nature and non-Abelian statistics, MZMs are theoretically protected from local perturbations, making them attractive for building robust quantum computers.

Abelian Anyons their exchange operators are commuted. Non-Abelian Anyons their exchange operators don't commute.

2 Anyons Model

3 Quantum Computation with Anyons

4 Spin Liquid

ferromagnet: every spin point at the same direction. paramagnet: spin pointing at an random direction at the high temperature.

Disorder means random directions of the spins, paramagnet. Order means the predictable directions of the spins, ferromagnet.

The directions of the spins affect by the temperature. At the high temperature, the directions of the spins are random. At the low temperature, the directions of the spins are the same. However, spin liquid is different it remains disorder even at the low temperature.

4.1 Resonate Valence Bond(RVB)

4.2 Hubbard Model

The Hubbard model is one of the most important simplified models in condensed matter physics for studying strongly correlated electron systems.

$$H = t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

1. $c_{i\sigma}^\dagger, c_{j\sigma}$: are the creation/annihilation operator for an electron with spin σ at site i .
2. t : hopping parameter (strength of electron motion between neighboring sites $\langle i, j \rangle$).
3. U : on-site Coulomb repulsion energy.
4. $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ (number operator).

The ideas of the Hubbard model's Hamiltonian are:

1. Electrons like to delocalize and move around the lattice sites, lowering their kinetic energy. This is described by the hopping strength t . Antiferromagnetic allows the electrons to move to its neighbor site, but ferromagnetic doesn't allow the electrons to move to its neighbor because of the Pauli exclusion principle.
2. Electrons like to repel each other if they occupied at the same sites, this is Coulomb repulsion(interaction). This is being characterized by on-site repulsion strength U .

This model is interesting because if $U \gg t$, then it describes a Mott insulator because the electrons can't move around and each site will have one electron. On the other hand, if $U \ll t$, then it describes a conductor because electrons are freely move around the sites.

If the limit of $U \gg t$, Hubbard model reduces to Heisenberg model where the spin interacts antiferromagnetically. If the underlying lattice geometry makes it impossible to satisfy all antiferromagnetic bonds simultaneously (e.g., triangular, kagome, or honeycomb lattices), then the system becomes frustrated. Frustration leads to quantum spin liquid. Frustration happens when spins cannot simultaneously satisfy all their interaction preferences because of the lattice geometry or competing interactions.

5 Project

If we only have two spin 1/2 particles, then Heisenberg Hamiltonian(only coupling terms, no one-body terms) will be the following:

$$\begin{aligned} H &= J_{12} \mathbf{S}_1 \cdot \mathbf{S}_2 \\ &= J_{12} (\sigma_{1x} \sigma_{2x} + \sigma_{1y} \sigma_{2y} + \sigma_{1z} \sigma_{2z}) \end{aligned}$$

$$\begin{aligned}
S_1 &= [S_{1x}, S_{1y}, S_{1z}] \\
S_2 &= [S_{2x}, S_{2y}, S_{2z}] \\
S_1 \cdot S_2 &= S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}
\end{aligned}$$

$$(S_{1x}) = S_x \otimes I = \frac{\hbar}{2} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (S_{2x}) = I \otimes S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$S_{1x} \cdot S_{2x} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$(S_{1y}) = S_y \otimes I = \frac{\hbar}{2} \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad (S_{2y}) = I \otimes S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}$$

$$S_{1y} \cdot S_{2y} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$(S_{1z}) = S_z \otimes I = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad (S_{2z}) = I \otimes S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$S_{1z} \cdot S_{2z} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (S_1 \cdot S_2) = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Ok, now let's do it with projectors. If we have two spin 1/2 particles, then:

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$$

We have spin= 1 and spin= 0 manifolds, and we can define projectors to project onto these two manifolds. A projector $P^{(s)}$ onto spin s gives 1 when acting on a collection of spins whose total spin is s, and 0 otherwise. The definition of

projector is $P^2 = P$, and the eigenvalue of P is either 0 or 1.
Proof:

$$\begin{aligned} P|v\rangle &= \lambda|v\rangle \\ P(P|v\rangle) &= \lambda^2|v\rangle \\ \lambda^2|v\rangle &= \lambda|v\rangle \\ (\lambda^2 - \lambda)|v\rangle &= 0 \end{aligned}$$

This implies $\lambda = \{1, 0\}$.

$$\begin{aligned} \hat{S} &= \hat{s}_1 + \hat{s}_2 \\ \hat{S}^2 &= (\hat{s}_1 + \hat{s}_2)(\hat{s}_1 + \hat{s}_2) \\ &= \hat{s}_1^2 + \hat{s}_2^2 + 2\hat{s}_1\hat{s}_2 \end{aligned}$$

We know that:

$$\hat{s}_i^2 = \frac{3}{4}\hbar^2 = \frac{3}{4}$$

rearrange the above equation, we will obtain the following:

$$\hat{s}_1\hat{s}_2 = \frac{1}{2}(\hat{S}^2 - \hat{s}_1^2 - \hat{s}_2^2)$$

The eigenvalues of these operators are:

$$\hat{s}_1\hat{s}_2 = \frac{1}{2}(S(S+1) - s_1(s_1+1) - s_2(s_2+1))$$

If we have two spin 1/2 particles, then:

$$\begin{aligned} \hat{s}_1\hat{s}_2 &= \frac{1}{2}(S(S+1) - s_1(s_1+1) - s_2(s_2+1)) \\ &= \frac{1}{2}(S(S+1) - \frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}(\frac{1}{2}+1)) \\ &= \frac{1}{2}(S(S+1) - \frac{6}{4}) \\ &= \frac{1}{2}S(S+1) - \frac{3}{4} \end{aligned}$$

If we are looking at $S = 1$ manifold:

$$\begin{aligned} \hat{s}_1\hat{s}_2 &= \frac{1}{2}1(1+1) - \frac{3}{4} \\ &= 1 - \frac{3}{4} \\ &= \frac{1}{4} \end{aligned}$$

If we are looking at $S = 0$ manifold:

$$\begin{aligned}\hat{s}_1 \hat{s}_2 &= \frac{1}{2}0(0+1) - \frac{3}{4} \\ &= -\frac{3}{4}\end{aligned}$$

Based on the definition of projector acting on certain manifold, then we can define the project as the following:

$$\begin{aligned}P^{(1)} &= \frac{3}{4} + \hat{s}_1 \hat{s}_2 \\ P^{(0)} &= \frac{1}{4} - \hat{s}_1 \hat{s}_2\end{aligned}$$

or we can define it in this way:

$$P_{\text{triplet}} = \sum_{m=-1}^1 |1, m\rangle \langle 1, m|, \quad P_{\text{singlet}} = |0, 0\rangle \langle 0, 0|.$$

then:

$$\hat{s}_1 \hat{s}_2 = \frac{\hbar^2}{4} P_{\text{triplet}} - \frac{3\hbar^2}{4} P_{\text{singlet}}$$

This ensures when acting on the appropriate state, it will yield the right eigenvalue. Based on the two projectors, we can re-define the Heisenberg interaction in terms of the projector:

$$\begin{aligned}H &= J_{12} \cdot P^{(0)}(\vec{S}_1 + \vec{S}_2) \\ &= J_{12} \left(\frac{1}{4} - \hat{s}_1 \hat{s}_2 \right)\end{aligned}$$

This give us the following matrix:

$$H = \frac{J_{12}}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

5.1 Four-Site Cluster

Now, we have 4 spin 1/2 particles with total angular momentum S :

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 0 \oplus 1 \oplus 1 \oplus 1 \oplus 2$$

The dimension of the direct sum representation will be:

$$0 \oplus 0 \oplus 1 \oplus 1 \oplus 1 \oplus 2 = 1 + 1 + 3 + 3 + 3 + 5 = 16$$

If we have 4 electrons, the dimension of the Hamiltonian will be $2^4 \times 2^4 = 16 \times 16$. However, we are only interested in the states that have $m_z = 0$, and they are the following:

$$|\uparrow\uparrow\downarrow\downarrow\rangle, |\uparrow\downarrow\uparrow\downarrow\rangle, |\uparrow\downarrow\downarrow\uparrow\rangle, |\downarrow\uparrow\uparrow\downarrow\rangle, |\downarrow\uparrow\downarrow\uparrow\rangle, |\downarrow\downarrow\uparrow\uparrow\rangle.$$

Each ket has eigenvalue of $\frac{1}{2}$ or $-\frac{1}{2}$. Based on these 6 states, we can construct the $m_z = 0$ block of the Hamiltonian ($H_{m_z=0}$):

$$H_{m_z=0} = \begin{pmatrix} -J_{1,1,2,2}^{3,4,3,4} & J_{3,2} & J_{4,2} & J_{3,1} & J_{4,1} & 0 \\ J_{3,2} & -J_{1,1,2,3}^{2,4,3,4} & J_{4,3} & J_{2,1} & 0 & J_{4,1} \\ J_{4,2} & J_{4,3} & -J_{1,1,2,3}^{2,3,4,4} & 0 & J_{2,1} & J_{3,1} \\ J_{3,1} & J_{2,1} & 0 & -J_{1,1,2,3}^{2,3,4,4} & J_{4,3} & J_{4,2} \\ J_{4,1} & 0 & J_{2,1} & J_{4,3} & -J_{1,1,2,3}^{2,4,3,4} & J_{3,2} \\ 0 & J_{4,1} & J_{3,1} & J_{4,2} & J_{3,2} & -J_{1,1,2,2}^{3,4,3,4} \end{pmatrix} \quad (1)$$

They are also can be constructed using projector $P_{m_z=0}$:

$$P_{m_z=0} = \sum_{i \in \sigma} |i\rangle \langle i|$$

σ is a set contains kets that have $m_z = 0$.

$$H_{m_z=0} = P_{m_z=0}^\dagger H P_{m_z=0}$$

What is the ket vector for $|\uparrow\uparrow\downarrow\downarrow\rangle$?

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

It is a 16 dimensional vector. Each row i of $H_{m_z=0}$ corresponds to the corresponding basis state, the

Note, $\sigma_{1z} \cdots \sigma_{nz}$ only contribute to the diagonal terms of the Hamiltonian. $\sigma_{1x} \cdots \sigma_{nx}$ and $\sigma_{1y} \cdots \sigma_{ny}$ only contribute to the right diagonal terms of the Hamiltonian.

Equation 1 doesn't manifest the SU(2) symmetry. We can decompose it into irreducible representations, where it is in the block diagonal form and we can see the SU(2) symmetry easily.

5.2 Bigger Picture

If we have 4 spin 1/2 particles, we can always decomposed it into the irreducible representation: $0 \oplus 0 \oplus 1 \oplus 1 \oplus 2$. With this we can look at $m_z = 0, \pm 1, \pm 2$ manifolds and their dimensions easily. In this case, we can use $S_{tot} = 0$ to be our qubits and it is 2 dimensional. In spin or superconducting qubits, people usually use energy splitting to distinguish logical qubit states $|0\rangle$ and $|1\rangle$. However, in topological qubit, the two logical state of the qubit $|0\rangle$ and $|1\rangle$ are exactly degenerate, they have the exact energy. They rely on the topology of the system to store quantum information.

5.3 How to construct equation 1?

First, determine the manifold that we are interested in. For example, $m_z = 0$, then there are 6 states that have $m_z = 0$. They are:

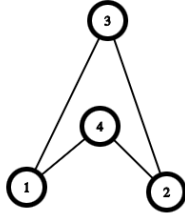
$$|\uparrow\uparrow\downarrow\downarrow\rangle, |\uparrow\downarrow\uparrow\downarrow\rangle, |\uparrow\downarrow\downarrow\uparrow\rangle, |\downarrow\uparrow\uparrow\downarrow\rangle, |\downarrow\uparrow\downarrow\uparrow\rangle, |\downarrow\downarrow\uparrow\uparrow\rangle.$$

Let's relabel them as the following:

$$|1\rangle, |2\rangle, |3\rangle, |4\rangle, |5\rangle, |6\rangle.$$

Second, construct the graph based on the states and geometry that we have. Node will be electron and edge will be the interaction coupling between its neighbors(geometry).

Focus on $|\uparrow\uparrow\downarrow\downarrow\rangle$:



Couplings are $J_{3,1}, J_{3,2}, J_{4,2}, J_{4,1}$, then:

$$\begin{aligned} \langle 1|H|1\rangle &= \frac{1}{2}(J_{3,1} + J_{3,2} + J_{4,2} + J_{4,1}), & \langle 1|H|2\rangle &= \frac{1}{2}J_{3,2}, & \langle 1|H|3\rangle &= \frac{1}{2}J_{4,2} \\ \langle 1|H|4\rangle &= \frac{1}{2}J_{3,1}, & \langle 1|H|5\rangle &= \frac{1}{2}J_{4,1}, & \langle 1|H|6\rangle &= 0. \end{aligned}$$

Combine them to form a vector:

$$\frac{1}{2} \begin{pmatrix} J_{3,1} + J_{3,2} + J_{4,2} + J_{4,1} & J_{3,2} & J_{4,2} & J_{3,1} & J_{4,1} & 0 \end{pmatrix}$$

When the bra and ket have the same indices, we basically sum the couplings. When they don't have the same indices, then

Repeat this process for all the states, and at the end combine all the row vectors to form a matrix.

5.3.1 General formula to calculate the number of $m_z = 0$ states for n particles

Suppose that we have n spin $\frac{1}{2}$ particles, we want to know how many states that can create $m_z = 0$. Each particle can only have $1/2$ or $-1/2$, which means in order to have $m_z = 0$, the state should have the same number spin up and down particles. This means from n particles we have to select $n/2$ of them and set them spin up, in this case the order doesn't matter which means $124 = 421$ in both cases particles 1,2,4 are spin up. Therefore, the total number of $m_z = 0$ states for n particles is:

$$\binom{n}{\frac{n}{2}}$$

If n is even. If n is odd, then there is no way to create $m_z = 0$ state. If we have 4 spin $1/2$ particles, then the answer will be:

$$\binom{4}{2} = \frac{4!}{2!2!} = 6$$

If we have 8 spin $1/2$ particles, then the answer will be:

$$\binom{8}{4} = \frac{8!}{4!4!} = 70$$

5.4 Transform uncoupled to coupled basis

We have:

$$\otimes_8 \frac{1}{2} = \oplus_{14} 0 \oplus_{28} 1 \oplus_{20} 2 \oplus_7 3 \oplus_1 4$$

We only want to look at the $S_{tot} = 0$ subspace. This gives us the 14×14 matrix. The question now is how to go from uncoupled to coupled basis in the matrix format? Let's listed out that 14 states in the uncoupled basis:

$$|\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\rangle$$

1. For the $m_z = 0$ block, we only know the dimension will be 70×70 . How to know which 14 of them are corresponds to the $S_{tot} = 0$? If we know these 14 states, then we can easily construct the cg coefficient to transform them in the coupled basis.

Things to do:

1. Construct $m_z = 0$ A matrix and the dimension will be 70×70 .
2. construct *c.g.* coefficients transformation matrix, and transform A into the block diagonal form to extract only the $S_{tot} = 0$ block.

5.5 Tasks

1. Perform perturbation theory.

6 Construct $m_z = 0$ block

Coupled basis:

$$S_{tot} = 0 : \{|0, 0, 1\rangle, \dots, |0, 0, 14\rangle\}$$

$$S_{tot} = 1 : \{|1, 0, 1\rangle, \dots, |1, 0, 28\rangle\}$$

$$S_{tot} = 2 : \{|2, 0, 1\rangle, \dots, |2, 0, 20\rangle\}$$

$$S_{tot} = 3 : \{|3, 0, 1\rangle, \dots, |3, 0, 7\rangle\}$$

$$S_{tot} = 4 : \{|4, 0, 1\rangle, \dots, |4, 0, 1\rangle\}$$

See one example: $|0, 0, 1\rangle = a_1 |\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\rangle + \dots + a_{70} |\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$

a_1, \dots, a_{70} are the c.g. coefficients.

We know that $[S^2, S_z] = 0$, this means they shared a common eigenbasis.

$$S^2 |s, m\rangle = \hbar s(s+1) |s, m\rangle, \quad S_z |s, m\rangle = \hbar m |s, m\rangle.$$

We can first construct S^2 matrix, then diagonalize it to obtain eigenvectors.

6.1 cg coefficients matrix

Two commuting sets of observables:

$$\{S_{1z}, S_{2z}\}, \quad \{S^2, S_z\}$$

The product basis diagonalizes the first set $|j_1 m_1\rangle \otimes |j_2 m_2\rangle$. $\{|J, M\rangle\}$ is also a complete orthonormal eigenbasis of $\{S^2, S_z\}$. We have two different complete set of orthonormal basis, one defined to be uncoupled basis and the other one defines as the coupled basis. We want to transform from one basis to another basis:

$$I = \sum_{m_1, m_2} |m_1, m_2\rangle \langle m_1, m_2|$$

$$I = \sum_{s, m_z} |s, m_z\rangle \langle s, m_z|$$

We can insert this into $|S, M\rangle$:

$$|J, M\rangle = \sum_{m_1, m_2} |m_1, m_2\rangle \langle m_1, m_2 | J, M\rangle$$

$$= \sum_{m_1, m_2} C_{m_1, m_2}^{J, M} |m_1, m_2\rangle$$

$C_{m_1, m_2}^{S, M}$ is the c.g. coefficients. We can construct an unitary U , its columns are in the coupled basis, and its rows are in the uncoupled basis. If we do:

$$U^\dagger S^2 U = \bigoplus_j H_j, \quad U^\dagger S_z U = \text{diag}(J(J+1)\hbar^2)$$

Each H_j forms a block, and we can concatenate them to form $U^\dagger S^2 U$. We have block diagonal instead of diagonal because each block contains equal eigenvalues and form a degenerate subspace. We have two basis: uncoupled basis $|J, M\rangle$, and coupled basis $|m_1, m_2\rangle$.

1. In the coupled basis, S^2 is block diagonal, and S_z is diagonal.
2. In the uncoupled basis, S_z is diagonal, but S^2 is not diagonal.

Suppose we have 2 spin 1/2 particles, then the cg coefficient matrix will be 4 by 4. The rows are the coupled basis, and the columns are the uncoupled basis. Rows read $\{|1, 1\rangle, |1, 0\rangle, |0, 0\rangle, |1, -1\rangle\}$, columns read $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$. For the cg coefficients matrix, there are 3 blocks because we allow 3 different values of m_z . They are:

1. The first block corresponds to $|1, 1\rangle \rightarrow |\uparrow\uparrow\rangle$. Dimension 1×1 .
2. The second block corresponds to $|1, 0\rangle \rightarrow a|\uparrow\downarrow\rangle + b|\downarrow\uparrow\rangle$. Dimension 2×2 .
3. The third block corresponds to $|0, 0\rangle \rightarrow a'|\downarrow\uparrow\rangle + b'|\uparrow\downarrow\rangle$. Dimension 1×1 .

Within each block, we can order them based on their S_{tot} (total spin number). If diagonalizing $S^2 = P^{-1}DP$, the columns of P are the eigenvectors, D is a diagonal matrix which consists of the eigenvalues/total spin number. Each column of P are the corresponding c.g. coefficients that transforms from uncoupled to coupled basis.

6.2 Intra-cluster and inter-cluster couplings

Each cluster contains 4 spin 1/2 particles and the intra-couplings are described above. Suppose now we have two clusters and we want to model the interactions between these two clusters, in other words, inter-couplings. This could be described by the following equation:

$$H = H_0 + V$$

It is basically the same interaction with the intra-couplings, but the coupling constants are weaker. H_0 can be understood as the intra-couplings and V can be understood as the inter-couplings. Let's define V explicitly:

$$V = \sum_{m, n=1}^4 J'_{m, n} S_m^{(1)} \cdot S_n^{(2)}$$

H_o can be constructed using the following:

$$H_0 = H_1 \otimes I + I \otimes H_2$$

6.3 Structure of the Hamiltonian

We have:

$$H, S_z, S_{1z}, S_{2z}, S^2, S_1^2, S_2^2.$$

m_z spin projection operators:

$$S_{1z} = I \otimes S_z, \quad S_{2z} = S_z \otimes I, \quad S_z = S_{1z} + S_{2z}.$$

Total spin projection operators:

$$S_1^2 = I \otimes S^2, \quad S_2^2 = S^2 \otimes I.$$

$$\begin{aligned} S^2 &= (S_1 + S_2)^2 \\ &= (I \otimes S + S \otimes I)^2 \\ &= (I \otimes S^2 + S \otimes S + S \otimes S + S^2 \otimes I) \\ &= S_1^2 + S_2^2 + 2S_1 \cdot S_2 \end{aligned}$$

$$S^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2$$

operators. The subscript denotes which cluster they belong to. Noticed that:

$$\begin{aligned} [H, S_z] &= 0, \quad [S^2, S_z] = 0. \\ [H_1, S_{1z}] &= 0, \quad [S_1^2, S_{1z}] = 0. \\ [H_2, S_{2z}] &= 0, \quad [S_2^2, S_{2z}] = 0. \end{aligned}$$

If an operator commutes with the Hamiltonian this means they shared a common eigenbasis, then both A and H are simultaneously block-diagonal.

Connection to our case:

1. If $[H, S^2] = 0$, then H can be block-diagonalized and each block is labeled by the S_{tot} number.
2. If $[H, S_1^2] = [H, S_2^2] = 0$, then within each S_{tot} , it can be further block-diagonalized and each block is labeled by the S_1 or S_2 number.

In our case, we want $[H, S_1^2] = [H, S_2^2] = 0$ to be true because within the $S_{tot} = 0$ manifold, we want it to be block-diagonal in order to apply the quasi-degenerate perturbation theory. If H commutes with both S_1^2 and S_2^2 , those subspaces do not mix, giving a block-diagonal structure, which means:

$$H_{s_{tot}=0} = H_{(S_1=S_2=0)} \oplus H_{(S_1=S_2=1)} \oplus H_{(S_1=S_2=2)}$$

Now, we know we have to satisfy 3 commutator relations, namely,

$$[H, S^2] = [H, S_1^2] = [H, S_2^2] = 0.$$

This will give us conditions to set the intra-couplings and inter-couplings.

6.3.1 Within each cluster

$$S_1 = S_{1x} + S_{1y} + S_{1z}, \quad S_2 = S_{2x} + S_{2y} + S_{2z}, \quad H_0 = J' S_1 \cdot S_2$$

We want $[H, S_1^2] = [H, S_2^2] = 0$. We know that $S_\alpha^2 (\alpha = 1, 2)$ commutes with each of its component, namely, S_x, S_y, S_z . We know that $[S_1^2, S_{1\beta}] = 0, (\beta = x, y, z)$, Proof:

$$\begin{aligned} S_1^2 &= [S_{1x}, S_{1y}, S_{1z}] \cdot [S_{1x}, S_{1y}, S_{1z}] \\ &= S_{1x}^2 + S_{1y}^2 + S_{1z}^2 \\ &= \frac{3}{4}I \\ [S_1^2, S_\beta] &= \frac{9}{16}(IS_\beta - S_\beta I) \\ &= \frac{9}{16}(S_\beta - S_\beta) \\ &= 0 \end{aligned}$$

6.4 Quasi-Degenerate Perturbation Theory

Suppose I have the Hamiltonian H in this form:

$$H = H^0 + H'$$

H^0 with the known eigenvalues E_n and eigenfunctions $|\psi_n\rangle$, and H' which is treated as a perturbation.

We assume that we can divide the set of eigenfunctions of H^0 into weakly we want use subset A to perform calculations that we're interested in and discard the subset B . This is basically the idea of quasi-degenerate perturbation theory, we want to construct a Hermitian matrix S and use it to perform the transformation to obtain \tilde{H} such that the eigenfunctions are partition into two subsets A and B . The transformation is depicted below(Similarity Transformation):

$$\tilde{H} = e^{-S} H e^S$$

Now the question is how do we construct that matrix S such that we have our desired transformation. First, let's Taylor expand e^S in the following way:

$$\begin{aligned} e^S &= \sum_{n=0}^{\infty} \frac{S^n}{n!} \\ &= 1 + S + \frac{1}{2!}S^2 + \frac{1}{3!}S^3 + \dots \end{aligned}$$

Substitute this back to the above equation:

$$\begin{aligned}
\tilde{H} &= (1 + S + \frac{1}{2!}S^2 + \frac{1}{3!}S^3 + \dots)H(1 + S + \frac{1}{2!}S^2 + \frac{1}{3!}S^3 + \dots) \\
&= (H + SH + \frac{1}{2!}S^2H + \frac{1}{3!}S^3H + \dots)(1 + S + \frac{1}{2!}S^2 + \frac{1}{3!}S^3 + \dots) \\
&= H + [H, S] + \frac{1}{2}[[H, S], S] + \dots \\
&= \sum_{n=0}^{\infty} \frac{[H, S]^{(n)}}{n!}
\end{aligned}$$

$[H, S]^{(n)} = [[H, S], S], S] \dots, S]$ nested commutator n times. This sort of means $\tilde{H} = e^{-S}He^S = e^{[H, S]}$. We can partition the H into three parts H^0, H^1, H^2 .

$$\tilde{H} = H^0 + H^1 + H^2 + [H^0, S^1] + O((H^2)^2)$$

H^0, H_1 are block-diagonal, and $H_2, [H^0, S^1]$ are off-block-diagonal. The block-diagonal part of

$$\tilde{H}_d = \sum_{j=1}^{\infty} \frac{1}{(2j)!} [H^0 + H^1, S]^{(2j)} + \sum_{j=0}^{\infty} \frac{1}{(2j+1)!} [H^2, S]^{2j+1}$$

The non-block-diagonal part of:

$$\tilde{H}_n = \sum_{j=1}^{\infty} \frac{1}{(2j+1)!} [H^0 + H^1, S]^{(2j+1)} + \sum_{j=0}^{\infty} \frac{1}{(2j)!} [H^2, S]^{2j}$$

We want the non-off-diagonal part to vanish, this means:

$$\begin{aligned}
[H^0, S^{(1)}] &= -H^2, \\
[H^0, S^{(2)}] &= -[H^1, S^{(1)}], \\
[H^0, S^{(3)}] &= -[H^1, S^{(2)}] - \frac{1}{3}[[H^2, S^{(1)}], S^{(1)}]
\end{aligned}$$

We assumed H^0 is block-diagonal and can be written as:

$$H^0 = \begin{pmatrix} H_{PP}^0 & 0 \\ 0 & H_{QQ}^0 \end{pmatrix}$$

And S is off-block-diagonal by construction and has the form of:

$$S^{(1)} = \begin{pmatrix} 0 & S_{PQ} \\ S_{QP} & 0 \end{pmatrix}$$

The $[H^0, S^{(1)}]$ will be a off-block-diagonal:

$$[H^0, S^{(1)}] = \begin{pmatrix} 0 & H_{PP}^0 S_{PQ}^0 - S_{PQ} H_{QQ}^0 \\ H_{QQ}^0 S_{QP}^0 - S_{QP} H_{PP}^0 & 0 \end{pmatrix}$$

Basically everytime when we have block-diagonal and off-block-diagonal, then the commutator of them will be off-block-diagonal. The idea of Quasi-Perturbation theory is that the unperturbed Hamiltonian is block-diagonal, but the perturbed Hamiltonian is not and it mixes the low (P) and high (Q) energy manifold. Quasi-degenerate perturbation theory systematically removes the couplings between P and Q up to some order in V .

7 Consequences of commuting operators

1. If an operator commutes with the Hamiltonian, this means the physical observable of that operator is conserved.
2. If two operators commute, this means they can be simultaneously diagonalized and they can be labeled with their eigenvalues, namely quantum numbers.

Let's focus on case 2, in the shared eigenbasis, every operator in the commuting set is block-diagonal and each block corresponds to a common eigenspace. Physically, this means you can label each basis state by m_1 and m_2 quantum numbers, and operators built from them won't mix states with different m_1 and m_2 .

Rule of Thumb:

Every Hermitian operator that commutes with the Hamiltonian adds another quantum number, and hence another block structure. There are two operators that commute with the Hamiltonian, then I can simultaneously diagonalize them and fully separate the corresponding subspaces.