Quantum Mechanics II Lecture 2

1 Introduction

- **Degenerate Perturbation Theory:** Discusses systems where degeneracy occurs in the unperturbed Hamiltonian.

2 Two-Fold Degeneracy

Two-Fold Degeneracy:

- Only two states are degenerate.
- Suppose:

$$H^{(0)}\,\psi_a^{(0)} = E^{(0)}\,\psi_a^{(0)}, \quad H^{(0)}\,\psi_b^{(0)} = E^{(0)}\,\psi_b^{(0)}, \quad \langle \psi_a^{(0)} | \psi_b^{(0)} \rangle = \delta_{a,b}$$

Theorem 1. ***Superposition of States:***

- *Any state can be written as a linear combination:*

$$\psi^{(0)} = \alpha\,\psi_a^{(0)} + \beta\,\psi_b^{(0)}$$

- *This is also an eigenstate of $H^{(0)}$.*

Proof. Note that

$$\begin{aligned}
\langle \psi^{(0)} | H^{(0)} | \, \psi^{(0)} \rangle &= \left(\alpha^* \langle \psi_a^{(0)} | + \beta^* \langle \, \psi_b^{(0)} | \right) H^{(0)} \left(\alpha\,\psi_a^{(0)} + \beta\,\psi_b^{(0)} \right) \\
&= \alpha^*\,\alpha\,\langle \psi_a^{(0)} | H^{(0)} | \, \psi_a^{(0)} \rangle + \alpha^*\,\beta\,\langle \psi_a^{(0)} | H^{(0)} | \, \psi_b^{(0)} \rangle \\
&\quad + \beta^*\,\alpha\,\langle \psi_b^{(0)} | H^{(0)} | \, \psi_a^{(0)} \rangle + \beta^*\,\beta\,\langle \psi_b^{(0)} | H^{(0)} | \, \psi_b^{(0)} \rangle \\
&= \alpha^*\,\alpha\,E^{(0)} + \beta^*\,\beta\,E^{(0)} = E^{(0)}
\end{aligned}$$

The last equality holds, since $H^{(0)}$ is diagonal in the degenerate subspace. □

Perturbation Theory:

Hamiltonian:

$$H = H^{(0)} + \lambda\,H'$$

where λ is the perturbation parameter.

Eigenvalue Equation:

$$H\,\psi = E\,\psi$$

Assumptions:

$$E = E^{(0)} + \lambda\,E^{(1)} + \lambda^2\,E^{(2)} + \cdots$$

$$\psi = \psi^{(0)} + \lambda\,\psi^{(1)} + \lambda^2\,\psi^{(2)} + \cdots$$

Diagonalization:

- To find "good states" that diagonalize H, assume:

$$\psi^{(0)} = \alpha\,\psi_a^{(0)} + \beta\,\psi_b^{(0)}$$

- Combine them:

$$H^{(0)}\,\psi^{(0)} + \lambda\,(H'\,\psi^{(0)} + H^{(0)}\,\psi^{(1)}) + \cdots = E^{(0)}\,\psi^{(0)} + \lambda\,[E^{(1)}\,\psi^{(0)} + E^{(0)}\,\psi^{(1)}] + \cdots$$

First-Order Approximation:

- At the first order of λ:

$$H^{(0)}\,\psi^{(1)} + H'\,\psi^{(0)} = E^{(1)}\,\psi^{(0)} + E^{(0)}\,\psi^{(1)}$$

Solution:

- Solve for $\psi^{(1)}$ and $E^{(1)}$ using the above equation.

Matrix Representation of the Perturbed Hamiltonian:

- The unperturbed Hamiltonian $H^{(0)}$ is diagonal in the degenerate subspace.
- The first-order perturbation H' is represented by the matrix W in the basis of degenerate states:

$$W = \begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix}$$

where

$$W_{ij} = \langle \psi_i^{(0)} | H' | \psi_j^{(0)} \rangle.$$

Eigenvalue Equation in Matrix Form:

- The eigenvalue problem for the perturbed system is written as:

$$W \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E^{(1)} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}.$$

- Using the determinant condition:

$$\det\,(W - E^{(1)}\,I) = 0,$$

where I is the identity matrix.

Solution for Eigenvalues:

- The eigenvalues $E^{(1)}$ are obtained by solving the characteristic equation:

$$\det \begin{bmatrix} W_{aa} - E^{(1)} & W_{ab} \\ W_{ba} & W_{bb} - E^{(1)} \end{bmatrix} = 0.$$

- This results in:

$$(W_{aa} - E^{(1)})\,(W_{bb} - E^{(1)}) - W_{ab}\,W_{ba} = 0.$$

- Solving for $E^{(1)}$:

$$E_{\pm}^{(1)} = \frac{W_{aa} + W_{bb}}{2} \pm \sqrt{\left(\frac{W_{aa} - W_{bb}}{2}\right)^2 + W_{ab}\,W_{ba}}.$$

References:

- See Chapter 4, Eq. (4.15) for the "Spin" problem as an example application.

Boxed Final Answer for Eigenvalues:

$$\boxed{E_{\pm}^{(1)} = \frac{W_{aa} + W_{bb}}{2} \pm \sqrt{\left(\frac{W_{aa} - W_{bb}}{2}\right)^2 + W_{ab}\, W_{ba}}}$$

Example 1. (Spin)

- The perturbation matrix W is:

$$W = \begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix}.$$

- Define $\Delta\, W = W_{bb} - W_{aa}$ and $W_{ab} = W_{ba}^{*}$.

Rotated Basis:

- The rotated basis is defined by the angle θ and phase ϕ:

$$\cos\theta = \frac{\Delta\, W}{\sqrt{(\Delta\, W)^2 + |W_{ab}|^2}}, \quad W_{ab} = |W_{ab}|\, e^{-i\phi}.$$

Good States:

- The "good states" $\psi_{+}^{(0)}$ and $\psi_{-}^{(0)}$ are:

$$\psi_{+}^{(0)} = \begin{pmatrix} \cos\frac{\theta}{2}\, e^{i\frac{\phi}{2}} \\ \sin\frac{\theta}{2}\, e^{-i\frac{\phi}{2}} \end{pmatrix}, \quad \psi_{-}^{(0)} = \begin{pmatrix} \sin\frac{\theta}{2}\, e^{-i\frac{\phi}{2}} \\ -\cos\frac{\theta}{2}\, e^{i\frac{\phi}{2}} \end{pmatrix}.$$

Orthogonality Check:

- Verify the orthonormal properties:

$$\langle \psi_{+}^{(0)} | \psi_{-}^{(0)} \rangle = 0, \quad \langle \psi_{+}^{(0)} | \psi_{+}^{(0)} \rangle = 1, \quad \langle \psi_{-}^{(0)} | \psi_{-}^{(0)} \rangle = 1.$$

Expectation Values:

- Compute the expectation values of the perturbation H' in the good states:

$$\langle \psi_{+}^{(0)} | H' |\, \psi_{+}^{(0)} \rangle = \bar{W} + \Delta\, W, \quad \langle \psi_{-}^{(0)} | H' |\, \psi_{-}^{(0)} \rangle = \bar{W} - \Delta\, W,$$

where $\bar{W} = \frac{W_{aa} + W_{bb}}{2}$.

Summary:

- The "good states" $\psi_{+}^{(0)}$ and $\psi_{-}^{(0)}$ are linear combinations of the degenerate states $\psi_{a}^{(0)}$ and $\psi_{b}^{(0)}$ that diagonalize the perturbation matrix W.
- The first-order corrections to the energy levels are given by:

$$E^{(1)} = \bar{W} \pm \Delta\, W,$$

where $\Delta\, W = \sqrt{\left(\frac{W_{aa} - W_{bb}}{2}\right)^2 + W_{ab}\, W_{ba}}$.

Boxed Final Answer:

$$\boxed{\psi_+^{(0)} = \begin{pmatrix} \cos\frac{\theta}{2}\, e^{i\frac{\phi}{2}} \\ \sin\frac{\theta}{2}\, e^{-i\frac{\phi}{2}} \end{pmatrix}, \quad \psi_-^{(0)} = \begin{pmatrix} \sin\frac{\theta}{2}\, e^{-i\frac{\phi}{2}} \\ -\cos\frac{\theta}{2}\, e^{i\frac{\phi}{2}} \end{pmatrix}}$$

3 Higher-Order Degeneracy

N-fold degeneracy = N-states with the same energy. Use the basis $\{\psi_1, \psi_2, \ldots, \psi_N\}$ to express H' as a matrix,

$$W_{ij} \equiv \langle \psi_i | H' | \psi_j \rangle$$

Example. (6.2) 3D cubic well

$$V(x, y, z) = \begin{cases} 0 & x, y, z \in [0, a] \\ \infty & \text{otherwise} \end{cases}$$

unperturbed statets

$$\psi_{n_x, n_y, n_z}^{(0)} = \left(\frac{2}{a}\right)^{3/2} \sin\!\left(\frac{n_x \pi}{a} x\right) \sin\!\left(\frac{n_y \pi}{a} x\right) \sin\!\left(\frac{n_z \pi}{a} x\right),$$

$$E_{n_x, n_y, n_z}^{(0)} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 (n_x^2 + n_y^2 + n_z^2).$$

Ground State Energy:

$$E_0^{(0)} = \frac{\pi^2 \hbar^2}{2\, m\, a^2} (1 + 1 + 1) = \frac{3\, \pi^2 \hbar^2}{2\, m\, a^2}$$

First Excited States:

$$\psi_a = \psi_{112}, \quad \psi_b = \psi_{121}, \quad \psi_c = \psi_{211}$$

$$E_1^{(0)} = \frac{\pi^2 \hbar^2}{2\, m\, a^2} (2^2 + 1 + 1) = \frac{3\, \pi^2 \hbar^2}{m\, a^2}$$

Perturbation:

- A perturbation H' is introduced as:

$$H' = \begin{cases} V_0, & x, y \in [0, \frac{a}{2}] \\ 0, & \text{elsewhere} \end{cases}$$

First-Order Correction to Energy:

- The first-order correction to the energy is given by:

$$E_0^{(1)} = \langle \psi_{111}^{(0)} | H' | \, \psi_{111}^{(0)} \rangle$$

- Explicitly, this becomes:

$$\boxed{E_0^{(1)} = \left(\frac{2}{a}\right)^3 V_0 \left(\int_0^{\frac{a}{2}} \sin^2\!\left(\frac{\pi}{a} x\right) d\, x\right)^2 \int_0^a \sin^2\!\left(\frac{\pi}{a} z\right) d\, z}$$

- Since the integral evaluates to a non-zero value, $E_0^{(1)} \neq 0$.

Perturbation Matrix Element W_{aa}

Definition:

$$W_{aa} = \langle \psi_a | H' | \psi_a \rangle$$

where $\psi_a = \psi_{112}$.

Expression:

$$W_{aa} = \left(\frac{2}{a}\right)^3 V_0 \int_0^a dx \sin^2\!\left(\frac{\pi}{a} x\right) \int_0^a dy \sin^2\!\left(\frac{\pi}{a} y\right) \int_0^a dz \sin^2\!\left(\frac{2\pi}{a} z\right)$$

Simplified:

$$W_{aa} = \frac{1}{6} V_0 \neq 0$$

Perturbation Matrix Element W_{ab}

Definition:

$$W_{ab} = \langle \psi_a | H' | \psi_b \rangle$$

where $\psi_a = \psi_{112}$ and $\psi_b = \psi_{121}$.

Expression:

$$W_{ab} = \left(\frac{2}{a}\right)^3 V_0 \int_0^a dx \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{\pi}{a} x\right) \int_0^a dy \sin\left(\frac{\pi}{a} y\right) \sin\left(\frac{2\pi}{a} y\right) \int_0^a dz \sin\left(\frac{2\pi}{a} z\right) \sin\left(\frac{\pi}{a} z\right)$$

Simplified:

$$W_{ab} = 0$$

Key Observations:

- H' does not couple ψ_a and ψ_b because $W_{ab} = 0$.
- Similarly, $W_{ac} = 0$, indicating that H' does not couple ψ_a and ψ_c.

Perturbation Matrix Element W_{bc}

Definition:

$$W_{bc} = \langle \psi_b | H' | \psi_c \rangle$$

where $\psi_b = \psi_{121}$ and $\psi_c = \psi_{211}$.

Expression:

$$W_{bc} = \left(\frac{2}{a}\right)^3 V_0 \int_0^a dx \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{2\pi}{a} x\right) \int_0^a dy \sin\left(\frac{2\pi}{a} y\right) \sin\left(\frac{\pi}{a} y\right) \int_0^a dz \sin^2\!\left(\frac{\pi}{a} z\right)$$

Simplified:

$$W_{bc} = \frac{16}{9\pi^2} V_0 \neq 0$$

Matrix Representation of $\boldsymbol{W}$

$$W = \begin{bmatrix} W_{aa} & W_{ab} & W_{ac} \\ W_{ba} & W_{bb} & W_{bc} \\ W_{ca} & W_{cb} & W_{cc} \end{bmatrix}$$

Substitution:

$$W = \begin{bmatrix} \frac{1}{6} V_0 & 0 & 0 \\ 0 & \frac{1}{6} V_0 & \frac{16}{9\pi^2} V_0 \\ 0 & \frac{16}{9\pi^2} V_0 & \frac{1}{6} V_0 \end{bmatrix}$$

Diagonalization of $\boldsymbol{W}$:

- The diagonal elements represent the unperturbed energy levels.
- The off-diagonal elements represent the coupling between states.

Eigenvalues:

- The eigenvalues of W give the first-order corrections to the energy levels.

Good States:

- The eigenstates of W correspond to "good states" that diagonalize the perturbation.

$$\boxed{W = \begin{bmatrix} \frac{1}{6} V_0 & 0 & 0 \\ 0 & \frac{1}{6} V_0 & \frac{16}{9\pi^2} V_0 \\ 0 & \frac{16}{9\pi^2} V_0 & \frac{1}{6} V_0 \end{bmatrix}}$$

The eigenstates ψ_2 and ψ_3 are written as column vectors:

$$\psi_2 = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{-i\phi} \end{pmatrix}, \quad \psi_3 = \begin{pmatrix} \sin\frac{\theta}{2} e^{i\phi} \\ -\cos\frac{\theta}{2} \end{pmatrix}$$

Derivation:

1. **Rotation Angle $\boldsymbol{\theta}$:**
    - The angle θ is defined as:

$$\cos\theta = \frac{1-\lambda}{\sqrt{1+\lambda^2}}$$

- This expression arises from the perturbation theory, where λ is a parameter related to the perturbation strength.

1. **Phase Factor ϕ:**

   - The phase ϕ is determined by the perturbation matrix elements. Here, it is given as:

$$\omega_{12}^{a} = s_{12}^{b} \cdot \sqrt{2}$$

- If k is zero, then $\phi = 0$.

Orthonormality of Eigenstates

The eigenstates ψ_2 and ψ_3 are orthonormal:

- **Normalization:**

$$\langle \psi_2 | \psi_2 \rangle = 1, \quad \langle \psi_3 | \psi_3 \rangle = 1$$

- **Orthogonality:**

$$\langle \psi_2 | \psi_3 \rangle = 0$$

Explicit Check:

Normalization of ψ_2:

$$\langle \psi_2 | \psi_2 \rangle = \left| \cos \frac{\theta}{2} \right|^2 + \left| \sin \frac{\theta}{2} e^{-i\phi} \right|^2 = \cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2} = 1$$

Normalization of ψ_3:

$$\langle \psi_3 | \psi_3 \rangle = \left| \sin \frac{\theta}{2} e^{i\phi} \right|^2 + \left| -\cos \frac{\theta}{2} \right|^2 = \sin^2 \frac{\theta}{2} + \cos^2 \frac{\theta}{2} = 1$$

Orthogonality:

$$\langle \psi_2 | \psi_3 \rangle = \cos \frac{\theta}{2} \left(-\cos \frac{\theta}{2} \right) + \sin \frac{\theta}{2} e^{-i\phi} \left(\sin \frac{\theta}{2} e^{i\phi} \right) = -\cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2} = 0$$

Linear Combinations of Original States

The eigenstates ψ_2 and ψ_3 can be expressed as linear combinations of the original degenerate states $\psi_2^{(0)}$ and $\psi_3^{(0)}$:

$$\psi_2^{(0)} = \frac{1}{\sqrt{2}} \psi_2 + \frac{1}{\sqrt{2}} \psi_3, \quad \psi_3^{(0)} = \frac{1}{\sqrt{2}} \psi_2 - \frac{1}{\sqrt{2}} \psi_3$$

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- **Orthogonality:**

$$\langle \psi_2 | \psi_3 \rangle = 0$$

Explicit Check:

Normalization of $\boldsymbol{\psi_2}$:

$$\langle \psi_2 | \psi_2 \rangle = \left|\cos\frac{\theta}{2}\right|^2 + \left|\sin\frac{\theta}{2}e^{-i\phi}\right|^2 = \cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} = 1$$

Normalization of $\boldsymbol{\psi_3}$:

$$\langle \psi_3 | \psi_3 \rangle = \left|\sin\frac{\theta}{2}e^{i\phi}\right|^2 + \left|-\cos\frac{\theta}{2}\right|^2 = \sin^2\frac{\theta}{2} + \cos^2\frac{\theta}{2} = 1$$

Orthogonality:

$$\langle \psi_2 | \psi_3 \rangle = \cos\frac{\theta}{2}\left(-\cos\frac{\theta}{2}\right) + \sin\frac{\theta}{2}e^{-i\phi}\left(\sin\frac{\theta}{2}e^{i\phi}\right) = -\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} = 0$$

Linear Combinations of Original States

The eigenstates ψ_2 and ψ_3 can be expressed as linear combinations of the original degenerate states $\psi_2^{(0)}$ and $\psi_3^{(0)}$:

$$\psi_2^{(0)} = \frac{1}{\sqrt{2}}\psi_2 + \frac{1}{\sqrt{2}}\psi_3, \quad \psi_3^{(0)} = \frac{1}{\sqrt{2}}\psi_2 - \frac{1}{\sqrt{2}}\psi_3$$

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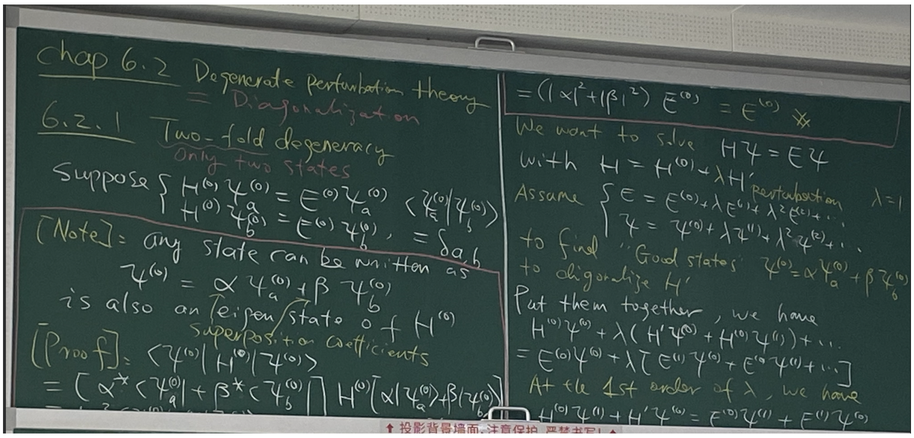

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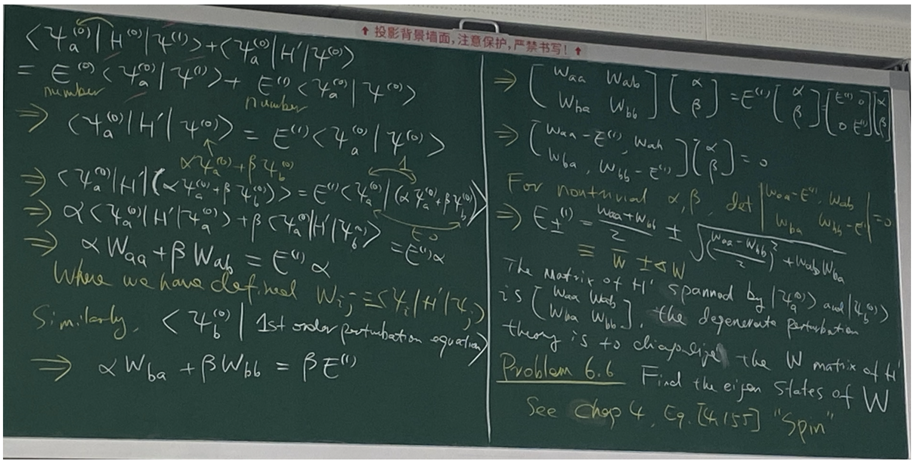

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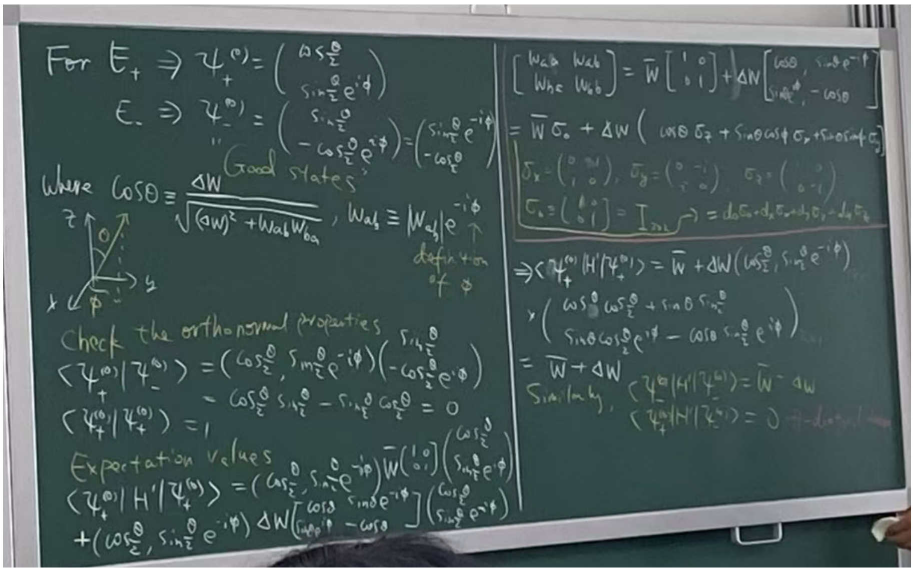

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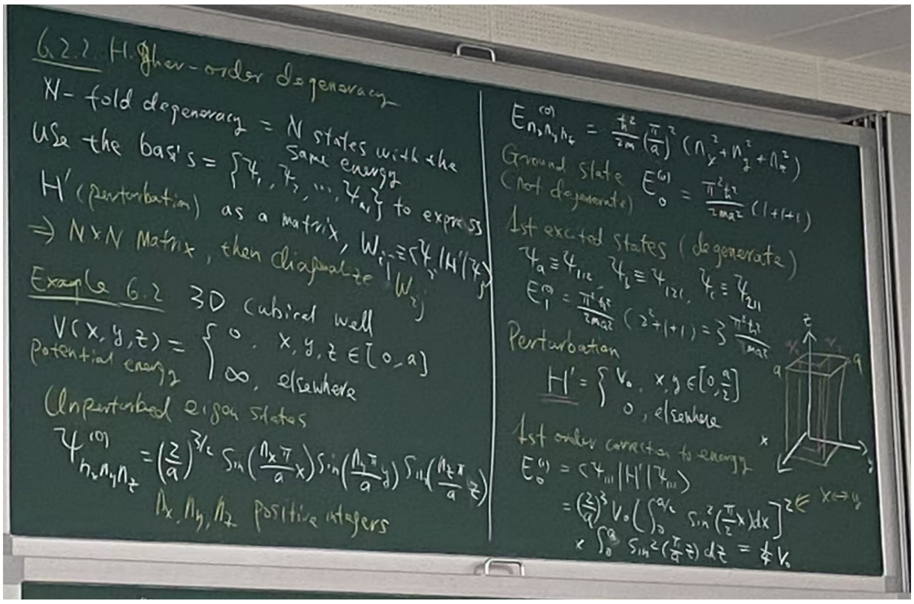

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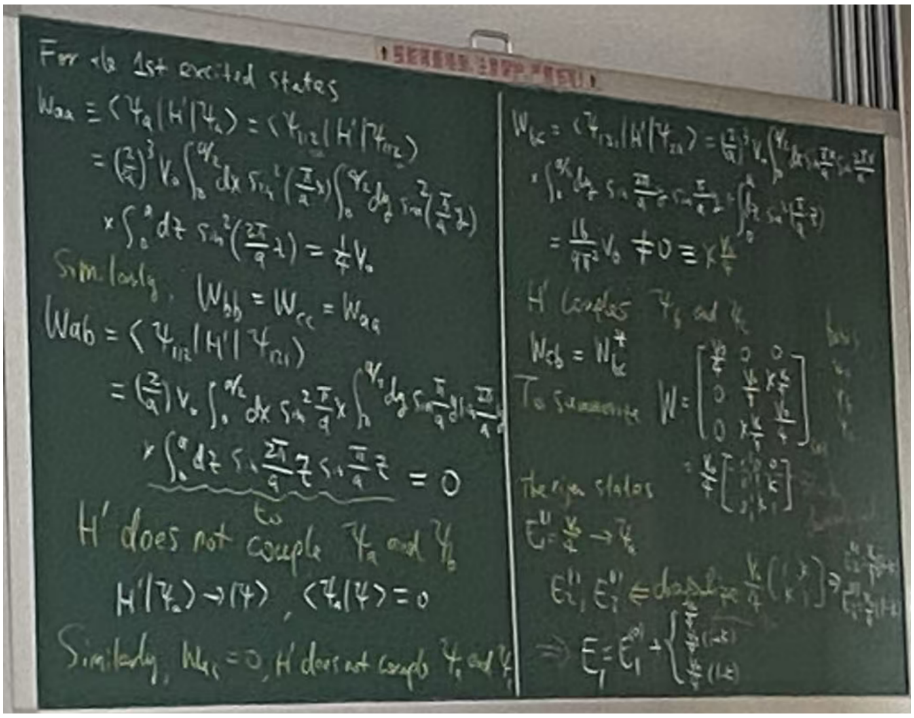

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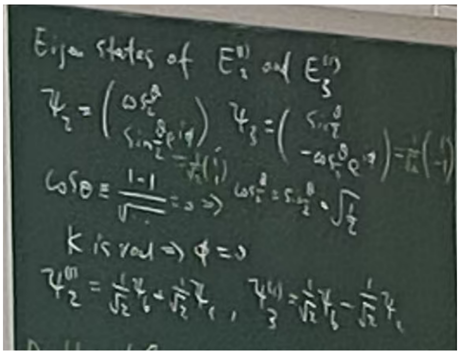

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