Lecture FYS4480/9480 August 21, 2025

$$\hat{\mathcal{H}}|\Psi_i\rangle = E_i|\Psi_i\rangle$$

split $\mathcal{H}$ into

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_I$$

non-interacting (perturbative)

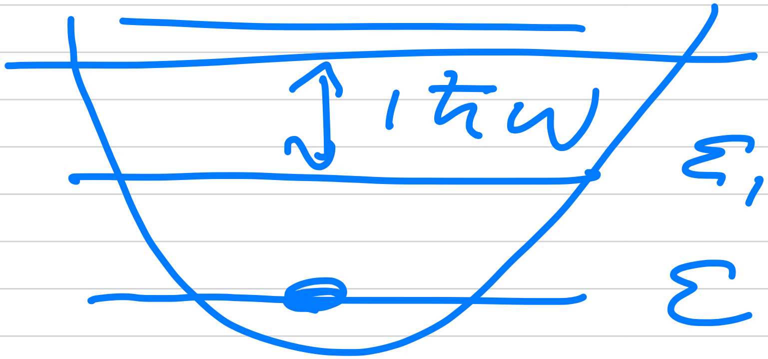
inter-acting part

Examples

Harmonic

ε_2 oscillator

1-dim

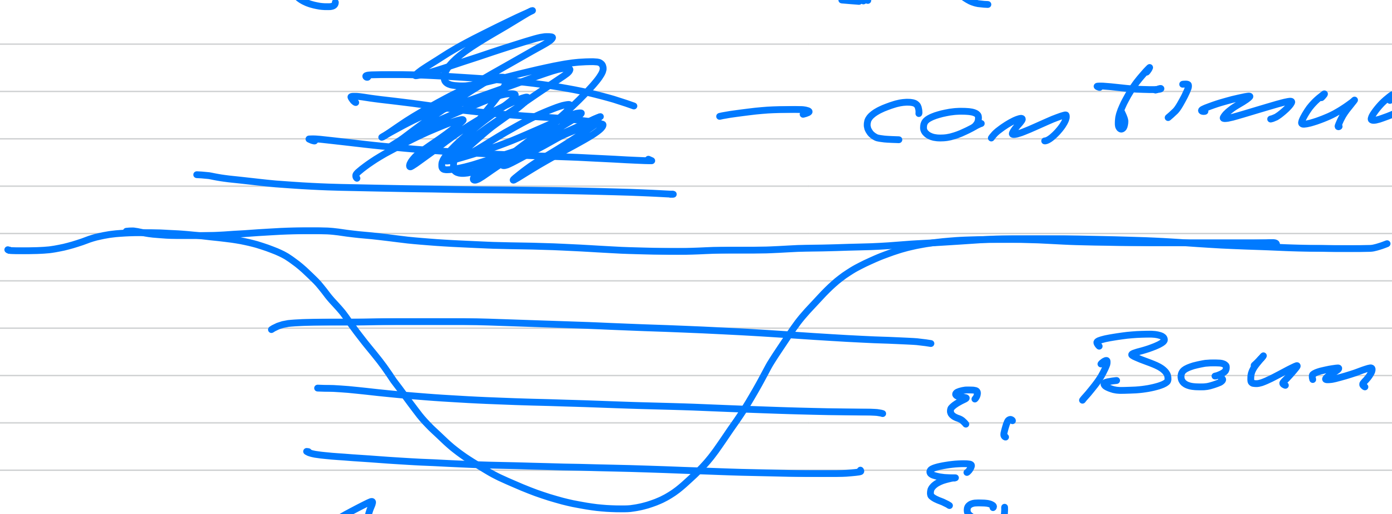


ε_1

ε_0

$i = 0, 1, 2, \ldots \infty$

$$\varepsilon_i = \hbar\omega\left(i + 1/2\right)$$



– continuum

$\varepsilon = 0$

Bound states

ε_1

ε_0

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$$

1-dim HO

$$\psi_n(x) = H_n(x)\, e^{-\alpha x^2/2}$$

$$E_n = \hbar\omega(n + 1/2)$$

$\psi_n(x)$ is $\boxed{\text{ONB}}$ $|\psi_n\rangle$

$$\langle \psi_n | \psi_m \rangle = \int_{-\infty}^{\infty} dx\, \psi_n^*(x)\, \psi_m(x)$$

$$= \delta_{mn}$$

start point to define computational basis computational basis

$$|\phi_i\rangle \qquad i = 0, 1, 2, \ldots \infty$$

$$\hat{h}_0 |\phi_i\rangle = \varepsilon_i |\phi_i\rangle$$

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}$$

$$\hat{\mathcal{H}} |\psi_i\rangle = E_i |\psi_i\rangle$$

$$\left(\hat{\mathcal{H}} |\phi_i\rangle \neq E_i |\phi_i\rangle \right)$$

$$|\psi_i\rangle = \sum_{j=0}^{\infty} u_{ij} |\phi_j\rangle$$

$$u_{ij} = \langle \psi_i | \phi_j \rangle$$

$$|\psi\rangle = U|\phi\rangle$$

unitary matrix

$$U^{\dagger}U = \mathbb{1} \qquad U^{\dagger} = U^{-1}$$

$$= UU^{\dagger} = \mathbb{1}$$

$$|\psi_i\rangle = \sum_{j=0}^{\infty} u_{ij}\,|\phi_j\rangle \simeq \sum_{j=0}^{d} u_{ij}\,|\phi_j\rangle$$

dimension of our reduced space

Two-level system

$$H_0 |\phi_i\rangle = \varepsilon_i |\phi_i\rangle$$

$$\text{———} \quad \varepsilon_1 \qquad |\phi_1\rangle \qquad \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\text{———} \quad \varepsilon_0 \qquad |\phi_0\rangle \qquad \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\langle \phi_0 | \phi_1 \rangle = 0 = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0$$

> computational basis

$$|\psi_0\rangle = \underbrace{\alpha}_{u_{00}} |\phi_0\rangle + \underbrace{\beta}_{u_{01}} |\phi_1\rangle$$

$$|\psi_1\rangle = \underbrace{\gamma}_{u_{10}} |\phi_0\rangle + \underbrace{\delta}_{u_{11}} |\phi_1\rangle$$

$$\mathcal{H}|\psi_i\rangle = E_i|\psi_i\rangle$$

Technicality:

$$|\phi_0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |\phi_1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Completeness

$$\mathbb{1} = \sum_{i=0}^{1} |\phi_i\rangle\langle\phi_i|$$

$$= \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}}_{|\phi_0\rangle\langle\phi_0|} + \underbrace{\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}}_{|\phi_1\rangle\langle\phi_1|}$$

$$\hat{P} = |\phi_0\rangle\langle\phi_0|$$

$$\hat{Q} = |\phi_1\rangle\langle\phi_1|$$

$$\mathbb{1} = \hat{P} + \hat{Q} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\hat{P}^2 = \hat{P} \qquad \hat{Q}^2 = \hat{Q}$$

$$[\hat{P}, \hat{Q}] = \hat{P}\hat{Q} - \hat{Q}\hat{P} = 0$$

$$\hat{P} \cdot \hat{Q} = 0$$

$$\hat{P}|\psi_0\rangle = \begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\left(\alpha\begin{bmatrix}1\\0\end{bmatrix}+\beta\begin{bmatrix}0\\1\end{bmatrix}\right.$$

$$= \alpha\begin{bmatrix}1\\0\end{bmatrix} = \alpha|\phi_0\rangle$$

$$\hat{Q}|\psi_0\rangle = \beta|\phi_1\rangle$$

$\begin{bmatrix}0\\1\end{bmatrix}$ ———— ε_1^B $\qquad\qquad$ $\begin{bmatrix}0\\1\end{bmatrix}$ ———— ε_1^B

$\begin{bmatrix}1\\0\end{bmatrix}$ ———— ε_0^A $\qquad\qquad$ $\begin{bmatrix}1\\0\end{bmatrix}$ ———— ε_0^B

A $\qquad\qquad\qquad\qquad$ B

Two-particle system

$$|\phi\rangle_{AB} = |\phi_0\rangle_A \otimes |\phi_0\rangle_B$$

$$= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = |00\rangle$$

$$= |0\rangle$$

$|x_0 x_1\rangle$

$$2 \cdot x_0 + x_1 = 0$$

$$\quad\;\; 0 \quad\;\; 0$$

$$|0\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |01\rangle \quad (= |1\rangle)$$

$$2 \cdot \underset{0}{x_0} + \underset{1}{x_1} = 1$$

$$|1\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |10\rangle = |2\rangle$$

$$|1\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |11\rangle = |3\rangle$$

$$\langle 00|01\rangle = 0 \quad \text{etc}$$

ONB

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle$$

$$+ \gamma|10\rangle + \delta|11\rangle$$

$$\hat{H}_0|00\rangle = E_{00}|00\rangle$$

$$H|00\rangle \neq E_0|00\rangle$$

Technical: Notation

single-particle degrees of freedom

$$\varphi_{\underbrace{\alpha}_{\beta\sigma}}(\vec{r}) = \phi_\beta(\vec{r}) \otimes \xi_{\sigma m_\sigma}$$

$\sigma = \frac{1}{2}$ $m_\sigma = \pm 1/2$ $(\uparrow \downarrow)$

$$x = (\vec{r}, \sigma)$$

$$|\varphi_{\alpha\sigma}\rangle = |\alpha\sigma\rangle$$

One way to obey the Pauli principle is to have an ansatz for the state in terms of a determinant

$$\begin{array}{c} \text{specific quantum number} \\ \\ \end{array} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = - \begin{bmatrix} a_{12} & a_{11} \\ a_{22} & a_{21} \end{bmatrix}$$

$$\begin{array}{cc} \uparrow & \uparrow \\ \text{particle } 1 & 2 \end{array}$$