1. Consider an operator A and its eigenfunctions ψ_a, defined over the interval $0 \le x \le L$, and satisfying the boundary conditions $\psi_a(x=0) = \psi_a(x=L)$
Determine the eigenvalues and eigenfunctions of A, if any, for the following cases :

(a) $A = \frac{d}{dx}$.

⇒ i) $A\psi_a(x) = a\psi_a(x)$

$$\frac{d}{dx}\psi_a(x) = a\psi_a(x) \rightarrow \frac{1}{\psi_a(x)} \cdot \frac{d\psi_a(x)}{dx} = a$$

$$\ln \frac{\psi_a(x)}{C} = ax + D$$

$$\therefore \psi_a(x) = N \cdot \exp(ax) \qquad (N = \text{const.})$$

ii) Boundary condition..

$$\psi_a(0) = \psi_a(L)$$

$$\therefore N = N \exp(aL) \quad \rightarrow \exp(aL) = 1$$

$$\therefore aL = i2\pi n \qquad (n = \text{integer})$$

$$\therefore a = i\frac{2\pi n}{L}$$

[∴ For the eigenvalue $a = i\frac{2\pi n}{L}$,
the eigenfunction $\psi_a(x)$ is..
$$\psi_a(x) = N\exp\left(i\frac{2\pi n}{L}x\right)$$]

(b) $A = i\frac{d}{dx} + k$, where k is real, positive and fixed.

⇒ i) $A\psi_a(x) = a\psi_a(x)$

$\downarrow$

$$\left(i\frac{d}{dx} + k\right)\psi_a(x) = a\psi_a(x).$$

$$\therefore \frac{d\psi_a(x)}{dx} = -i(a-k)\psi_a(x).$$

$$\therefore \psi_a(x) = N\exp[-i(a-k)x].$$

ii) B.C. 만족?

$$\psi_a(0) = N$$
$$\psi_a(L) = N\exp[-i(a-k)L]$$ =

$$\therefore \exp[-i(a-k)L] = 1$$

$$\therefore (a-k)L = 2n\pi \quad (n = 정수)$$

$$\therefore a-k = \frac{2n\pi}{L} \qquad a_n = k + \frac{2n\pi}{L}.$$

iii) $\therefore \psi_{a_n}(x) = N \exp\left[-i(a_n - k)x\right]$

where $a_n = k + \dfrac{2n\pi}{L}$. $(n = 정수)$.

eigenvalue

(c) A= the integral operator defined by...

$A\psi = i\int_a^x \psi(y)\,dy$.

⇒ i) eigenvalue 를 α 라 하자.

$\therefore i\int_a^x \psi_\alpha(y)\,dy = \alpha\,\psi_\alpha(x)$

일단 $x = a$ 에서 좌변 0. $\therefore \psi_\alpha(x=a) = 0$

양변 x에 관해 미분.

$i\,\psi_\alpha(x) = \alpha \cdot \dfrac{d\psi_\alpha(x)}{dx} \rightarrow \dfrac{d\psi_\alpha(x)}{dx} = i\dfrac{1}{\alpha}\psi_\alpha(x)$

$\therefore \psi_\alpha(x) = N \cdot \exp\left[i \cdot \dfrac{1}{\alpha}x\right]$

$x = a$ 에서 $\psi_\alpha(x)$는 0이 될 수 없으므로.

$(\exp(ix) \neq 0)$. eigenfunction 존재 X.

2. Consider the eigenvalue equation

$$A\psi_a(x) = a\psi_a(x),$$

defined over the interval $-L \leq x \leq L$ and subject to the boundary conditions.

$$\psi_a(-L) = \psi_a(+L) = 0.$$

(a) If $A = (d/dx)^n$, for what values of n, if any, is A Hermition?

$\Rightarrow$ i) 어떠한 operator $\hat{Q}$가 hermitian 이려면.. 다음 조건을 만족해야 한다.

$$\langle \phi | \hat{Q}\psi \rangle = \langle \hat{Q}\phi | \psi \rangle.$$

이때.. $|\phi\rangle$ 와 $|\psi\rangle$는 가능한 임의의 state.

이를 position space에서 보면..

$$\begin{aligned}\langle \phi | \hat{Q}\psi \rangle &= \langle \phi | \int dx\, |x\rangle\langle x | \hat{Q}\psi \rangle \\ &= \int dx\, \langle x|\phi\rangle^* \, Q(x)\, \langle x|\psi\rangle \\ &= \int dx\, \phi^*(x)\, Q(x)\, \psi(x).\end{aligned}$$

$\hookrightarrow$ $\hat{Q}$의 position space representation

마찬가지 방법으로..

$$\langle \hat{Q}\phi | \psi \rangle = \langle \hat{Q}\phi | \int dx\, |x\rangle\langle x | \psi \rangle$$

$$= \int dx \left[Q(x)\, \phi^*(x) \right] \cdot \psi(x).$$

∴ $\hat{Q}$가 hermitian 이려면..

$$\int dx\, \phi^*(x) \left[Q(x)\, \psi(x) \right] = \int dx \left[Q(x)\, \phi^*(x) \right] \psi(x).$$

ii) 우리 문제의 경우 관심 있는 domain은 $-L \sim L$ 이고.

$Q(x) = \left(\frac{d}{dx}\right)^n$ 이다.

∴ $\left(\frac{d}{dx}\right)^n$ 이 hermitian 이려면 다음식 만족해야 한다.

$$\int_{-L}^{L} dx\, \phi^*(x) \left(\frac{d}{dx}\right)^n \psi(x) = \int_{-L}^{L} \left(\frac{d}{dx}\right)^n \phi^*(x) \cdot \psi(x).$$

좌변을 하나 하나씩 integration by parts해서..

우변으로 만들어보자.

iii)
$$\int_{-L}^{L} \phi^*(x)\left(\frac{d}{dx}\right)^n \psi(x)\, dx$$

$$= \cancel{\phi^*(x)\left(\frac{d}{dx}\right)^{n-1} \psi(x) \Big]_{-L}^{L}} - \int_{-L}^{L} dx \left(\frac{d}{dx}\phi^*(x)\right)\left(\frac{d}{dx}\right)^{n-1}\psi(x)$$

↳ ∵ $\underline{\phi^*(\pm L)=0}$

일단 $n=1$ 일때.. $-$ 부호로 인해 $\left(\frac{d}{dx}\right)$는 hermitian이 아님을 알 수 있다.

iv)
$$\int_{-L}^{L} \phi^*(x)\left(\frac{d}{dx}\right)^n \psi(x)\, dx$$

$$= -\int_{-L}^{L} dx \left(\frac{d}{dx}\right)\phi^*(x) \cdot \left(\frac{d}{dx}\right)^{n-1}\psi(x)$$

$$= -\left(\frac{d}{dx}\right)\phi^*(x) \cdot \left(\frac{d}{dx}\right)^{n-2}\psi(x) \Big]_{x=-L}^{x=L}$$

$$+ \int_{-L}^{L} dx \left(\frac{d}{dx}\right)^2 \phi^*(x) \cdot \left(\frac{d}{dx}\right)^{n-2}\psi(x).$$

이때 만약 $n=2$ 라면.. $\psi(\pm L)=0$ 이므로.. boundary term 이 사라지고.. 따라서 $\left(\frac{d}{dx}\right)^2$ 는 hermitian 임을 알수있다.

ii) fixed ends boundary condition ($\psi(-L) = \psi(L) = 0$)

때문에.. $\left(\frac{d}{dx}\right)^2$ 의 eigenfunction은.. 다음과 같이 주어지게 된다..

$$\text{even} \rightarrow \psi_n^{(even)}(x) = \sqrt{\frac{1}{L}} \cos\left[\frac{(2n+1)\pi}{2L} x\right]$$

$$\text{odd} \rightarrow \psi_n^{(odd)}(x) = \sqrt{\frac{1}{L}} \sin\left[\frac{2n\pi}{2L} \cdot x\right]$$

$$(n = 1, 2, 3, \cdots)$$

여기. 임의의 state를 위 $\left(\frac{d}{dx}\right)^2$ (hermition) 의 eigenfunction 들의 linear combination 으로 쓸 수 있고..
(hermition operator의 eigenfunction은 complete)

따라서

$$\psi(x) = \sum_n \left[\alpha_n \psi_n^{(even)}(x) + \beta_n \psi_n^{(odd)}(x)\right]$$

$$\phi(x) = \sum_n \left[\gamma_n \psi_n^{(even)}(x) + \delta_n \psi_n^{(odd)}(x)\right]$$

로 임의의 state $\psi(x)$, $\phi(x)$ 를 표현할 수 있다.

이제.. 위 state를 이용하면..

$$\int_{-L}^{L} dx\, \phi^*(x) \left[\left(\frac{d}{dx}\right)^{2n} \psi(x)\right] = \int_{-L}^{L} dx \left[\left(\frac{d}{dx}\right)^{2n} \phi^*(x)\right] \psi(x)$$

(n = integer)

임을 보일 수 있다. ∴ $\underline{\left(\frac{d}{dx}\right)^{2n} \text{ 은 hermitian}}$

(b) Find the eigenfunctions of A corresponding to $a=0$ for each of the cases $n=3,4,5$. If there are any degeneracies for a given n, use the Gramm-Schmidt procedure to orthogonalize the degenerate states.

⇒ i) $\left(\frac{d}{dx}\right)^n \psi_0(x) = 0.$ 주어진 eigenvalue problem.

ii) $n=3$

$$\psi_0(x) = ax^2 + bx + c.$$

$n=4$

$$\psi_0(x) = ax^3 + bx^2 + cx + d.$$

$n=5$

$$\psi_0(x) = ax^4 + bx^3 + cx^2 + dx + e.$$

iii) n=3

일단. boundary condition 맞춘다.

$$\psi_0(\pm L) = aL^2 \pm bL + c = 0.$$

간단한 해로.. $a=1$.. $b=0$. $c=-L^2$.

$$\psi(x) = x^2 - L^2.$$

자유도가 3개 (a, b, c), boundary condition이

2개 이므로.. degeneracy 있다?

normalize

$$\int_{-L}^{L} dx \, |N|^2 (x^2-L^2)^2$$

$$= |N|^2 \int_{-L}^{L} dx \left(x^4 - 2L^2x^2 + L^4 \right)$$

$$= 2|N|^2 \cdot \int_0^L dx \, (x^4 - 2L^2x^2 + L^4)$$

$$= 2|N|^2 \left(\frac{1}{5}x^5 - \frac{2}{3}L^2x^3 + L^4x \right) \Big]_{x=0}^{x=L}$$

$$= |N|^2 \cdot 2 \cdot \left[\frac{L^5}{5} - \frac{2}{3}L^5 + L^5 \right].$$

$$= |N|^2 \cdot L^5 \cdot 2 \cdot \frac{3-10+15}{15} = |N|^2 \cdot L^5 \cdot \frac{16}{15}$$

$\therefore \int_{-L}^{L} |N|^2 (x^2-L^2)^2 = |N|^2 \cdot \frac{16}{15} L^5 = 1.$

$\therefore |N|^2 = \frac{1}{L^5} \cdot \frac{15}{16} \rightarrow \underline{N = L^{-5/2} \cdot \frac{\sqrt{15}}{4}}$

$\therefore \underline{\psi(x) = L^{-5/2} \cdot \frac{\sqrt{15}}{4} (x^2-L^2)}$

iv) $n=4$

$\psi(x) = ax^3 + bx^2 + cx + d.$

$\psi(L) = aL^3 + bL^2 + cL + d = 0.$

$\psi(-L) = -aL^3 + bL^2 - cL + d = 0.$

자유도 4개 (a, b, c, d), B.C. 2개.

$\therefore$ 2개의 degenerary 존재.

간단한 두개 의 solution (B.C 만족).

$a=1. \quad b=0. \quad c=-L^2 \quad d=0.$

$a=0. \quad b=1. \quad c=0 \quad d=-L^2$

$\therefore \psi_1(x) = x^3 - L^2 x$

$\psi_2(x) = x^2 - L^2$

이 두 solution 을 Gramm-Schmidt procedure 로. orthogonalize 할 것임.

일단..

$$\psi_0(x) = L^{-5/2}\frac{\sqrt{15}}{4}(x^2-L^2)$$

$$\psi_1'(x) = \psi_1(x) - \left[\int dx\, \psi_0^*(x)\,\psi_1(x)\right]\cdot \psi_0(x)$$

이 계산은 자동으로. $\psi_0(x)$와 orthogonal.

$$\int_{-L}^{L} dx\, L^{-5/2}\frac{\sqrt{15}}{4}(x^2-L^2)\cdot x(x^2-L^2)$$

$$= L^{-5/2}\frac{\sqrt{15}}{4}\underbrace{\int_{-L}^{L} dx\,(x^5 - 2L^2x^3 + L^4x)}_{=0}$$

$=0.$ 이미 orthogonal!

$$\psi_1(x) = N(x^3 - L^2x.)$$

normalization

$$\int_{-L}^{L} dx \ |N|^2 \cdot x^2 (x^2-L^2)^2$$

$$= 2|N|^2 \cdot \int_0^L dx \left(x^6 - 2L^2x^4 + L^4x^2\right)$$

$$= 2|N|^2 \cdot \left[\frac{1}{7}L^7 - \frac{2}{5}L^7 + \frac{1}{3}L^7\right]$$

$$= |N|^2 \cdot 2 \cdot \frac{15-42+35}{105} L^7$$

$$= |N|^2 \cdot L^7 \cdot \frac{16}{105} = 1.$$

$$\therefore N = L^{-7/2} \cdot \frac{\sqrt{105}}{4}.$$

$$\left[\begin{array}{l} \psi_1(x) = L^{-7/2} \dfrac{\sqrt{105}}{4} (x^3 - L^2 x) \\ \psi_2(x) = L^{-5/2} \dfrac{\sqrt{15}}{4} (x^2 - L^2). \end{array}\right.$$

v) $n=5$

$\psi(x) = ax^4 + bx^3 + cx^2 + dx + e$

$\psi(L) = 0$

$\psi(-L) = 0$

자유도 5개. B.C. 2개 → 3개의 degeneracy
존재!

앞선 두 개의 degeneracy는..

$$\left[\begin{array}{l} \psi_1(x) = L^{-7/2} \dfrac{\sqrt{105}}{4} (x^3 - L^2 x) \\ \psi_2(x) = L^{-5/2} \cdot \dfrac{\sqrt{15}}{4} (x^2 - L^2) \end{array}\right.$$

이라고 하자..

나머지 하나를..

$\psi_3(x) = N \cdot (x^4 - L^2 x^2)$ 이라고 정하자.

이제 이놈을.. ψ_1, ψ_2 와 orthogonal 하게

만들것!

$$\psi_3^{(new)}(x) = \psi_3(x) - \overbrace{\left[\int dx\, \psi_1^*(x)\, \psi_3(x) \right]}^{①} \psi_1(x)$$

$$- \underbrace{\left[\int dx\, \psi_2^*(x)\, \psi_3(x) \right]}_{②} \psi_2(x).$$

$$① = \underbrace{\int_{-L}^{L} dx\, L^{-7/2} \frac{\sqrt{105}}{4} (x^3 - L^2 x) \cdot N \cdot (x^4 - L^2 x^2)}_{\text{odd}}$$

$$= 0.$$

$$② = \int_{-L}^{L} dx\, L^{-5/2} \frac{\sqrt{15}}{4} (x^2 - L^2) \cdot x^2 (x^2 - L^2)\, N$$

$$= N \cdot \frac{\sqrt{15}}{4} L^{-5/2}\, 2 \cdot \int_0^L dx\, (x^6 - 2L^2 x^4 + L^4 x^2)$$

$$= N \cdot \frac{\sqrt{15}}{2} L^{-5/2} \cdot \left[\frac{1}{7} L^7 - \frac{2}{5} L^7 + \frac{1}{3} L^7 \right]$$

$$= N \cdot \frac{\sqrt{15}}{2} L^{-5/2} \cdot \frac{15 - 42 + 35}{105} L^7$$

$$= N \cdot \frac{\sqrt{15}}{2} L^{9/2} \cdot \frac{8}{105} = N \cdot \sqrt{15} \frac{4}{105} L^{9/2}$$

$$\psi_3^{(new)}(x) = N(x^4 - L^2x^2)$$

$$- N\cdot\sqrt{15}\cdot\frac{4}{105}L^{9/2}\cdot L^{-5/2}\frac{\sqrt{15}}{4}(x^2-L^2)$$

$$= N\cdot\left[x^4 - L^2x^2 - \frac{1}{7}L^2(x^2-L^2)\right]$$

$$= N\left[x^4 - \frac{8}{7}L^2x^2 + \frac{1}{7}L^4\right].$$

normalization

$$|N|^2\cdot\int_{-L}^{L}dx\,\left[x^4 - \frac{8}{7}L^2x^2 + \frac{1}{7}L^4\right]^2$$

$$= |N|^2\cdot\frac{64L^9}{2205} = 1.$$

$$\therefore N = \frac{21}{8}\sqrt{5}\,L^{-9/2}.$$

$$\therefore \begin{cases} \psi_1(x) = L^{-7/2}\dfrac{\sqrt{105}}{4}(x^3-L^2x) \\ \psi_2(x) = +L^{-5/2}\dfrac{\sqrt{15}}{4}(x^2-L^2) \\ \psi_3(x) = +L^{-9/2}\dfrac{21\sqrt{5}}{8}\left(x^4-\dfrac{8}{7}L^2x^2+\dfrac{1}{7}L^4\right) \end{cases}$$

3. Let ϕ_n denote the orthonormal stationary states of a system corresponding to energy E_n. At time $t=0$, the normalized state function of the system is $\Psi = \sum c_n \phi_n$. Assuming the ϕ_n and c_n to be given,

(a) write the state function of the system for $t>0$.

⇒ i) $\Psi(t) = \sum_n c_n \phi_n \cdot \exp\left[-i \frac{E_n}{\hbar} t\right]$.

(b) What is the probability that a measurement of the energy at time t will yield the value E_n?

⇒. ii) $|c_n|^2$. (ϕ_n 이 등장할 확률은 time evolution 에 있어도 변화 X)

(c) What is the expectation value of the energy at any time t?

→ (b)와 마찬 가지 이유로.. 확률이 변하지 않기 때문에..

$$\langle E \rangle_t = \sum_n |c_n|^2 \cdot E_n$$

4. Show that the expectation value of the square of an Hermitian operator can never be negative.

⇒ 가정) 임의의 state $|\alpha\rangle$ 가 있다고 하고..

이떠한 hermitian operartor 를 A 라 하자.

그리고.. A의 eigen state 들을 $|n\rangle$ 이라 하자.

(그 eigenvalue a_n (real))

9°)

$$\therefore \langle\alpha| A^2 |\alpha\rangle$$

$$= \langle\alpha| A^2 \mathbb{1} |\alpha\rangle = \langle\alpha| A^2 \cdot \sum_n |n\rangle\langle n|\alpha\rangle$$

$$= \langle\alpha| \sum_n \underbrace{A^2 |n\rangle}_{a_n^2 |n\rangle} \langle n|\alpha\rangle$$

$$= \sum_n a_n^2 \langle\alpha|n\rangle\langle n|\alpha\rangle$$

$$= \sum_n \underbrace{a_n^2 \, |\langle n|\alpha\rangle|^2}_{\text{real \& positive}} \Rightarrow \underline{\underline{\text{real \& positive}}}$$