Week 12, Lecture 1

Wednesday 23/04. **NOT EXAMINABLE**

Application of PIEs – Quantum Mechanics

Schrödinger eq$^{\underline{n}}$ in one spatial dimension

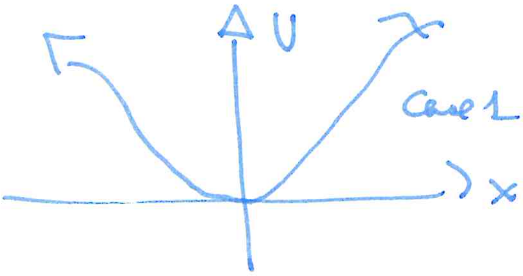
$$(1) \quad i\frac{\partial \psi}{\partial t} = \hat{H}\psi, \quad \psi(x, t=0) = \psi_0(x),$$

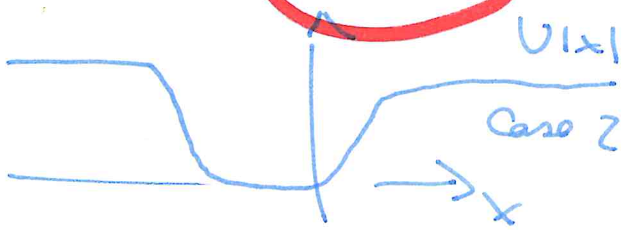
$x \in (-\infty, \infty)$.

$$\hat{H} = -\frac{\partial^2}{\partial x^2} + U(x).$$

$U(x)$ is the potential function:

- $U(x)$ continued into the complex plane is analytic
- $U(x) \sim \begin{cases} C x^{2p} & |x| \to \infty \quad \text{Case 1} \\ C & |x| \to \infty \quad \text{Case 2} \end{cases}$ **KEY**





- Assume WLOG that U is even in x.

Laplace transform :

$$\left[i \frac{\partial \psi}{\partial t} = \hat{H} \psi \right] e^{-\lambda t}$$

$$\int_0^\infty i \, e^{-\lambda t} \frac{\partial \psi}{\partial t} \, dt = \int_0^\infty \hat{H} \psi e^{-\lambda t} \, dt$$

$$\int_0^\infty \left[\frac{\partial}{\partial t} \left(i e^{-\lambda t} \psi \right) + i \lambda \psi e^{-\lambda t} \right] dt$$
$$= \int_0^\infty \hat{H} \psi e^{-\lambda t} \, dt$$

$$\hat{\psi}_\lambda(x) = \int_0^\infty e^{-\lambda t} \psi(x,t) \, dt$$

provided $|\psi(x,t)| \le M e^{\lambda_0 t}$, $M, \lambda_0 \in \mathbb{R}^+$.

Hence :

$$\lim_{L \to \infty} i e^{-\lambda t} \psi \Big|_L - i \overbrace{\psi_0(x)}^{= \psi(x, t=0)} + i \lambda \hat{\psi}_\lambda = \hat{H} \hat{\psi}_\lambda$$

Take $\mathrm{Re}(\lambda) > \lambda_0$.

$$\boxed{i \lambda \hat{\psi}_\lambda - i \psi_0(x) = \hat{H} \psi_\lambda} \quad (2)$$

Notation : use $\lambda = -i\omega$

$$\Psi_\omega(x) = \hat{\psi}_\lambda(x), \quad \lambda = -i\omega .$$

$$\boxed{\omega \Psi_\omega - i \psi_0(x) = \hat{H} \Psi_\omega} \quad (3)$$

Green's Functions:

$$[-\partial_{xx} + U(x)]\,\Phi_\omega^1(x) = \omega\,\Phi_\omega^1(x) - i\,\psi_0(x)$$

Homogeneous problem:

$$[-\partial_{xx} + U(x)]\,\Phi^1 = 0.$$

Method of variation of parameters gives Green's function for corresponding inhomogeneous problem, valid on an interval $(-\infty,\infty)$. Call the Green's Function $g(x,y)$:

$$[-\partial_{xx} + U(x)]\,\Phi_\omega^1(x) = \underbrace{\omega\,\Phi_\omega^1(x) - i\,\psi_0(x)}_{S(x)}$$

$$\Phi_\omega^1(x) = \int_0^\infty g(x,y)\,[-i\,\psi_0(y)]\,dy$$

$$+\ \omega \int_0^\infty g(x,y)\,\Phi_\omega^1(y)\,dy$$

Here, we integrate over $[0,\infty)$ and use the symmetry of $\Phi_\omega^1(x)$, valid for an even potential function.

Identify

$$\mathcal{K}\,\psi_1(x) = \int_0^\infty g(x,y)\,\psi_1(y)\,dy.$$

The operator K is the inverse of $\hat{H}$, in the following sense:

$$\hat{H} K \psi_1(x) = \hat{H} \int_0^\infty G(x,y)\,\psi_1(y)\,dy$$

$$= \int_0^\infty \hat{H}_x G(x,y)\,\psi_1(y)\,dy$$

$$\overset{\text{Thm 6.1 \#2}}{=} \int_{x-\epsilon}^{x+\epsilon} \hat{H}_x G(x,y)\,\psi_1(y)\,dy$$

$$= -\int_{x-\epsilon}^{x+\epsilon} \frac{\partial}{\partial x}\frac{\partial G}{\partial x}(x,y)\,\psi_1(y)\,dy$$

$$= -\left.\frac{\partial G}{\partial x}\right|_{x-\epsilon}^{x+\epsilon} \psi_1(x)$$

$$\cancel{= -\left(\frac{1}{p_2(x)}\right)\psi_1(x)}$$

Eq. 14.106

$$= -\left(\frac{-W}{W}\right)\psi_1(x)$$

(4)

$$= \psi_1(x).$$

$\cancel{\hat{H}\psi_1}$

$$\therefore \hat{H} K \psi_1(x) = \psi_1(x)$$

$$\boxed{\hat{H} K = \delta}$$

$\hat{H}$ and K are inverses.

Using (4), the Schödinger Eq^{n} (3) is converted into a FIE:

$$\omega K \Psi_\omega + \underbrace{K(-i\psi_0(x))}_{\hat{f}_0(x)} = \overbrace{\Psi_\omega}^{= K\hat{H}\Psi_\omega}$$

$\hat{f}_0(x)$, can be written as a condition.

$$\boxed{\Psi_\omega(x) = f(x) + \omega K \Psi_\omega(x)}$$

ψ_0 is broken up into two parts, $\psi_0 = \psi_1 + \psi_2$

- $\psi_1 \in L^2((0,\infty))$
- $|\psi_2| \le M \quad |x| \to \infty$.

Hence:

$$f_1 = K(-i\psi_1)$$
$$f_2 = K(-i\psi_2)$$

Linear problems:

$$(\mathbb{I} - \omega K)\chi_1 = f_1 \qquad \text{(5a)}$$
$$(\mathbb{I} - \omega K)\chi_2 = f_2 \qquad \text{(5b)}$$

$$\Psi_\omega = \chi_1 + \chi_2 .$$

Part (5a): Since $\mathcal{F}_1 = K(-i\psi_1)$ $\underline{\text{VI}}$

we can expand everything in terms of eigenfunctions of FIE: $\chi_n = \omega_n K \chi_n$.

$\iff$ $\hat{H}\chi_n = \omega_n \chi_n$ ... Eigenvalues of Schrödinger Eq$^{\underline{n}}$.

$$(\mathbb{I} - \omega K)\sum_n \chi_n \cdot a_n = \sum_n \langle f_1, \chi_n \rangle \chi_n$$

$\Rightarrow$ $\cancel{\omega_n = \omega}$

$$\left(I - \frac{\omega}{\omega_n}\right)\chi_n \cdot a_n = \langle f_1, \chi_n \rangle \cdot \chi_n$$

$$\frac{\omega_n - \omega}{\omega_n} a_n = \langle f_1, \chi_n \rangle$$

$$a_n = \frac{\omega_n \langle f_1, \chi_n \rangle}{\omega_n - \omega}$$

$$\mathcal{X}_1 = \sum_n \frac{\omega_n}{\omega_n - \omega} \langle f_1, \chi_n \rangle$$

$$= \sum_n \frac{\omega_n \langle K(-i\psi_1), \chi_n \rangle}{\omega_n - \omega}$$

$$= \sum_n \frac{\omega_n \langle -i\psi_1, \overbrace{K\chi_n}^{1/\omega_n \chi_n} \rangle}{(\omega_n - \omega)}$$

$$\Rightarrow \boxed{\mathcal{X}_1 = \sum_n \frac{\langle -i\psi_1, \chi_n \rangle}{\omega_n - \omega}} \qquad \omega \neq \omega_n$$

Part (5b)

$$(\mathbb{I} - \omega K) X_2 = f_2$$

$$\Leftrightarrow \quad (\hat{H} - \omega) X_2 = \hat{H}(-iK\psi_{02})$$

Hence $(\hat{H} - \omega) X_2 = -i\psi_{02}$.

Method of variation of parameters:

$$X_2(x;\omega) = \frac{F(x,\omega)}{W(\omega)}.$$

General sol^n:

$$\Psi_\omega(x) = \sum_n \frac{\langle -i\psi_0, X_n \rangle}{\omega_n - \omega} + \frac{F(x,\omega)}{W(\omega)}$$

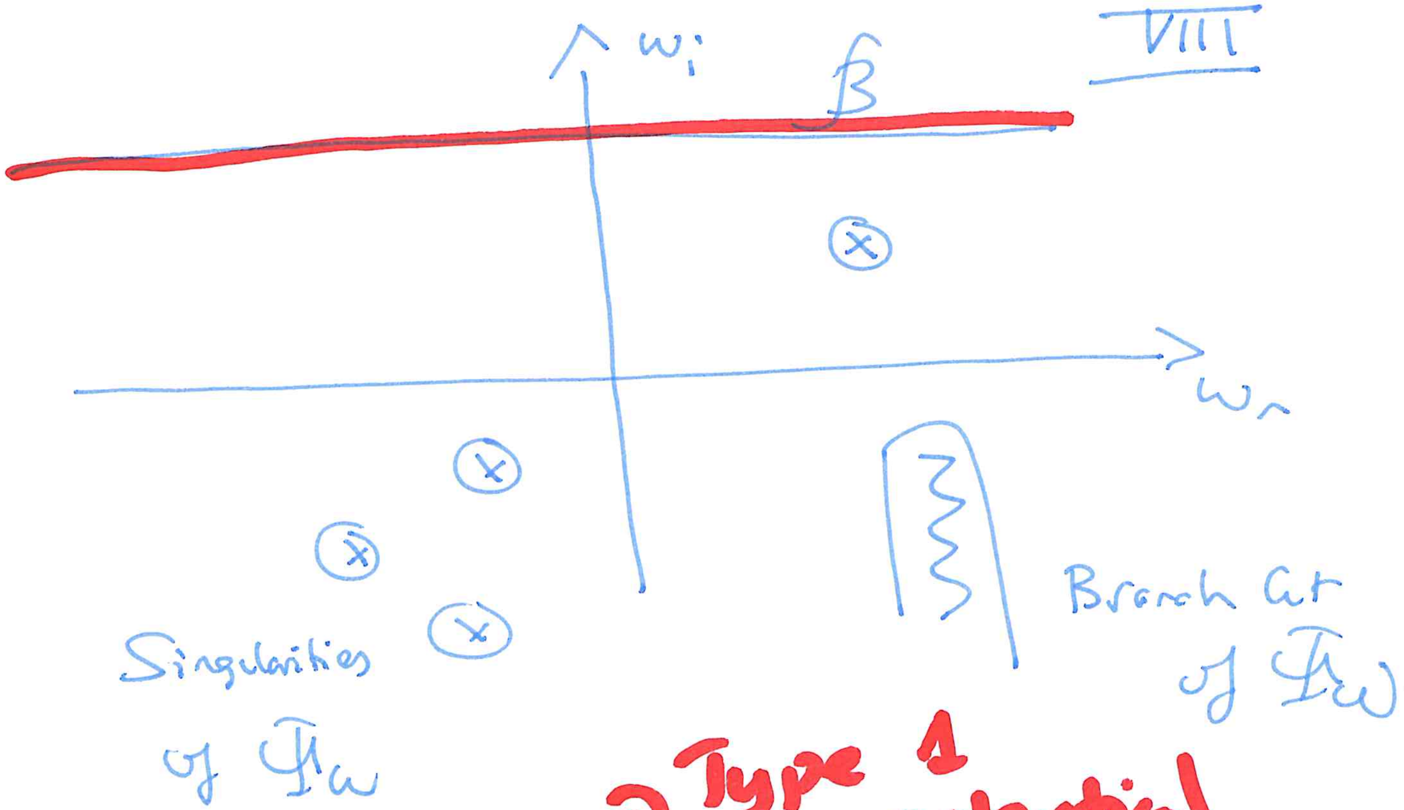
Non L^2-component of initial wavef^{n}.

But $\Psi_\omega(x) = \int_0^\infty e^{-\lambda t} \psi(x,t)\,dt$, $\lambda = -i\omega$.

Invert to get

$$\psi(x,t) = \frac{1}{2\pi} \int_\beta [-\Psi_\omega(x)] e^{-i\omega t}\, d\omega$$

$\longrightarrow$



Type 1 potential

Since $F(x,\omega)$ and $W(\omega)$ are analytic in ω and $W(\omega)$ is never zero, singularities in $\Psi_\omega(x)$ occur only at $\omega = \omega_n$ (eigenvalues).

Hence, by Cauchy's Residue Theorem:

$$\psi_1(x,t) = \sum_n \frac{\langle -i\psi_0, \chi_n \rangle \chi_n(x)}{2\pi} \cdot 2\pi i \, e^{-i\omega_n t} (-1)$$

or

$$\psi_1(x,t) = \sum_n \langle \psi_0, \chi_n \rangle e^{-i\omega_n t} \chi_n(x)$$

Remark: A type 2 potential gives a contribution from the continuous spectrum ⟶

$$\psi(x,t) = \sum_n \langle \psi_0, \chi_n \rangle \chi_n(x) e^{-i\omega_n t} + \int_c^{\infty} Q(\omega) e^{-i\omega t} d\omega$$

Bound states

Travelling waves.