Diffusion equation in $\mathbb{R}^m$

$$u_t = k\Delta u \quad \text{on } \mathbb{R}^m \times (0,\infty)$$

$$u(x,t) \to 0 \quad |x| \to \infty$$

$$u(x,0) = \phi(x) \quad \text{on } \mathbb{R}^m \qquad u \in C^0(\mathbb{R}^m \times [0,\infty))$$

Theorem: The solution of the diff eqn in $\mathbb{R}^m$ is given by

$$u(x,t) = \int_{\mathbb{R}^m} \underbrace{\frac{1}{(4\pi kt)^{m/2}} e^{-|x-y|^2/4kt}}_{S_m(x-y,t)} \phi(y)\,dy$$

Remark: $S_m(x,t) = \prod_{i=1}^{m} \frac{1}{\sqrt{4\pi kt}} e^{-x_i^2/4kt}$

If $\phi(x) = \prod_{i=1}^{m} \phi_i(x_i) \Rightarrow u(x,t) = \prod_{i=1}^{m} \int_{\mathbb{R}^m} S_1(x_i-y_i,t)\,\phi_i(y_i)\,dy_i$

Proof: (Sketch)

① $\frac{\partial}{\partial t} S_n(x,t) = k \Delta S_n(x,t) \quad (x,t) \in \mathbb{R}^n \times (0,\infty)$

② $\frac{\partial}{\partial x_i} \int S_n(x-y,t)\, \phi(y)\, dy = \int \frac{\partial}{\partial x_i} S(x-y,t)\, \phi(y)\, dy$

Similar for any variable

$\Rightarrow \quad u \in C^2(\mathbb{R}^n \times (0,\infty)) \quad u_t = k \Delta u$

③ exercise + previous Remark.

$\boxed{}$

Schrödinger equation

$$-i u_t = \frac{1}{2} k \Delta u + V \cdot u \quad \text{on } \mathbb{R}^s \times [0, \infty)$$

(*)

$$u(x,t) \to 0 \quad |x| \to \infty$$

$$u(x,0) = \phi(x)$$

Sep. of Variables: $u(x,t) = T(t)\, X(x)$

$$\left[i\lambda = \frac{T_\lambda'(t)}{T_\lambda(t)} \right. \implies T_\lambda(t) = e^{i\lambda t}$$

$\in \mathbb{C}$

$\boxed{k = 2}$

$$\left.\begin{aligned} &\Delta X + V \cdot X = -\lambda X \quad \text{on } \mathbb{R}^n \\ &LX := -\Delta X - V \cdot X = +\lambda X \\ &X(x) \to 0 \quad |x| \to \infty \end{aligned}\right\} \quad (**)$$

(time independent Schrödinger equ)

If $(**)$ is solvable for λ, then λ is called energy level of QM system described by operator L.

Goal: Find energy levels λ_n and corresponding V_n that solve $(**)$.

Team

We can write sol. of (x) as $u(x,t) = \sum_{k=0}^{\infty} A_k T_{\lambda_k}(t) v_k(x)$

<u>Harmonic oscillator</u>: $V(x) = -|x|^2$

$n=1$: $(x.x) \Rightarrow v'' - x^2 \cdot v + \lambda v = 0$ on $\mathbb{R}$

$\lambda = 1$: $e^{-x^2/2}$ solves (xx) and $e^{-x^2/2} \to 0$ $|x| \to \infty$

$\lambda \neq 1$: $v(x) = w(x) \cdot e^{-x^2/2}$

$\Rightarrow v'(x) = w' e^{-x^2/2} - x w e^{-x^2/2}$

$\Rightarrow v'' = w'' e^{-x^2/2} - x w' e^{-x^2/2} - x w' e^{-x^2/2}$

$- w e^{-x^2/2} + w x^2 e^{-x^2/2}$

$\Rightarrow (x^2 - \lambda) w \cdot \cancel{e^{-x^2/2}} = (w'' - 2x w' - w + x^2 w) \cancel{e^{-x^2/2}}$

$\Rightarrow 0 = w'' - 2x w' + (\lambda - 1) w$

(Hermite's diff. eqn.)

Power series method

Assume $w(x) = \sum_{k=0}^{\infty} a_k x^k$

$$\Longrightarrow \quad 0 = \underbrace{\sum_{k=0}^{\infty} a_k \, k(k-1) x^{k-2}}_{\sum_{k=2}} - \sum_{k=0}^{\infty} a_k \, 2x \underbrace{k x^{k-1}}_{k x^{k}} + \sum_{k=0}^{\infty} (\lambda-1) a_k x^k$$

$$\Longrightarrow \quad 0 = \sum_{k=0}^{\infty} a_{k+2} (k+2)(k+1) x^k + \sum_{k=0}^{\infty} a_k (\lambda - 2k - 1) x^k$$

$$\Longrightarrow \quad a_{k+2} (k+2)(k+1) = (2k+1-\lambda) a_k \qquad \forall k \in \mathbb{N}_0$$

$a_0 = 0 \quad \Longrightarrow \quad a_k = 0 \quad \forall k = 2, 4, 6, \dots$

$a_1 = 0 \quad \Longrightarrow \quad a_k = 0 \quad \forall k = 3, 5, 7, \dots$

If $\lambda = 2k+1 \Rightarrow 0 = a_{k+2} = a_{k+4} = \dots$

$\Rightarrow$ if $a_0 \neq 0$. $a_1 = 0$ and $\lambda = 2k+1$ k even

$\Rightarrow$ w is even Polynomial of degree k

if $a_0 = 0$ $a_1 \neq 0$ and $\lambda = 2k+1$ k odd

$\Rightarrow$ w is odd Polynomial of degree k

$H_0(x) = 1$ $\lambda = 1$ $a_0 = 1$. $a_1 = 0$

$H_1(x) = 2x$ $\lambda = 3$ $a_0 = 0$ $a_1 = 2$

$H_2(x) = 4x^2 - 2$ $\lambda = 5$ $a_0 = -2$ $a_1 = 0$

$$a_2 = \frac{1-5}{2 \cdot 1} \cdot -2 = 4$$

$\vdots$

Hermite Polynomials

$\Rightarrow$ $v_k(x) = H_k(x) \cdot e^{-x^2/2}$

<u>Remark</u>: ① v_n satisfies the Cdy at infinity

② if $\lambda \neq 2n+1$, no power series sol. satisfies the condition at infinity

③ The following formula holds: $H_n(x) = (-1)^n e^{x^2} \cdot \frac{d^n}{dx^n} e^{-x^2}$

④ $(v_n)_{n \in \mathbb{N} \cup \{0\}}$ are mutually orthogonal

$$\int_{\mathbb{R}} H_n(x) \cdot e^{-x^2/2} \cdot H_l(x) \cdot e^{-x^2/2} \, dx = 0 \quad \text{if } n \neq l$$

⑤ $(v_k)_{k \in \mathbb{N}}$ is complete: $\forall f \in \mathbb{R} \to \mathbb{R}$ s.t $\int f^2 dx < \infty$

$$\Rightarrow \quad f \overset{L^2}{=} \sum_{k=0}^{\infty} A_k v_k \qquad A_k = \frac{(v_k, f)}{(v_k, v_k)}$$

$$\int u \cdot v \, dx = (u, v)$$

Solutions of $(*)$ are

$$u(x,t) = \sum_{k=0}^{\infty} A_k \, T_{\lambda_k}(t) \cdot v_k(x)$$

where $u(x,0) = \Phi(x) \overset{L^2}{=} \sum_{k=0}^{\infty} A_k v_k$

<u>Remark</u>: Higher dimension

$$\Delta v - |x|^2 \cdot v = -\lambda v$$

$$\Rightarrow \sum_{i=1}^{m} \left(v_{x x_i} + |x_i|^2 v \right) = -\lambda v$$

$$\Rightarrow v = \prod_{j=1}^{m} H_{k_j}(x_j) \, e^{-(x_j)^2/2}$$ solves the equat.

for $\lambda_{\vec{k}} = \sum_{j=1}^{m} \lambda_{k_j}$ $\quad \vec{k} = (k_1, \ldots, k_m) \in \mathbb{N}^m$.

Hydrogen Atom : $V(x) = \frac{1}{|x|}$

$\boxed{k=1}$ $\quad -\Delta v - \frac{2}{|x|} v - \lambda v = 0 \quad$ on $\mathbb{R}^3$

Spherical coord. : $-\tilde{v}_{rr} - \frac{2}{r}\tilde{v}_r - \frac{1}{r^2}(\ldots) - \frac{2}{|x|}v - \lambda v = 0$

derivatives w.r.t. ϕ, θ

Assume v spherical symmetric

$\Longrightarrow \quad R'' + \frac{2}{r}R' + \frac{2}{r}R + \lambda R = 0 \quad (xxx)$

Laguerre's diff eqn

$R(0) < \infty \qquad R(x) \longrightarrow 0 \quad |x| \longrightarrow \infty$

Assume $\lambda < 0$

Asymptotic behavior of (xxx) is $\quad R'' + \lambda R = 0$

$\rightsquigarrow \quad R(r) = e^{\pm \beta r}$

$\beta = \sqrt{-\lambda}$

$$* \quad R(r) = w(r) \cdot e^{-\beta r}$$

$$\Longrightarrow \quad w'' + 2\left(\beta - \frac{1}{r}\right) w' + \left(2(\beta - 1)\frac{1}{r}\right) w = 0$$

$$\Longrightarrow \quad \frac{1}{2} r w'' + \beta \cdot r w' + w' + (\beta - 1) w = 0$$

Power series method. $w(r) = \sum a_k x^k$

$$\Longrightarrow 0 = \frac{1}{2} \sum_{k=0}^{\infty} a_k (k-1) k r^{k-1} - \underbrace{\beta \sum_{k=0}^{\infty} k a_k r^k}_{\sum_{k=1}} + \sum_{k=0}^{\infty} k a_k r^{k-1} + (1-\beta) \sum_{k=0}^{\infty} a_k r^k$$

$$\Longrightarrow 0 = \frac{1}{2} \sum_{k=0}^{\infty} a_k \Big(\underbrace{(k-1)k + k}_{k(k+1)} \Big) r^{k-1} + \sum_{k=1}^{\infty} a_{k-1} \Big(\underbrace{(1-\beta) - \beta(k-1)}_{-\beta k + 1} \Big) r^{k-1}$$

$$\Longrightarrow \quad a_k \frac{k(k+1)}{2} = (\beta k - 1) a_{k-1} \qquad k = 1, \ldots$$

if $\beta = \frac{1}{n}$ $\Longrightarrow$ $0 = a_n = a_{n+1} = \dots$

$\Longrightarrow$ Polynomial w_n of degree $n-1$

$\Longrightarrow$ $\tilde{v}_k(r) = R_n(r) = w_n(r) \cdot e^{-\beta r}$

$\rightsquigarrow$ Spherical symmetric sol of HA equa.

$$u(x,t) = \sum_{n=0}^{\infty} e^{2\lambda_n t} \cdot v_n(x) \qquad -\lambda_n = \beta_n^2 = \frac{1}{n^2}$$

$\Longrightarrow$ $\left\{\frac{1}{n^2}\right\}$ energy level of the Hydrogen Atom

Remarks

(1) But v_k are not complete.

two reason: 1. We assumed that spectrum of v_k spherical symmetric

2. The operator $-\Delta v - \frac{1}{|x|} \cdot v = Lv$

has besides λ_k a continuous part that is $[0, \infty)$

(2) Assume power series of w is not finite

$(\beta \neq \frac{1}{k})$

$\Rightarrow$ if k is very big $\rightsquigarrow$ $a_k = \beta \frac{2}{k} a_{k-1}$

$\Rightarrow$ $e^{2\beta r} = w(r)$ does not satisfy condition at infinity