1.9.2 Existence of Dynamics

From Stone's Theorem, we can thus conclude the following existence result for the Schrödinger equ

$$i\dot{\Psi} = H\Psi \qquad \text{(TDSE)}$$

where H is self-adjoint on an appropriate domain $D \subseteq \mathbb{H}$, with a Hilbert space $\mathbb{H}$

<u>Theorem</u>: Assume that H is a self-adjoint operator on a Hilbert space $\mathbb{H}$. Then, there exists a unique family of unitary operators e^{-itH}, $t \in \mathbb{R}$, with the following properties;

1) The operators e^{-itH} satisfy the group property:
$$e^{-i(t+s)H} = e^{-itH} e^{-isH}, \quad \forall s,t \in \mathbb{R}$$

2) The mapping $t \mapsto e^{-itH}$ is <u>strongly continuous</u>, i.e.
$$\|e^{-itH}\Psi_0 - \Psi_0\| \to 0 \text{ as } t \to 0 \quad \forall \Psi_0 \in \mathbb{H}$$

3) (TDSE) with initial value $\Psi_0 \in D(H)$ has the solution $\Psi(t) = e^{-itH}\Psi_0$:
$$i\frac{d}{dt} e^{-itH}\Psi_0 = He^{-itH}\Psi_0$$
(the expressions on both sides are well-defined!)

1.9.3 Perturbation Theory for Self-Adjoint Operators

Theorem The operator $-\frac{1}{2}\Delta$ is self-adjoint with domain $\mathbb{H} = H^2$.

Proof: [19]

1.9.4 Mathematical Supplement: Sobolev spaces

Consider the Hilbert space $\mathcal{H} = L^2$ with inner product

$$\langle u | v \rangle = \int_{\mathbb{R}^3} \bar{u}(x)\, v(x)\, dx$$

Def: $u \in L^2$ has a weak derivative $\partial u \in L^2$ if

$$\langle w | \partial u \rangle = - \langle \partial w | u \rangle$$

for all test functions w, i.e. $w \in C^\infty$ with compact support

Def.: The set of all functions in L^2 having weak derivatives up to order $\leq k$ is denoted as the Sobolev space H^k. It is equipped with the norm

$$\| u \|_{H^k} := \left(\sum_{\alpha} \| \partial^\alpha u \|^2 \right)^{1/2},$$

where the sum is over all weak partial derivatives up to order k.

Def: $\| u \|_{L^\infty}$ denotes the supremum norm of functions u bounded almost everywhere

Theorem: Let T be selfadjoint. If A is symmetric and T-bounded with bound < 1, i.e., $D(A) \supseteq D(T)$ &

$$\|Au\| \le a\|u\| + b\|Tu\| \quad \forall u \in D(T)$$

with $b < 1$, then $T + A$ is selfadjoint on $D(T)$.

Proof: [10].

Theorem: $\nabla \ll \Delta$, $\frac{1}{|x|} \ll \Delta$ (i.e., T-bounded with arbitrarily small bound b)

Proof: [19, 20].

Corollary: The Hamiltonian H for an atom with f electrons interacting by Coulomb force is self-adjoint with domain $D(H) = H^2$.

Proof: The Hamiltonian is given by

$$H = \sum_{k=1}^{f} \left(-\frac{1}{2} \Delta^{(k)} + \sum_{\ell \neq k} \frac{1}{|x_k - x_\ell|} \right).$$

With the last Theorem, the proposition is proven. //

II The Quantum Harmonic Oscillator

§ 2.1. The position and momentum operators

Def: Define operators (for $x \in \mathbb{R}$)

$p: \phi \mapsto -i \cdot \phi'$ "momentum operator"

$q: \phi \mapsto x\phi(x)$ "position operator"

"Canonical commutator relations"

$$\frac{1}{i}[q,p](\phi) = \frac{1}{i}(qp - pq)\cdot\phi$$

$$= \frac{1}{i} x(-i\phi') - \frac{1}{i}(-i(x\phi(x))' =$$

$$= -x\phi' + x\phi' + \phi = \phi$$

$$\Rightarrow \frac{1}{i}[q,p] = 1 \quad \text{(Identity operator)}$$

§2.2

Def: "Ladder operators"

$$A = \frac{1}{\sqrt{2}}(q+ip), \ A^+ = \frac{1}{\sqrt{2}}(q-ip)$$

$$A^+A = \frac{1}{2}(p^2+q^2) - \frac{1}{2}, \ AA^+ = \frac{1}{2}(p^2+q^2) + \frac{1}{2}$$

Remark: Thus, A^+A and AA^+ have the same eigenfunctions as the "quantum harmonic oscillator", defined by $H := \frac{1}{2}(p^2+q^2)$, see below.

Eigenfunctions of A: Gaussian $\phi_0(x) = e^{-x^2/2}$.

Proof: $A\phi_0 = \frac{1}{\sqrt{2}}\left(x e^{-x^2/2} + i\left(-i \frac{d}{dx}\left(e^{-x^2/2}\right)\right)\right) =$

$$= \frac{1}{\sqrt{2}}\left(x e^{-x^2/2} + e^{-x^2/2}(-x)\right) = 0$$

Lemma (without proof):

a) $c \cdot \phi_0$ only fcns. in Kernel of A.

b) A^+ has only the trivial kernel 0.

c) $AA^+ = A^+A + 1$ (trivial)

d) $A^* = A^+$, i.e. $\langle A^+\varphi | \psi\rangle = \langle \varphi | A\psi\rangle$

(formal argument for symmetry by integration by parts)

From $AA^+\phi_0 = A^+A\phi_0 + \phi_0 = \phi_0$ it follows that

ϕ_0 is an eigenfcn of AA^+ to

the eigenvalue 1.

Furthermore

$$A^+A\underbrace{A^+\phi_0}_{=\phi_1} = A^+A^+A\phi_0 + A^+\phi_0 = \underbrace{A^+\phi_0}_{=\phi_1}$$

$\Rightarrow \phi_1 := A^+\phi_0$ is eigenfcn. of A^+A to EV 1

$\Rightarrow AA^+\phi_1 = A^+A\phi_1 + \phi_1 = \phi_1 + \phi_1 = 2\phi_1$

$\Rightarrow \phi_1$ is eigenfcn. of AA^+ to EV 2.

Continuing inductively we construct

$$\phi_{k+1} = A^+ \phi_k \quad , k \geq 0 .$$

ϕ_k is an eigenfunction of A^+A to EV k
AA^+ to EV $k+1$.

Normalization:

$$\| A^+ \phi_k \|^2 = \langle A^+ \phi_k | A^+ \phi_k \rangle = \langle \phi_k | AA^+ \phi_k \rangle =$$
$$= (k+1) \| \phi_k \|^2$$

We therefore obtain eigenfcns of AA^+ and A^+A of unit L^2 norm by setting

$$\phi_0(x) := \frac{1}{\pi^{1/4}} e^{-x^2/2}$$

$$\phi_{k+1} := \frac{1}{\sqrt{k+1}} A^+ \phi_k \quad , k \geq 0.$$

$$A \phi_{k+1} = \frac{1}{\sqrt{k+1}} AA^+ \phi_k = \sqrt{k+1}\, \phi_k \implies$$

$$\implies \phi_{k-1} = \frac{1}{\sqrt{k}} A \phi_k \quad , k \geq 0$$

"A^+ ... raising operator"

"A ... lowering operator"

"ladder operators"

$$\phi_{k+1} = \frac{1}{\sqrt{k+1}} A^+ \phi_k \qquad \Big| \cdot \sqrt{k+1}$$

$$\sqrt{k+1}\,\phi_{k+1} = A^+ \phi_k$$

$$\phi_{k-1} = \frac{1}{\sqrt{k}} A \phi_k \qquad \Big| \cdot \sqrt{k}$$

$$\sqrt{k}\,\phi_{k-1} = A \phi_k$$

$$\sqrt{k+1}\,\phi_{k+1} + \sqrt{k}\,\phi_{k-1} = A^+ \phi_k + A \phi_k$$

$$= \frac{1}{\sqrt{2}}(q - ip)\phi_k + \frac{1}{\sqrt{2}}(q + ip)\phi_k =$$

$$= \frac{2}{\sqrt{2}}(x\phi_k)$$

$\Rightarrow \sqrt{k+1}\,\phi_{k+1} = \sqrt{2}\, x \phi_k - \sqrt{k}\,\phi_{k-1}$ ... three-term recurrence.

<u>Definition</u>: (The Quantum Harmonic Oscillator)

Is defined by the Hamiltonian

$$H = \frac{1}{2}(p^2 + q^2).$$

<u>Definition</u>: (Hermite basis in 1D)

The <u>Hermite functions</u>

$$\varphi_k(x) = \frac{1}{\sqrt[4]{\pi}} \frac{1}{\sqrt{2^k k!}} H_k(x) e^{-x^2/2}.$$

H_k is the <u>Hermite polynomial</u> of degree k, i.e. the k-th orthogonal polynomial w.r.t. the weight fcn e^{-x^2} on $\mathbb{R}$.