1.7 Conserved Quantities of TDSE

1) The Hamiltonian operator H is selfadjoint

Define $\langle f | g \rangle := \int_{\mathbb{R}^3} \bar{f}(x) g(x) \, dx$

A ... operator : $\langle f | A | g \rangle := \langle f | Ag \rangle$

Then $\langle \psi | H | \Phi \rangle = \langle \psi | H\Phi \rangle = \langle H\psi | \Phi \rangle$

(Proof: Integration by parts)

Remark: This shows that H is symmetric, in fact it turns out that H is self-adjoint with domain $D(H) = H^2$ (see [10])

2) Conservation of Norm:

$$\frac{d}{dt} \|\psi\|^2 = \langle \dot{\psi} | \psi \rangle + \langle \psi | \dot{\psi} \rangle = \langle \dot{\psi} | \psi \rangle + \overline{\langle \dot{\psi} | \psi \rangle}$$

$$= 2\mathrm{Re}(\langle \dot{\psi} | \psi \rangle) = 2\mathrm{Re}(\langle -iH\psi | \psi \rangle) =$$

$$= -2\mathrm{Re}(i \langle \psi | H | \psi \rangle) = 0$$, see 4) below

3) Conservation of Energy $\langle \psi | H | \psi \rangle$

$$\frac{d}{dt} \langle \psi | H | \psi \rangle = \langle \dot{\psi} | H\psi \rangle + \langle \psi | H\dot{\psi} \rangle =$$

$$= \langle -iH\psi | H\psi \rangle + \langle H\psi | \dot{\psi} \rangle =$$

$$= i\|H\psi\|^2 + \langle H\psi | -iH\psi \rangle =$$

$$= i\|H\psi\|^2 - i\|H\psi\|^2 = 0$$

4) Energy real: $\overline{\langle \psi | H\psi \rangle} = \langle H\psi | \psi \rangle = \langle \psi | H\psi \rangle$

4) Let A ... self-adjoint linear operator, commuting with H, i.e. $[A,H] = AH - HA = 0$

$[A,H]$ ... commutator

($\rightarrow$ we will encounter commutators with nonlinear operators later in the analysis of split-step time integrators)

Then $\langle \psi | A | \psi \rangle$ is conserved:

$$\frac{d}{dt}\langle \psi | A | \psi \rangle = \langle \dot{\psi} | A\psi \rangle + \langle \psi | A\dot{\psi} \rangle =$$

$$= \langle -iH\psi | A\psi \rangle + \langle \psi | -A\, iH\psi \rangle =$$

$$= +i\langle \psi | HA\psi \rangle - i\langle \psi | AH\psi \rangle =$$

$$= i\langle \psi | (HA - AH)\psi \rangle = i\langle \psi | [H,A]\psi \rangle = 0$$

5) In particular: Higher moments, $\frac{d}{dt}\langle \psi | H^p | \psi \rangle = 0$

Proof: Choose $A = H^p$ in 4)

<u>Geometric Integration</u> Numerical method such that similar conservation properties hold!

1.8 Propagation of the free TDSE

1.8.1 Math. Supplement: Fourier transform

Define the map $\mathcal{F}: \psi \mapsto \hat{\psi}$,

$$\hat{\psi}(k) := \frac{1}{(2\pi)^{D/2}} \int_{\mathbb{R}^D} e^{-ik\cdot x} \psi(x)\, dx,$$

where $\psi: \mathbb{R}^D \to \mathbb{C}$, $\hat{\psi}: \mathbb{R}^D \to \mathbb{C}$

$\mathcal{F}$ is well-defined for $\psi \in L^1(\mathbb{R}^D)$

Useful properties:

1) Plancherel Theorem: $\mathcal{F}$ is a unitary map from $L^2(\mathbb{R}^D) \to L^2(\mathbb{R}^D)$

(Note: Initially $\mathcal{F}$ is defined only on $L^1(\mathbb{R}^D)$!)

$$\|\mathcal{F}\psi\|_{L^2} = \|\psi\|_{L^2}$$

2) Inversion formula: Adjoint $\mathcal{F}^* = \mathcal{F}^{-1}: \psi \mapsto \check{\psi}$,

$$\check{\psi}(x) = \frac{1}{(2\pi)^{D/2}} \int_{\mathbb{R}^d} e^{ix\cdot k} \psi(k)\, dk.$$

3) $-i\,\widehat{\nabla_x \psi}(k) = k\hat{\psi}(k)$.

4) $\widehat{x\psi}(k) = i\nabla_k \hat{\psi}(k)$.

5) $\widehat{\phi\psi} = \frac{1}{(2\pi)^{D/2}} \hat{\phi} * \hat{\psi}$

6) $\widehat{\phi * \psi} = (2\pi)^{D/2} \hat{\phi}\hat{\psi}$

with the convolution

$$(f*g)(x) := \int_{\mathbb{R}^D} f(y) g(x-y)\, dy$$

1.8.2 Evolution Operator of the free TDSE

The free Schrödinger equation in $\mathbb{R}^D$

$$i\dot{\psi} = -\frac{1}{2}\Delta\psi \,, \quad \psi(0) = \psi_0$$

has the solution

$$\boxed{\psi(x,t) = \frac{1}{(2\pi)^{D/2}} \int_{\mathbb{R}^D} e^{ik\cdot x - i|k|^2 t/2}\, \hat{\psi}_0(k)\, dk \,,}$$

where

$$\hat{\psi}_0(k) = \frac{1}{(2\pi)^{D/2}} \int_{\mathbb{R}^D} e^{-ik\cdot x}\, \psi_0(x)\, dx$$

Proof: $\psi(x,0) = \psi_0(x)$ ✓

$$\frac{\partial\psi}{\partial t} = \left(\frac{1}{2\pi}\right)^{D/2} \int_{\mathbb{R}^D} e^{ik\cdot x - i|k|^2 t/2}\, \hat{\psi}_0(k) \left(-\frac{i}{2}|k|^2\right) dk$$

$$\nabla_x \psi = \left(\frac{1}{2\pi}\right)^{D/2} \int_{\mathbb{R}^D} e^{ik\cdot x - i|k|^2 t/2}\, \hat{\psi}_0(k)\, (ik)\, dk$$

$$\Delta_x \psi = \left(\frac{1}{2\pi}\right)^{D/2} \int_{\mathbb{R}^D} e^{ik\cdot x - i|k|^2 t/2}\, \hat{\psi}_0(k) \left(-|k|^2\right) dk$$

$$i\dot{\psi} = \left(\frac{1}{2\pi}\right)^{D/2} \int_{\mathbb{R}^D} e^{ik\cdot x - i|k|^2 t/2}\, \hat{\psi}_0(k) \left[\frac{1}{2}|k|^2\right] dk$$

$$-\frac{1}{2}\Delta_x \psi = \left(\frac{1}{2\pi}\right)^{D/2} \int_{\mathbb{R}^D} e^{ik\cdot x - i|k|^2 t/2}\, \hat{\psi}_0(k) \left[\frac{1}{2}|k|^2\right] dk \quad //$$

1.9 Existence of Dynamics (with Potential)

1.9.1 Math. Supplement: Semigroups of unbounded Operators

Def: A one-parameter family $S(t)$ of linear operators on a Banach space X is a "semigroup" of operators on X if

(i) $S(0) = I$ and (ii) $S(t+s) = S(t)S(s)$

$S(t)$ is "strongly continuous" if $\lim_{t\to 0} S(t)x = x \quad \forall x \in X$.

The linear operator A defined by

$$Ax := \lim_{t\to 0} \left(S(t)x - x \right)/t$$

with domain equal to all x such that this limit exists, is denoted as the "infinitesimal generator" of $S(t)$.

We write $S(t) = e^{At}$

Properties of strongly continuous semigroups:

1) $\lim_{s\to 0} \| S(t+s)x - S(t)x \| = \lim_{s\to 0} \| S(t)\left(S(s) - S(0)\right)x \| = 0$

2) $\lim_{h\to 0} \frac{1}{h} \int_t^{t+h} S(s)x \, ds = S(t)x$

Proof: $t \mapsto S(t)x$ is continuous!

3) $\int_0^t S(s)x\,ds \in D(A)$ $\forall x \in X$, and

$A\left(\int_0^t S(s)x\,ds\right) = S(t)x - x$

Proof: $\frac{S(h)-I}{h}\int_0^t S(s)x\,ds = \frac{1}{h}\int_0^t [S(s+h)x - S(s)x]\,ds$

$= \frac{1}{h}\int_h^{t+h} S(s)x\,ds - \frac{1}{h}\int_0^t S(s)x\,ds =$

$= \frac{1}{h}\int_h^{t} S(s)x\,ds + \frac{1}{h}\int_t^{t+h} S(s)x\,ds - \frac{1}{h}\int_0^t S(s)x\,ds =$

$= \cancel{\frac{1}{h}\int_0^t S(s)x\,ds} - \frac{1}{h}\int_0^h S(s)x\,ds + \frac{1}{h}\int_t^{t+h} S(s)x\,ds -$

$\cancel{- \frac{1}{h}\int_0^t S(s)x\,ds} \to$

$\to S(t)x - S(0)x = S(t)x - x$ //

4) $S(t)x \in D(A)$ for $x \in D(A)$ and

$\frac{d}{dt} S(t)x = AS(t)x = S(t)Ax$

Proof: For $x \in D(A)$, $h > 0 \Rightarrow$

$\frac{S(h)-I}{h} S(t)x = S(t)\left(\frac{S(h)-I}{h}\right)x \to S(t)Ax$, $h \to 0$

$\Rightarrow S(t)x \in D(A)$ and $AS(t)x = S(t)Ax$

and $\frac{d^+}{dt} S(t)x = AS(t)x = S(t)Ax$

(this is the right derivative, which is the simple part)

For the left derivative, first show left-continuity:

$\lim_{h\to 0} S(t-h)x - S(t)x = \lim_{h \to 0} S(t-h)(x - S(h)x)$

$\to 0$ (left continuity follows from right continuity)

Thus for the left derivative:

$$\lim_{h\to 0}\left[\frac{S(t)x - S(t-h)x}{h} - S(t)Ax\right] =$$

$$= \lim_{h\to 0} S(t-h)\left[\frac{S(h)x - x}{h} - Ax\right] +$$

$$+ \lim_{h\to 0}\left[S(t-h)Ax - S(t)Ax\right] =$$

$$= \lim_{h\to 0}\left[S(t-h) - S(t)\right]\left[\frac{S(h)x-x}{h} - Ax\right] +$$

$$+ \lim_{h\to 0} S(t)\Big[\underbrace{\frac{S(h)x-x}{h}}_{\to Ax} - Ax\Big] + \lim_{h\to 0}\Big[\underbrace{S(t-h)Ax}_{\to S(t)Ax} - S(t)Ax\Big]$$

$$= 0$$

Theorem of Stone: An operator A on a Hilbert space $\mathcal{H}$ generates a unitary group of operators on $\mathcal{H}$ iff iA is self-adjoint.

Proof: [4, p. 89].