MA4A7 Quantum Mechanics: Basic Principles and Probabilistic Methods

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Chapter 1

Introduction

1.1 Basic Axioms

The Quantum Mechanics description of a 'point particle' is given by three hypothesis:

H1 The state of a particle at time t is described by a function $\psi(\cdot, t) : \mathbb{R}^3 \to \mathbb{C}$ (the *wavefunction*). The time evolution is given by the *Schrödinger equation*

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\Delta\psi(x,t) + V(x)\psi(x,t) \tag{1.1}$$

where $\hbar = \frac{h}{2\pi}$, where h is *Planck's constant.* m is the mass of the particle and $V : \mathbb{R}^3 \to \mathbb{R}$ is the potential in which the particle moves. Δ is the Laplace operator.

H2 The probability to find the particle at time t in a region $A \subset \mathbb{R}^3$ is given by

$$\int_A |\psi(x,t)|^2 dx$$

$|\psi(x,t)|^2 = \psi(x,t)\overline{\psi(x,t)}$ is interpreted as the probability density, thus

$$\int_{\mathbb{R}^3} |\psi(x,t)|^2 dx = 1$$

We can compare this to Newton's law:

$$\left.\begin{array}{l} m\dot{x} = p \\ \dot{p} = -\nabla V(x(t)) \end{array}\right\} m\ddot{x} = -\nabla V(x(t))$$

Classical mechanics gives us a path along which the particle travels, whereas Quantum mechanics gives us a 'path of probability' densities which correspond to the particles position. V is the same in quantum and classical mechanics

H3 The probability to find the value of the particle momentum in the set $B \subset \mathbb{R}^3$, at time t is given by

$$\int_B \left| \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \hat{\psi}(\frac{p}{\hbar}, t) \right|^2 dp \tag{1.2}$$

where $\hat{\psi}(k,t) = \int_{\mathbb{R}^3} e^{-ik\cdot x}\psi(x,t)dx$ is the Fourier transform of ψ with respect to x. Thus the momentum is related to the oscillation of frequencies of ψ. We will see later that H3 makes sense as the analogue of momentum

Axioms H1-H3 only give probabilities, not trajectories. In classical mechanics initial position and momentum determine the trajectory, whereas in quantum mechanics, initial wave function determines $\psi(x,t)$ for every t.

1.2 Consistency of the Axioms

Since $|\psi(x,t)|^2$ and $|\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\hat{\psi}(\frac{p}{\hbar},t)|^2$ are interpreted as probability densities, they have to have total integral 1, for all times. We now prove this under somewhat restrictive conditions. It holds for greater generality.

Definition 1.1. Assume $V:\mathbb{R}^3\to\mathbb{R}$ is continuous, a function $\psi:\mathbb{R}^3\times\mathbb{R}\to\mathbb{C}$ is called a *classical solution* to (1.1) if $\psi(x,\cdot)\in C^1(\mathbb{R})$ for every x and $\psi(\cdot,t)\in C^2(\mathbb{R}^3)$ for every t and if (1.1) holds for every x and t. (Later we shall study *weak* solutions which are not C^2)

A classical solution is not good enough. We need $\int|\psi(x,t)|^2dx<\infty$ for H2 and H3, i.e. we need $|\psi(x,t)|\to 0$ as $|x|\to\infty$ fast enough. (i.e. we need boundary conditions). A convenient assumption is:

Assume that for all time intervals $[a,b]$ there exists $C_{a,b}<\infty$ and $\alpha>\frac{3}{2}$ with

$$|\psi(x,t)|\le\frac{C_{a,b}}{|x|^{\alpha}}\qquad|\nabla\psi(x,t)|\le\frac{C_{a,b}}{|x|^{\alpha-1}}\tag{1.3}$$

for every $x\in\mathbb{R}^3$, $t\in[a,b]$.

We remark that $\alpha=\frac{3}{2}$ is the borderline integrability of $|\psi(x,t)|^2$

$$\int|\psi(x,t)|^2dx\sim\int_0^{\infty}|\psi(r,t)|^2r^2dr\cdot 2\pi$$

i.e. so need $|\psi(r,t)|$ to have at least $r^{-\frac{3}{2}}$ decay at ∞. So as a decay rate, (1.3) is optimal.

Lemma 1.2. *Assume that V is continuous, ψ is a classical solution to (1.1) and satisfies (1.3) then*

$$t\mapsto\int|\psi(x,t)|^2dx$$

is constant.

Proof. First we rewrite (1.1) as

$$\partial_t\psi(x,t)=i\beta\Delta\psi(x,t)+i\gamma V(x)\psi(x,t)\tag{1.4}$$

with $\beta = \frac{\hbar}{2m}$ and $\gamma = \frac{-1}{\hbar}$. Now for $B_R = \{x \in \mathbb{R}^3 : |x| < R\}$

$$\begin{aligned}
\frac{d}{dt}\int_{B_R} |\psi(x,t)|^2 dx &= \frac{d}{dt}\int_{B_R} \psi(x,t)\overline{\psi(x,t)}dx = \int_{B_R} (\dot{\psi}(x,t)\overline{\psi(x,t)} + \psi(x,t)\overline{\dot{\psi(x,t)}})dx \\
&\overset{(1.1)}{=} \int_{B_R} [i\beta\Delta\psi + i\gamma V\psi]\overline{\psi} + \psi[(-i)\beta\overline{\Delta\psi} + (-i)\gamma\overline{V\psi}]dx \\
&= \int_{B_R} (i\beta(\Delta\psi)\overline{\psi} - i\beta\psi\Delta\overline{\psi})dx \qquad \text{since } V = \overline{V} \\
&\overset{IBP}{=} i\beta\left[-\int_{B_R} \cancel{(\nabla\psi\nabla\overline{\psi} - \nabla\psi\nabla\overline{\psi})}dx + \int_{\partial B_R} [(\nabla\psi)\overline{\psi} - \psi\nabla\overline{\psi}]\frac{x}{|x|}ds\right]
\end{aligned}$$

Now integrating this over t gives

$$\int_{B_R} |\psi(x,t)|^2 dx - \int_{B_R} |\psi(x,0)|^2 dx = \beta\left|\int_0^t \left[\int_{\partial B_R} (\nabla\psi\overline{\psi} - \psi(\nabla\overline{\psi})\tfrac{x}{|x|}ds\right]d\tau\right| \tag{1.5}$$

Then since

$$\text{Area of } \partial B_R = 4\pi R^2 \qquad |\nabla\psi||\psi| \le \frac{C_{0,t}^2}{R^{2\alpha-1}}$$

where $\alpha > \frac{3}{2}$. Then

$$(1.5) \le \beta C_{0,t}^2 \frac{8\pi}{R^{2\alpha-3}} \overset{R\to\infty}{\to} 0$$

The limit of the LHS of (1.5) is $\int |\psi(x,t)|^2 dx - \int |\psi(x,0)|^2 dx$ and so it follows that

$$\int |\psi(x,t)|^2 dx = \int |\psi(x,0)|^2 dx$$

for every t □

Thus if $\int |\psi(x,0)|^2 dx = 1$ then $\int |\psi(x,t)|^2 dx = 1$ for all t.

Theorem 1.3 (Uniqueness)**.** *If two solutions to (1.1) and (1.3) agree at time $t = 0$, then they are agree for all time.*

Proof. If ψ, ϕ solves (1.1), then $\psi - \phi$ solves (1.1), and $\psi(x,0) - \phi(x,0) = 0$ for every x by assumption. Then $\int |\psi(x,t) - \phi(x,t)|^2 dx = 0$ for all time t and so $\psi(x,t) - \phi(x,t) = 0$ for all t and x. □

We remark that this theorem implies causality.

1.3 Solution to the Free Schrödinger equation

The 'free' refers to the fact that we have linear motion, no external forces. In Newtonian mechanics, either the particle stays still or moves in a straight line. We consider (1.1) with $V = 0$, and in *atomic units*, we can assume $\hbar = m = 1$.

$$i\partial_t(x,t) = -\frac{1}{2}\Delta\psi(x,t) \tag{1.6}$$

A simple solution can be guessed:

$$\psi(x,t) = e^{i(k\cdot x+\frac{1}{2}|k|^2 t)}$$

called *de Broglie's wave*. But $|\psi(x,t)|^2 = 1$ and so $\int |\psi(x,t)|^2 dx = \infty$. To find square integrable solutions, we need a more systematic approach. Recall the Fourier transform:

$$(\mathcal{F}\psi)(k,t) = \hat{\psi}(k,t) = \int_{\mathbb{R}^3} e^{-ik\cdot x}\psi(x,t)dx$$

and its inverse

$$(\mathcal{F}^{-1}\psi)(x,t) = \check{\psi}(k,t) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e^{ik\cdot x}\hat{\psi}(k,t)dk \vee \wedge$$

Moreover, $\mathcal{F}\partial x_j \mathcal{F}^{-1} = ik_j$:

$$\begin{aligned}
[\mathcal{F}\partial x_j \mathcal{F}^{-1}\psi](k) &= \frac{1}{(2\pi)^3}\left[\mathcal{F}\partial x_j \int e^{i\tilde{k}\cdot x}\psi(\tilde{k})d\tilde{k}\right](k) \\
&= \frac{1}{(2\pi)^3}\left[\mathcal{F}\int e^{i\tilde{k}\cdot x}\underbrace{[i\tilde{k}_j\psi(\tilde{k})]}_{g(\tilde{k})}d\tilde{k}\right](k) \\
&= \mathcal{F}\mathcal{F}^{-1}g(k) = g(k) = ik_j\psi(k)
\end{aligned}$$

and thus it follows $\mathcal{F}\Delta\mathcal{F}^{-1} = -|k|^2$, where we think of $\mathcal{F}, \Delta, \partial x_j, \mathcal{F}^{-1}$ as operators of functions. One can say that Δ is diagonal in Fourier space. By viewing $f(x)$ as a 'vector' with index x (think spectrum!), then

$$\mathcal{F}\Delta\mathcal{F}^{-1}f(k) = -|k|^2 f(k)$$

So, we can solve (1.6) by looking at it in Fourier space:

$$\begin{aligned}
&i\partial_t\widehat{\psi(x,t)} = -\frac{1}{2}\widehat{\Delta\psi(x,t)} \\
&\Leftrightarrow i\partial_t\hat{\psi}(k,t) = -\frac{1}{2}\mathcal{F}\Delta\mathcal{F}^{-1}\mathcal{F}\psi = \frac{1}{2}|k|^2\hat{\psi}(k,t)
\end{aligned}$$

The solution to this is trivial for fixed k:

$$\hat{\psi}(k,t) = e^{-i\frac{|k|^2 t}{2}}\hat{\psi}(k,0)$$

and is well defined if $\hat{\psi}(k,0) \in L^2$ (equivalently $\psi(x,0) \in L^2$). Recall that the Fourier representation is good for studying momentum from (1.2). Note that we have immediately Newton's first law - *conservation of momentum*, using $|e^{-i\frac{|k|^2}{2}t}| = 1$

$$\int_B \left|\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\hat{\psi}(\tfrac{k}{\hbar},t)\right|^2 dk = \int_B \left|\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\hat{\psi}(\tfrac{k}{\hbar},0)\right|^2 dk$$

This also means that wavepackets are spread over time.

We are interested in position space, so we need to do an inverse Fourier transform.

$$\begin{aligned}
\psi(x,t) = \mathcal{F}^{-1}\hat{\psi}(k,t) &= \frac{1}{(2\pi)^d}\int e^{ik\cdot x}e^{-i\frac{|k|^2}{2}t}\hat{\psi}(k,0)dk \\
&= \frac{1}{(2\pi)^d}\int e^{ik\cdot x}e^{-i\frac{|k|^2 t}{2}}\left[\int e^{-ik\cdot y}\psi(y,o)dy\right]dk
\end{aligned}$$

Now do the integral over k:

$$\begin{aligned}\int e^{ik\cdot(x-y)}e^{-i\frac{|k|^2t}{2}}dk &= \frac{e^{\frac{i}{2t}(x-y)^2}}{(2\pi)^d}\int e^{-\frac{it}{2}(k-\frac{1}{t}(x-y))^2}dk \\ &= \frac{e^{\frac{i}{2t}(x-y)^2}}{(2\pi it)^{\frac{d}{2}}}\end{aligned}$$

Where for the last inequality we have used that the integral is in Gaussian form with mean $\frac{1}{t}(x-y)$ and variance $\sqrt{\frac{1}{it}}$. And thus

$$\psi(x,t) = \frac{1}{(2\pi it)^{\frac{d}{2}}}\int e^{\frac{i}{2t}(x-y)^2}\psi(y,0)dy \tag{1.7}$$

We define an operator $P_t : \psi(\cdot,0) \to \psi(\cdot,t)$, called the *propagator*. It is given by integrating against the kernel

$$K(x-y,t) = \frac{1}{(2\pi it)^{\frac{d}{2}}}e^{\frac{i}{2t}(x-y)^2} \tag{1.8}$$

An important special case is the Gaussian wavepacket (in d dimensions). It is given by the initial condition:

$$\psi(x,0) = \frac{1}{2\pi\sigma^2}\frac{1}{4}e^{iv_0\cdot(x-x_0)-\frac{|x-x_0|^2}{4\sigma^2}}$$

The integral in (1.7) can now be done explicitly to give

$$\psi(x,t) = (\frac{\sigma^2}{2\pi})^{\frac{d}{4}}\frac{1}{(\sigma^2+\frac{it}{2})^{\frac{3}{2}}}\exp\left[\frac{|\sigma^2 v_0 + i\frac{|x-x_0|^2}{2}|^2}{\sigma^2+i\frac{t}{2}} - \sigma^2 v_0^2\right]$$

What does $\psi(x,t)$ look like? $\psi(x,0)$ is a Gaussian, with total probability 1, mean position x_0 and standard deviation (or 'uncertainty') σ. Furthermore it can be shown that $\psi(x,t)$ has mean x_0+tv_0 and standard deviation $\sigma(t) = \sqrt{\sigma^2+(\frac{t}{2\sigma})^2}$. Note that

(i) The mean solves

$$\begin{cases} m\ddot{x} = 0 \\ x(0) = x_0 \\ \dot{x}(0) = v_0 \end{cases} \quad \text{Newton's equations - i.e. behaves classically}$$

(ii) uncertainty increases over time

(iii) speed is encoded by oscillations. Note that

$$\mathrm{Re}(\psi(x,0)) = \frac{1}{2\pi\sigma^2}^{\frac{d}{4}}\cos(v_0-(x-x_0))e^{-\frac{|x-x_0|^2}{4\sigma^2}}$$

i.e. faster oscillations = bigger v_0 = faster wavefunction.

1.4 Ehrenfest equations

We've seen that the mean position of a Gaussian wavepacket solves free Newton's equation (for the free Schrodinger equation). A similar thing holds fore more general wavepackets and potentials.

Definition 1.4. For a wavefunction $\psi(x,t)$ with $\int |\psi(x,t)|^2 = 1$ the *expected position* and *expected momentum* are vectors given by

$$\begin{aligned}\langle X(t)\rangle &= \int_{\mathbb{R}^d} x|\psi(x,t)|^2 dx\\ \langle P(t)\rangle &= \int_{\mathbb{R}^d} k|\frac{1}{(2\pi\hbar)^{\frac{d}{2}}}\hat{\psi}(\frac{k}{\hbar},t)|^2 dk\end{aligned}$$

respectively.
The idea is that $|\psi(x,t)|^2$ is the position probability density and $|\frac{1}{(2\pi\hbar)^{\frac{d}{2}}}\hat{\psi}(\frac{k}{\hbar},t)|^2$ the momentum probability density. Taking derivatives of $\langle X(t)\rangle$ and $\langle P(t)\rangle$ we might expect that they satisfy

$$\langle \ddot{X}(t)\rangle = \partial_t^2\langle X(t)\rangle \overset{?}{=} \frac{1}{m}(-\nabla V\langle X(t)\rangle)$$

similar to $m\ddot{x}(t) = -\nabla V(x(t))$. But *this is not true.* However, we do have the following

Proposition 1.5.

$$\frac{d}{dt}\langle X_j(t)\rangle = \frac{1}{m}\langle P_j(t)\rangle$$

Proof.

$$\begin{aligned}\frac{d}{dt}\langle X_j(t)\rangle &= \int_{\mathbb{R}^d}\frac{d}{dt}[x_j\psi(x,t)\overline{\psi}(x,t)]dx\\ &= \int_{\mathbb{R}^d} x_j[(\partial_t\psi)\overline{\psi} + \psi\partial_t\overline{\psi}]dx\\ &= \int_{\mathbb{R}^d} x_j[(i\beta\Delta\psi + i\gamma V\psi)\overline{\psi} + \psi(\overline{i\beta\Delta\psi + i\gamma V\psi})]dx\\ &= i\beta\int_{\mathbb{R}^d} x_j[(\Delta\psi)\overline{\psi} - \psi(\Delta\overline{\psi})]dx\\ &= -i\beta\int_{\mathbb{R}^d}\nabla x_j\cdot[(\nabla\psi)\overline{\psi} - \psi\nabla\overline{\psi}]dx \quad \text{IBP}\\ &= -i\beta\int_{\mathbb{R}^d}(\partial_{x_j}\psi)\overline{\psi} - \psi(\partial_{x_j}\overline{\psi})dx\end{aligned}$$

and by integration by parts on the second term we get

$$\begin{aligned}&= -2i\beta\int_{\mathbb{R}^d}(\partial_{x_j}\psi)\overline{\psi}dx \qquad (1.9)\\ &= \frac{1}{m}\int_{\mathbb{R}^d}(\frac{\hbar}{i}\partial_{x_j}\psi)\overline{\psi}dx\\ &= \frac{1}{m}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\widehat{\frac{\hbar}{i}\partial_{x_j}\psi}\hat{\overline{\psi}}dk \quad \text{Plancherel}\\ &= \frac{1}{m}\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\hbar k_j\hat{\psi}\hat{\overline{\psi}}dk\\ &= \frac{1}{m}\int_{\mathbb{R}^d} p_j|\frac{1}{(2\pi\hbar)^{\frac{d}{2}}}\hat{\psi}(\frac{p}{\hbar})|^2 dp = \frac{1}{m}\langle P_j(t)\rangle\end{aligned}$$

□

Consider (1.9) again, taking one more derivative and (1.4) using and integration by parts

$$\begin{aligned}
\frac{d^2}{dt^2}\langle X_j(t)\rangle &= -2i\beta\int_{\mathbb{R}^d}\dot{\overline{\psi}}\partial_{x_j}\psi+\overline{\psi}\partial_{x_j}\dot{\psi}dx\\
&= -2i\beta\int_{\mathbb{R}^d}(-i\beta\Delta\overline{\psi}-i\gamma V\overline{\psi})\partial_{x_j}\psi+\overline{\psi}\partial_{x_j}[i\beta\Delta\psi+i\gamma V\psi]dx\\
&= -2i\beta\int_{\mathbb{R}^d}-i\gamma V\overline{\psi}\psi'+i\gamma(V\psi)'\overline{\psi}dx\\
&= 2\gamma\beta\int_{\mathbb{R}^d}(V'\overline{\psi}\psi+V\overline{\psi}'\psi-\overline{\psi}'V\psi dx\\
&= 2\gamma\beta\int_{\mathbb{R}^d}V'|\psi|^2dx=-\frac{1}{m}\int(\partial_{x_j}V)(x)|\psi(x,t)|^2dx\\
&\overset{\text{Def}}{=} -\frac{1}{m}\langle\partial x_jV(t)\rangle
\end{aligned}$$

Thus, we have shown that

$$\frac{d^2}{dt^2}\langle X(t)\rangle=-\frac{1}{m}\langle\nabla V(t)\rangle$$

where the right hand side is *not* the same as $\nabla V(\langle X(t)\rangle)$. We can compare this to Newton's equation

$$\frac{d^2}{dt^2}x(t)=-\frac{1}{m}V(x(t))$$

So the mean function fulfils a Newton equation but the force is given by the mean value of the potential with respect to the wave function, not by the potential at the mean position. We have proved

Theorem 1.6 (Ehrenfest's Equations)**.** *Let $V:\mathbb{R}^d\to\mathbb{R}$ be in C^1, $\psi\in C^2$ be a solution to the (1.1) satisfying*

$$\int|\psi|^2dx=1\quad\int|x||\psi|^2dx<\infty\quad\int(\nabla V(x))|\psi|^2dx<\infty$$

Then

(i) $\frac{d}{dt}\langle X(t)\rangle=\frac{1}{m}\langle P(t)\rangle$

(ii) $\frac{d}{dt}\langle P(t)\rangle=-\langle\nabla V(t)\rangle$

Now the mean value of the energy

$$\begin{aligned}
\langle E(t)\rangle &= \langle\frac{|P(t)|^2}{2m}\rangle+\langle V(t)\rangle\\
&= \int\frac{|k|^2}{2m}|\frac{1}{(2\pi\hbar)^{\frac{d}{2}}}\hat{\psi}(\frac{k}{\hbar},t)|^2dk+\int V(x)|\psi(x,t)|^2dx
\end{aligned}$$

Classically $E(t)=\frac{|p(t)|^2}{2m}+V(x,t)$ and

$$\begin{aligned}
\partial_tE(t) &= \frac{1}{m}p(t)\dot{p}(t)+\nabla V(x,t)\cdot\dot{x}(t)\\
&= \frac{1}{m}p(t)[\dot{p}(t)+\nabla V(x,t)]=0
\end{aligned}$$

This is also true in quantum mechanics.

Theorem 1.7. *Let $\psi(x,t)$ be a solution of (1.1) with*

$$\int |-\frac{1}{2}\Delta\psi + V\psi|^2 dx < \infty$$

then $\partial_t \langle E(t) \rangle = 0$

Proof. Exercise $\square$

Chapter 2

Quantum Mechanics via Operators

2.1 Hilbert spaces and operators

2.1.1 Hilbert spaces

If we have the equation (the Schrödinger equation with $\hbar = m = 1$)

$$i\partial_t \psi = (-\frac{1}{2}\Delta + V)\psi = H\psi$$

then it is reasonable to suspect that the solution will be of the form

$$\psi(t) = e^{-itH}\psi_0$$

but we need to make sense of an exponential of an operator. In this section we study operators from functional analysis and apply them to the study of the Schrödinger equation.

Definition 2.1. An *inner product* on a vector space X is a map $\langle \cdot, \cdot \rangle : X \times X \to \mathbb{C}$, that satisfies the following for every $\alpha, \beta \in \mathbb{C}$ and $v, w, z \in X$

(i) Linearity in second term: $\langle v, \alpha w + \beta z\rangle = \alpha\langle v, w\rangle + \beta\langle v, z\rangle$

(ii) Conjugate symmetry: $\langle v, w\rangle = \overline{\langle w, v\rangle}$

(iii) Positivity: $\langle v, v\rangle \geq 0$ and $\langle v, v\rangle = 0$ if and only if $v = 0$.

The above implies that $\langle \alpha v+\beta w, z\rangle = \overline{\alpha}\langle v, w\rangle + \overline{\beta}\langle v, z\rangle$. Also the map $v \mapsto ||v|| := \sqrt{\langle v, v\rangle}$ is a norm.

A complex vector space X with an inner product is called *Hilbert* if it is complete with respect to this inner product. A *Hilbert-Schmidt basis* is a set of mutually orthogonal vectors that is big enough to construct X. Formally it is a family $\{v_n : n \in \mathbb{N}\}$ of mutually orthogonal vectors such that the set of finite linear combinations

$$\{\sum_{j=1}^{n} \alpha_j v_{n_j} : n \in \mathbb{N}, \alpha_j \in \mathbb{R}, \{n_j\} \subset \mathbb{N}\}$$

is dense in X. If $\{v_n\}$ is a Hilbert-Schmidt basis then

Parseval relation: $||w||^2 = \sum_{n\in\mathbb{N}} |\langle w, v_n\rangle|^2$

Fourier series : $w = \sum_{n\in\mathbb{N}} \langle w, v_n\rangle v_n$

2.1.2 Operators

Unfortunately many operators that we come across in physics are unbounded maps $A : \mathcal{H} \to \mathcal{H}$. These are defined on a a subset $\mathcal{D}(A) \subset \mathcal{H}$.

We look at some common operators:

(i) $I, 1, id : \psi \mapsto \psi$

(ii) Multiplication by a co-ordinate ('position operator is unbounded')

$$x_j : \psi \mapsto x_j\psi$$

(iii) Multiplication by a function $V : \mathbb{R}^d \to \mathbb{C}$

$$M_V, V : \psi \mapsto V\psi; \quad (V\psi)(x) = V(x)\psi(x)$$

(iv) Momentum operator (unbounded)

$$P_j : \psi \mapsto -i\hbar\partial_{x_j}\psi$$

(v) Laplace operator (unbounded)

$$\Delta : \psi \mapsto \sum_{j=1}^{n} \partial_{x_j}^2\psi$$

(vi) Integral Operators

$$(K\psi)(x) = \int K(x,y)\psi(y)dy$$

for some kernel $K(x,y) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$

(vii) Schrödinger operator (unbounded)

$$H : \psi \mapsto -\frac{\hbar^2}{2m}\Delta\psi + V\psi$$

If an operator is bounded, then the operator norm is given by

$$||A|| := \sup_{\psi\in\mathcal{H}, ||\psi||=1} ||A\psi|| \equiv \sup_{\psi\in\mathcal{H}\setminus\{0\}} \frac{||A\psi||}{||\psi||} < \infty$$

2.1.3 Commutators

Definition 2.2. The *commutators* of A and B is

$$[A, B] = AB - BA$$

e.g. $[\partial_x, x] = 1$

$$\partial_x(xf(x)) - x\partial_x f(x) = f(x) + xf'(x) - xf'(x) = 1f(x)$$

(Note that there are some domain issues here as not all functions are differentiable).

2.2 Existence of solution to the Schrödinger equation

We reformulate the Schrödinger equation (1.1) in language of operators:

$$\begin{aligned} i\partial_t\psi &= H\psi \\ \psi(0) &= \psi_0 \end{aligned} \tag{2.1}$$

with $H = -\frac{1}{2}\Delta + V$ (take $\hbar = m = 1$). If H were a number the solution would be trivial: $\psi(t) = e^{-itH}\psi_0$. If H was a matrix we could define define

$$U_t = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} H^n =: e^{-itH}$$

and check that

$$\frac{\partial}{\partial t} U_t\psi_0 = -iHU_t\psi_0 \qquad U_0\psi_0 = \psi_0$$

So $U_t\psi_0$ solves (2.1). The same works for bounded operators. An operator U_t such that $U_t\psi_0$ solves (2.1) is called a *propagator* of (2.1).

Problems arise when H is unbounded, since $\sum_{n=0}^{\infty} \frac{(-it)^n}{n!} H^n$ may not make sense. For example if $H = -\frac{1}{2}\Delta$, then H^n is defined only for $\psi \in C^{2n}$. Thus we need at least $\psi_0 \in C^\infty$. We could try to define

$$e^{itH} := \lim_{n\to\infty} (1 - \frac{it}{n} H)^n$$

but we have the same problem. What does work, however, is

$$e^{itH} := \lim_{n\to\infty} (1 + \frac{it}{n} H)^{-n} \tag{2.2}$$

because $(1 + \frac{it}{n}H)^{-1}$ exists and is bounded. Before continuing we make a few more definitions.

Definition 2.3. An operator is *symmetric* if

$$\langle A\psi, \phi\rangle = \langle \psi, A\phi\rangle \quad \forall \psi, \phi \in \mathcal{D}(A)$$

For example the operator M_V is symmetric if and only if V is real. Since

$$\langle M_V\psi, \phi\rangle = \int \overline{V(x)\psi(x)}\phi(x)dx = \int \overline{\psi(x)V(x)}\phi(x)dx = \langle \psi, M_{\overline{V}}\phi\rangle$$

Note that using integration by parts, ∂_x is anti-symmetric, $i\partial_x$ is symmetric and ∂_x^2 is symmetric. In particular Δ is symmetric, and thus H is also symmetric.

Lemma 2.4. *Let A be a symmetric operator. For every $\phi \in \mathcal{D}(A)$, $\delta > 0$*

$$||(i\delta + A)\phi||^2 \geq \delta^2||\phi||^2 \tag{2.3}$$

Proof.

$$\begin{aligned} ||(i\delta + A)\phi||^2 &= \langle (i\delta + A)\phi, (i\delta + A)\phi\rangle \\ &= \delta^2||\phi||^2 + ||A\phi||^2 + i\delta\langle\phi, A\phi\rangle - i\delta\langle A\phi, \phi\rangle \\ &= \delta^2||\phi||^2 + ||A\phi||^2 \geq \delta^2||\phi||^2 \end{aligned}$$

□

So in particular $(i\delta + H)$ is always injective. However, as an operator $(i\delta + H) : C^2 \to L^2$ it is *not* onto (the domain is too small).

Definition 2.5. The *adjoint* A^* of an operator A is the unique operator with

$$\langle A^*\psi, \phi\rangle = \langle \psi, A\phi\rangle \quad \forall \phi \in \mathcal{D}(A), \psi \in \mathcal{D}(A^*)$$

where $\mathcal{D}(A^*) = \{\psi \in L^2 : |\langle \psi, A\phi\rangle| \le C_\psi ||\phi||\}$ for some constant C_ψ and for all $\phi \in \mathcal{D}(A)\}$. A symmetric operator is called *self-adjoint* if $\mathcal{D}(A) = \mathcal{D}(A^*)$

The good news is that H is self-adjoint on suitable domains for all physically relevant potentials V (but not, for example, for $V(x) = -\frac{C}{|x|^2}$ with $C > \frac{1}{4}$).

Proposition 2.6. *Assume that A is self-adjoint then for all $\delta \in \mathbb{R}\backslash\{0\}$ $(i\delta + A)^{-1}$ is bounded and $||(i\delta + A)^{-1}|| < \frac{1}{|\delta|}$.*

So, for example if for $\phi \in L^2$ put $u = (i\delta - \frac{1}{2}\Delta)^{-1}\phi$, then u is the solution to the inhomogeneous equation.

$$i\delta u - \frac{1}{2}\Delta u = \phi$$

We now return to constructing e^{-itH}.

Theorem 2.7. *Let H be self-adjoint with $\mathcal{D}(H)$ dense in L^2. Then for each $\phi \in L^2$*

$$U_t\phi := \lim_{n\to\infty} (1 + \frac{it}{n}H)^{-n}\phi$$

exists in L^2

Proof. Set $V_n(t) = (1 + \frac{it}{n}H)^{-n}$. By proposition 2.6 and the fact that $1 + aH = a(\frac{1}{a} + H)$ then $(1 + aH)^{-1} = \frac{1}{a}(\frac{1}{a} + H)^{-1}$. Thus we have

$$||(1 + \frac{it}{n}H)^{-1}|| = ||\frac{n}{it}(\frac{n}{it} + H)^{-1}|| \le \frac{n}{t}\frac{t}{n} = 1$$

It follows $||V_n(t)|| \le 1$ for every $n \in \mathbb{N}$. Furthermore we have

$$\lim_{t\to 0} V_n(t)\phi = \phi \tag{2.4}$$

To see this, for $\phi \in \mathcal{D}(H)$ compute

$$\begin{aligned} V_1(t)\phi - \phi &= \big((1 + itH)^{-1} - 1\big)\phi = \frac{1 - 1 - itH}{1 + itH}\phi = \frac{-itH}{1 + itH}\phi \\ &= -it(1 + itH)^{-1}H\phi \end{aligned}$$

It follows that $||V_1(t)\phi - \phi|| \le t||(1 + itH)^{-1}||||H\phi||$. For general ϕ, by denseness of $\mathcal{D}(H)$ in L^2 take $\tilde{\phi} \in \mathcal{D}(H)$ with $||\tilde{\phi} - \phi|| < \epsilon$. Then

$$\begin{aligned} ||V_1(t)\phi - \phi|| &= ||(V_1(t) - 1)\phi|| \le ||(V_1(t) - 1)\tilde{\phi}|| + ||(V_1(t) - 1)(\phi - \tilde{\phi})|| \\ &\le t||H\tilde{\phi}|| + 2||\phi - \tilde{\phi}|| \overset{t\to 0}{\to} 2\epsilon \end{aligned}$$

for every ϵ. For general n note

$$(V_n(t)-1)\phi = (V_1(\tfrac{t}{n})^n - 1)\phi = (V_1(\tfrac{t}{n})-1)\sum_{k=0}^{n-1}(V_1(\tfrac{t}{n}))^k\phi$$

This implies

$$||(V_n(t)-1)\phi|| \le ||V_1(\tfrac{t}{n})-1||\sum_{k=0}^{n-1}||V_1(\tfrac{t}{n})||^k \le nt \overset{t\to 0}{\to} 0$$

We now show that $\{V_n(t)\phi\}_{\in\mathbb{N}}$ is a Cauchy sequence for every ϕ. That is

$$||V_n(t)-V_m(t)||_{L^2} \overset{m,n\to\infty}{\to} 0 \qquad \forall\psi\in L^2$$

and so this implies strong convergence. Note

$$\begin{aligned}
(V_n(t)-V_m(t))\phi &= \lim_{\epsilon\to 0}\int_{\epsilon}^{t-\epsilon}\frac{d}{ds}[V_m(t-s)V_n(s)\phi]ds \\
&= \lim_{\epsilon\to 0}\int_{t}^{t-\epsilon}[-V_m'(t-s)V_n(s)+V_m(t-s)V_m'(s)]\phi ds \qquad (2.5)
\end{aligned}$$

Now

$$\begin{aligned}
V_m'(t-s)V_n(s)-V_m(t-s)V_n'(s) &= -iH\left[\frac{1}{(1+\frac{i(t-s)}{m}H)^{m+1}}\frac{1}{(1+\frac{is}{n}H)^n}-\frac{1}{(1+i\frac{t-s}{m}H)^m}\frac{1}{(1+\frac{is}{n}H)^{n+1}}\right] \\
&= -iH\left[\frac{1+\frac{is}{n}H-1-\frac{i(t-s)}{m}H}{(1+\frac{i(t-s)}{m}H)^{m+1}(1+\frac{is}{n}H)^{n+1}}\right] \\
&= H^2\underbrace{\left(\frac{s}{n}-\frac{t-s}{m}\right)}_{\to 0\text{ as }n,m\to\infty}\underbrace{\left(1+\frac{i(t-s)}{m}H\right)^{-m-1}\left(1+\frac{is}{n}H\right)^{-n-1}}_{\text{bounded by }1}
\end{aligned}$$

But what about H^2? Assume $\phi\in\mathcal{D}(H^2)$, then

$$\begin{aligned}
||2.5|| &\le \int_0^t||(\frac{s}{n}-\frac{t-s}{m})\underbrace{(1+\frac{i(t-s)}{m}H)^{-m-1}(1+\frac{is}{n}H)^{-n-1}}_{||\cdot||\le 1}H^2\phi|| \\
&\le \frac{t^2}{2}(\frac{1}{n}+\frac{1}{m})||H^2\phi|| \overset{m,n\to\infty}{\to} 0 \qquad (2.6)
\end{aligned}$$

So $(V_n(t)\phi)$ is Cauchy for $\phi\in\mathcal{D}(H^2)$. For general ϕ we use denseness of $\mathcal{D}(H^2)$. We claim the following (proof is left as an exercise)

$$\left.\begin{array}{l}\text{(i) }\mathcal{D}(H^2)=(H+i)^{-1}\mathcal{D}(H)\\ \text{(ii) range}((H+i)^{-1}=\mathcal{D}(H)\end{array}\right\}\Rightarrow\ \mathcal{D}(H^2)\text{ dense}$$

With this we get $\{V_n(t)\}_{\in\mathbb{N}}$ is a Cauchy sequence and so a limit exists. □

Later we shall write $U_t=e^{-itH}$ but for it to warrant the notation we need to check that it actually behaves like an exponential. So far we have shown that the operator U_t defined as

$$U_t\phi := \lim_{n\to\infty}V_n(t)\phi$$

actually exists.

Theorem 2.8. *Define U_t as above. Then*

(i) U_t is strongly continuous i.e.

$$L^2 - \lim_{t \to t_0} U_t \phi = U_{t_0} \phi \quad \forall \phi \in L^2.$$

(i) For every $\phi \in \mathcal{D}(H)$

$$U_t H \phi = H U_t \phi.$$

So in particular $U_t \phi \in \mathcal{D}(H)$ for each t and $\phi \in \mathcal{D}(H)$.

(iii) For $\phi \in \mathcal{D}(H)$

$$i \partial_t (U_t \phi) = H(U_t \phi).$$

So $\phi(x,t) = U_t \phi_0(x)$ solves (2.1) with initial condition ϕ_0.

Proof. (a) $V_n(t)\phi \overset{t \to t_0}{\to} V_n(t_0)\phi$ as the resolvent is analytic (for $t_0 > 0$) or by direct computation for $t_0 = 0$ (see above). By (2.6) convergence is uniform in t on on compact intervals.

(b) Let $\phi \in \mathcal{D}(H)$ Then

$$U_t H \phi = \lim_{n \to \infty} V_n(t) H \phi = \lim_{n \to \infty} H V_n(t) \phi.$$

Now let $\psi_n = V_n(t)\phi$ Then we have

(i) $\psi_n \overset{n \to \infty}{\to} U_t \phi$

(ii) $(H\phi_n)_{n \in \mathbb{N}}$ is convergent in L^2

Since H is a closed operator we have $U_t \phi \in \mathcal{D}(H)$ and $HU_t\phi = \lim_{n \to \infty} H\phi_n = U_t H \phi$.

(c) By part (b) the claim is that

$$i \partial_t (U_t \phi) = H(U_t \phi) = U_t H \phi$$

Consider the limit

$$\begin{aligned} \lim_{n \to \infty} V_n'(t) &= \lim_{n \to \infty} \partial_t (1 + \tfrac{it}{n} H)^{-n} \phi \\ &= \lim_{n \to \infty} \tfrac{i}{n} H(-n)(1 + \tfrac{it}{n} H)^{-n-1} \phi \\ &= \lim_{n \to \infty} -iH(1 + \tfrac{it}{n} H)^{-1} V_n(t) \phi \end{aligned}$$

□

We will now show that U_t behaves like an exponential.

Definition 2.9. An operator U is *unitary* if $U^*U = UU^* = 1$. If U is unitary then

$$||U\phi||^2 = \langle U\phi, U\phi \rangle = \langle \phi, U^*U\phi \rangle = ||\phi||^2.$$

So unitaries are always isometries.

Theorem 2.10. $U_t = \lim_{n \to \infty} V_n(t)$ *is unitary for every* $t \in \mathbb{R}$.

Proof. Clearly the adjoint of $V_n(t)$ is given by

$$V_n^*(t) = (1 - \tfrac{it}{n}H)^{-n}$$

Now consider $W_n(t) := V_n^*(t)V_n(t) = (1 + \frac{t^2}{n^2}H^2)^{-n}$. We will show that $W_n(t) \to 1$ strongly. For $\phi \in \mathcal{D}(H^2)$,

$$(W_n(t) - 1)\phi = (W_1(\tfrac{t}{n})^n - 1)\phi = (W_1(\tfrac{t}{n}) - 1)\sum_{k=0}^{n-1}(W_1(\tfrac{t}{n}))^k\phi \tag{2.7}$$

Now, since

$$\begin{aligned}||(1 + \tfrac{t^2}{n^2}H^2)\phi||^2 &\geq ||\phi||^2 + 2\tfrac{t^2}{n^2}||H\phi||^2 + \tfrac{t^4}{n^4}||H^2\phi||^2 \\ &\geq ||\phi||^2\end{aligned}$$

we have that $||(1 + \frac{t^2}{n^2}H^2)^{-1}|| \leq 1$. Also

$$(W_1(\tfrac{t}{n}) - 1)\phi = \left(\frac{1}{1 + \frac{t^2}{n^2}H^2} - 1\right)\phi = \left(\frac{-\frac{t^2}{n^2}H^2}{1 + \frac{t^2}{n^2}H^2}\right)\phi.$$

This shows the norm of $(W_1(\frac{t}{n}) - 1)\phi$ is bounded by $||\frac{t^2}{n^2}H^2\phi||$. So we can bound the norm of (2.7) by

$$\tfrac{t^2}{n^2}n||H^2\phi||$$

which tends to zero as $n \to \infty$. For general ϕ, we use an approximation argument. □

Corollary 2.11 (Conservation of probability)**.** *For all $\psi_0 \in \mathcal{D}(H)$ the solution $\psi(x,t)$ of (2.1) with initial condition ψ_0 fulfils*

$$||\psi(\cdot,t)||^2 = ||\psi_0||^2 \tag{2.8}$$

Finally we show that $t \mapsto U_t$ is a group.

Theorem 2.12. *For every $t, s \in \mathbb{R}$ we have*

$$U_tU_s = U_{t+s}$$

Proof. Using the fact $HU_t\phi = U_tH\phi$ for $\phi \in \mathcal{D}(H)$

$$\frac{d}{ds}(U_{t-s}U_s) = -U'_{t-s}U_s + U_{t-s}U'_s = -HU_{t-s}U_s + U_{t-s}HU_s = 0.$$

So $s \mapsto U_{t-s}U_s$ is constant. The result follows. □

So we conclude that $e^{-itH} := U_t$ is a unitary group of operators with $(e^{-itH})^* = e^{itH}$ and $e^{-itH}\psi_0$ solves

$$i\partial_t\psi = H\psi \qquad \psi(0) = \phi_0 \in \mathcal{D}(H)$$

2.3 Observables and Eigenvalues

An *observable* is a self-adjoint operator on the Hilbert space L^2. For example:

(i) Poisson operator X

$$(X_j\psi)(x) = x_j\psi(x)$$

(ii) Momentum operator

$$P_j : \psi \mapsto -i\hbar\partial_{x_j}\psi$$

(iii) Energy operator E

$$(E\psi)(x) = (-\frac{\hbar^2}{2m}\Delta + M_V)\psi(x)$$

(iv) Angular momentum L

$$L_{x_1}\phi = -i\hbar(x_2\partial_{x_3} - x_3\partial_{x_2})$$

Definition 2.13. The *mean* of an operator A with respect to the wave function ψ is

$$\langle A\rangle_\psi = \langle\psi, A\psi\rangle$$

Theorem 2.14 (Evolution of the mean)**.** *If ψ solves (2.1) then*

$$\begin{aligned}\frac{d}{dt}\langle A\rangle_{\psi(t)} &= \langle\psi, \frac{i}{\hbar}[H,A]\psi\rangle \\ &= \langle\frac{i}{\hbar}[H,A]\rangle_{\psi(t)}\end{aligned}$$

Proof.

$$\begin{aligned}\frac{d}{dt}\langle\psi, A\psi\rangle &= \frac{d}{dt}\int \psi(x,t)(A\psi)(x,t)dx \\ &= \langle\partial_t\psi, A\psi\rangle + \langle\psi, \partial_t A\psi\rangle \\ &= \langle\tfrac{1}{i\hbar}H\psi, A\psi\rangle + \langle\psi, A\tfrac{1}{i\hbar}H\psi\rangle \\ &= \langle A\psi, -\tfrac{1}{i\hbar}(HA - AH)\psi\rangle \\ &= \langle A\psi, \tfrac{i}{\hbar}[H,A]\psi\rangle\end{aligned}$$

□

Corollary 2.15. *The energy*

$$E(t) := \langle H\rangle_\psi = \langle P^2 + V\rangle_\psi$$

is conserved.

If $[A,H] = 0$ for any observable, then $\langle A\rangle_{\psi(t)}$ = constant and we call A a *conserved quantity.* For example, $P = \frac{\hbar}{i}\partial_x$ is conserved in the free Schrödinger equation.

Definition 2.16. An element $\psi \in L^2\backslash\{0\}$ is called an *eigenvector* (or *eigenfunction*) of A if there exists an eigenvalue λ such that $H\psi = \lambda\psi$.

Each eigenfuntion ψ gives rise to a conserved operator, P_ψ defined by

$$P_\psi \phi = \langle \psi, \phi \rangle \psi$$

i.e. the one-dimensional projection onto the subspace spaced by ϕ. Then

$$\begin{aligned} HP_\psi \phi &= H\langle \psi, \phi\rangle \psi = \langle \psi, \phi\rangle H\psi = \langle \psi, \phi\rangle \lambda\psi \\ P_\psi H\phi &= \langle \psi, H\phi\rangle \psi = \langle H\psi, \phi\rangle \psi = \langle \lambda\psi, \phi\rangle\psi = \overline{\lambda}\langle \psi, \phi\rangle \psi. \end{aligned}$$

since λ is an eigenvalue of a symmetric operator H, $\lambda||\psi||^2 = \langle \psi, H\psi\rangle = \langle H\psi, \psi\rangle = \overline{\lambda}||\psi||^2$, i.e. $\lambda \in \mathbb{R}$. It follows that for $a_j \in \mathbb{R}$

$$\sum_{j=1}^{N} \alpha_j P_{\psi_j}$$

for eigenfunctions ψ_j is a conserved quantity and more generally it can be shown that all spectral projections are conserved.

We can use eigenfunctions to study dynamics. For ψ_0 an eigenfunction with eigenvalue λ we have

$$e^{-itH}\psi_0 = e^{-it\lambda}\psi_0$$

since $i\partial_t \psi_0 = H\psi_0 = \lambda\psi_0$. So ψ_0 is a stationary solution of (2.1). As such $e^{it\lambda}\psi_0$ produces the same expected values as ψ_0. More precisely

$$\begin{aligned} \langle A\rangle_{e^{-it\lambda}\psi_0} &= \langle e^{-it\lambda}\psi_0, Ae^{-it\lambda}\psi_0\rangle = \langle \psi_0, e^{+it\lambda}Ae^{-it\lambda}\psi_0\rangle \\ &= \langle \psi_0, Ae^{+it\lambda}e^{-it\lambda}\psi_0\rangle = \langle \psi_0, A\psi_0\rangle = \langle A\rangle_{\psi_0} \end{aligned}$$

wave functions that differ only by a constant (non-x-dependent) phase describe the same physical state.

Proposition 2.17. *Assume that* $\psi(x,0) = \sum_{n=1}^{\infty} \alpha_n\psi_n(x)$ *with* $H\psi_n = \lambda_n\psi_n$. *Then*

(a) $\psi \in \mathcal{D}(A)$ *if and only if* $\sum_{n=1}^{\infty} |\lambda_n\alpha_n|^2 < \infty$

(a) If even

$$\sum_{n=1}^{\infty} |\lambda_n|^4|\alpha_n|^2 < \infty$$

then $\psi(0,t) = \sum \alpha_n e^{-it\lambda_n}\psi_n$ *is the unique solution of (2.1)*

2.4 Heisenberg Picture of Quantum Dynamics

Recall that for any observable we have

$$\begin{aligned} \langle A\rangle_{\psi(t)} &= \langle e^{-\frac{i}{\hbar}tH}\phi_0, Ae^{-\frac{i}{\hbar}tH}\phi_0\rangle = \langle \phi_0, \underbrace{e^{+\frac{i}{\hbar}tH}Ae^{-\frac{i}{\hbar}tH}}_{A(t)}\phi_0\rangle \\ &= \langle A(t)\rangle_{\phi_0}. \end{aligned}$$

So instead of solving (2.1) we can solve the following equation in the space of operators:

$$\frac{d}{dt}A(t) = \frac{i}{\hbar}[H, A(t)]$$

This gives

$$\frac{i}{\hbar}He^{\frac{i}{\hbar}Ht}Ae^{\frac{-i}{\hbar}Ht} + e^{\frac{i}{\hbar}Ht}A(-\frac{i}{\hbar})He^{-\frac{i}{\hbar}Ht} = \frac{i}{\hbar}[H, A(t)] \tag{2.9}$$

2.5 Uncertainty Principle

Fundamental properties in probability theory

$$\textit{Mean value: } E(X) = \int x d\mu(x) \qquad \textit{Standard deviation: } \sigma(X) = \left(\int (x - E(X))^2 d\mu(x)\right)^{\frac{1}{2}}$$

In Quantum Mechanics, the position mean value is

$$\langle X \rangle_\psi = \int x|\psi(x)|^2 dx$$

or more generally

$$\langle A \rangle_\psi = \langle \psi, A\psi \rangle$$

For position it's clear that

$$\int (x - \langle X \rangle_\psi)^2 |\psi(x)|^2 dx = \langle X^2 \rangle_\psi - \langle X \rangle_\psi^2$$

is the variance. So $\sqrt{\langle X^2 \rangle_\psi - \langle X \rangle_\psi^2}$ is the standard deviation. In general

$$\blacktriangle A := \sqrt{\langle A^2 \rangle_\psi - \langle A \rangle_\psi^2}$$

is the *uncertainty* (i.e. standard deviation) of A.

Consider the Gaussian wave packets with zero mean value and zero mean momentum. That is

$$\psi(x) = \frac{1}{2\pi\sigma^2}e^{\frac{|x|^2}{4\sigma^2}}.$$

It can be easily check that $\langle X_j \rangle_\psi = 0$ and $\langle P_j \rangle_\psi = 0$. Furthermore

$$\begin{aligned}
\langle \blacktriangle X_j \rangle^2 &= \int x_j^2 \frac{1}{(2\pi\sigma^2)^{\frac{d}{2}}} e^{\frac{-|x|^2}{2\sigma^2}} dx \\
&= \underbrace{1 \cdot \ldots \cdot 1}_{d-1} \int x_j^2 \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} e^{-\frac{x_j^2}{2\sigma^2}} dx_j = \sigma^2 \\
\langle \blacktriangle P_j \rangle^2 &= \langle P_j^2 \rangle_\psi = \langle \psi, P_j^2 \psi \rangle \\
&= \int \overline{\psi(x)}(-\hbar^2 \partial_j^2 \psi(x)) dx \overset{\text{IBP}}{=} \hbar^2 \int \partial_j \overline{\psi} \partial_j \psi dx \\
&= \hbar^2 \int (\overline{\frac{x_j}{2\sigma^2}\psi})(\frac{x_j}{2\sigma^2}\psi) dx = \frac{\hbar^2}{4\sigma^4} \int x_j^2 |\psi(x)|^2 dx = \frac{\hbar^2}{4\sigma^2}
\end{aligned}$$

So either we make σ small and get good information about position or we make σ large and get good information about momentum, but we cannot have both. In particular

$$\langle \blacktriangle X_j \rangle_\psi \langle \blacktriangle P_j \rangle_\psi = \frac{\hbar}{2}$$

The following theorem shows that this is the best we can hope for:

Theorem 2.18 (Heisenberg's Uncertainty Principle)**.** *For any* $\psi \in \mathcal{D}(X_j^2) \cap \mathcal{D}(P_j^2)$ *we have*

$$\langle_\psi \blacktriangle X_j \rangle_\psi \langle \blacktriangle P_j \rangle_\psi \geq \frac{\hbar}{2}$$

Implication: it is *in principle* impossible to measure both position and speed of a particle to arbitrary accuracy. To prove theorem 2.18 we will need the canonical commutation relation (CCR): $[P_j, X_j] = \frac{\hbar}{i} 1$ which follows from the observation

$$\begin{aligned} P_j X_j f &= \partial_{x_j}(x_i f(x)) = f(x) + x_j f'(x) \\ X_j P_j f &= x_j \partial_{x_j}(f(x)) = x_j f'(x) \end{aligned}$$

Theorem theorem 2.18 follows immediately from

Theorem 2.19 (Abstract Uncertainty Principle)**.** *Let A, B be self-adjoint operators. Then for any* $\psi \in \mathcal{D}(A) \cap \mathcal{D}(A^2) \cap \mathcal{D}(B) \cap \mathcal{D}(B^2)$ *we have*

$$\langle \blacktriangle A \rangle_\psi \langle \blacktriangle B \rangle_\psi \geq |\frac{1}{2} \langle [A, B] \rangle_\psi|$$

Proof. We use

$$\begin{aligned} |\langle [X, Y] \rangle_\psi| &= |\langle \psi, (XY - YX)\psi \rangle| = |\langle X\psi, Y\psi \rangle - \langle Y\psi, X\psi \rangle| \\ &= |\langle X\psi, Y\psi \rangle - \overline{\langle X\psi, Y\psi \rangle}| \\ &= |2 \operatorname{Im} \langle X\psi, Y\psi \rangle| \leq 2|\langle X\psi, Y\psi \rangle| \\ &\leq 2||X\psi||||Y\psi|| \end{aligned}$$

Now use

$$X = A - \underbrace{\langle A \rangle_\psi}_{\alpha} 1 \qquad Y = B - \underbrace{\langle B \rangle_\psi}_{\beta} 1$$

Then

$$\begin{aligned} [X, Y] &= [A - \alpha 1, B - \beta 1] = [A, B] - [A, \beta 1] - [\alpha 1, B] + \alpha\beta[1, 1] \\ &= [A, B] \end{aligned}$$

and

$$\begin{aligned} ||X\psi||^2 &= \langle (A - \alpha I)\psi, (A - \alpha I)\psi \rangle = \langle A\psi, A\psi \rangle - \langle A\psi, \alpha\psi \rangle - \langle \alpha\psi, A\psi \rangle + \langle \alpha\psi, \alpha\psi \rangle \\ &= \langle \psi, A^2\psi \rangle - \alpha \langle \psi, A\psi \rangle - \alpha \langle \psi, A\psi \rangle + \alpha^2 ||\psi||^2 \\ &= \langle A^2 \rangle_\psi - \langle A \rangle_\psi^2 \end{aligned}$$

$\square$

The equality

$$\langle [X, Y] \rangle_\phi = 2i \operatorname{Im} \langle X\psi, Y\psi \rangle \tag{2.10}$$

can be used to prove the following:

2.6 The Stability of the Hydrogen Atom

In classical mechanics there is a nucleus and one electron. The nucleus is much heavier, so we consider its position fixed and calculate the motion of the electron. They interact vis the *Coulomb potential*

$$V(x) = \frac{-e^2}{|x - x_{\text{nuc}}|} = \frac{-e^2}{|x|}. \tag{2.11}$$

This means that the classical energy is given by

$$E = \frac{\rho^2}{2} - \frac{1}{|x|} \overset{x \to 0}{\to} -\infty.$$

This means that if the electron falls into the nucleus, it gains infinite energy, which is impossible in the real world. The same problem seems to exist in celestial mechanics, but there, the planets can be shown to go on stable orbits around the sun for a very long time. The situation is different for an electron orbiting around a nucleus: As it moves on a curved orbit, it will always accelerate, therefore emit radiation and be slowed down. So a classical electron orbiting a classical nucleus would crash into that nucleus sooner rather than later.

In quantum mechanics this does not happen. What do you mean? Again H is the Hamiltonian operator, in this example with potential given above, i.e.

$$H = -\frac{\hbar}{2m}\Delta - \frac{e^2}{|x|^2}$$

We need that

$$\langle H \rangle_\psi = \langle \psi, H\psi \rangle = \langle \psi, -\frac{\hbar}{2m}\Delta\psi \rangle - \langle \psi, \frac{e^2}{|x|^2}\psi \rangle$$

is bounded from below in the variable ψ. More precisely we want

$$\inf\{\langle H \rangle_\psi : \psi \in L^2\} > -\infty$$

The key is

Theorem 2.20. *For all ψ in a d dense subspace of $\mathcal{D}(H)$ we have the following*

$$|\langle \psi, -\Delta\psi \rangle| \geq |\langle \psi, \frac{1}{4|x|^2} \rangle|$$
$$\int |\nabla\psi(x)|^2 dx \geq \frac{1}{4} \int |\psi(x)|^2 \frac{1}{|x|^2} dx$$

Proof. First we prove

$$\frac{1}{|x|^2} = \frac{i}{\hbar d} \sum_{j=1}^{d} [\frac{1}{|x|} P_j \frac{1}{|x|}, X_j] \tag{2.12}$$

(note $\partial_{x_j} \frac{1}{|x|} = \frac{-x_j}{|x|^3}$).

$$\frac{1}{|x|}\partial_j \frac{1}{|x|} x_j f(x) = \frac{1}{|x|}\left[\frac{-x_j^2}{|x|^3} + \frac{1}{|x|}\right] + \frac{x_j}{|x|^2}\partial_j f(x)$$

and

$$\frac{x_j}{|x|}\partial_j \frac{1}{|x|} f(x) = \frac{x_j}{|x|}\left[\frac{-x_j}{|x|^3} f(x) + \frac{1}{|x|}\partial_j f(x)\right] + \frac{x_j}{|x|^2}\partial_j f(x)$$

subtracting and summing over j from 1 to d gives the right-hand side of (2.12). This equality and (2.10) allows us to express

$$\hbar d\langle\psi,\frac{1}{|x|^2}\psi\rangle = -2\sum_{j=1}^{d}\mathrm{Im}(\langle\frac{1}{|x|}P_j\frac{1}{|x|}\psi,x_j\psi\rangle)$$

Now using the equality $P_j\frac{1}{|x|}=\frac{1}{|x|}P_j+[P_j,\frac{1}{|x|}]=\frac{1}{|x|}P_j+i\hbar\frac{x_j}{|x|^3}$. This gives us

$$\begin{aligned}\langle\frac{1}{|x|}P_j\frac{1}{|x|}\psi,x_j\psi\rangle &= \langle\frac{1}{|x|}(\frac{1}{|x|}P_j+i\hbar\frac{x_j}{|x|^3})\psi,x_j\psi\rangle\\ &= \langle\frac{1}{|x|^2}P_j\psi,x_j\psi\rangle - i\hbar\langle\frac{x_j}{|x|^4}\psi,x_j\psi\rangle\\ &= \langle P_j\psi,\frac{x_j}{|x|^2}\psi\rangle - i\hbar\langle\psi,\frac{x_j^2}{|x|^4}\psi\rangle\end{aligned}$$

Summing over j gives

$$\hbar d\langle\psi,\frac{1}{|x|^2}\psi\rangle = -2\,\mathrm{Im}\sum_{j=1}^{d}\langle P_j\psi,\frac{x_j}{|x|^2}\psi\rangle + 2\hbar\langle\psi,\frac{1}{|x|^2}\psi\rangle$$

We use this and then the Cauchy-Schwarz inequality

$$\begin{aligned}|\langle\psi,\frac{1}{|x|^2}\psi\rangle|^2 &= \frac{4}{(\hbar(d-2))^2}|\,\mathrm{Im}(\sum_{j=1}^{d}\langle P_j\psi,\frac{x_j}{|x|^2}\psi\rangle)|^2\\ &\leq \frac{4}{(\hbar(d-2))^2}|\sum_{j=1}^{d}\langle P_j\psi,\frac{x_j}{|x|^2}\psi\rangle|^2\\ &= \frac{4}{(\hbar(d-2))^2}|\langle\vec{P}\psi,\frac{\vec{x}}{|x|^2}\psi\rangle|^2\\ &\overset{C-S}{\leq} \frac{4}{(\hbar(d-2))^2}\langle\vec{P}\psi,\vec{P}\psi\rangle\langle\frac{\vec{x}}{|x|^2}\psi,\frac{\vec{x}}{|x|^2}\psi\rangle\\ &= \frac{4}{(\hbar(d-2))^2}|\langle\psi,\underbrace{\sum_{j=1}^{d}P_j^2}_{\hbar^2\Delta}\psi\rangle||\langle\psi,\sum_{j=1}^{d}\frac{x_j^2}{|x|^4}\psi\rangle|\\ &= \frac{4}{(\hbar(d-2))^2}|\langle\psi,-\hbar^2\Delta\rangle||\langle\psi,\frac{1}{|x|^2}\psi\rangle|\end{aligned}$$

It follows

$$|\langle\psi,\frac{1}{|x|^2}\psi\rangle|^2 \leq \frac{4}{(d-2)^2}|\langle\psi,-\Delta\psi\rangle||\langle\psi,\frac{1}{|x|^2}\psi\rangle|$$

which gives the claim ($d=3$). □

In the above proof we have used Cauchy-Schwarz inequalitys on $L^2(\mathbb{R}^d,\mathbb{R}^d)$ with

$$\langle\vec{f},\vec{g}\rangle = \sum_{j=1}^{d}\langle f_i,g_i\rangle_{L^2(\mathbb{R}^d,\mathbb{R})}$$

For the Hydrogen atom in $\mathbb{R}^3$ we find

$$\begin{aligned}\langle\psi, H\psi\rangle &= \langle\psi, (-\frac{\hbar}{2m}\Delta - \frac{e^2}{|x|})\psi\rangle = \langle\psi, -\frac{\hbar}{2m}\Delta\psi\rangle - \langle\psi, \frac{e^2}{|x|})\psi\rangle \\ &\geq \frac{\hbar^2}{8m}\langle\psi, \frac{1}{|x|^2}\psi\rangle = \langle\psi, f(x)\psi\rangle\end{aligned}$$

with $f(x) = \frac{\hbar^2}{8m}\frac{1}{|x|^2} - \frac{e^2}{|x|} \geq \frac{2me^4}{\hbar^2}$ which proves stability.

Chapter 3

The Harmonic Oscillator

The quantum harmonic oscillator is the quantum mechanical analogue of the classical harmonic oscillator. It is one of the few quantum mechanical systems for which a simple exact solution is known. Furthermore it is one of the most most important model systems in quantum mechanics because an arbitrary potential can be approximated as a harmonic potential at the vicinity of a stable equilibrium point. This is because particles move very little if they sit close to a potential energy minimum and have low kinetic energy. In this case we can approximate energy by its Taylor expansion.

$$V \approx V(x_0) + (x - x_0)V'(x_0) + \frac{1}{2}(x - x_0)^2 V''(x_0)$$

The $V(x_0)$ can be set to zero by an 'energy shift' and $V'(x_0) = 0$ as we are at a minimum. Thus we get the following

$$V(x) = \frac{\kappa}{2}x^2$$

where κ is some constant.

3.1 Classical Harmonic Oscillator

Using the classical relations

$$\begin{aligned} \dot{x}(t) &= \frac{1}{m}\rho(t) \\ \dot{\rho}(t) &= -\kappa x(t) \end{aligned}$$

Setting $\omega = \sqrt{\frac{\kappa}{m}}$ we get the solutions

$$\begin{aligned} x(t) &= A\sin(\omega t - b) \\ \rho(t) &= m\omega A\cos(\omega t - b) \end{aligned}$$

The energy of the system is given by

$$H_{\text{class}} = \frac{\rho^2}{2m} + \frac{\kappa}{2}x^2$$

3.2 Quantum Harmonic Oscillator

In quantum mechanics in one dimension

$$H = -\frac{\hbar^2}{2m}\partial_x^2 + \frac{\kappa}{2}x^2 \tag{3.1}$$

and in d dimensions

$$H = -\frac{\hbar^2}{2m}\Delta + xAx$$

where A is a positive definite matrix, but we shall be dealing only with one dimension. We can simplify the expression by scaling. For $\psi \in L^2(\mathbb{R})$ satisfying (3.1) define

$$\tilde{\psi}(\lambda x, \omega t) = \psi(x,t) \qquad \text{with } \lambda = \sqrt{\tfrac{mw}{\hbar}},\ \omega = \sqrt{\tfrac{\kappa}{m}}$$

Put $y = \lambda x$, and $\tau = \omega t$ then

$$\begin{aligned}
\partial_x^2 \psi(x) &= \partial_x^2(\tilde{\psi}(\lambda x, \omega t)) = \lambda^2 \psi''(y,\tau) = \frac{m\omega}{\hbar}\tilde{\psi}''(y,\tau) \\
x^2\psi(x,t) &= \frac{1}{\lambda^2}(\lambda x)^2 \tilde{\psi}(\lambda x, \omega t) = \frac{\hbar}{m\omega} y^2 \tilde{\psi}(y,\tau) \\
\partial_t \psi(x,t) &= \partial_t \tilde{\psi}(\lambda x, \omega t) = \omega \partial_\tau \tilde{\psi}(y,\tau)
\end{aligned}$$

Thus we have

$$\begin{aligned}
H\psi(x,t) &= -\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\tilde{\psi}''(y,\tau) + \frac{\kappa}{2}\frac{\hbar}{m\omega}\tilde{x}^2\tilde{\psi}(y,\tau) \\
&= -\frac{\hbar\omega}{2}\tilde{\psi}''(y,\tau) + \frac{\omega^{\cancel{2}}\cancel{m}}{2}\frac{\hbar}{\cancel{m\omega}} y^2 \tilde{\psi}(y,\tau) \\
&= \frac{\hbar\omega}{2}(-\tilde{\psi}''(y,\tau) + y^2\tilde{\psi}(\tilde{x})) \\
i\partial_t\psi(x,t) &= i\omega\partial_\tau\tilde{\psi}(y,\tau)
\end{aligned}$$

This gives us the more simplified quantum harmonic oscillator equation of

$$\frac{1}{2}(-\tilde{\psi}''(y,\tau) + y^2\tilde{\psi}(y,\tau)) = i\partial_\tau\tilde{\psi}(y,\tau) \tag{3.2}$$

In a similar way the above we can use scaling to put $m = \hbar = 1$ in the general Schrödinger equation (1.1).

3.3 Eigenvalues and Eigenvectors

We want to solve

$$H\psi = \lambda\psi \tag{3.3}$$

For this a different scaling workings better:

$$\tilde{\psi}(x) = \psi(\frac{x}{\lambda_0}) \qquad \text{with } \lambda_0 = \tfrac{\sqrt{m}}{\hbar},\ \omega = \hbar\sqrt{\tfrac{k}{m}}.$$

Then if ψ solves (3.3), then $\tilde{\psi}$ solves

$$-\frac{1}{2}\partial_x^2\tilde{\psi} + \frac{1}{2}\omega^2 x^2\tilde{\psi} = \lambda\tilde{\psi}$$

We drop the $\tilde{}$ notation and study

$$-\frac{1}{2}\partial_x^2\psi + \frac{1}{2}\omega^2 x^2\psi = \lambda\psi \tag{3.4}$$

and we will find all its solutions. We shall use the following strategy:

(i) Find one eigenfunction

(ii) Find the operators A_+, A_- that map each eigenfunction to the 'next higher' (or 'next lower') energy eigenfunction. This give us infinitely many eigenfunctions.

(iii) Show this gives them all

We start with (ii) and define

Definition 3.1. The *creation operator* (at frequency ω) is

$$A_+ := \frac{1}{\sqrt{2}}(-\frac{d}{dx} + \omega x)$$

and the *annihilation operator* (at frequency ω) is

$$A_- := \frac{1}{\sqrt{2}}(\frac{d}{dx} + \omega x)$$

In fact it can be easily shown that $A_- = A_+^*$. So we write $A = A_-$, $A^* = A_+$

Lemma 3.2.

$$A^*A = H - \frac{\omega}{2} \qquad AA^* = H + \frac{\omega}{2}$$

Proof.

$$\begin{aligned}
AA^*\psi &= \frac{1}{2}(\frac{d}{dx} + \omega x)(-\frac{d}{dx} + \omega x)\psi \\
&= \frac{1}{2}(\frac{d}{dx} + \omega x)(\omega x\psi - \frac{d\psi}{dx}) \\
&= \frac{1}{2}(\omega\psi + \omega x\frac{d\psi}{dx} - \frac{d^2\psi}{dx^2} - \omega^2 x^2\psi - \omega x\frac{d\psi}{dx} \\
&= (-\frac{1}{2}\frac{d^2\psi}{dx^2} + \frac{1}{2}\omega^2 x^2)\psi + \frac{\omega}{2}\psi \\
&= (H + \frac{\omega}{2})\psi
\end{aligned}$$

The proof of the other is similar. □

Before we implement step (ii), we shall first prove the following propositions:

Proposition 3.3. *Any eigenvalue of H is greater than or equal to $\frac{\omega}{2}$.*

Proof. Suppose λ is an eigenvalue of H. Then

$$\begin{aligned}
\lambda = \lambda||\psi||^2 &= \langle\psi, \lambda\psi\rangle = \langle\psi, H\psi\rangle = \langle\psi, (A^*A + \frac{\omega}{2})\psi\rangle \\
&= \langle\psi, (A^*A)\psi\rangle + \langle\psi, \frac{\omega}{2}\psi\rangle \\
&= ||A\psi|| + \frac{w}{2} \geq \frac{w}{2}
\end{aligned}$$

□

Proposition 3.4. *Assume $H\psi = \lambda\psi$ for some $\lambda \geq \frac{\omega}{2}$. Then*

(a) $A^*\psi$ is an eigenfunction of H with eigenvalue of $\lambda + \omega$

(b) For $\lambda > \frac{\omega}{2}$, $A\psi$ is an eigenfunction of H with eigenvalue of $\lambda - \omega$

(c) $\lambda = \frac{\omega}{2}$ if and only if $A\psi = 0$

Proof. Start with (c). Assume $H\psi = \lambda\psi$. Then

$$||A\psi||^2 = \langle \psi, A^*A\psi \rangle = \langle \psi, (H - \frac{\omega}{2})\psi \rangle = \langle \psi, (\lambda - \frac{\omega}{2})\psi \rangle = (\lambda - \frac{\omega}{2})||\psi||^2$$

which is zero if and only if $\lambda = \frac{\omega}{2}$.

For (b), assume again $H\psi = \lambda\psi$ then

$$\begin{aligned} H(A\psi) &= (AA^* - \frac{\omega}{2})A\psi = A(A^*A\psi - \frac{\omega}{2})\psi \\ &= (H - \frac{\omega}{2})\psi - \frac{\omega}{2}\psi = (\lambda - \frac{\omega}{2})\psi - \frac{\omega}{2}\psi \\ &= (\lambda - \omega)\psi \end{aligned}$$

For (a)

$$\begin{aligned} H(A^*\psi) &= (A^*A + \frac{\omega}{2})A^*\psi = A^*(AA^*\psi - \frac{\omega}{2})\psi \\ &= (H + \frac{\omega}{2})\psi + \frac{\omega}{2}\psi = (\lambda + \frac{\omega}{2})\psi + \frac{\omega}{2}\psi \\ &= (\lambda + \omega)\psi \end{aligned}$$

We need to check that $A^*\psi \neq 0$. Note that

$$\begin{aligned} ||A^*\psi|| &= \langle \psi, AA^*\psi \rangle = \langle \psi, (H + \frac{\omega}{2})\psi \rangle \\ &= \langle \psi, \lambda\psi \rangle + \frac{\omega}{2}||\psi||^2 > 0 \end{aligned}$$

□

So step (ii) is complete. For step (iii):

Proposition 3.5. *If λ is an eigenvalue of H then $\lambda \in \{\frac{\omega}{2} + n\omega : n \in \mathbb{N}\}$*

Proof. Assume by way of contradiction, $\lambda = \omega(\gamma + n)$, $\gamma \in (\frac{1}{2}, \frac{3}{2})$ $n \in \mathbb{N}$. Let ψ be the corresponding eigenfunction. Then $A^n\psi$ is an eigenfunction with eigenvalue $\lambda - \omega n = \omega\gamma$. So $H(A^n\psi) = \gamma\omega A^n\psi$. Now apply A again to find $H(A^{n+1})\psi = (\gamma - 1)wA^{n+1}\psi$ and since $\gamma - 1 < \frac{1}{2}$ this contradicts proposition 3.3. □

So we have shown A^* is a bijection from the eigenspace with eigenvalues $\frac{\omega}{2} + n\omega$ to the eigenspace with eigenvalues $\frac{\omega}{2} + (n+1)\omega$. Similarly A is a bijection from the $(\frac{1}{2} + n + 1)\omega$-eigenspace to the $(\frac{1}{2} + n)\omega$-eigenspace. It now remains to find one eigenspace, i.e. eigenfunctions corresponding to $\lambda = \frac{\omega}{2}$ (step 1). They are given, by part (c) of proposition 3.4 to be exactly the functions for which $A\psi = 0$. Thus

$$\begin{aligned} A\psi = \frac{1}{\sqrt{2}}(\psi'(x) + \omega x\psi(x)) = 0 \\ \Leftrightarrow \frac{\psi'(x)}{\psi(x)} = -\omega x \\ \Leftrightarrow \log(\psi(x)) = -\frac{\omega}{2}x^2 + c \\ \Leftrightarrow \psi(x) = e^{-\frac{\omega}{2}x^2}e^c \end{aligned}$$

We need $||\psi||^2 = 1$, so we find $1 = e^{2c}\int e^{-\omega x^2}dx = e^{2c}(\frac{\pi}{\omega})^{\frac{1}{2}}$. Thus

$$\phi(x) = (\frac{\omega}{\pi})^{\frac{1}{4}} e^{-\frac{\omega}{2}x^2}$$

Theorem 3.6. *The eigenvalues of the (scaled, one dimensional) quantum harmonic oscillator equation*

$$H_{osc} = -\frac{1}{2}\partial_x^2 + \frac{\omega^2}{2}x^2$$

are given by $\lambda_n = (\frac{1}{2}+n)\omega$ *for* $n \in \mathbb{N}\cup\{0\}$. *The corresponding normalised eigenfunctions are*

$$\phi_n = \frac{\omega^{\frac{1}{4}-\frac{n}{2}}}{\pi^{\frac{1}{4}}\sqrt{n!}}(-\frac{d}{dx} + wx)^n e^{-\frac{\omega}{2}x^2}$$

Proof. For $n = 0$ see above. Then by way of induction assume for $n \geq 0$, then

$$A^*\psi_n = \frac{1}{\sqrt{2}}(-\frac{d}{dx} + \omega x)\psi_n$$

is an eigenfunction, but not normalised. We have

$$||A^*\psi_n||^2 = \langle\psi_n, AA^*\psi\rangle = (\lambda_n + \omega)||\psi_n||^2 = (n+1)\omega.$$

So it follows that

$$\psi_{n+1} = \frac{1}{\sqrt{n+1}\sqrt{\omega}}A^*\psi_n$$

is an eigenfunction and normalised. □

A direct calculation of the above gives

$$(-\frac{d}{dx} + \omega x)^n e^{-\frac{\omega}{2}x^2} = H_n e^{-\frac{\omega}{2}x^2} \qquad \text{with } H_0(x) = 1, H_2 = 2x, H_3 = 4x^2 - 2, ...$$

$H_n(x)$ is called the n^{th} *Hermite polynomial.* Note that $\psi_0(x) > 0$ for all x and is the only eigenfunction with that property.

3.4 Dynamics

We want to solve

$$\frac{1}{2}(-\partial_x^2 + x^2)\psi(x,t) = i\partial_t\psi(x,t) \tag{3.5}$$

with $\psi(x,0) = \psi_0(x)$.

3.4.1 Periodicity

Let us write

$$\psi_0(x) = \sum_{n=0}^{\infty}\alpha_n\psi_n(x)$$

with ψ_n eigenfunctions to $H = \frac{1}{2}(-\partial_x^2 + x^2)$

$$H\psi_n = (\frac{1}{2} + n)\psi_n$$

(where we are considering $\omega = 1$). It can be shown that $\{\psi_n\}_{n\in\mathbb{N}}$ is an orthonormal basis of $L^2(\mathbb{R})$. Then by proposition 2.17

$$\begin{aligned}\psi(x,t) &= \sum_{n=0}^{\infty} \alpha_n e^{-i(n+\frac{1}{2})t}\psi_n(x) \\ &= \left[\sum_{n=0}^{\infty} \alpha_n e^{int} c_n H_n(x)\right] e^{-\frac{x^2}{2} - \frac{i}{2}t}\end{aligned}$$

Thus $\psi(x,t)$ is 2π periodic up to a global phase, which is invisible to all observables.

3.4.2 Dynamics of mean values

Recall the Ehrenfest equations

$$\frac{d}{dt}\langle X(t)\rangle_\psi = \langle P(t)\rangle_\psi \qquad \frac{d}{dt}\langle P(t)\rangle_\psi = -\langle \nabla V(t)\rangle_\psi$$

For the harmonic oscillator

$$\langle \nabla V(x)\rangle_\psi = \langle \psi, (\frac{1}{2}x^2)'\psi\rangle = \langle \psi, x\psi\rangle = \langle x\rangle_\psi = \nabla V(\langle x\rangle_\psi)$$

so in this case (but *not* in general) the mean values follow precisely the classical trajection.

3.4.3 Dynamics of observables

For the mean values we now know

$$\frac{d^2}{dt^2}\langle X(t)\rangle_\psi = \langle X(t)\rangle_\psi.$$

Solving this we get

$$\begin{aligned}\langle X(t)\rangle &= \cos(t)\langle X(0)\rangle + \sin(t)\langle P(0)\rangle \\ \langle P(t)\rangle &= \cos(t)\langle P(0)\rangle - \sin(t)\langle X(0)\rangle\end{aligned} \tag{3.6}$$

The trick is to note that (3.6) $\Leftrightarrow$

$$\langle \psi(t), X\psi(t)\rangle = \langle e^{-itH}\psi_0, Xe^{-itH}\psi_0\rangle = \cos(t)\langle \psi(0), X\psi(0)\rangle + \sin(t)\langle \psi(0), P\psi(0)\rangle$$

Thus defining:

$$X(t) := e^{itH}Xe^{-itH} = cos(t)X + sin(t)P$$

This implies

$$X^2(t) := e^{itH}X^2e^{-itH} = e^{itH}X\underbrace{e^{-itH}e^{itH}}_{=1}Xe^{-itH}$$

It is the same for all powers, so this implies

$$\begin{aligned}e^{iX(t)} &= \langle \psi, e^{iX}\psi\rangle = \int |\psi(x,t)|^2 e^{iX}dx \\ &= \sum_{n=0}^{\infty} \frac{i^n}{n!}X^n(t) = \exp(i(\cos(t)X + \sin(t)P))\end{aligned}$$

This becomes useful together with the *Weyl relation* (proof as exercise):

$$e^{i(aX+bP)} = e^{iaX}e^{ibP}e^{i\frac{ab}{2}}$$

Theorem 3.7. *[Mehler Kernel] The solution* $\psi(x,t)$ *of (3.5) is given by*

$$\psi(x,t) = \int K_t(x,y)\psi_0(y)dy$$

where

$$K_t(x,y) = \frac{e^{-i\frac{t}{2}}}{\sqrt{\pi(1-e^{-2it}}} \exp\left[\frac{(e^{-it}x-y)^2-(e^{-it}y-x)^2}{2(1-e^{-2it})}\right]$$

is the Mehler Kernel

Proof. See later (uses Feynman-Kac formula) □

Note that for $t=\frac{\pi}{2}$, $e^{-it}=-i$, $e^{-2it}=-1$. So

$$K_t(x,y) = \frac{e^{-i\frac{\pi}{4}}}{\sqrt{2\pi}} \exp\left[\frac{1}{4}((ix+y)^2+(iy+x)^2)\right] = e^{-i\frac{\pi}{4}}\frac{1}{\sqrt{2\pi}}e^{ixy}$$

and so K_t is the kernel of the Fourier transform, i.e. turns position into momentum and vice-versa. For $t=k\pi$ the kernel is undefined. But for $t\to k\pi$ it converges to a $\delta-$kernel.

Chapter 4

The Feynman-Kac Formula

4.1 Feynman integral

The aim of this section is to compute the integral kernel for e^{-itH} in general, i.e. find a function $K_t(x,y)$ such that
$$e^{-itH}f(x) = \int K_t(x,y)f(y)dy.$$
Why? Because then the solution of (1.6) is given by an integral.

4.1.1 Trotter Product Formula

We know

(a) $H = -\frac{1}{2}\Delta \Rightarrow K_t(x,y) = \frac{1}{(2\pi it)^{\frac{1}{2}}}e^{\frac{i}{2t}(x-y)^2}$ (free motion)

(b) $H = -\frac{1}{2}\Delta + \frac{x^2}{2} \Rightarrow K_t(x,y) =$ Mehler Kernel

and that's all. We *do* know the kernel of $e^{-it(-\frac{1}{2}\Delta)}e^{-itV}$:
$$K_t(x,y) = \frac{1}{(2\pi it)^{\frac{1}{2}}}e^{\frac{i}{2t}(x-y)^2}e^{-itV(y)}$$
but unfortunately
$$e^{-it(-\frac{1}{2}\Delta+V)} \neq e^{-it(-\frac{1}{2}\Delta)}e^{-itV}$$
But what is true is the following

Theorem 4.1 (Trotter Product Formula)**.** *Let A,B be operators. Assume, alternatively*

(i) either A or B are bounded

(ii) or A, B and $A+B$ are self-adjoint and bounded below.

Then for any $\lambda \in \mathbb{C}$ with $\mathrm{Re}(\lambda) \leq 0$ *and any $\psi \in \mathcal{D}(A) \cap \mathcal{D}(B) \cap \mathcal{D}(A+B)$ we have*
$$e^{\lambda(A+B)}\psi = \lim_{n\to\infty}(\exp(\frac{\lambda}{n}A)\exp(\frac{\lambda}{n}B))^n\psi$$

Proof. Only for (i). In this case the theorem is called the *Lie product formula*. Without loss of generality let $\lambda = 1$. And let $S_n = e^{\frac{A+B}{n}}$ and $T_n = e^{\frac{A}{n}} e^{\frac{B}{n}}$ then

$$\begin{aligned} e^{A+B} - (e^{\frac{1}{n}A} e^{\frac{1}{n}B})^n &= S_n^n - T_n^n = S_n^n - T_n S_n^{n-1} + T_n S_n^{n-1} - T_n^2 S_n^{n-2} + T_n^2 S_n^{n-2} ... + ... - T_n^n \\ &= \sum_{k=0}^{n-1} T_n^k (S_n - T_n) S_n^{n-k-1} \end{aligned}$$

Thus,

$$\begin{aligned} ||e^{A+B} - (e^{\frac{1}{n}A} e^{\frac{1}{n}B})^n|| &\leq \sum_{k=0}^{n-1} ||T_n^k|| ||(S_n - T_n)|| ||S_n||^{n-k-1} \\ &\leq \sum_{k=0}^{n-1} ||(S_n - T_n)|| (\max\{||T_n||, ||S_n||\})^{n-1} \\ &= n||(S_n - T_n)|| (\max\{||T_n||, ||S_n||\})^{n-1} \\ &\leq n||(S_n - T_n)|| (e^{\frac{||A||}{n}} e^{\frac{||B||}{n}})^{n-1} \end{aligned}$$

Since,

$$\begin{aligned} ||S_n|| &\leq e^{\frac{||A+B||}{n}} \leq e^{\frac{||A||}{n}} e^{\frac{||B||}{n}} \\ ||T_n|| &= ||e^{\frac{A}{n}} e^{\frac{B}{n}}|| \leq ||e^{\frac{A}{n}}|| ||e^{\frac{B}{n}}|| \leq e^{\frac{||A||}{n}} e^{\frac{||B||}{n}} \end{aligned}$$

Finally since S_n and T_n are bounded operators,

$$\begin{aligned} S_n &= 1 + \frac{A+B}{n} + \frac{(A+B)^2}{2!n^2} + ... \\ T_n &= (1 + \frac{A}{n} + \frac{A^2}{2!n^2} + ...)(1 + \frac{B}{n} + \frac{B^2}{2!n^2} + ...) = 1 + \frac{A+B}{n} + \frac{A^2 + 2AB + B^2}{2n^2} + ... \end{aligned}$$

So

$$||S_n - T_n|| = \sum_{k=2}^{\infty} |\frac{1}{k!n^k} \text{ something in } A, B| \leq \frac{c}{n^2} \overset{n\to\infty}{\to} 0$$

□

Let us apply this to $H = -\frac{1}{2}\Delta + V$ and $\lambda = -it$ (so $A = -\frac{1}{2}\Delta,\ B = V$). Then we know $exp(\frac{\lambda}{n}A)exp(\frac{\lambda}{n}B)$ has kernel with

$$K_{\frac{t}{n}}(x, y) = \frac{1}{(2\pi i \frac{t}{n})^{\frac{1}{2}}} e^{\frac{i}{2\frac{t}{n}}|x-y|^2} e^{-i\frac{t}{n}V(y)}.$$

It follows,

$$[\text{ Kernel of } e^{-itH}](x, y) \quad = \quad \lim_{n\to\infty} \int K_{\frac{t}{n}}(x, x_1)...K_{\frac{t}{n}}(x_{n-2}, x_{n-1}) K_{\frac{t}{n}}(x_{n-1}, y) dx_1...dx_{n-1}$$

since, letting $H_0 = -\frac{1}{2}\Delta$

$$
\begin{aligned}
e^{-itH}f(x) &\overset{\text{trotter}}{=} \lim_{n\to\infty} e^{-i\frac{t}{n}H_0}e^{-i\frac{t}{n}V}\cdot e^{-i\frac{t}{n}H_0}e^{-i\frac{t}{n}V}\cdot \underbrace{...}_{n\text{ times}} \cdot e^{-i\frac{t}{n}H_0}e^{-i\frac{t}{n}V}f(x)\\
&= \lim_{n\to\infty}\int dx_1 K_{\frac{t}{n}}(x,x_1)...\int dx_{n-1}K_{\frac{t}{n}}(x_{n-2},x_{n-1})\int dy K_{\frac{t}{n}}(x_{n-1},y)f(y)\\
&\overset{\text{Fubini}}{=} \lim_{n\to\infty}\int dx_1...dx_{n-1}dyK_{\frac{t}{n}}(x,x_1)K_{\frac{t}{n}}(x_1,x_2)...K_{\frac{t}{n}}(x_{n-2},x_{n-1})K_{\frac{t}{n}}(x_{n-1},y)f(y)\\
&= \lim_{n\to\infty}\int\left[\int ...\int dx_1...dx_{n-1}K_{\frac{t}{n}}(x,x_1)K_{\frac{t}{n}}(x_1,x_2)...K_{\frac{t}{n}}(x_{n-2},x_{n-1})K_{\frac{t}{n}}(x_{n-1},y)\right]f(y)dy\\
&= \lim_{n\to\infty}\int\left[\int ...\int dx_1...dx_{n-1}\exp\left(i\sum_{k=0}^{n-1}(\frac{1}{2}\frac{1}{\frac{t}{n}}|x_{k+1}-x_k|^2 - V(x_{k+1})\frac{t}{n})\right)(\frac{2\pi it}{n})^{\frac{-nd}{2}}\right]f(y)dy
\end{aligned}
\tag{4.1}
$$

with $x_0 = x$, $x_n = y$.

4.1.2 Feynman's ingenious interpretation

We now consider the part inside the exponential

$$S_n = \sum_{k=0}^{n-1}(\frac{1}{2}\frac{1}{\frac{t}{n}}|x_{k+1}-x_k|^2 - V(x_{k+1})\frac{t}{n})$$

and Feynman's interpretation of it.

Let $\phi_n : \mathbb{R}\to\mathbb{R}^d$ be piecewise linear with $\phi_n(\frac{kt}{n}) = x_k$ for $k = 0,1,...,n$ and $x_0 = x$ and $x_n = y$. Then

$$S_n = \frac{t}{n}\sum_{k=0}^{n-1}\frac{1}{2}\left(\frac{\phi_n(\frac{k+1}{n}t)-\phi_n(\frac{k}{n}t)}{\frac{t}{n}}\right)^2 - V(\phi_n(\frac{k+1}{n}t))$$

and instead of integrating over x_i we can integrate over functions that start at x and finish at y. What's more, S_n converges as a Riemann sum to

$$\int\frac{1}{2}|\phi'(s)|^2 - V(\phi(s))ds =: S(\phi,t).$$

So by taking the limit in the exponent only, gives an answer. $S(\phi,t)$ is the classical action corresponding to the classical Newton equation $\ddot{x} = -\nabla V(x)$. So we can get the integral kernel of e^{-itH} by

(i) evaluating the classical action 'all' possible paths

(ii) averaging over the results.

So in a sense, the final integral should be over $(\mathbb{R}^d)^\infty$ or rather $(\mathbb{R}^d)^{[0,t]}$ (the space of all functions $[0,t]\to\mathbb{R}^d$.

Great heuristic advantage: Since $S(\phi,t)$ is stationary at the classical solution those paths that are 'close' to it shall count most ('stationary phase argument'). Feynman went one step further than (4.1) and took the limit $n\to\infty$ also in the measure. The result:

$$e^{\frac{i}{\hbar}tH}(x,y) = \int e^{\frac{i}{\hbar}S(\phi,t)}d\phi$$

where '$d\phi$' is the 'Lebesgue' measure on all functions from x to y. The bad news is that it can be shown that there is no way to make sense of such a measure. This does not stop physicists! And the Feynman integral is used widely (e.g. for guessing results that have to be proved by other means). We want a rigorous general theory, and have to settle for less.

4.1.3 Feynman integrals for imaginary time

Marc Kac noticed that Feynman integrals make mathematical sense for imaginary time. Put differently

$$e^{-tH} = e^{-i(-itH)}$$

has kernel given by a space of functions. So from now on we aim to find the kernel of e^{-tH} for $t \in \mathbb{R}$.

Idea: Incorporate the $\frac{1}{2}\int_0^t |\phi'(s)|^2 ds$ term into the measure. So consider the measure on functions by

$$\begin{aligned}
&\mu_n(\phi(\tfrac{t}{n}) \in A_1, \phi(\tfrac{2t}{n}) \in A_2, ..., \phi(\tfrac{(n-1)t}{n}) \in A_{n-1}) \\
&= (\tfrac{2\pi t}{n})^{-\frac{nd}{2}} \int dx_1...dx_{n-1} e^{-\frac{1}{2\frac{t}{n}}|x-x_1|^2} 1_{A_1}(x_1) e^{-\frac{1}{2\frac{t}{n}}|x_2-x_1|^2} 1_{A_2}(x_2)...1_{A_{n-1}}(x_{n-1}) e^{-\frac{1}{2\frac{t}{n}}|y-x_{n-1}|^2} \\
&= \int dx_1...dx_{n-1} g_{\frac{t}{n}}(x,x_1) 1_{A_1}(x_1) g_{\frac{t}{n}}(x_1,x_2) 1_{A_2}(x_2)...1_{A_{n-1}}(x_{n-1}) g_{\frac{t}{n}}(x_{n-1},y) \qquad (4.2)
\end{aligned}$$

where

$$g_s(x,y) = \frac{1}{(2\pi s)^{\frac{d}{2}}} e^{-\frac{1}{2s}|x-y|^2}$$

Note that this function satisfies

$$\int g_s(x,y) g_t(y,z) dy = g_{t+s}(x,z)$$

and replacing the $1_{A_n}(x)$ in (4.2) with $e^{-\frac{t}{n}V(\frac{xt}{n})}$ gives back the 'real time' of (4.1). What about the limit $n \to \infty$? The idea is to view the measures μ_n as the finite dimensional distributions of some 'big' measure. So the question is: Is there a measure μ on functions $\phi : [0,t] \to \mathbb{R}^d$ such that for all $t_1 < ... < t_n$ we have

$$\begin{aligned}
&\mu_n(\phi(t_1) \in A_1, \phi(t_2) \in A_2, ..., \phi(t_n) \in A_n) \\
&\quad = \int g_{t_1}(x,x_1) 1_{A_1}(x_1) g_{t_2-t_1}(x_1,x_2) 1_{A_2}(x_2) g_{t_3-t_2}(x_3,x_2) 1_{A_3}(x_3)...g_{t-t_n}(y,x_n) dx_1...dx_n?
\end{aligned}$$

The answer is yes by Kolmogorov's consistency (sometimes extension or existence) theorem:

Theorem 4.2 (Kolmogorov consistency theorem). *Let $\{\mu_{t_1,...,t_n} : 0 \le t_1 < t_2 < ... < t_n < t\}$ be a family of finite measures (e.g. probability measures). Each $u_{t_1,...,t_n}$ is assumed to be on $(\mathbb{R}^d)^n$ and we assume the consistency condition*

$$\mu_{t_1,..,t_k,\tau,t_{k+1},...t_n}(A_1 \times ... \times A_k \times \mathbb{R}^d \times A_{k+1} \times ... \times A_n) = \mu_{t_1,..,t_k,t_{k+1},...t_n}(A_1 \times ... \times A_k \times A_{k+1} \times ... \times A_n)$$

for every $t_j \in (0,t)$ and $\tau \in [0,t]$ with $t_k < \tau < t_{k+1}$ and $A_j \in \mathbb{R}^d$ measurable. Then there exists a measure μ on $(\mathbb{R}^d)^{[0,t]}$ (i.e. functions from $[0,t]$ to $\mathbb{R}^d$) such that

$$\mu(\phi(t_1) \in A_1, ..., \phi(t_n) \in A_n) = \mu_{t_1,...,t_n}(A_1 \times ... \times A_n)$$

Let us check that our measures are consistent.

$$\begin{aligned}
&\mu_4(\phi(\tfrac{t}{4}) \in A, \phi(\tfrac{2t}{4}) \in \mathbb{R}, \phi(\tfrac{3t}{4}) \in B) = \mu_{\frac{1}{4},\frac{2}{4},\frac{3}{4}}(A \times \mathbb{R} \times B) \\
&= \int dx_1 \frac{e^{-\frac{1}{\frac{2t}{4}}|x-x_1|^2}}{(2\pi\frac{t}{4})^{\frac{d}{2}}} 1_A(x_1) \int dx_2 \frac{e^{-\frac{1}{\frac{2t}{4}}|x_2-x_1|^2}}{(2\pi\frac{t}{4})^{\frac{d}{2}}} 1_{\mathbb{R}}(x_2) \int dx_3 \frac{e^{-\frac{1}{\frac{2t}{4}}|x_3-x_2|^2}}{(2\pi\frac{t}{4})^{\frac{d}{2}}} 1_B(x_3) \underbrace{\frac{e^{-\frac{1}{\frac{2t}{4}}|y-x_3|^2}}{(2\pi\frac{t}{4})^{\frac{d}{2}}}}_{=:h_y(x_3)} \\
&= [e^{-\frac{t}{4}H_0} 1_A e^{-\frac{t}{4}H_0} 1_{\mathbb{R}^d} e^{-\frac{t}{4}H_0} h_y](x) \\
&= [e^{-\frac{t}{4}H_0} 1_A e^{-\frac{t}{2}H_0} h_y](x) \\
&= \mu_{\frac{1}{4},\frac{3}{4}}(A \times B)
\end{aligned}$$

The measure μ will turn out to be the conditional Brownian motion from x to y in time t. We write $W_t^{x,y}(d\phi)$ for it. Then formally

$$\begin{aligned}
e^{-tH}(x,y) &= \lim_{n\to\infty} \int e^{-\frac{t}{n}\sum_{k=0}^{n-1} V(\phi(\frac{k+1}{n}t)} \mu_n(d\phi) \\
&= \int e^{-\int_0^t V(\phi(s))ds} W_t^{x,y}(d\phi) \qquad (4.3)
\end{aligned}$$

Note that the term inside the exponential converges to $\int_0^t V(\phi(s))ds)$ but we need to be careful about the limit of μ_n. We will prove this rigorously later. (4.3) is called the *Feynman-Kac formula.* We aim to prove it.

4.2 Brownian Motion

Classical Construction: Let $\{X_i\}_{i\in\mathbb{N}}$ be independent random variables with probability $\mathbb{P}(X_i = 1) = \mathbb{P}(X_i = -1) = \frac{1}{2}$. Put $S_n = \sum_{i=1}^n X_i$. So S_n can be viewed as piecewise linear function, just as before.

Actually if X_i is Gaussian random variable rather than Bernoulli we get precisely the picture we had in the imaginary time Feynman integrals.

$$\mathbb{P}(S_1 \in A_1, ..., S_n \in A_n) = \int g_1(0,x_1)1_{A_1}(x_1)g_1(x_1,x_2)1_{A_2}(x_2)...g_1(x_n,x_{n-1})1_{A_n}(x_n)dx_1...dx_n$$

Now we want to make the grid finer. Identify $i \in \mathbb{N}$ with $\frac{i}{N}t \in \mathbb{R}$ and send $N \to \infty$. Keeping step size 1 would make the function to rough. Try jump size $\frac{1}{N}$, but then

$$\sum_{i=1}^{N} \frac{1}{N} X_i = \frac{1}{N} S_n \overset{\text{law of large numbers}}{\to} E(X_1) = 0$$

So this step size is too small!. The central limit theorem implies.

$$\sum_{i=1}^{N} \frac{1}{\sqrt{N}} X_i \overset{\text{distribution}}{\to} \mathcal{N}(0,1)$$

Now formalise this: Define a map $G : \{-1,1\}^N \to C([0,t];\mathbb{R})$, $(X_i)_{i\le N} \mapsto B^{(N)} : [0,t] \to \mathbb{R}$, where

$$B_s^{(N)} \begin{cases} \frac{1}{\sqrt{N}} \sum_{i=1}^k X_i & \text{if } s = t\frac{k}{n} \\ \text{linear interpolation} & \text{otherwise} \end{cases}$$

Let $W^{(N)}$ be the image measure of the Bernoulli measure $(\mathcal{B}(-1,1))^N$ under G i.e. for a subset of A of $C([0,1];\mathbb{R})$ we define W^N to be the pushforward measure

$$W^{(N)}(A) = (\mathcal{B}(-1,1))^N[G^{-1}(A)] \tag{4.4}$$

Note that the $\sigma-$algebra on $C([0,T];\mathbb{R})$ will always be the one generated by point evaluations $f \mapsto f(t)$ for some t.

Facts about $W^{(N)}$:

(i) It is concentrated on piecewise linear functions with corners at $t\frac{k}{N}$ and slopes $\frac{1}{t}\sqrt{N}$

(ii) Each possible path has weight $\frac{1}{2^N}$

Theorem 4.3 (Donsker)**.** *$W^{(N)}$ converges weakly (with respect to the topology of local uniform convergence) to a probability measure W^0 on $C([0,T];\mathbb{R})$*

W^0 is called *Brownian motion* starting at 0. The same construction works on $C(\mathbb{R}^+,\mathbb{R})$ or $C(\mathbb{R}^+,\mathbb{R}^d)$. Shifting the starting point of the random walk to $x \in \mathbb{R}^d$ gives W^x - Brownian motion starting at x. Since W^0 is a measure on $C(\mathbb{R}^+,\mathbb{R}^d)$ we can say things about almost all paths $q : \mathbb{R}^+ \to \mathbb{R}^d$. A remark on notation: a *path* is a (random) function drawn according to W^x. We will use $q(s)$ or q_s for a path (evaluated at time s).

Remarks

(a) $q(0) = x$ for W^x-almost all paths

(b) $t \mapsto q_t$ is nowhere differentiable W^x-almost surely. Since the finite approximations slope $\sqrt{N}$ we could expect that $|q_t - q_s| \sim |t-s|^{\frac{1}{2}}$ for small $|t-s|$. This is almost correct. The reality is a bit more involved.

$$\limsup_{t\to t_0} \frac{q_t - q_{t_0}}{\sqrt{2|t-t_0|ln(ln(\frac{1}{|t-t_0|}))}} = 1 \text{ almost surely}$$

$$\limsup_{\delta\to 0} \left\{ \frac{q_s - q_t}{\sqrt{2|t-s|ln(\frac{1}{|t-s|})}} \right\} = 1 \text{ almost surely}$$

Theorem 4.4 (Finite Dimensional Distributions on Brownian Motion)**.** *For $0 < t_1 < t_2 < ... < t_n$ and $A_1, A_2, ..., A_n \in \mathcal{B}(\mathbb{R}^d)$ (Borel sets) where $\mathbb{P}(A) = W^x(A)$. Then*

$$\begin{aligned}
& W^x(q_{t_1} \in A_1, ..., q_{t_n} \in A_n) \\
= & \int \frac{1}{(2\pi t_1)^{\frac{d}{2}}} e^{-\frac{1}{2t_1}|x-x_1|^2} 1_{A_1}(x_1) \frac{1}{(2\pi(t_2-t_1))^{\frac{d}{2}}} e^{-\frac{1}{2(t_2-t_1)}|x_2-x_1|^2} 1_{A_2(x_2)} \cdots \\
& \cdots \frac{1}{(2\pi(t_n-t_{n-1}))^{\frac{d}{2}}} e^{-\frac{1}{2(t_n-t_{n-1})}|x_n-x_{n-1}|^2} 1_{A_n(x_n)} dx_1 ... dx_n \\
= & [e^{-t_1 H_0} 1_{A_1} e^{-(t_2-t_1)H_0} 1_{A_2} e^{-(t_3-t_2)H_0} ... e^{-(t_n-t_{n-1})H_0} 1_{A_n}](x) \qquad (4.5)
\end{aligned}$$

where $H_0 = -\frac{1}{2}\Delta$

Sketch Proof. Use Donsker's Theorem 4.3 with Gaussian jumps: Start with jumps of size $t_1, t_2 - t_1, t_3 - t_2, ..$ and then *refine* the grid (retaining original points $t_1, t_2, ...$). By the semi-group property of $(W^x)^{(N)}(q_{t_1} \in A_1, ..., q_{t_n} \in A_n) =$ right hand side of (4.5) for all N and the left hand side converges to W^x by Donsker. □

An equivalent definition of *Brownian motion* is the unique probability measure W^x on $C(\mathbb{R}^+, \mathbb{R}^d)$ such that

$$W^x(q_{t_1} \in A_1, ..., q_{t_n} \in A_n) = [e^{-t_1 H_0} 1_{A_1} e^{-(t_2 - t_1)H_0} 1_{A_2} ... e^{-(t_n - t_{n-1})H_0} 1_{A_n}](x)$$

for all $t_1 < t_2 < ... < t_n \in \mathbb{R}^+$, $A_1, ..., A_n \subset \mathbb{R}^d$ open where $H_0 = -\frac{1}{2}\Delta$.

4.2.1 Markov Property

Intuitively the behaviour of a path q for times after t_1 depends only on $q_{t_1} \equiv q(t_1)$. Formally, cylinder sets are sets of functions for the form

$$C_t(A) = \{q \in C(\mathbb{R}^+, \mathbb{R}^d) : q(t) \in A\}$$

for some $A \in \mathcal{B}(\mathbb{R}^d)$ (Borel set). Generate the $\sigma-$algebra

$$\mathcal{F}_{\{t\}} = \sigma(\{C_t(A) : A \in \mathcal{B}(\mathbb{R}^d)\})$$

A subset B of $C(\mathbb{R}^+, \mathbb{R}^d)$ is in $\mathcal{F}_{\{t\}}$ if it can be decided for any function, $q \in B$, whether q belongs to B or not by knowledge of $q(t)$ alone. Define

$$\mathcal{F}_{[a,b]} = \sigma(\{C_t(A) : A \in \mathcal{B}(\mathbb{R}^d), t \in [a, b]\})$$

Definition 4.5. Let $F : C(\mathbb{R}^+, \mathbb{R}^d) \to \mathbb{R})$ be measurable. Then for $a \leq b$ we define *conditional expectation*, $W^x(F|\mathcal{F}_{[a,b]})$, to be the (almost surely) unique random variable $C(\mathbb{R}^+, \mathbb{R}^d) \to \mathbb{R}$ such that

(i) $W^x(F|\mathcal{F}_{[a,b]})$ is $\mathcal{F}_{[a,b]}$ measurable

(ii) For all $\mathcal{F}_{[a,b]}$ measurable functions G we have

$$\int W^x(F|\mathcal{F}_{[a,b]})(q) G(q) dW^x(q) = \int F(q) G(q) dW^x(q)$$

We can think of $\mathcal{F}_{[a,b]}$ measurable functions, F ($F \in m\mathcal{F}_{[a,b]}$), as functions that depend only on q_s for $a \leq s \leq b$. For example:

$$F(q) = \int_a^b q(s) ds \text{ is } \mathcal{F}_{[a,b]} \text{ measurable}$$

$$F(q) = \int_0^1 q(s) q(1-s) ds \text{ is } \mathcal{F}_{[0,1]} \text{ measurable}$$

If

$$F(q) = \int_0^t q^2(s) ds$$

Then

$$\begin{aligned}
W^0(\int_0^t q_s^2 ds) &= \int\int_0^t q_s^2 ds dW^0(q) = \int_0^t \left(\int q_s^2 dW^0(q)\right) ds \\
&= \int_0^t \left(\tfrac{1}{\sqrt{2\pi s}}\int x^2 e^{-\frac{1}{2s}|x|^2} dx\right) ds \text{ integrating over all paths, looking only at } q(s). \\
&= \int_0^t \left(s^2\right) ds = \frac{1}{3}t^3
\end{aligned}$$

Intuitively $W^x(q_t \in A|\mathcal{F}_{[a,b]})(\overline{q})$ is the probability that $q_t \in A$ if we know that $q_s = \overline{q}_s$ for $s \in [a,b]$.

Theorem 4.6. *Conditional expectation exists.*

Theorem 4.7 (Conditional Expectation of Brownian Motion)**.** *For $f \in L^\infty$, set $y \in \mathbb{R}^d$ we have*

$$W^y(f(q_t)|\mathcal{F}_{\{s\}})(\overline{q}) = (e^{-(t-s)H_0}f)(\overline{q}_s) = W^{\overline{q}_s}(f(q_{t-s}))$$

the last expression is the expectation with respect to a standard Brownian motion started at the point $\overline{q}(s)$ at time s.

Proof. $[e^{-(t-s)H_0}f](\overline{q}_s)$ depends only on $\overline{q}_s$ and so is $\mathcal{F}_{\{s\}}$ measurable. Now for $g \in m\mathcal{F}_{\{s\}}$ we find

$$W^y([e^{-(t-s)H_0}f](\overline{q}_s)g(\overline{q}_s)) \overset{\text{Thm. 4.4}}{=} (e^{-sH_0}ge^{-(t-s)H_0}f)(y) \overset{\text{Thm. 4.4}}{=} W^y(g(q_s)f(q_t))$$

□

The moral is that Brownian motion starts a fresh at $x \in \mathbb{R}^d$ when conditioned to be at $x \in \mathbb{R}^d$.

Theorem 4.8 (Markov Property)**.** *For all $F \in m\mathcal{F}_{[t,\infty)}$ $t > 0$ we have*

$$W^y(F|\mathcal{F}_{[0,t]}) = W^y(F|\mathcal{F}_{\{t\}})$$

Proof. Since $\mathcal{F}_{\{t\}} \subset \mathcal{F}_{[0,t]}$, then clearly $W^y(F|\mathcal{F}_{\{t\}}) \in m\mathcal{F}_{[0,t]}$. For $G \in m\mathcal{F}_{[0,t]}$ we first consider

$$G(q) = g_1(q_{t_1})g_2(q_{t_2})...g_n(q_{t_n})$$

with $t_1 < t_2 < ... < t_n = t$ and

$$F(q) = f_1(q_{t_{n+1}})f_2(q_{t_{n+2}})...f_m(q_{t_{n+m}}).$$

Then

$$\begin{aligned}
W^y(GW^y(f|\mathcal{F}_{\{t\}})) &\overset{\text{Thm. 4.7}}{=} W^y(g_1(q_{t_1})g_2(q_{t_2})...g_n(q_{t_n}) \times [e^{-(t_{n+1}-t_n)H_0}f_1e^{-(t_{n+2}-t_{n+1})H_0}f_2... \\
&\qquad ...e^{-(t_{n+m}-t_{n+m-1})H_0}f_m](q_{t_n}) \\
&\overset{\text{Thm. 4.4}}{=} [e^{-t_1H_0}g_1e^{-(t_2-t_1)H_0}g_2.. \\
&\qquad ...g_ne^{-(t_{n+1}-t_n)H_0}f_1e^{-(t_{n+2}-t_{n+1})H_0}f_2...e^{-(t_{n+m}-t_{n+m-1})H_0}f_m](y) \\
&= W^y(FG)
\end{aligned}$$

□

Define $\tau_t : L^1(C(\mathbb{R}^+, \mathbb{R}^d)) \to L^1(C(\mathbb{R}^+, \mathbb{R}^d))$

$$(\tau_t h)(q) = h(\{q_{t+s} : s \in \mathbb{R}\})$$

which translates Brownian motion. For example:

$$F : g \mapsto \int_0^T q_s^2 ds \qquad (\tau_t F)(q) = F(q_{\cdot+t}) = \int_0^T q_{t+s}^2 ds$$

We will need the following consequence of this

Lemma 4.9. *Let $f, g : C(\mathbb{R}^+, \mathbb{R}) \to \mathbb{R}^+$ with $f \in m\mathcal{F}_{[0,t]}$, $W^x(|f|) < \infty$ and $\sup_y W^y(|g|) < \infty$. Then*

$$W^x(f\tau_t g) \leq W^x(f) \sup_y W^y(g)$$

Proof. By the definition of conditional expectation (ii):

$$\begin{aligned}
W^x(f\tau_t G) &\overset{f\in m\mathcal{F}_{[0,t]}}{=} W^x(fW^x(\tau_t g : \mathcal{F}_{[0,t]})) \\
&\overset{\text{Markov}}{=} W^x(fW^x(\tau_t g : \mathcal{F}_{\{t\}})) \\
&\overset{\text{Thm4.7}}{=} W^x(fW^{q(t)}(g)) \\
&\leq W^x(f \sup_y W^y(g)) \\
&= W^x(f) \sup_y W^y(g)
\end{aligned}$$

□

4.3 Feynman-Kac Formula

Theorem 4.10. *Assume $V : \mathbb{R}^d \to \mathbb{R}$ is bounded above and below and continuous. Then for each $f, g \in L^2(\mathbb{R}^d)$ we have*

$$\begin{aligned}
\langle f, e^{-t(H_0+V)} \rangle &= \int_{\mathbb{R}^d} f(x) W^x \left(e^{-\int_0^t V(q_s)ds} g(q_t) \right) dx \\
&= \int_{\mathbb{R}^d} f(x) \left(\int e^{-\int_0^t V(q_s)ds} g(q_t) dW^x \right) dx
\end{aligned}$$

this means that

$$e^{-t(H_0+V)} = W^x \left(e^{-\int_0^t V(q_s)ds} g(q_t) \right)$$

in L^2 sense

Proof. exercise - using Trotter and DCT □

But what we really want is difficult potentials like $V(x) = \frac{1}{|x|}$ in $\mathbb{R}^3$. For instances does the integral with respect to Brownian motion of $e^{-\int_0^t V(q_s)ds} g(q_t)$ make sense? For example $V(x) = -\frac{1}{|x|}$. Where the integrand is infinite we hope that such paths have measure zero. A key result is:

Theorem 4.11 (Kashminski)**.** *Let* $V : \mathbb{R}^d \to \mathbb{R}$*,* $V \geq 0$ *be measurable with*

$$\sup_{x\in\mathbb{R}^d} W^x \left(\int_0^t V(q_s)ds \right) = \alpha < 1$$

then

$$\sup_x W^x \left(e^{\int_0^t V(q_s)ds} \right) \leq \frac{1}{1-\alpha}$$

Proof. We will show that

$$I_n := \sup_{x\in\mathbb{R}^d} W^x \left(\frac{1}{n!} (\int_0^t V(q_s)ds)^n \right) \leq \alpha^n \tag{4.6}$$

Then $\sup_{x\in\mathbb{R}^d} W^x \left(e^{\int_0^t V(q_s)ds} \right) \leq \sum_{n=0}^{\infty} I_n = \frac{1}{1-\alpha}$. To show that note:

$$\begin{aligned}
I_n &= \frac{1}{n!} \sup_{x\in\mathbb{R}^d} W^x \left(\int_0^t ds_1 ... \int_0^t ds_n V(q_{s_1}) ... V(q_{s_n}) \right) \\
&= \sup_{x\in\mathbb{R}^d} W^x \left(\int_0^t ds_1 \int_{s_1}^t ds_2 ... \int_{s_{n-1}}^t ds_n V(q_{s_1}) V(q_{s_1}) ... V(q_{s_n}) \right) \\
&= \sup_{x\in\mathbb{R}^d} W^x \left(\int_{\substack{s\in[0,1]^n \\ s_1 \leq s_2 \leq ... \leq s_n}} V(q_{s_1}) ... V(q_{s_n}) ds_1 ... ds_n \right) \\
&\overset{\text{Fubini}}{=} \sup_{x\in\mathbb{R}^d} \int_0^t ds_1 \int_{s_1}^t ds_2 ... \int_{s_{n-2}}^t ds_{n-1} W^x \left(V(q_{s_1}) V(q_{s_1}) ... V(q_{s_{n-1}}) \int_{s_{n-1}}^t V(q_{s_n})) ds_n \right)
\end{aligned}$$

The second equality follows since the integrand is symmetric in $s_1, ..., s_n$, so we can integrate over the lower triangle, i.e. over the set $\{(s_1, ..., s_n) : s_n \geq ... \geq s_1\}$ and multiply by the number of different orderings $n!$. That is, there are $n!$ permutations of $s_1, ..., s_n$ and

$$V(s_1) ... V(s_n) = V(s_{\pi(1)}) ... V(s_{\pi(n)})$$

for all permutations $\pi : \{1, ..., n\} \to \{1, ..., n\}$. Now, using conditional expectation and the fact that $V(q_{s_1}) V(q_{s_1}) ... V(q_{s_{n-1}})$ is $\mathcal{F}_{s_{n-1}}$ measurable then,

$$\begin{aligned}
W^x \left(V(q_{s_1}) V(q_{s_1}) ... V(q_{s_{n-1}}) \int_{s_{n-1}}^t V(q_{s_n})) ds_n \right) &\leq W^x \left(V(q_{s_1}) ... V(q_{s_{n-1}}) \underbrace{\sup_y W^y \int_0^{t-s_{n-1}} V(q_r) dr}_{\leq \alpha} \right) \\
&\leq \alpha W^x \left(V(q_{s_1}) ... V(q_{s_{n-1}}) \right)
\end{aligned}$$

repeat n times to get result. $\square$

Definition 4.12. A measurable function $V : \mathbb{R}^d \to \mathbb{R}$ is *Kato class*, $V \in \mathcal{K}(\mathbb{R}^d)$ if

(i) $\sup_{x\in\mathbb{R}^d} \int 1_{\{|x-y|\leq 1\}} |V(y)| dy < \infty$ if $d = 1$

(ii) $\lim_{r\to 0} \sup_{x\in\mathbb{R}^d} \int 1_{\{|x-y|\leq r\}} g(x-y) |V(y)| dy = 0$ if $d \geq 2$

where

$$g(x) = \begin{cases} -ln|x| & d = 2 \\ \frac{1}{|x|^{d-2}} & d \geq 3 \end{cases}$$

$V \in \mathcal{K}(\mathbb{R}^d)$ can be locally singular but not too much. Check this for $V(x) = \frac{1}{|x|^q}$ in $\mathbb{R}^3$:

$$\lim_{r\to 0} \sup_{x\in\mathbb{R}^d} \int 1_{\{|x-y|<r\}} \frac{1}{|x-y|} \frac{1}{|y|^q} dy \overset{x=0}{=} \lim_{r\to 0} \int_{|y|\leq r} \frac{1}{|q|^{q+1}} dy = 0$$

So $\frac{1}{|x|} \in \mathcal{K}(\mathbb{R}^3)$ but $\frac{1}{|x|^2} \notin \mathcal{K}(\mathbb{R}^3)$.

Definition 4.13. V is *locally Kato-class*, $V \in \mathcal{K}_{\text{loc}}$, if $1_K V \in \mathcal{K}$ for every compact set K. V is *Kato-decomposable*,$V \in \mathcal{K}_{\pm}$, if $V = V^+ - V^-$ with $V^+, V^- \geq 0$ and $V^+ \in \mathcal{K}_{\text{loc}}$ and $V^- \in \mathcal{K}$.

Remember that we want $W^x \left(e^{-\int_0^t V(q_s)ds}\right) < \infty$ so we don't care too much about what V^+ does at infinity.

Theorem 4.14. *A non-negative function $V \in \mathcal{K}(\mathbb{R}^d)$ if and only if*

$$\lim_{t\downarrow 0} \sup_{x\in\mathbb{R}^d} W^x \left(\int_0^t V(q_s)ds\right) = 0$$

Proof for $d = 4$. By Fubini

$$\begin{aligned} W^x \left(\int_0^t V(q_s)ds\right) &= \int_0^t W^x(V(q_s))ds = \int_0^t \int e^{-\frac{1}{2s}|x-y|^2} \frac{1}{(2\pi s)^{\frac{d}{2}}} V(y)dyds \\ &\overset{\text{Fubini}}{=} \int \left[\int_0^t e^{-\frac{1}{2s}|x-y|^2} \frac{1}{(2\pi s)^{\frac{d}{2}}} ds\right] V(y)dy \end{aligned}$$

Then by using the substitution $\frac{|x-y|^2}{2s} =: u(s)$, then

$$\int_0^t e^{-\frac{|x-y|^2}{2s}} \frac{1}{(2\pi s)^{\frac{d}{2}}} ds = \frac{|x-y|^{2-d}}{(2\pi)^{\frac{d}{2}}} \int_{\frac{|x-y|^2}{2t}}^{\infty} e^{-u} u^{\frac{d}{2}-2} du =: Q(|x-y|, t)$$

So

$$\lim_{t\to 0} \sup_{x\in\mathbb{R}^4} W^x \left(\int_0^t V(q_s)ds\right) = \lim_{r\to 0} \sup_{x\in\mathbb{R}^4} \int Q(|x-y|, r)V(y)dy$$

We show that the right hand side of the above equation is equal to

$$\lim_{r\to 0} \sup_{x\in\mathbb{R}^4} \int g|x-y| 1_{\{|x-y|<r\}} V(y)dy$$

where g is as in the definition of Kato-class (definition 4.12). To see this, note that

$$Q(|x-y|, r) \approx g(|x-y|) \text{ for } |x-y|^2 \leq 2r$$

while $Q(|x-y|, r) \ll 1$ if $|x-y|^2 \gg r$. We only look at $d = 4$, then

$$\begin{aligned} Q(|x-y|, r) &= \frac{1}{(2\pi)^2(x-y)^2} e^{-\frac{|x-y|^2}{2t}} \\ &\geq \frac{1}{(2\pi)^4} e^{-\frac{t}{2}} 1_{\{|x-y|\leq t\}} \end{aligned}$$

So

$$\begin{aligned}
4\pi^2 e^{-r} \int g(x-y) 1_{\{|x-y|\leq r\}} V(y)dy &\leq \int Q(|x-y|, r) V(y) dy \\
&\leq 4\pi^2 e^{-r} \int g(x-y) 1_{\{|x-y|\leq r^{\frac{1}{4}}\}} V(y)dy \\
&\quad + 4\pi^2 \int_{\{|x-y|\geq r^{\frac{1}{4}}\}} e^{-\frac{|x-y|^2}{2r}} g(x-y)V(y)dy
\end{aligned}$$

The first inequality shows that

$$\lim_{t\to 0} \sup_{x\in\mathbb{R}^4} W^x \left(\int_0^t V(q_s)ds \right) = 0 \Rightarrow V \in \mathcal{K}(\mathbb{R}^4)$$

For $V \in \mathcal{K}(\mathbb{R}^4)$, the first term in the last line vanishes when taking $lim_{r\to 0} \sup_{x\in\mathbb{R}^4}$. The second term also vanishes: if $V \in \mathcal{K}(\mathbb{R}^4)$, there exists r_0 such that

$$\sup_{x\in\mathbb{R}^4} \int_{|x-y|<r} g(x,y)V(y)dy < 1$$

for all $r < r_0$. We partition $\mathbb{R}^d$ into cubes of size r_0 and find on each cube that the second term

$$\leq \max\{e^{-\frac{|x-y|^2}{2r}} : y \in \text{ cube } \} \underbrace{\int V(y)g(x-y)dy}_{\leq 1}$$

summing up over all the cubes gives a finite results (since the function decays very quickly) which vanishes as $r \to 0$. □

Corollary 4.15. *Assume $V \in \mathcal{K}(\mathbb{R}^d)$. Then for any $t \geq 0$*

$$\sup_{x\in\mathbb{R}^d} W^x \left(\exp \int_0^t V(q_s)ds \right) < \infty \tag{4.7}$$

Proof. By theorems 4.14, 4.11, for sufficiently small $t > 0$ we find

$$\sup_x W^x \left(\exp \int_0^t V(q_s)ds \right) < \frac{1}{1-\alpha}$$

where $\alpha < 1$. Now, via conditional expectation

$$\begin{aligned}
W^x \left(\exp(\int_0^{2t} V(q_s)ds) \right) &= W^x \left(W^x \left(\exp(\int_0^t V(q_s)ds) \exp(\int_t^{2t} V(q_s)ds) \middle| \mathcal{F}_{[0,t]} \right) \right) \\
&= W^x \left(\exp(\int_0^t V(q_s)ds W^x \left(\exp(\int_t^{2t} V(q_s)ds \middle| \mathcal{F}_{[0,t]} \right) \right) \\
&= W^x \left(\exp(\int_0^t V(q_s)ds W^{q_t} \left(\exp(\int_0^{2t-t} V(q_s)ds \right) \right) \\
&\leq \frac{1}{1-\alpha} W^x \left(\exp(\int_0^t V(q_s)ds \right) \\
&\leq \frac{1}{(1-\alpha)^2}.
\end{aligned}$$

Iterate for arbitrary time intervals. □

Corollary 4.16. *Assume $V \in \mathcal{K}_\pm(\mathbb{R}^d)$. Then for any $t \geq 0$*

$$\sup_{x\in\mathbb{R}^d} W^x\left(\exp - \int_0^t V(q_s)ds\right) < \infty \tag{4.8}$$

Proof. Proof exercise. Note we have a negative exponential so V^+ only makes things small, but why is $\int_0^t V(q_s)ds$ finite for almost all Brownian motion paths? □

This corollary means we can make the following definition:

Definition 4.17. For $V \in \mathcal{K}_\pm(\mathbb{R}^d)$, $f \in L^\infty(\mathbb{R}^d)$ define

$$(P_t f)(x) := W^x\left(e^{-\int_0^t V(q_s)ds} f(q_t)\right)$$

$\{P_t\}_{t\geq 0}$ is called the *Feynman-Kac semigroup*

The aim is show that $P_t f = e^{-t(-\frac{1}{2}\Delta + V)} f$. To achieve this we will first show that $\{P_t\}_{t\geq 0}$ is a strongly continuous symmetric semi-group in L^2. Strong continuity means that

$$\lim_{t\to 0} ||P_t f - f||_{L^2} = 0 \quad \forall f \in L^2$$

We fist show that P_t is symmetric.

Lemma 4.18. *If*

$$\int f(x) P_t g(x) dx < \infty$$

then

$$\int f(x) P_t g(x) dx = \int g(x) P_t f(x) dx$$

Thus, in L^2, this means $\langle f, P_t g\rangle = \langle P_t f, g\rangle$. For the proof, recall the measure introduced just before Kolmogorov's Consistency Theorem 4.2.

$$W_t^{x,y}(g_{t_1} \in A_1, ..., g_{t_n} \in A_n) = \left(\frac{1}{\prod_{i=1}^{n+1} 2\pi(t_{i+1} - t_i)}\right)^{\frac{1}{2}} \int dx_1 ... dx_n e^{-\sum_{i=1}^{n+1} \frac{1}{2|t_j - t_{j-1}|}|x_j - x_{j-1}|^2} 1_{A_1}(x_1) ... 1_{A_n}(x_n)$$

with $0 = t_0 < t_1 < ... < t_n < t_{n+1} = t$ and $x_0 = x_1$, $x_{n+1} = y$. This is called *Conditional Brownian Motion from x to y in time t.*

Proof of lemma 4.18. Note that for $s < t$

$$\int W_t^{x,y}(f(q_s)) g(y) dy = W_t^x(f(q_s) g(q_t))$$

(we can prove this using a denseness argument)

$$\int f(x) W^x\left(e^{-\int_0^t V(q_s)ds} g(q_t)\right) dx = \int\int f(x) g(y) W_t^{x,y}\left(e^{-\int_0^t V(q_s)ds} g(q_t)\right) dxdy \tag{4.9}$$

We use the following fact of Brownian Motion (see exercise): *time reversibility*

$$W_t^{x,y}(q_{t_1} \in A_1, ..., q_{t_n} \in A_n) = W_t^{y,x}(q_{t-t_1} \in A_1, ..., q_{t-t_n} \in A_n)$$

which extends to general functions of paths. Then

$$\begin{aligned}
\text{RHS of 4.9} &= \int\int f(x)g(y)W_t^{y,x}\left(e^{-\int_0^t V(q_{t-s})ds}\right)dxdy \qquad \text{using substitution } s \mapsto t-s \\
&= \int g(y)W^y\left(e^{-\int_0^t V(q_s)ds}f(q_t)\right) \\
&= \int g(y)P_tf(y)dy
\end{aligned}$$

□

Next we show that P_t acts on L^2 as a bounded operator. In fact, we show more.

Theorem 4.19 (Simon-1982)**.** *Let $f \in L^p(\mathbb{R}^d)$ with $1 \le p \le \infty$. Then for every $q \ge p$*

$$P_tf \in L^q(\mathbb{R}^d) \quad \textit{and} \quad \sup\{||P_tf||_{L^q} : ||f||_{L^p} \le 1\} < \infty.$$

We say that P_t is bounded from L^p to L^q.

Proof. The proof uses the Riesz-Thorin interpolation theorem: If an operator A is bounded from $L^{p_j} \to L^{q_j}$ for $p_1, ..., p_n$ and $q_1, ..., q_n$ with $1 \le p_j, q_j \le \infty$ then it is bounded from L^r to L^s such that $(\frac{1}{r}, \frac{1}{s})$ is in the convex hull of

$$\{(\frac{1}{p_j}, \frac{1}{q_j}) : j = 1, ..., n\}$$

So we only need to prove it is bounded

(i) from L^1 to L^1

(ii) from L^1 to L^∞

(iii) from L^∞ to L^∞

and we have already seen (iii). For (i), let $f \in L^1$

$$\begin{aligned}
\int |P_tf|dx &= \int |W^x\left(e^{-\int_0^t V(q_s)ds}f(q_t)\right)|dx \\
&\le \int W^x\left(e^{-\int_0^t V(q_s)ds}|f(q_t)|\right)dx
\end{aligned}$$

Now

$$\begin{aligned}
\infty &> \int |f(x)| \underbrace{W^x\left(e^{-\int_0^t V(q_s)ds}1(q_t)\right)}_{\sup_x \ldots < \infty \text{ by Kashminski's theorem 4.11}} dx \\
&\stackrel{\text{Lemma 4.18}}{=} \int 1W^x\left(e^{-\int_0^t V(q_s)ds}|f(q_t)|\right) \\
&= \int (P_t|f|)dx
\end{aligned}$$

Thus $||P_tf||_{L^1} \le \int P_t|f|dx \le \sup_x W^x\left(e^{-\int_0^t V(q_s)ds}1(q_t)\right)||f||_{L^1}$.

For (ii), first show that $P_t f \in L^\infty$ for $f \in L^2$.

$$
\begin{aligned}
||P_t f||_\infty^2 \quad &= \quad \sup_x \left(\int e^{-\int_0^t V(q_s)ds} f(q_t) dW^x(q) \right)^2 \\
&\overset{\text{Cauchy-Schwarz}}{\leq} \quad \sup_x \left(\int e^{-2\int_0^t V(q_s)ds} dW^x(q) \right) \left(\int (f(q_t))^2 dW^x(q) \right) \\
&\leq \quad \underbrace{\sup_x \int e^{-2\int_0^t V(q_s)ds} dW^x(q)}_{\leq C \text{ since } 2V \in \mathcal{K}_\pm} \underbrace{\sup_x \int \frac{1}{(2\pi t)^{\frac{d}{2}}} e^{-\frac{|x-y|^2}{2t}} (f(y))^2 dy}_{\frac{1}{(2\pi t)^{\frac{d}{2}}} ||f||_2^2}
\end{aligned}
$$

Finally we show that $P_t f \in L^2$ for each $f \in L^1$. For each $g \in L^2$

$$\langle P_t f, g \rangle = \int P_t f(x) g(x) dx = \int \underbrace{P_t g(x)}_{\in L^\infty} f(x) < \infty$$

which justifies the use of lemma 4.18, and so by above,

$$\langle P_t f, g \rangle \leq ||P_t g||_\infty ||f||_1 \leq C_1 ||g||_2 ||f||_1$$

A general fact:

$$f \in L^2 \Leftrightarrow \sup\{ \int f(x) g(x) dx : g \in L^2, ||g||_2 = 1 \} < \infty$$

So $P_t f \in L^2$, $||P_t f||_{L^2} \leq C_2 ||f||_{L^2}$ and finally

$$||P_t f||_{L^2} = ||P_{\frac{t}{2}} P_{\frac{t}{2}} f||_{L^2} \leq C_1 C_2 ||f||_2$$

□

Once we know that $P_t = e^{-tH}$ this shows the amazing statement that

Corollary 4.20. *Suppose that u solves*

$$
\begin{aligned}
&\partial_t u(x,t) = -\tfrac{1}{2}\Delta u + Vu \\
&u(x,0) - u_0
\end{aligned}
$$

with $V \in \mathcal{K}_\pm$. Then $u_0 \in L^p$ implies $u(x,t) \in L^q$ for all $t \geq 0$ and $q \geq p$

So P_t takes L^p functions in L^q for $q \geq p$. In fact, even more is true:

Theorem 4.21. *Let $V \in \mathcal{K}_\pm(\mathbb{R}^d)$. Then for each $f \in L^p$, $1 \leq p \leq \infty$ and each $t > 0$, $P_t f$ is a continuous function.*

For the proof we need

Lemma 4.22. *For $V \in \mathcal{K}$ we have*

$$\lim_{t \to 0} \sup_{x \in \mathbb{R}^d} W^x \left(\left| 1 - e^{-\int_0^t V(q_s)ds} \right| \right) = 0$$

Proof. Note that

$$W^x\left(\left|1-e^{-\int_0^t V(q_s)ds}\right|\right) \leq \sum_{k=1}^{\infty} \frac{1}{k!} W^x\left(\left[\int_0^t |V(q_s)|ds\right]^k\right) \tag{4.10}$$

Put $\alpha(t) = \sup_x W^x(\int_0^t |V(q_s)|ds)$. By theorem (4.14) $\lim_{t\to 0} \alpha(t) = 0$. By Kashminski theorem 4.11

$$\sup_x \text{ RHS of (4.10)} \leq \sum_{k=1}^{\infty} \alpha(t)^k = \frac{\alpha(t)}{1-\alpha(t)} \overset{t\to 0}{\to} 0$$

□

Proof of theorem 4.21. Note that $P_t = P_{\frac{t}{2}} P_{\frac{t}{2}}$, so by theorem 4.19, we only need to consider $f \in L^\infty$. Assume first that $V \in \mathcal{K}(\mathbb{R}^d)$. Define

$$g_\tau(x) = W^x\left(e^{-\int_\tau^t V(q_s)ds} f(q_t)\right)$$

Then

$$\begin{aligned} g_\tau(x) &\overset{\text{Markov}}{=} W^x\left(W^{q_\tau}\left(e^{-\int_0^{t-\tau} V(q_s)ds} f(q_{t-\tau})\right)\right) \\ &= [e^{-\tau H_0}(P_{t-\tau})]f(x) \end{aligned}$$

So $x \mapsto g_\tau(x)$ is continuous as it solves the heat equation

$$\begin{aligned} \partial_t g_\tau &= -\frac{1}{2}\Delta g_\tau \\ g_\tau(0) &= P_{t-\tau} f \in L^\infty \end{aligned}$$

Now

$$\begin{aligned} ||g_\tau - P_t f||_{L^\infty} &= \sup_x W^x\left((1-e^{-\int_0^\tau V(q_s)ds})e^{-\int_\tau^t V(q_s)ds} f(q_t)\right) \\ &\overset{\text{Markov}}{=} \sup_x W^x\left((1-e^{-\int_0^\tau V(q_s)ds}) W^{q_\tau}(e^{-\int_0^{t-\tau} V(q_s)ds} f(q_t))\right) \\ &\leq \sup_x W^x\left(\left|1-e^{-\int_0^\tau V(q_s)ds}\right|\right) \sup_y \sup_{r\leq t} W^y\left(e^{-\int_0^r V(q_s)ds}\right) ||f||_{L^\infty} \end{aligned}$$

On the right hand side, the first term tends to zero as $\tau \to 0$. The second term is bounded by a constant, by corollary 4.16 and $||f||_\infty$. So $P_t f$ is the uniform limit of continuous functions and therefore continuous. For $V \in \mathcal{K}_\pm$ the proof is completed by showing that in this case P_t is the uniform limit on compact sets of continuous functions, and therefore again continuous. Thus the proof is completed by the following lemma. □

Lemma 4.23. *Let $V \in \mathcal{K}_\pm$. Put*

$$V_n(x) = V(x) 1_{\{|x|\leq n\}} \in \mathcal{K}(\mathbb{R}^d)$$

and put

$$P_{t,n}(x) = W^x\left(e^{-\int_0^t V_n(q_s)ds} f(q_t)\right)$$

Then for $f \in L^\infty$, $\lim_{n\to\infty} P_{t,n} f(x) = P_t f(x)$ uniformly on compact subsets of $\mathbb{R}^d$.

Proof. For all paths q_s that never leave $\{x \in \mathbb{R}^d : |x| \leq n\}$ clearly

$$\int_0^t V(q_s)ds = \int_0^t V_n(q_s)ds$$

Put $A_n = \{w \in C(\mathbb{R}^+, \mathbb{R}^d) : \sup_{0 \leq s \leq t} |w_s| \leq n\}$. Then by Cauchy-Schwarz inequality

$$\begin{aligned} |P_t f(x) - P_{t,n} f(x)| &= \left| W^x \left(\left(e^{-\int_0^t V(q_s)ds} - e^{-\int_0^t V_n(q_s)ds} \right) (\cancel{1_{A_n}} + 1^c_{A_n}) f(q_t) \right) \right| \\ &\leq \left[W^x \left(\left(e^{-\int_0^t V(q_s)ds} - e^{-\int_0^t V_n(q_s)ds} \right)^2 |f(q_t)|^2 \right) \right]^{\frac{1}{2}} \left[W^x (1_{A_n^c}) \right]^{\frac{1}{2}}. \end{aligned}$$

Notice that the second term on the right hand side is equal to

$$W^x \left(\{w \in C(\mathbb{R}^+, \mathbb{R}^d) : \sup_{0 \leq s \leq t} |w_s| > n\} \right)^{\frac{1}{2}} \xrightarrow{n \to \infty} 0$$

by properties of Brownian motion. We now show that the supremum over $x \in \mathbb{R}^d$ of the first term on the right hand side is finite, independently of n. This is because

$$\begin{aligned} & W^x \left(e^{-2\int_0^t V(q_s)ds} + e^{-2\int_0^t V_n(q_s)ds} - 2e^{-\int_0^t V_n(q_s) + V(q_s)ds} \right) \\ = \; & \underbrace{W^x \left(e^{-2\int_0^t V(q_s)ds} \right)}_{<\infty \text{ by Kashminski's 4.11}} + W^x \left(e^{-2\int_0^t V_n(q_s)ds} \right) + \text{ cross terms} \end{aligned}$$

and the second term is bounded

$$W^x \left(e^{-2\int_0^t V_n^-(q_s)ds} \right) \leq W^x \left(e^{-2\int_0^t V^-(q_s)ds} \right) < \infty$$

as $V \in \mathcal{K}_\pm(\mathbb{R}^d)$. Similarly the cross terms are bounded uniformly in x and n. Taking $\sup_{x \in M}$ for compact sets $M \subset \mathbb{R}^d$ above proves the lemma. $\square$

Next we show

Theorem 4.24. *Assume that V is Kato-decomposable. Then the semigroup P_t is* strongly continuous, *i.e.*

$$\lim_{t \to 0} \|P_t f - f\|_{L^2} = 0 \qquad \text{for all } f \in L^2.$$

Proof. We first consider f bounded with compact support, say $|f(x)| \leq D$ and $f(x) = 0$ when $|x| > R$. We write

$$Q_t = e^{-tH_0}, \qquad \text{with } H_0 = -\frac{1}{2}\Delta$$

for the propagator of the heat equation. Recall that

$$Q_t f(x) = \frac{1}{(2\pi t)^{d/2}} \int e^{-\frac{|x-y|^2}{2t}} f(y)\, dy.$$

It is a classical result of the heat equation (and can be checked using the above formula) that $\lim_{t \to 0} \|Q_t f - f\|_{L^2} = 0$ for all $f \in L^2$. The strategy of this proof is to compare P_t with Q_t. Lemma (4.22) gives

$$|Q_t f(x) - P_t f(x)| = \left| \int \left(1 - e^{-\int_0^t V(q_s)\, ds} \right) dW^x(q) \right| \to 0$$

as $t \to 0$, for all x. So if we can find a function that dominates $|Q_t f(x) - P_t f(x)|$ and is square integrable, the dominated convergence will prove the claim. It is enough to study the case $t \leq 1$. We find

$$\begin{aligned}(P_t f(x) - Q_t f(x))^2 &= \left(\int \left(e^{-\int_0^t V(q_s) ds} - 1 \right) f(q_t) dW^x(q) \right)^2 \\ &\leq \int \left(e^{-\int_0^t V(q_s) ds} - 1 \right)^2 dW^x(q) \int f_0^2(q_t) dW^x(q),\end{aligned}$$

by the Cauchy-Schwarz inequality. Now the first factor above is bounded uniformly in x (by C, say), by Kasminskiis Lemma, and the integrand $f^2(q_t)$ in the second factor is bounded by D, and zero whenever $|q_t| \geq R$. We conclude

$$\begin{aligned}(P_t f(x) - Q_t f(x))^2 \leq CDW^x(|q_t| \leq R) &= CD \frac{1}{(2\pi t)^{d/2}} \int_{|y| \leq R} e^{-|x-y|^2/2t} \, dy \\ &\leq CD \sup_{|y| \leq R} e^{-|x-y|^2/4t} \frac{1}{(2\pi t)^{d/2}} \int_{|y| \leq R} e^{-|x-y|^2/4t} \, dy.\end{aligned}$$

The last factor above is bounded in x by a constant independent of x, and the first factor decays quicker than exponentially for $|x| > R$. So $P_t f(x) - Q_t f(x)$ is bounded by a square integrable function, and dominated convergence shows the claim for all bounded, compactly supported f. For general $f \in L^2$, we use the old triangle inequality trick: Let $f \in L^2$ be given. Since bounded, compactly supported functions are dense in L^2, we can find f_0 bounded and compactly supported with $\|f - f_0\|_{L^2}^2 < \varepsilon$. Then,

$$\|P_t f - f\| \leq \|P_t f - P_t f_0\| + \|P_t f_0 - f_0\| + \|f - f_0\|.$$

The first term above is bounded by $\|P_t\| \|f - f_0\| \leq \varepsilon \|P_t\|$, where $\|P_t\|$ is the operator norm. It is not difficult to see that this operator norm is finite uniformly in $0 \leq t \leq t_0$ for each fixed t_0. The second term converges to zero as $t \to 0$ by our argument above. The third term is bounded by ε. So, we have shown that

$$\limsup_{t \to 0} \|P_t f - f\| < (1 + \sup_{0 \leq s \leq t_0} \|P_t\|) \varepsilon.$$

Since ε was arbitrary, this finishes the proof. □

We can now state the main result: the general Feynman-Kac formula.

Theorem 4.25. *Assume V is Kato-deomposable. Then $Af := \lim_{t \to 0} \frac{1}{t}(P_t f - f)$ exists for all f from a dense subset of $L^2(\mathbb{R}^d)$. A is a self-adjoint operator on the domain $D(A) := \{f : \lim_{t \to \infty} \frac{1}{t}(P_t f - f)$ exists.$\}$. For smooth functions $f_0 \in D(A)$ with compact support, we have $Af_0 = Hf_0$, where $H = -\frac{1}{2}\Delta + V$ is as usual the Schrödinger operator. Thus, we can write $P_t = e^{-tH}$.*

Proof. We have just seen that P_t is a strongly continuous semigroup on $L^2(\mathbb{R}^d)$. Now, all of the statements except the one about $Af_0 = hf_0$ follow from general theory, see Reed/Simon, Methods of Modern Mathematical Physics, Volume 2, Chapter X.8, page 236.

For the last remaining statement, we restrict to bounded, continuous V for simplicity. The statement is true for general Kato-decomposable potentials, but the proofs become much more technical then. For bounded continuous V, put (as above) $H_0 = -\frac{1}{2}\Delta$ and $Q_t = e^{-tH_0}$. Then

$$\frac{1}{t}(P_t f - f) = \frac{1}{t}(P_t f - Q_t f) + \frac{1}{t}(Q_t f - f).$$

The last term converges to $-\frac{1}{2}\Delta f$ by the theory of the heat equation, for smooth f. For the first term on the right hand side, we use the expansion (for small t)

$$e^{-\int_0^t V(q_s) \, ds} \approx 1 - \int_0^t V(q_s) \, ds,$$

which is also the place where we need that V is bounded. Then,

$$\begin{aligned}\frac{1}{t}(P_t f - Q_t f)(x) &= \frac{1}{t}\int \left(e^{-\int_0^t V(q_s)\,ds} - 1\right) f(q_t) dW^x(q) \\ &\approx -\frac{1}{t}\int\int_0^t V(q_s)\,ds\, f(q_t) dW^x(q) = \\ &-\frac{1}{t}\int_0^t W^x(V(q_s)f(q_t))\,ds \to -V(x)f(x)\end{aligned}$$

as $t \to 0$. The last statement can be shown by examining the explicit expression for the expectation under W^x of the two time-point function $V(q_s)f(q_t)$. This finishes the proof in the easy case where V is bounded and continuous (the latter is needed so that the evaluation $V(x)$ makes sense). For general V several things need to be done more carefully; we need to show that Brownian paths usually do not hit the singularities of V, we need to localize the argument (to allow for V that grow at infinity), and we need to make sure that we understand the implications of the requirement $f \in D(A)$; this may e.g. mean that f has to vanish where the potential V has a particularly bad singularity. We will not do any of this here and declare the proof as finished. $\square$

Finally, let us state a nice property of the integral kernel of $P_t f$:

Theorem 4.26. *Assume that V is Kato-decomposable, $H = -\frac{1}{2}\Delta$. Then e^{-tH} is an integral operator with kernel*

$$K_t(x,y) = \int e^{-\int_0^t V(q_s)ds} dW_t^{x,y}(q).$$

Moreover, $(x,y) \mapsto K_t(x,y)$ is continuous.

Proof. We already know that $e^{-tH}f(x) = \int K_t(x,y)f(y)\,dy$, so the first statement is true almost everywhere. The proof will thus be finished once we show the continuity statement. For this, we use a nice little trick. Let $s = t/3$. Then, by the Markov property,

$$K_t(x,y) = \int K_s(x,z)K_s(z,w)K_s(w,y)\,dz\,dw. \tag{4.11}$$

Now, $K_s(w,y) = K_s(y,w)$ by the time reversibility of Brownian motion, and

$$K_s(x,z)K_s(y,w) = \int e^{-\int_0^s (V(q_r)+V(\tilde{q}_r)\,dr} dW^{(x,y),(z,w)}(q,\tilde{q}).$$

Here, $W^{(x,y),(z,w)}$ is the measure of $2d$-dimensional conditional Brownian motion starting at (x,y) and ending at (z,w), and we denote its paths by $(q_r, \tilde{q}_r)$. Thus $K_s(x,z)K_s(y,w)$ is the kernel of a Schrödinger operator in $L^2(\mathbb{R}^{2d})$, with potential $\mathbf{V}(x,y) = V(x) + V(y)$. You should check that Kato-decomposability of V implies that of $\mathbf{V}$, in the higher dimensional space. Thus, the Schrödinger semigroup $e^{-t\mathbf{H}}$ with $\mathbf{H} = -\frac{1}{2}\Delta + \mathbf{V}$ takes bounded functions into continuous functions, by our earlier results. Since e^{-sH} is bounded as an operator from L^1 to L^∞, its kernel $K_s(z,w)$ is bounded (to see this, note first that boundedness from L^1 to L^∞ means $|\int K_s(x,y)f(y)dy| \leq C\|f\|_{L^1}$, and then approximate a delta distribution at y by functions $f_n \in L^1$ with $\|f_n\|_{L^1} = 1$). So, (4.11) means that $K_t(x,y) = e^{-t\mathbf{H}}K_s(x,y)$, and is therefore continuous. $\square$

Corollary 4.27. *Assume that $f(x) \geq 0$ and $f(x) > 0$ for all x from some set of positive measure. Then $e^{-tH}f(x) > 0$ for every $x \in \mathbb{R}^d$.*

Proof. Assume $f(x) > \epsilon$ on $A \subset \mathbb{R}^d$, with $\int_A dx \geq \delta$. Without loss of generality we can assume A is compact. Then $K_t(x,y) > c$ on A, since $K_t(x,y)$ is continuous and pointwise positive. Then

$$e^{-tH}f(x) := \int K_t(x,y)f(y)dy \geq \int_A K_t(x,y)f(y) \geq \epsilon c\delta > 0$$

$\square$

4.4 Some applications of the Feynman-Kac formula

The first application is the Perron-Frobenius theorem. It says that quantum minimal energy states are unique and that the wave function can be chosen to be strictly positive. Let us give some necessary preparations.

The *spectrum* of an operator H is, by definition,

$$\sigma(H) = \{z \in \mathbb{C} : zI - H \text{ is not invertible }\}.$$

Here I is the identity operator. For example, all eigenvalues are in $\sigma(H)$, but the spectrum can be larger than that. It is known that for self-adjoint H, $\sigma(H)$ is contained in the real line. Furthermore, for Kato-decomposable V and $H = -\frac{1}{2}\Delta + V$, $\lambda = \inf \sigma(H) > -\infty$. This follows from the fact

$$e^{-t \inf \sigma(H)} = \|e^{-tH}\|_{L^2 \to L^2},$$

where the latter is the operator norm of e^{-tH} as an operator on L^2, which as we know is finite.

The main ingredient for the following theorem is the fact that e^{-tH} improves positivity. This means that for any $f \in L^2$ such that $f(x) \geq 0$ almost everywhere and $f \neq 0$, we have $P_t f(x) > 0$ everywhere. This is what we have seen in Corollary 4.27. We state the main theorem for a general operator.

Theorem 4.28 (Perron-Frobenius)**.** *Let T be a bounded operator on L^2, and assume that T improves positivity. Assume further that $\lambda = \|T\| = \sup \sigma(T)$ is an eigenvalue of T. Then it has multiplicity one, and the eigenfunction can be chosen to be strictly positive (remember, it is only determined up to a complex constant). In other words, there exists $\psi \in L^2$ with $\psi(x) > 0$ for all x such that $H\psi(x) = \lambda\psi(x)$.*

Proof. Since T improves positivity, in particular it maps real-valued functions into real-valued functions. Thus, we may assume that all of its eigenfunctions are real: namely, for any (possibly complex valued) eigenfunction ϕ, also the real and imaginary part of ϕ are eigenfunctions, and obviously $\phi = \mathrm{Re}(\phi) + i\mathrm{Im}(\phi)$ is in the linear span of its real sand imaginary part. So, each possibly complex valued eigenfunction can be replaced by at most two real-valued ones (or only one, if real and imaginary part are not independent).

Let us therefore assume that ψ is a real-valued eigenfunction to the eigenvalue $\lambda = \|T\|$. Since obviously $|\psi(x)| - \psi(x) \geq 0$, we find

$$0 \leq T(|\psi| - \psi)(x) = T|\psi|(x) - T\psi(x). \tag{4.12}$$

Equality only holds if $\psi = |\psi|$ almost everywhere. Furthermore, we have

$$\begin{aligned} \langle \psi, T\psi \rangle &= \int \psi(x) T\psi(x)\, dx \leq \int |\psi(x)||T\psi(x)|\, dx \\ &\leq \int |\psi(x)| T|\psi|(x)\, dx \leq \|\psi\|\|T\psi\| \leq \|\psi\|^2 \|T\| = \lambda \|\psi\|^2. \end{aligned}$$

The inequality at the line break follows from (4.12). But now notice that since $T\psi = \lambda\psi$, the very left hand side of the above string of inequalities is also equal to $\lambda\|\psi\|^2$, and thus all the inequalities are in fact equalities. We have thus found

$$\langle T|\psi|, |\psi| \rangle = \langle T\psi, \psi \rangle. \tag{4.13}$$

We now decompose ψ into positive and negative part: $\psi(x) = \psi_+(x) - \psi_-(x)$, with $\psi_+(x) \geq 0$ and $\psi_-(x) \geq 0$. Then (4.13) reads

$$\langle T\psi^+, \psi^+ \rangle - 2\langle T\psi^+, \psi^- \rangle + \langle T\psi^-, \psi^- \rangle = \langle T\psi^+, \psi^+ \rangle + 2\langle T\psi^+, \psi^- \rangle + \langle T\psi^-, \psi^- \rangle,$$

and we conclude that $\langle T\psi^+, \psi^- \rangle = 0$. Now if $\psi^+ \neq 0$, then $T\psi^+$ is strictly positive, so in this case ψ^- must be zero almost everywhere (both are non-negative). It follows that ψ is either non-negative or non-positive, and by multiplying with -1 if necessary we may assume that $\psi \geq 0$. But $\psi = \frac{1}{\lambda} T\psi$, and since T improves positivity, it follows that indeed $\psi(x) > 0$ for all x.

Let us now assume that there is another linearly independent eigenvector for the eigenvalue λ. Then in particular, there is another eigenvector ϕ to λ that is orthogonal to ψ. But by the argument above, we would find that $\phi(x) > 0$. But it is impossible for two strictly positive functions to be orthogonal in L^2, thus the multiplicity of λ is one. □

When we apply the above theorem to $P_t = e^{-tH}$, we find that

Corollary 4.29. *Assume that $H = -\frac{1}{2}\Delta + V$, V is Kato-decomposable, and $\lambda = \inf \sigma(H)$ is an eigenvalue. Then the corresponding eigenspace has dimension one, and the eigenvector can be chosen to be strictly positive.*

Proof. It is enough to note that an eigenvector of H for the eigenvalue λ is also an eigenvalue of P_t for the eigenvalue $e^{-\lambda}$, and vice versa, and that $\|P_t\| = e^{-t\lambda}$. Now apply the theorem to P_t. □

The final result will deal with the spatial decay of eigenstates. Assume that V is Kato-decomposable, and that $H\psi = E\psi$ for some $E \in \mathbb{R}$. To see how we can estimate the decay rate of ψ, let us start by writing

$$\psi(x) = e^{tE} e^{-tH}\psi(x) = e^{tE} \int e^{-\int_0^t V(q_s)ds} \psi(q_t) dW^x(q).$$

If V grows as $|x| \to \infty$, then the last term becomes small as $|x| \to \infty$; this is because the Brownian motion travels a distance of $\sqrt{t}$ in time t (roughly), so if t is not too large, the path q_s will not be able to leave the region where V is large.

To formalize this, we first separate positive and negative part of the potential:

$$\begin{aligned}
|\psi(x)|^2 &= e^{2tE} \left(\int e^{-\int_0^t V(q_s)ds} \psi(q_t) dW^x(q) \right)^2 \\
&\leq e^{2tE} \|\psi\|_{L^\infty} \left(\int e^{-\int_0^t V_+(q_s)ds} e^{\int_0^t V_-(q_s)ds} dW^x(q) \right)^2 \\
&\leq e^{2tE} \|\psi\|_{L^\infty} \int e^{-2\int_0^t V_+(q_s)ds} dW^x(q) \int e^{2\int_0^t V_-(q_s)ds} dW^x(q),
\end{aligned}$$

where in the last line we used the Cauchy-Schwarz inequality on $L^2(dW^x)$. The second term is bounded by $e^{C_K t}$ for some constant C_K, by Kashminskiis Lemma. To tackle the first term we introduce

$$A_r(t) = \{q \in C(\mathbb{R}^+, \mathbb{R}^d) : \sup_{s \leq t} |q_s - q_0| < r\},$$

i.e. the set of continuous functions that deviate no more than r from their value at $t = 0$ inside the interval $[0, t]$. It is a fact about Brownian motion that there is a constant D such that

$$W^x(A_r^c(t)) \leq D \int_{r/\sqrt{t}} u^{d-1} e^{-u^2/2}\, du.$$

Here $A_r^c(t)$ denotes the complement of $A_r(t)$. Thus,

$$\begin{aligned}
\int e^{-2\int_0^t V_+(q_s)ds} dW^x(q) &= \int e^{-2\int_0^t V_+(q_s)ds} 1_{A_r(t)}(q) dW^x(q) + \int e^{-2\int_0^t V_+(q_s)ds} 1_{A_r^c(t)}(q) dW^x(q) \leq \\
&\leq \exp\left(-2t \inf\{V(y) : |x-y| \leq r\}\right) + D \int_{r/\sqrt{t}} u^{d-1} e^{-u^2/2}\, du.
\end{aligned}$$

In the last inequality, we used $e^{-2\int_0^t V_+(q_s)ds} \leq 1$. In order to make further progress, we now need to make assumptions about the growth of V at infinity.

Theorem 4.30 (Carmonas Estimate)**.** *Let V be Kato-decomposable, and assume $V_+(x) \geq \gamma|x|^{2m}$ for some $\gamma > 0$, $m > 0$, and all x outside of some compact set. Let $H = -\frac{1}{2}\Delta + V$, and let ψ be any eigenfunction of H. Then there exist constants $\delta, D > 0$ such that*

$$|\psi(x)| \leq D\exp(-\delta|x|^{m+1}) \qquad \text{for all } x \in \mathbb{R}.$$

Proof. By the calculations above,

$$|\psi(x)|^2 \leq e^{(2E+C_K)t}\left(e^{-2t\inf\{V(y):|x-y|\leq r\}} + D\int_{r/\sqrt{t}} u^{d-1}e^{-u^2/2}\,du\right).$$

Since $\int_{r/\sqrt{t}} u^{d-1}e^{-u^2/2}\,du \leq C_I(r/\sqrt{t})^{d-1}e^{-r^2/2t}$, and $\inf\{V(y) : |x-y| \leq r\} \geq \gamma(|x|-r)^{2m}$, this implies

$$|\psi(x)|^2 \leq e^{(2E+C_K)t}\left(e^{-\gamma t(|x|-r)^{2m}} + C_I(r/\sqrt{t})^{d-1}e^{-r^2/2t}\right).$$

We ignore the prefactor $(r/\sqrt{t})^{d-1}$ for now and try to maximize the negative exponent

$$M(r,t) = t\gamma(|x|-r)^{2m} + r^2/2t.$$

For r, we just fix $r = \alpha|x|$ with some $0 < \alpha < 1$. For t, we differentiate and find

$$M'(\alpha|x|,t) = \gamma(1-\alpha)|x|^{2m} - \frac{\alpha^2|x|^2}{2t^2}.$$

Equating this zero gives $t_* = \sqrt{\frac{\alpha^2}{\gamma(1-\alpha)}}|x|^{1-m}$, and putting this back into M gives

$$M(\alpha|x|,t_*) = \alpha\sqrt{(1-\alpha)\gamma}|x|^{1-m}|x|^{2m} + \frac{1}{2}\alpha\sqrt{\gamma(1-\alpha)}|x|^2|x|^{m-1} = \frac{3}{2}\alpha\sqrt{(1-\alpha)\gamma}|x|^{m+1}.$$

We can now optimize over α and find $\alpha_* = 2/3$. This finally gives $M(\alpha_*,t_*) = \sqrt{\gamma/3}|x|^{m+1}$. With the choices of α_* and t_*,

$$r/\sqrt{t} = \frac{\alpha_*|x|}{(\alpha_*^2/\gamma(1-\alpha_*))^{1/4}|x|^{(m+1)/2}} = \sqrt{2/3}(\gamma/3)^{-1/4}|x|^{1/2-m/2},$$

and $e^{(2E+C_K)t_*} = e^{2/3(2E+C_K)\sqrt{3/\gamma}|x|^{1-m}}$. Altogether,

$$|\psi(x)|^2 \leq \left(1 + C_I\sqrt{2/3}(\gamma/3)^{-1/4}|x|^{1/2-m/2}\right)e^{2/3(2E+C_K)\sqrt{3/\gamma}|x|^{1-m}}e^{-\sqrt{\gamma/3}|x|^{m+1}}.$$

As $m > 0$, the decaying exponential term decays faster than the growing exponential term grows. The prefactor $|x|^{1/2-m/2}$ grows if $m < 1$, but only like a power law, so this is irrelevant for the exponential decay. The claim follows. □

The above theorem is only a first taste of Carmonas technique. Lower bounds on the decay, and sharper constants on it, can be found in [R. Carmona, Commun. Math. Phys. **62**, 97-108 (1978)].