Introduction to Quantum Physics

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Introduction

This document provides a summary of basic concepts from quantum mechanics, organized roughly by concepts, and provides a list of selected problems.

1 Position, Momentum, and k-space

The Fourier transform is given by

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x) dx \qquad f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \tilde{f}(k) dk$$

We define the momentum space to be

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ikx}{\hbar}} \psi(x) dx$$

Claim. 1

For the k-space, we have

$$\langle f(\hat{p}) \rangle = \int_{-\infty}^{\infty} f(\hbar k) |\tilde{\psi}(k)|^2 \, dk$$

For the momentum space, we have

$$\langle f(\hat{p}) \rangle = \int_{-\infty}^{\infty} f(\hbar k) |\phi(p)|^2 \, dp$$

Proof.

$$\begin{aligned}
\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \overline{\psi}\hat{p}\psi\, dx &= \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{iqx}\tilde{\psi}(q)dq \right)^* \frac{\hbar}{i}\frac{\partial}{\partial x} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx}\tilde{\psi}(k)dk \right) dx \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} e^{-iqx}\tilde{\psi}^*(q)dq \right) \left(\int_{-\infty}^{\infty} \frac{\hbar}{i}\frac{\partial}{\partial x} e^{ikx}\tilde{\psi}(k)dk \right) dx \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{\psi}^*(q)\tilde{\psi}(k) e^{-iqx} \frac{\hbar}{i}\frac{\partial}{\partial x} e^{ikx} dxdqdk \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{\psi}^*(q)\tilde{\psi}(k) \left(\int_{-\infty}^{\infty} e^{-iqx}\hbar k e^{ikx} dx \right) dqdk \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{\psi}^*(q)\tilde{\psi}(k)\hbar k \underbrace{\left(\int_{-\infty}^{\infty} e^{i(k-q)x} dx \right)}_{=2\pi\delta(k-q)} dqdk \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{\psi}^*(q)\tilde{\psi}(k)\hbar k\delta(k-q)dqdk \\
&= \int_{-\infty}^{\infty} \tilde{\psi}^*(k)\hbar k\tilde{\psi}(k)dk \\
&= \int_{-\infty}^{\infty} |\tilde{\psi}(k)|^2 \hbar k dk
\end{aligned}$$

We see that for $\langle \hat{p} \rangle$ is multiplicative – $\langle \hat{p}^n \rangle \mapsto \frac{1}{\sqrt{2\pi}} \int |\tilde{\psi}|^2 (\hbar k)^n$. Now we generalize this to any $\langle f(\hat{p}) \rangle$. Consider the power series expansion

$$\begin{aligned}
\langle f(\hat{p}) \rangle &= \left\langle f(0) + \hat{p}f'(0) + \frac{\hat{p}^2}{2!}f''(0) + \dots \right\rangle \\
&= f(0) + \langle \hat{p} \rangle f'(0) + \frac{\langle \hat{p}^2 \rangle}{2!}f''(0) + \dots
\end{aligned}$$

Calculating each $\langle \hat{p}^n \rangle$:

$$\begin{aligned}
\langle f(\hat{p}) \rangle &= f(0) + f'(0) \int_{-\infty}^{\infty} |\tilde{\psi}(k)|^2 \hbar k dk + \frac{1}{2!}f''(0) \int_{-\infty}^{\infty} |\tilde{\psi}(k)|^2 (\hbar k)^2 dk + \dots \\
&= \int_{-\infty}^{\infty} |\tilde{\psi}(k)|^2 \left(f(0) + \hbar k f'(0) + \frac{(\hbar k)^2}{2!}f''(0) + \dots \right) dk \\
&= \int_{-\infty}^{\infty} |\tilde{\psi}(k)|^2 f(\hbar k) dk
\end{aligned}$$

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If we work in momentum space, this is analo gous:

$$\langle f(\hat{p}) \rangle = \int p|\phi(p)|^2 dp$$

Claim. 2

For k-space,

$$\langle f(\hat{x}) \rangle = \int_{-\infty}^{\infty} f\left(i\frac{\partial}{\partial k}\right) |\tilde{\psi}(k)|^2 dk$$

For momentum space,

$$\langle f(\hat{x}) \rangle = \int_{-\infty}^{\infty} f\left(i\hbar\frac{\partial}{\partial p}\right) |\phi(p)|^2 dp$$

Proof.

$$
\begin{aligned}
\langle \hat{x} \rangle &= \int_{-\infty}^{\infty} \overline{\psi(x)} x \psi(x) dx \\
&= \int_{-\infty}^{\infty} \overline{\left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ik'x} \tilde{\psi}\left(k'\right) dk' \right]} x \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \tilde{\psi}(k) dk \right] dx \\
&= \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik'x} \overline{\tilde{\psi}(k')} dk' \right] \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x e^{ikx} \tilde{\psi}(k) dk \right] dx \\
&= \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik'x} \overline{\tilde{\psi}(k')} dk' \right] \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{i} \frac{\partial}{\partial k} e^{ikx} \right) \tilde{\psi}(k) dk \right] dx \\
&= \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik'x} \overline{\tilde{\psi}(k')} dk' \right] \frac{1}{i} \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} \left(\frac{\partial}{\partial k} e^{ikx} \right) \tilde{\psi}(k) dk \right] dx \\
&= \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik'x} \overline{\tilde{\psi}(k')} dk' \right] \frac{1}{i} \frac{1}{\sqrt{2\pi}} \left[e^{ikx} \tilde{\psi}(k) \big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} e^{ikx} \frac{\partial \tilde{\psi}(k)}{\partial k} dk \right] dx \\
&= \frac{i}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-ik'x} \overline{\tilde{\psi}\left(k'\right)} e^{ikx} \frac{\partial \tilde{\psi}(k)}{\partial k} dk' dk dx \\
&= \int_{-\infty}^{\infty} \overline{\tilde{\psi}(k)} \left(i \frac{\partial}{\partial k} \right) \tilde{\psi}(k) dk
\end{aligned}
$$

The same exact reasoning gives

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} \left(i\hbar \frac{\partial}{\partial p} \right) |\phi(p)|^2 dp$$

Furthermore we can generalize this to any $\|f(\hat{x})\|$.

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Wavefunction collapse

Operator	Eigenvalue	Eigenfunction
$\hat{x}$	$y \in \mathbb{R}$	$y\delta(x-y)$
$\hat{p}$	$\hbar k$	Ae^{ikx}
$\hat{H}$	E_n	ϕ_E

Depending on which observable, the wavefunction changes to the associated eigenfunction upon measurement.

2 Probability Current

The probability is defined as:

$$\mathcal{J}(x,t) = \frac{i\hbar}{2m}\left(\psi\overline{\frac{\partial \psi}{\partial x}} - \overline{\psi}\frac{\partial \psi}{\partial x}\right) = \frac{\hbar}{m}\operatorname{Im}\left(\overline{\psi}\frac{\partial \psi}{\partial x}\right)$$

Claim. 3

$$\frac{dP_{ab}}{dt} = \mathcal{J}(a,t) - \mathcal{J}(b,t)$$

Proof.

$$\begin{aligned}
P_{ab}(t) &= \int_a^b |\psi(x,t)|^2 dx = \int_a^b \psi^*(x,t)\psi(x,t)dx \\
\frac{dP_{ab}}{dt} &= \frac{d}{dt}\int_a^b \psi^*(x,t)\psi(x,t)dx = \int_a^b \frac{\partial}{\partial t}\left[\psi^*(x,t)\psi(x,t)\right]dx = \int_a^b \left[\psi^*\frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi\right]dx
\end{aligned}$$

From the Schrodinger's equation, we get

$$\begin{aligned}
i\hbar\frac{\partial \psi(x,t)}{dt} &= -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \\
-i\hbar\frac{\partial \psi^*(x,t)}{dt} &= -\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*(x,t)}{\partial x^2} + V(x)\psi^*(x,t)
\end{aligned}$$

Substituting,

$$\begin{aligned}
\frac{dP_{ab}}{dt} &= \frac{1}{i\hbar}\int_a^b \left[\psi^*\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi\right) - \left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + V\psi^*\right)\psi\right]dx \\
&= \frac{1}{i\hbar}\int_a^b \left[-\frac{\hbar^2}{2m}\left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right) + (\psi^*V\psi - V\psi^*\psi)\right]dx \\
&= \frac{i\hbar}{2m}\int_a^b \left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right)dx \\
&= \frac{i}{2m}\int_a^b \left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right)dx \\
&= \frac{i}{2m}\int_a^b \left[\psi^*\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\right) - \psi\frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}\right)\right]dx \\
&= \frac{i}{2m}\left[\left(\psi^*\frac{\partial\psi}{\partial x}\right)\Big|_a^b - \left(\psi\frac{\partial\psi^*}{\partial x}\right)\Big|_a^b - \int_a^b \frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x}dx + \int_a^b \frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x}dx\right] \\
&= \frac{i}{2m}\left[\left(\psi^*\frac{\partial\psi}{\partial x}\right)\Big|_a^b - \left(\psi\frac{\partial\psi^*}{\partial x}\right)\Big|_a^b\right] \\
&= \frac{i}{2m}\left[\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right)\Big|_{x=a} - \left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right)\Big|_{x=b}\right] \\
&= \mathcal{J}(a,t) - \mathcal{J}(b,t)
\end{aligned}$$

■

Claim. 4
For
$$\psi(x) = A(x)e^{i\theta(x)}$$
the probability current is given by
$$\mathcal{J} = |A(x)|^2 \frac{\hbar}{m}\frac{\partial}{\partial x}\theta(x)$$

Proof.
$$\frac{\partial \psi}{\partial x} = A(x)i\frac{\partial \theta}{\partial x}e^{i\theta(x)} + \frac{\partial A}{\partial x}e^{i\theta(x)} \quad \text{and} \quad \frac{\partial \psi^*}{\partial x} = -A(x)i\frac{\partial \theta}{\partial x}e^{-i\theta(x)} + \frac{\partial A}{\partial x}e^{-i\theta(x)}$$
By definition of $\mathcal{J}(x,t)$ we get
$$\mathcal{J}(x,t) = \frac{i\hbar}{2m}\left(-|A|^2 i\frac{\partial \theta}{\partial x} + A\frac{\partial A}{\partial x} - |A|^2 i\frac{\partial \theta}{\partial x} - A\frac{\partial A}{\partial x}\right) = |A(x)|^2\frac{\hbar}{m}\frac{\partial \theta}{\partial x}$$
■

An easy consequence is that real wavefunctions have $\mathcal{J}(x,t) = 0$.
For a plane wave $\psi(x) = Ae^{i(kx-\omega t)}$, we have $\frac{d\psi}{dx} = ikAe^{ikx}$ and so
$$\mathcal{J}(x,t) = \frac{\hbar k}{m}|A|^2 \tag{2.0.1}$$

3 Operators

Basic facts

Claim. 5

If A, B are normal and $[\hat{A}, \hat{B}] = 0$, then they have common basis of eigenfunctions. Furthermore, if $\hat{A}$ and $\hat{B}$ share a complete set of eigenbasis, then $[\hat{A}, \hat{B}] = 0$.

An immediate consequence is the contrapositive of the second part: if, say, $[\hat{A}, \hat{B}] = 1$, then they share no complete set of eigenfunctions. This explains the Heisenberg uncertainty principle since $[\hat{x}, \hat{p}] = i\hbar$. Similarly, $[\hat{x}, \hat{H}] = [\hat{x}, \frac{\hat{p}^2}{2m}] = \frac{i\hbar}{m}\hat{p}$, implying there are no common normalizable eigenfunctions. This is the time-energy uncertainty principle.

Claim. 6

If $[\hat{A}, \hat{B}] = \lambda\hat{B}$, then for any eigenfunction of A satisfying $\hat{A}\psi = a\psi$, we have that $(a + \lambda)$ is an eigenvalue of $\hat{A}$ corresponding to the eigenvector $\hat{B}\psi$.

Proof.

$$
\begin{aligned}
[\hat{A}, \hat{B}]\psi = \hat{A}\hat{B}\psi - \hat{B}\hat{A}\psi &= \lambda\hat{B}\psi \\
\hat{A}\hat{B}\psi - a\hat{B}\psi &= \lambda\hat{B}\psi \\
\hat{A}(\hat{B}\psi) &= (a + \lambda)(\hat{B}\psi)
\end{aligned}
$$

∎

Translation operator

Define

$$\hat{T}_L f(x) = f(x - L)$$

and $\hat{D}$ be the differential operator. The eigenfunctions of $\hat{T}_L$ can be found by setting

$$\phi(x - L) = \hat{T}_L\phi = \lambda\phi$$

Introducing $\phi_\beta = e^{\beta L}g(x)$ where $\beta \in \mathbb{C}$ one gets

$$
\begin{aligned}
e^{\beta(x-L)}g(x - L) &= \alpha e^{\beta x}g(x) \\
e^{-\beta L}g(x - L) &= \alpha g(x)
\end{aligned}
$$

Set $\alpha = e^{-\beta L}$ gives

$$g(x - L) = g(x)$$

Thus we obtain that the eigenstates of $\hat{T}_L$ are of the form

$$\phi_\beta(x) = e^{\beta x}g(x)$$

where $g(x - L) = g(x)$, and the corresponding eigenvalue is $\alpha = e^{-\beta L}$.

Momentum is the generator of translations:

$$\begin{aligned}\hat{T}_a\psi(x) &= \psi(x-a)\\ &= \sum_{n=0}^{\infty}\frac{1}{n!}D^n\psi(x)(-a)^n\\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-ia}{\hbar}\hat{p}\right)^n\\ &= e^{-\frac{ia}{\hbar}\hat{p}}\end{aligned}$$

The adjoint of $\hat{T}_L$ is $\hat{T}_{-L}$:

$$\hat{T}_{-L}f(x) = f(x+L) = e^{i\frac{L}{\hbar}\hat{p}}f(x) = \left(e^{-i\left(\frac{L}{\hbar}\hat{p}\right)}\right)^{\dagger} = T_L^{\dagger}f(x)$$

Properties

Proposition.

$$\left[\hat{T}_L,\hat{x}\right] = -L\hat{T}_L$$

Proof.

$$\begin{aligned}\left[\hat{T}_L,\hat{x}\right]f(x) &= \hat{T}_L(\hat{x}f(x)) - \hat{x}\hat{T}_Lf(x)\\ &= \hat{T}_L(xf(x)) - x\hat{T}_Lf(x)\\ &= (x-L)f(x-L) - xf(x-L)\\ &= -Lf(x-L) = -L\hat{T}_Lf(x)\end{aligned}$$

■

Proposition.

$$[\hat{T}_L,\hat{D}] = 0$$

Proof.

$$\hat{T}_L\hat{D}f(x) = \hat{T}_L\frac{\partial}{\partial x}f(x) = \hat{T}_Lf'(x) = f'(x-L)$$

$$\hat{D}\hat{T}_Lf(x) = \hat{D}f(x-L) = \frac{\partial}{\partial x}f(x-L) = f'(x-L)$$

■

Proposition.

$$\hat{T}_L = e^{-L\hat{D}} = e^{-L\frac{i}{\hbar}\hat{p}}$$

Proof.

$$e^{-L\frac{\partial}{\partial x}} = 1 - L\frac{\partial}{\partial x} + \frac{L^2}{2}\frac{\partial^2}{\partial x^2} - \dots$$

Apply to f:

$$e^{-L\frac{\partial}{\partial x}}f(x) = f(x) - L\frac{\partial f}{\partial x} + \frac{L^2}{2}\frac{\partial^2 f}{\partial x^2} - \dots$$

This is Taylor's theorem applied to $f(x-L)$ at x.

Hence

$$e^{-L\frac{\partial}{\partial x}}f(x) = f(x-L) = \hat{T}_L f(x)$$

■

Proposition.

$$[\hat{D}, \hat{x}] = 1$$

Proof.

$$\left[\hat{T}_L, \hat{x}\right] = -L\hat{T}_L = -L(1 - L\hat{D} + \cdots)$$

Also,

$$\left[\hat{T}_L, \hat{x}\right] = [1 - L\hat{D} + \cdots, \hat{x}] = [1, \hat{x}] + [-L\hat{D} + \cdots, \hat{x}] = -L[\hat{D} + \cdots, \hat{x}]$$

Comparing coefficients of L, we see that $[\hat{D}, \hat{x}] = 1$.

In general,

$$\left[\hat{T}_L, \hat{x}\right] = -L\hat{T}_L = -L\sum_{n=0}^{\infty}\frac{1}{n!}(-L\hat{D})^n = \sum_{n=1}^{\infty}\frac{1}{(n-1)!}(-L)^n\hat{D}^{n-1}$$

Also,

$$\left[\hat{T}_L, \hat{x}\right] = \left[\sum_{n=0}^{\infty}\frac{1}{n!}(-L\hat{D})^n, \hat{x}\right] = \sum_{n=0}^{\infty}\frac{1}{n!}(-L)^n\left[\hat{D}^n, \hat{x}\right]$$

Comparing coefficients of L:

$$\frac{1}{(n-1)!}\hat{D}^{n-1} = \frac{1}{n!}\left[\hat{D}^n, \hat{x}\right]$$

Hence,

$$\left[\hat{D}^n, \hat{x}\right] = n\hat{D}^{n-1}.$$

■

Proposition.

$$\hat{T}_L\tilde{f}(k) = e^{-ikL}\tilde{f}(k)$$

Proof.

$$\begin{aligned}\hat{T}_L \tilde{f}(k) &= \hat{T}_L \frac{1}{\sqrt{2\pi}} \int e^{-ikx} f(x)\, dx \\ &= \frac{1}{\sqrt{2\pi}} \int e^{-ikx} \hat{T}_L f(x)\, dx \\ &= \frac{1}{\sqrt{2\pi}} \int e^{-ikx} f(x-L)\, dx \\ &= \frac{1}{\sqrt{2\pi}} \int e^{-ikx} e^{-ikL} f(x)\, dx \\ &= e^{-ikL} \tilde{f}(k)\end{aligned}$$

■

Proposition.

$$\hat{D}\tilde{f}(k) = ik\tilde{f}(k)$$

Proof. First, Taylor expand $\hat{D}$ to get:

$$\hat{T}_L \tilde{f}(k) = e^{-L\hat{D}} \tilde{f}(k) = (1 - L\hat{D} + \cdots)\tilde{f}(k)$$

Then, use the last proposition:

$$\hat{T}_L \tilde{f}(k) = e^{-iLk} \tilde{f}(k) = (1 - ikL + \cdots)\tilde{f}(k)$$

Match the linear term:

$$\hat{D}\tilde{f}(k) = ik\tilde{f}(k).$$

■

Proposition.

$$\hat{x}\tilde{f}(k) = i\frac{\partial}{\partial k}\tilde{f}(k)$$

Proof.

$$\begin{aligned}\hat{x}\tilde{f}(k) &= \hat{x}\frac{1}{\sqrt{2\pi}} \int e^{-ikx} f(x)\, dk \\ &= \frac{1}{\sqrt{2\pi}} \int \hat{x} e^{-ikx} f(x)\, dk \\ &= \frac{1}{\sqrt{2\pi}} \int i\frac{\partial}{\partial k} e^{ikx} f(x)\, dk \\ &= i\frac{\partial}{\partial k}\frac{1}{\sqrt{2\pi}} \int e^{-ikx} \tilde{f}(x)\, dk = i\frac{\partial}{\partial k}\tilde{f}(k)\end{aligned}$$

■

Boost-by-q Operator

Define

$$\hat{B}_q f(x) = e^{iqx/\hbar} f(x)$$

We have

$$\langle \hat{x} \rangle_{\hat{B}_q f} = \int x \left(e^{iqx/\hbar} f(x)\right)^* e^{iqx/\hbar} f(x)\, dx = \langle \hat{x} \rangle_f$$

And

$$\begin{aligned}
\langle \hat{p} \rangle_{\hat{B}_q f} &= -i\hbar \int dx \left(e^{iqx/\hbar} f(x)\right)^* \frac{\partial}{\partial x} \left(e^{iqx/\hbar} f(x)\right) \\
&= -i\hbar \int dx f^*(x) e^{-iqx/\hbar} \left(\frac{iq}{\hbar} e^{iqx/\hbar} f(x) + e^{iqx/\hbar} \frac{\partial}{\partial x} f(x)\right) \\
&= -i\hbar \int dx f^*(x) \frac{iq}{\hbar} f(x) - i\hbar \int dx f^*(x) \frac{\partial}{\partial x} f(x) = q + \langle \hat{p} \rangle_f
\end{aligned}$$

Similar to $\hat{T}_L$, the adjoint $\hat{B}_q^\dagger = \hat{B}_{-q}$.

Time evolution operator

Define

$$\hat{U}_t \psi(x, 0) = \psi(x, t)$$

Claim. 7

U_t is unitary.

Proof.

$$\begin{aligned}
&\int |\psi(x,t)|^2 dx = \langle U_t \psi(x,0) | U_t \psi(x,0) \rangle = \langle U_t^\dagger U_t \psi(x,0) | \psi(x,0) \rangle = 1 \\
&U_t^\dagger U_t = 1
\end{aligned}$$

by isometry properties. This implies

$$\hat{U}_t^\dagger \hat{U}_t \psi(x,0) = \hat{U}_t^\dagger \psi(x,t) = \psi(x,0)$$

Hence $\hat{U}_t^\dagger(t) = \hat{U}_{-t}$, so the adjoint of the time-evolution operator is reverse time evolution. ■

From the Schrodinger's equation we get

$$\begin{aligned}
(\partial_t \hat{U}_t)\psi(x,0) &= -\frac{i}{\hbar} \hat{H} \hat{U}_t \psi(x,0) \\
\Rightarrow \partial_t \hat{U}_t &= -\frac{i}{\hbar} \hat{H} \hat{U}_t
\end{aligned}$$

Solving, we get

$$\hat{U}_t = e^{-\frac{i}{\hbar}\hat{H}t} \hat{U}_0 \tag{3.0.1}$$
$$1 = e^{\frac{i}{\hbar}\hat{H}t} \hat{U}_0^\dagger e^{-\frac{i}{\hbar}\hat{H}t} \hat{U}_0 \tag{3.0.2}$$
$$1 = \hat{U}_0^\dagger \hat{U}_0 \tag{3.0.3}$$

Write $\hat{U}_{t_2} = \hat{U}_{t_1+t_2} \hat{U}_{t_1}^\dagger$, we get

$$e^{-\frac{i}{\hbar}\hat{H}t_2} \hat{U}_0 = e^{-\frac{i}{\hbar}\hat{H}(t_1+t_2)} \hat{U}_0 \hat{U}_0^\dagger e^{\frac{i}{\hbar}\hat{H}t_1} = e^{-\frac{i}{\hbar}\hat{H}t_2} \Rightarrow \hat{U}_0 = 1$$

So

$$\hat{U}_t = e^{-\frac{i}{\hbar}\hat{H}t} \tag{3.0.4}$$

and $\hat{U}_0 = 1$.

4 Quantum Harmonic Oscillator

Classically, the harmonic oscillator satisfies the following formula for energy:

$$E(x) = \frac{1}{2}mw^2x^2 + \frac{p^2}{2m}$$

where $k = mw^2$, and the solution for the initial condition $x(0) = 0$ is

$$x(t) = A\sin(wt)$$

At $t = 0$, $V = 0$, and we can calculate the kenetic energy to be

$$E = T(0) = \frac{1}{2}mv^2 = \frac{1}{2}mA^2w^2\cos^2(wt) = \frac{1}{2}mw^2A^2$$

Since energy is conserved, this will be the system's energy.

The quantum counterpart corresponds $H \to \hat{H} = \frac{1}{2m}[\hat{p}^2 + (mw\hat{x})^2]$. This gives the following Schrodinger's equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}mw^2x^2\psi = E\psi$$

Define the following operators [1]

$$\hat{a} = \frac{1}{\sqrt{2\hbar mw}}(mw\hat{x} + i\hat{p}) \qquad a^\dagger = \frac{1}{\sqrt{2\hbar mw}}(mw\hat{x} - i\hat{p})$$

Clearly they are Hermitian conjugates, and

$$\begin{aligned}\hat{a}\hat{a}^\dagger &= \frac{1}{2\hbar mw}(\hat{p}^2 + (mw\hat{x})^2 - imw(\hat{x}\hat{p} - \hat{p}\hat{x})) \\ &= \frac{1}{2\hbar mw}(\hat{p}^2 + (mw\hat{x})^2) - \frac{i}{2\hbar}[\hat{x}, \hat{p}] \\ &= \frac{1}{\hbar w}\hat{H} + \frac{1}{2}\end{aligned}$$

To summarize:

$$\hat{a}\hat{a}^\dagger = \frac{1}{\hbar w}\hat{H} + \frac{1}{2} \tag{4.0.1}$$

$$\hat{a}^\dagger\hat{a} = \frac{1}{\hbar w}\hat{H} - \frac{1}{2} \tag{4.0.2}$$

$$[\hat{a}, \hat{a}^\dagger] = 1 \tag{4.0.3}$$

$$\hat{H} = \hbar w(\hat{a}\hat{a}^\dagger - \frac{1}{2}) = \hbar w(\hat{a}^\dagger\hat{a} + \frac{1}{2}) \tag{4.0.4}$$

The above defintions also give

$$\hat{x} = \sqrt{\frac{\hbar}{2mw}}(\hat{a} + \hat{a}^\dagger) \qquad \hat{p} = i\sqrt{\frac{\hbar mw}{2}}(\hat{a}^\dagger - \hat{a}) \tag{4.0.5}$$

[1] In Griffiths, we have the following definition: $\hat{a}_\pm = \frac{1}{\sqrt{2\hbar mw}}(\mp i\hat{p} + mwx)$ I've basically made the substitution $\hat{a}_+ \to \hat{a}^\dagger$ and $\hat{a}_- \to \hat{a}$. Note Wikipedia uses the definitions $a = \sqrt{\frac{mw}{2\hbar}}(\hat{x} + \frac{i}{mw}\hat{p})$ and $a = \sqrt{\frac{mw}{2\hbar}}(\hat{x} - \frac{i}{mw}\hat{p})$, which is the same.

This implies

$$\langle \hat{x} \rangle_{\phi_n} = \sqrt{\frac{\hbar}{2mw}} \int \overline{\phi_n} (\hat{a} + \hat{a}^\dagger) \phi_n = \sqrt{\frac{\hbar}{2mw}} \int \overline{\phi_n} (\sqrt{n} \phi_{n-1} + \sqrt{n+1} \phi_{n+1}) = 0$$
$$\langle \hat{p} \rangle_{\phi_n} = i \sqrt{\frac{\hbar}{2mw}} \int \overline{\phi_n} (\hat{a}^\dagger - \hat{a}) \phi_n = i \sqrt{\frac{\hbar}{2mw}} \int \overline{\phi_n} (\sqrt{n+1} \phi_{n+1} - \sqrt{n} \phi_{n-1}) = 0$$

Similarly, we have

$$\begin{aligned} \left\langle \hat{x}^2 \right\rangle_{\phi_n} &= \frac{\hbar}{2mw}(2n+1) \\ \left\langle \hat{p}^2 \right\rangle_{\phi_n} &= \frac{\hbar mw}{2}(2n+1) \end{aligned}$$

Hence we can calculate the uncertanties:

$$\Delta x \Delta p = \sqrt{\frac{\hbar}{2mw}(2n+1)\frac{\hbar mw}{2}(2n+1)} = \frac{\hbar}{2}(2n+1)$$

Due to minimal uncertainty wavefunctions, we know that wavefunctions with uncertainties $\frac{\hbar}{2}$ corresponds to Gaussians, which is confirmed in this case with $\phi_0(x) = \left(\frac{mw}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\frac{mwx^2}{2\hbar}}$, while higher energy states are not Gaussians.

Claim. 8 (Ladder operation)
If ϕ_E is an eigenfunction of $\hat{H}$, then so is $\hat{a}^\dagger \phi_E = (E + \hbar w) \phi_{E+\hbar w}$. Similarly $\hat{a} \phi_E = (E - \hbar w) \phi_{E-\hbar w}$.

Proof.

$$\begin{aligned} \hat{H}(\hat{a}^\dagger \phi_E) &= \hbar w (\hat{a}^\dagger \hat{a} + \frac{1}{2})(\hat{a}^\dagger \phi_E) = \hbar w (\hat{a}^\dagger \hat{a} \hat{a}^\dagger + \frac{1}{2} \hat{a}^\dagger) \phi_E \\ &= \hbar w \hat{a}^\dagger (\hat{a} \hat{a}^\dagger + \frac{1}{2}) \phi_E = \hbar w \hat{a}^\dagger (\hat{a}^\dagger \hat{a} + 1 + \frac{1}{2}) \phi_E \\ &= \hat{a}^\dagger (\hat{H}^\dagger + \hbar w) \phi_E = \hat{a}^\dagger (E \phi_E + \hbar w \phi_E) = (E + \hbar w)(\hat{a}^\dagger \phi_E) = (E + \hbar w) \phi_{E+\hbar w} \end{aligned}$$

■

Similarly

$$\hat{H}(\hat{a}\phi_E) = (E - \hbar w)\phi_{E-\hbar w}$$

Using this ladder operation, there will be a minimum for the eigenvalue. When that occurs, we will have $\hat{a}\phi_{E_0} = 0$. Backtracking, we get

$$\begin{aligned} \frac{1}{\sqrt{2\hbar mw}}(\hbar \frac{d}{dx} + mw\hat{x})\phi_{E_0}(x) &= 0 \\ \frac{d\phi_{E_0}}{dx} &= -\frac{mw}{\hbar} x \phi_{E_0}(x) \end{aligned}$$

$$\psi_0(x) := \phi_{E_0}(x) = \left(\frac{mw}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{mw}{2\hbar}x^2} \tag{4.0.6}$$

Claim. 9 (Energy)
The ground state $E_0 = \frac{1}{2}\hbar w$, and each successive state $E_n = \hbar w(n + \frac{1}{2})$.

Proof. From (4) we get

$$\hat{H}\phi_{E_0} = \hbar w(\hat{a}^\dagger\hat{a}\phi_{E_0} + \frac{1}{2}\phi_{E_0}) = \frac{1}{2}\hbar w\phi_{E_0}$$

As $n \to n+1$, we have $E_n \to E_{n+1} = E_n + \hbar w$, which proves the second part. ∎

Claim. 10 (Normalization)
The following properties holds:

$$\hat{a}^\dagger\hat{a}\psi_n = n\psi_n \qquad \hat{a}\hat{a}^\dagger\psi_n = (n+1)\psi_n$$

And this implies normalization for each $\psi_n = A_n(\hat{a}^\dagger)^n\psi_0$ with $A_n = \frac{1}{\sqrt{n!}}$.

Proof.

$$\begin{aligned}
\hat{H}\psi_n = E_n\psi_n &\Rightarrow \hbar w(\hat{a}^\dagger\hat{a} + \frac{1}{2})\psi_n = \hbar w(n + \frac{1}{2})\psi_n \\
&\Rightarrow \hat{a}^\dagger\hat{a}\psi_n = n\psi_n \\
\hat{H}\psi_n = E_n\psi_n &\Rightarrow \hbar w(\hat{a}\hat{a}^\dagger - \frac{1}{2})\psi_n = \hbar w(n + \frac{1}{2})\psi_n \\
&\Rightarrow \hat{a}\hat{a}^\dagger\psi_n = (n+1)\psi_n
\end{aligned}$$

Hence

$$\begin{aligned}
\left\|\hat{a}^\dagger\psi_n\right\|^2 &= \left\langle \hat{a}^\dagger\psi_n \middle| \hat{a}^\dagger\psi_n \right\rangle = \left\langle \hat{a}\hat{a}^\dagger\psi_n \middle| \psi_n \right\rangle = (n+1)\left\langle \psi_n | \psi_n \right\rangle = n+1 \\
\left\|\hat{a}\psi_n\right\|^2 &= \left\langle \hat{a}\psi_n | \hat{a}\psi_n \right\rangle = \left\langle \hat{a}^\dagger\hat{a}\psi_n \middle| \psi_n \right\rangle = n\left\langle \psi_n | \psi_n \right\rangle = n
\end{aligned}$$

Since $\hat{a}^\dagger\psi_n = c_n\psi_{n+1}$ and $\hat{a}\psi_n = d_n\psi_{n-1}$, we know that $c_n = n+1$ and $d_n = n$. To summarize:

$$\hat{a}^\dagger\psi_n = \sqrt{n+1}\psi_{n+1} \qquad \hat{a}\psi_n = \sqrt{n}\psi_{n-1} \tag{4.0.7}$$

$$\psi_n = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\psi_0 \tag{4.0.8}$$

∎

Define the number operator

$$\hat{N} = \hat{a}^\dagger\hat{a}$$

We have

$$[\hat{N}, \hat{a}] = \hat{a}^\dagger\hat{a}\hat{a} - \hat{a}\hat{a}^\dagger\hat{a} = (\hat{a}\hat{a}^\dagger - 1)\hat{a} - \hat{a}\hat{a}^\dagger\hat{a} = -\hat{a} \tag{4.0.9}$$

$$[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}^\dagger\hat{a} = \hat{a}^\dagger(1 + \hat{a}^\dagger\hat{a}) - \hat{a}^\dagger\hat{a}^\dagger\hat{a} = \hat{a}^\dagger \tag{4.0.10}$$

The eigenstates of $\hat{N}$ are given as follows:

$$\begin{aligned}
\hat{N}\psi &= \hat{a}^\dagger\hat{a}\psi = \lambda\psi \\
\left(\frac{1}{\hbar w}\hat{H} - \frac{1}{2}\psi\right) &= \lambda\psi \\
\hat{H}\psi &= \hbar w\left(\lambda + \frac{1}{2}\right)\psi
\end{aligned}$$

We also have

$$\hat{N}(\hat{a}^\dagger |n\rangle) = (n+1)\hat{a}^\dagger |n\rangle \tag{4.0.11}$$

Hence the eigenvalues are precisely the quantum numbers, and eigenvectors are just ϕ_{E_n}, the energy eigenstates. In other words

$$\hat{H} = \hbar w \left(\hat{N} + \frac{1}{2}\right) \tag{4.0.12}$$

which is what we derived previously.

A note on parity

The energy eigenstates $\psi_0, \psi_1, \ldots$ corresponds to an alternating parity: even, odd, even, ...

In general, let's define the parity operator $\hat{P} : \psi(x) \mapsto \psi(-x)$. Since $\hat{P}^2 = 1$, we have that the eigenvalues of $\hat{P}$ is ± 1, which corresponds to even/odd eigenstates.

Claim. 11 (Parity)
For a symmetric potential $V(x) = V(-x)$, we have $[\hat{H}, \hat{P}] = 0$. Hence there are common eigenfunctions that can be either even or odd.

The closed form of the eigenstates are given by:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{mw}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{mwx^2}{2\hbar}} H_n\left(\sqrt{\frac{mw}{\hbar}} x\right)$$

where H_n are the Hermite polynomials

$$H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n}\left(e^{-z^2}\right)$$

For n even, H_n is an even function. For n odd, H_n is an odd function. Hence the basis $\psi_0, \psi_1, \ldots$ is a set of common eigenfunction of both operators.

Problems

Problem. 1
Consider the initial wave function $\psi(x, 0) = \frac{1}{\sqrt{2}}[\phi_0(x) + i\phi_1(x)]$, where ϕ_n corresponds to the eigenstates.

1. Calculate $\psi(x, t)$ and $|\psi(x, t)|^2$.
2. Find $\langle x \rangle$.
3. Show that the probability returns to its original shape after the classical period $T = \frac{2\pi}{w_0}$. In general, when does it occur?

Solution. 1.

$$|\psi(x, t)| = \frac{1}{\sqrt{2}} \phi_0 e^{-\frac{1}{2} i w_0 t} + \frac{1}{\sqrt{2}} i\phi_1 e^{-\frac{3}{2} i w_0 t}$$

And

$$\begin{aligned}
|\psi(x, t)|^2 &= \left(\frac{1}{\sqrt{2}} \overline{\phi_0} e^{\frac{1}{2} i w_0 t} - \frac{1}{\sqrt{2}} i\overline{\phi_1} e^{\frac{3}{2} i w_0 t}\right)\left(\frac{1}{\sqrt{2}} \phi_0 e^{-\frac{1}{2} i w_0 t} + \frac{1}{\sqrt{2}} i\phi_1 e^{-\frac{3}{2} w i w_0 t}\right) \\
&= \frac{1}{2}|\phi_0|^2 + \frac{1}{2}|\phi_1|^2 + \frac{1}{2} i\overline{\phi_0}\phi_1 e^{-i w_0 t} - \frac{1}{2} i\overline{\phi_1}\phi_0 e^{i w_0 t}
\end{aligned}$$

Here, we use the fact that we can always take energy eigenstates to be real. Hence $\overline{\phi_0} = \phi_0$, and $\overline{\phi_1} = \phi_1$, and we also use the fact that $\sin(z) = \frac{e^{iz}-e^{-iz}}{2i}$ to get:

$$= \frac{1}{2}|\phi_0|^2 + \frac{1}{2}|\phi_1|^2 + \phi_0\phi_1 \sin(w_0 t)$$

2.
$$\langle \hat{x} \rangle = \int x|\psi|^2 = \frac{1}{2}\int x|\phi_0|^2 + \frac{1}{2}\int x|\phi_1|^2 + \int \phi_0\phi_1 \sin(w_0 t)$$

Since $V(x)$ is even, we can take ϕ_n to be even or odd. Hence, the first two integrals evaluate to zero. The last one evaluate to $\sqrt{\frac{\hbar}{2mw_0}}\sin(w_0 t)$.

3. Consider

$$\begin{aligned}\psi(x,t) &= \sum c_n\phi_n e^{-\frac{iE_n t}{\hbar}} = \sum c_n\phi_n e^{-iw_0(n+\frac{1}{2})t} \\ &= e^{-\frac{1}{2}iw_0 t}\sum c_n\phi_n e^{-inw_0 t}\end{aligned}$$

Hence, $\psi(x,t)$ is a superposition of eigenstates with period $\frac{2\pi}{nw_0}$, which is $\frac{1}{n}$ of the classical period $T = \frac{2\pi}{w_0}$. Therefore after $t \to t+T$, all eigenstates to the original position.

Let's define the angular frequency $w_n = \frac{E_n}{\hbar}$ and redefine $\tilde{w}$ to be our original harmonic oscillator frequency.

Claim. 12

If our potential satisfies $w_n - w_0 = \tilde{w}a$, where $a \in \mathbb{Q}$, then $\psi(x,t)$ is periodic in t. In this case $V(x) = \frac{1}{2}m\tilde{w}^2x^2$, we have $w_n - w_0 = \tilde{w}n$, and all energies are spaced evenly apart.

Proof. Write

$$\begin{aligned}\psi(x,t) &= \sum c_n\phi_n e^{-i(w_n-w_0)t-iw_0 t} \\ &= e^{-iw_0 t}\sum c_n\phi_n e^{-i(w_n-w_0)t} \\ &= e^{-iw_0 t}\sum c_n\phi_n e^{-i\tilde{w}at}\end{aligned}$$

each ϕ_n has period $\frac{2\pi}{a\tilde{w}}$, compared with the classical period $T = \frac{2\pi}{\tilde{w}}$. Write $a = \frac{c}{d}$, then after a period of dT, it returns to its original state. Let's just hope that $\text{lcm}(d_1, d_2, \dots)$ doesn't explode. If $a \in \mathbb{Z}$ everything is easy, since T is just an integer multiple of each period of ϕ_n. ■

■

Problem. 2

Show that if $[\hat{A},\hat{B}] = \lambda\hat{B}$, then for any eigenfunction of A satisfying $\hat{A}\psi = a\psi$, we have that $(a+\lambda)$ is an eigenvalue of $\hat{A}$ corresponding to the eigenvector $\hat{B}\psi$. In this case, we have $[\hat{H},\hat{a}^\dagger] = \hbar w\hat{a}^\dagger$, which corresponds to our discussion of the ladder operators.

Solution.

$$\begin{aligned}[\hat{A},\hat{B}]\psi = \hat{A}\hat{B}\psi - \hat{B}\hat{A}\psi &= \lambda\hat{B}\psi \\ \hat{A}\hat{B}\psi - a\hat{B}\psi &= \lambda\hat{B}\psi \\ \hat{A}(\hat{B}\psi) &= (a+\lambda)(\hat{B}\psi)\end{aligned}$$

An energy eigenfunction ϕ_n then follows the ladder $(E_n, \phi_n) \to (E_{n+1} = E_n + \hbar w, \phi_{n+1})$. ■

5 Finite and infinite square well

5.1 Infinite square well

Define

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

Outside the wall the wave function is 0. Hence in that case our particle is free, and WLOG we can write

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

The boundary conditions state

$$0 = \psi(0) = B \qquad\qquad 0 = \psi(a) = A\sin(ka)$$

This implies $ka = n\pi \Rightarrow k = \frac{n\pi}{a}$ for $n \geq 1$. Normalizing gives

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{(n+1)\pi}{a}x\right)} \tag{5.1.1}$$

Solving for energy gives

$$\boxed{E_n = \frac{\hbar^2(n+1)^2\pi^2}{2mL^2}} \tag{5.1.2}$$

Note this satisfies

$$\begin{aligned} E_n &= \frac{\hbar^2(n+1)^2\pi^2}{2mL^2} \\ &= \frac{\hbar^2\pi^2n^2}{2mL^2} + \frac{2\hbar^2\pi^2n}{2mL^2} + \frac{\hbar^2\pi^2}{2mL^2} \\ &= E_{n-1} + \frac{2}{n}E_{n-1} + \frac{1}{n^2}E_{n-1} \\ &= \left(1 + \frac{1}{n}\right)^2 E_{n-1} \end{aligned}$$

Hence the telescoping series

$$E_n = \frac{(n+1)^2}{n^2} \cdot \frac{n^2}{(n-1)^2} \cdot \cdots \cdot \frac{2^2}{1^2}E_0 = (n+1)^2E_0$$

5.2 Finite square well

Define

$$V(x) = \begin{cases} -V_0 & \text{if } -a \leq x \leq a \\ 0 & \text{if } |x| > a \end{cases}$$

Bound states

$E < V(\pm\infty) = 0$. For $x > a$, this is just the free particle, which gives

$$\psi(x) = Be^{kx}$$

for $k = \frac{\sqrt{-2mE}}{\hbar}$.

For $|x| \leq a$, we have $k' = \frac{\sqrt{2m(E+V_0)}}{\hbar}$. Note this construction ensures $k, k' \in \mathbb{R}$. Schrodinger becomes

$$\frac{\partial^2 \psi}{\partial x^2} = -k'^2 \psi$$

Like the finite case we can WLOG to get

$$\psi(x) = D\cos(k'x) + C\sin(k'x)$$

Since V_0 is even, we can take ψ to be either even or odd. Note that for any ψ we can simply do $\psi \to \frac{\psi(x)+\psi(-x)}{2}$ to make it even and $\psi \to \frac{\psi(x)-\psi(-x)}{2}$ to make it odd. Hence we can break up all our ψ_n's into even and odd cases. More specfically, our 2 cases are:

$$\psi(x) = \begin{cases} Fe^{-kx} & x > a \\ D\cos(k'x) & 0 \leq x \leq a \\ \psi(x) & x < 0 \end{cases} \qquad \psi(x) = \begin{cases} Fe^{-kx} & x > a \\ C\sin(k'x) & 0 \leq x \leq a \\ -\psi(x) & x < 0 \end{cases} \tag{5.2.1}$$

For both cases we have 4 boundary conditions. But since parity takes care of 2, we have 2 on the positive number line. For the **even**, they are

$$Fe^{-ka} = D\cos(k'a) \qquad -kF^{-ka} = -k'D\sin(k'a)$$

Divide the second one by the first one we get

$$k = k'\tan(k'a)$$

We now derive a transcendental equation to solve for energy Define $z = k'a$, $z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$. These imply $k^2 + k'^2 = \frac{2mV_0}{\hbar}$, $ka = \sqrt{z_0^2 - z^2}$, and

$$\tan(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

For a very deep well (z_0 large), the intersections occur at $z_n = \frac{n\pi}{2}$, which corresponds to $E_n + V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$, which is the energy for the infinite case.

Note there is always one bound even state.

For the **odd** case we have

$$Fe^{-ka} = C\sin(k'a) \qquad -kFe^{-ka} = k'\cos(k'a)$$

Divide it out, we get

$$-k = k'\cot(k'a)$$

Using the same definitions as above, we find

$$\cot(z) = -\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

The intersections for a deep well is $z_n = n\pi$, which corresponds to $E_n + V_0 \approx \frac{n^2\pi^2\hbar^2}{2ma^2}$.

Note that there isn't an odd bound state when $z_0 < \frac{\pi}{2} \Leftrightarrow a < \frac{\hbar\pi}{2\sqrt{2mV_0}}$.

Scattering states

Since $E > 0$, k is real. $E + V_{min} > 0$ still holds. Hence we get

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ C\sin(k'x) + D\cos(k'x) & -a \leq x \leq a \\ Fe^{ikx} + Ge^{-ikx} & x > a \end{cases} \tag{5.2.2}$$

If we're scattering from the left, $G = 0$. We also have 4 boundary conditions. All of these give

$$F = \frac{e^{2ika}A}{\cos(2k'a) - i\frac{(k^2+l^2)}{2kl}\sin(2k'a)}$$

From this we get

$$T = \frac{j_F}{j_A} = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)}\sin^2(\frac{2a}{\hbar}\sqrt{2m(E+V_0)})} \tag{5.2.3}$$

When $T = 1$, we get

$$\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi \Leftrightarrow E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

the case of the infinite square well.

Barrier

If we switch $-V_0 \to V_0$, $E + V_{min} > 0$ still holds, so we can essentially only change expression in T. Note this splits into 2 cases. For $E > V_0$:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)}\sin^2(\frac{2a}{\hbar}\sqrt{2m(E-V_0)})} \tag{5.2.4}$$

For $E < V_0$ and using $\sin(ix) = i\sinh(x)$ we get:

$$\begin{aligned} T &= \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)}\sin^2(i\frac{2a}{\hbar}\sqrt{2m(V_0-E)})} \\ &= \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)}\sinh^2(\frac{2a}{\hbar}\sqrt{2m(V_0-E)})} \end{aligned} \tag{5.2.5}$$

6 Delta potentials

Define

$$V(x) = \alpha\delta(x-a)$$

If we plug this into the Schrodinger equation and integrate both sides while taking the limit of the integrand to a i.e. $\lim_{\epsilon\to 0}\int_{a-\epsilon}^{a+\epsilon}$, we find that for an energy eigenstate ϕ_E

$$\lim_{x\to a^+}\frac{d\phi_E}{dx} - \lim_{x\to a^-}\frac{d\phi_E}{dx} = \frac{2m\alpha}{\hbar^2}\phi_E(a) \tag{6.0.1}$$

bound states

For $x < a$, we have $\psi(x) = Be^{kx}$, where $k = \frac{\sqrt{-2mE}}{\hbar} \in \mathbb{R}$. Note $A = 0$ due to normalization constraints. Similarly for $x > a$, we have $\psi(x) = Fe^{-kx}$. Due to continuity at a: $Be^{ka} = Fe^{-ka} \Rightarrow F = Be^{2ka}$. Using equation (16), we get

$$\begin{aligned}
-kFe^{-ka} - kBe^{ka} &= \frac{2m\alpha}{\hbar^2}Be^{ka} \\
-2kBe^{ka} &= \frac{2m\alpha}{\hbar^2}Be^{ka} \\
k &= -\frac{m\alpha}{\hbar^2} \\
E &= -\frac{\hbar^2k^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}
\end{aligned} \tag{6.0.2}$$

To normalize ψ:

$$\begin{aligned}
\int_{-\infty}^{a} B^2e^{2kx}dx + \int_{a}^{\infty} B^2e^{4ka}e^{-2kx}dx &= 1 \\
\frac{B^2}{2k}e^{2ka} - \frac{B^2e^{4ka}}{-2k}e^{-2ka} &= 1 \\
\frac{1}{k}B^2e^{2ka} &= 1 \\
B = \sqrt{ke^{-2ka}} &= \sqrt{k}e^{-ka}
\end{aligned}$$

To summarize

$$\psi(x) = \begin{cases} \sqrt{k}e^{k(x-a)} & x < a \\ \sqrt{k}e^{k(a-x)} & x \geq a \end{cases} \tag{6.0.3}$$

Scattering state

To simplify things we'll take $V(x) = -\alpha\delta(x)$. Similar to the finite well, we have for $k = \frac{\sqrt{2mE}}{\hbar} \in \mathbb{R}$

$$\psi(x)\begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Fe^{ikx} & x > 0 \end{cases}$$

The 2 continuity conditions imply

$$\begin{aligned}
&A + B = F \\
&F = A(1+2i\beta) - B(1-2i\beta)
\end{aligned}$$

for $\beta = \frac{m\alpha}{\hbar^2 k}$. A bit of algebra shows

$$\frac{B}{A} = \frac{i\beta}{1-i\beta} \qquad\qquad \frac{F}{A} = \frac{1}{1-i\beta}$$

The scattering matrix can be written as

$$S = \begin{pmatrix} \frac{i\beta}{1-i\beta} & \frac{1}{1-i\beta} \\ \frac{1}{1-i\beta} & \frac{i\beta}{1-i\beta} \end{pmatrix}$$

The matrix is symmetric for reasons outlined in the next section. We can calculate transmission and reflection rates easily:

$$R = \frac{|j_B|}{|j_A|} = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2} = \frac{1}{1+\frac{2\hbar^2 E}{m\alpha^2}}$$
$$T = \frac{|j_F|}{|j_A|} = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2} = \frac{1}{1+\frac{m\alpha^2}{2\hbar^2 E}}$$

Notice there is one pole for the S-matrix at $\beta = -i$ or $E = -\frac{m\alpha^2}{2\hbar^2}$, which is the exact energy of the bound state. This always happens, as will be explained below.

7 Scattering

A plane wave is scattered from the left: $\psi(x) = Ae^{ikx} + Be^{-ikx}$, and plane waves are scattered from the right: $\psi(x) = Ce^{ikx} + De^{-ikx}$. All these waves corresponds to the same energy, and hence the same wave number. Define the S-matrix:

$$S(E) = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix}$$

where

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}$$

Under this definition, we see that from the **left** when $D = 0$:

$$B = rA \Rightarrow R = \frac{|B|^2}{|A|^2} = |r|^2 \tag{7.0.1}$$

$$C = tA \Rightarrow T = \frac{|C|^2}{|A|^2} = |t|^2 \tag{7.0.2}$$

When scattering from the **right** ($A = 0$):

$$B = \tilde{t}D \Rightarrow T = \frac{|B|^2}{|D|^2} = |\tilde{t}|^2 \tag{7.0.3}$$

$$C = \tilde{r}D \Rightarrow R = \frac{|C|^2}{|D|^2} = |\tilde{r}|^2 \tag{7.0.4}$$

If we write $t = |t|e^{i\phi}$, then for scattering from the left we see that the plane wave going out (Ce^{ikx}) shifts its phase by ϕ.

Since S is unitary, one automatically has

$$|r|^2 + |t|^2 = 1, \quad |\tilde{t}|^2 + |\tilde{r}|^2 = 1, \quad r^*\tilde{t} + t^*\tilde{r} = 0.$$

Claim. 13

If $V(x)$ is even, S is a symmetric matrix.

Proof. If V is symmetric scattering from the left and right doesn't matter. This allows us to do $A \leftrightarrow D$ and $B \leftrightarrow C$. Since the system is invariant under parity, we have $S \to S$. Hence,

$$\begin{pmatrix} C \\ B \end{pmatrix} = S \begin{pmatrix} D \\ A \end{pmatrix}$$

Bashing this out and comparing with the original definition gives $r = \tilde{r}$ and $t = \tilde{t}$. Another property of symmetric potentials is if $r = |r|e^{i\theta}$:

$$tr^* + rt^* = 0 \Rightarrow |t|e^{-i\phi}|r|e^{-i\theta} + |t|e^{i\phi}|r|e^{i\theta} = 0 \Rightarrow e^{2i\theta} = -e^{-2i\phi} \Rightarrow e^{i\theta} = \pm ie^{-i\phi}$$

Hence we have

$$r = \pm i|r|e^{-i\varphi}$$

■

Claim. 14 (S is unitary)
S satisfies $S^\dagger S = 1$.

Proof. First let's calculate the probability current from the left and right.

$$j_{left} = \frac{\hbar}{2mi}\left(\overline{\psi}\frac{\partial\psi}{\partial x} - \psi\overline{\frac{\partial\psi}{\partial x}}\right) = \frac{\hbar k}{m}(|A|^2 - |B|^2) \tag{7.0.5}$$

$$j_{right} = \frac{\hbar k}{m}(|C|^2 - |D|^2) \tag{7.0.6}$$

Since we're in a stationary state,

$$0 = \frac{d}{dt}|\rho(x,t)|^2 = -\frac{\partial j}{\partial x}$$

This implies j is constant with respect to position, so $j_{left} = j_{right}$, meaning $|A|^2+|C|^2 = |B|^2+|D|^2$. Hence, S preserves norms, so is unitary. ∎

Claim. 15
Bound state energies correspond with poles of the S-matrix.

Proof. If $E < 0$, then $k = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2m(-E)}}{\hbar} = i\frac{\sqrt{2mE}}{\hbar}$. Hence, our plane waves become exponentials: $Ae^{-kx} + Be^{kx}$ and $Ce^{-kx} + De^{kx}$. But to be normalizable, $A = D = 0$. This gives

$$\begin{pmatrix} B \\ C \end{pmatrix} = S_b(E)\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

This forces S_b to diverge at the bound state energies E.

$$S_b(E) \sim \sum_n \frac{s_n}{E - E_n}$$

∎

Transmission and Reflection Coefficients for General systems

Scattering that goes from free particle $\rightarrow$ potential $V(x)$ $\rightarrow$ free particle has a simple formula

$$T = \frac{|C|^2}{|A|^2} = |t|^2 \qquad\qquad R = \frac{|B|^2}{|A|^2} = |r|^2$$

as given above. But the unphysical cases where the potential is nonzero at infinity (like an infinite step) the transmitted wave may have a different wavenumber than the incident wave. In this general case we use

$$T = \frac{|j_C|}{|j_A|} \qquad\qquad R = \frac{|j_B|}{|j_A|}$$

Problem. 3
Derive scattering off a potential step

$$V(x) = \begin{cases} 0 & x \leq 0 \\ V_0 & x > 0 \end{cases}$$

for both scattering states $E < V_0$ and $E > V_0$. What about scattering down hill?

Solution. Begin with $E > V_0$. Then we have

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x < 0 \\ Ce^{ik_2x} & x > 0 \end{cases}$$

with $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$. Boundary conditions give:

$$\begin{aligned} A + B &= C \\ ik_1(A - B) &= ik_2C \end{aligned}$$

Solving gives

$$\begin{aligned} B &= \frac{k_1 - k_2}{k_1 + k_2}A \Rightarrow r = \frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \\ C &= \frac{2k_1}{k_1 + k_2}A \Rightarrow t = \frac{C}{A} = \frac{2k_1}{k_1 + k_2} \end{aligned}$$

Caculating probability densities:

$$\begin{aligned} R &= \frac{|j_B|}{|j_A|} = \frac{|B|^2\frac{k_1}{m}}{|A|^2\frac{k_1}{m}} = \frac{|B|^2}{|A|^2} = |r|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2, \\ T &= \frac{|j_C|}{|j_A|} = \frac{|C|^2\frac{k_2}{m}}{|A|^2\frac{k_1}{m}} = \frac{|B|^2k_2}{|A|^2k_1} = |t|^2\frac{k_2}{k_1} = \frac{4k_1k_2}{(k_1 + k_2)^2} \end{aligned}$$

When $E < V_0$, k_2 becomes imaginary. Our wavefunction becomes

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x < 0 \\ Ce^{-k_2x} & x > 0 \end{cases}$$

Doing the same calculation again, we find

$$\begin{aligned} A + B &= C \\ ik_1(A - B) &= k_2C \end{aligned}$$

The calculation of R still follows from (2.1), but we need to resort the actual definition of the transmission probability for T since j_C no longer corresponds to a plane wave.

$$j_C = |C|^2\frac{i}{2m}\left[e^{-|k_2|x}\frac{\partial\left(e^{-|k_2|x}\right)}{\partial x} - e^{-|k_2|x}\frac{\partial\left(e^{-|k_2|x}\right)}{\partial x}\right] = 0$$

Scattering downhill is essentially changing $k_1 \mapsto k_2$ and $k_2 \mapsto k_1$. When $E > V_0$ this yields the same R, T. But if $E < V_0$, realize that we have

$$\psi(x) = \begin{cases} Ae^{-k_2x} + Be^{k_2x} & x < 0 \\ Ce^{ik_1x} & x > 0 \end{cases}$$

This forces $A = 0$ due to normalization. Hence it's kind of a trivial case. ∎

8 Uncertainty principle

For any observable A, we can calculate the standard deviation:

$$\sigma_A^2 = \langle (\hat{A} - \langle A \rangle)\psi \mid (\hat{A} - \langle A \rangle)\psi \rangle$$

Let $f = (\hat{A} - \langle A \rangle)\psi$, and we get

$$\sigma_A^2 = \langle f \mid f \rangle$$

Similarly for an observable B we can define $g = (\hat{B} - \langle B \rangle)\psi$ so that

$$\sigma_A^2 \sigma_B^2 = \langle f \mid f \rangle \langle g \mid g \rangle \geq |\langle f \mid g \rangle|^2$$

By Cauchy-Schwartz. Also, for any complex number $z \in \mathbb{C}$, we have $z \geq (\operatorname{Im} z)^2 = (\frac{1}{2i}(z - \overline{z}))^2$. By the Hermiticity of A,

$$\begin{aligned}
\langle f \mid g \rangle &= \langle \psi \mid (\hat{A} - \langle A \rangle)(\hat{B} - \langle B \rangle)\psi \rangle \\
&\ldots \\
&= \left\langle \hat{A}\hat{B} \right\rangle - \langle A \rangle \langle B \rangle \\
\langle g \mid f \rangle = \cdots &= \left\langle \hat{B}\hat{A} \right\rangle - \langle A \rangle \langle B \rangle
\end{aligned}$$

Hence, $\langle f \mid g \rangle - \langle g \mid f \rangle = \left\langle [\hat{A}, \hat{B}] \right\rangle$, so

$$\sigma_A \sigma_B \geq \frac{1}{2i} \left\langle [\hat{A}, \hat{B}] \right\rangle \tag{8.0.1}$$

We recover the Heisenberg uncertainty principle if we set $\hat{A} = \hat{x}$ and $\hat{B} = -i\hbar \frac{d}{dx}$ we get $\langle [\hat{x}, \hat{p}] \rangle = i\hbar$ and

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \tag{8.0.2}$$

Similarly, energy-time uncertainty principle states:

$$\sigma_E \sigma_t \geq \frac{\hbar}{2}$$

The physical interpretation of the uncertainty principle states that if $[\hat{A}, \hat{B}] \neq 0$, they are **incompatible**. Hence their uncertainty is nonzero, meaning that you can't measure them simultaneously. For example, if you collapse the wavefunction to a position eigenstate (to a delta function, which is the eigenstate of the position operator), then the momentum function becomes more scattered (think about the fourier transform of a delta function). Conversely, if $[\hat{A}, \hat{B}] = 0$, then both observables can be measured at the same time, both being determined.

Minimum uncertainty wave packet

When does the above calculation become an equality? First, Cauchy-Schwartz requires $g(x) = cf(x)$ for $c \in \mathbb{C}$. Also we need $\operatorname{Re}\langle f \mid g \rangle = \operatorname{Re} c\langle f \mid f \rangle = 0 \Rightarrow c = ia$ for $a \in \mathbb{R}$.

Going back to the Heisenberg principle, we see that

$$iaf(x) = g(x) \Rightarrow ia(-i\hbar \frac{d}{dx} - \langle p \rangle)\psi = ia(x - \langle x \rangle)\psi$$

We get

$$\psi(x) = Ae^{-\frac{a(x - \langle x \rangle)^2}{2\hbar}} e^{\frac{i\langle p \rangle x}{\hbar}} \tag{8.0.3}$$

which is a Gaussian multiplied by a phase. Note that in the above calculations we treated $\langle x \rangle, \langle p \rangle$ as constants.

Ehrenfest Theorem

For any observable Q, we have

$$\frac{d}{dt}\langle Q\rangle = \frac{d}{dt}\langle\psi\,|\,\hat{Q}\psi\rangle = \langle\frac{\partial\psi}{\partial t}\,|\,\hat{Q}\psi\rangle + \langle\psi\,|\,\frac{\partial\hat{Q}}{\partial t}\psi\rangle + \langle\psi\,|\,\hat{Q}\frac{\partial\psi}{\partial t}\rangle$$

By Schrodinger's equation, $i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$, so

$$\frac{d}{dt}\langle Q\rangle = -\frac{1}{i\hbar}\langle\hat{H}\psi\,|\,\hat{Q}\psi\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle + \frac{1}{i\hbar}\langle\psi\,|\,\hat{Q}\hat{H}\psi\rangle$$

We get

$$\frac{d\langle Q\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle \tag{8.0.4}$$

The latter term is often zero. An immediate consequence is if H commutes with Q, then Q is a conserved quantity.

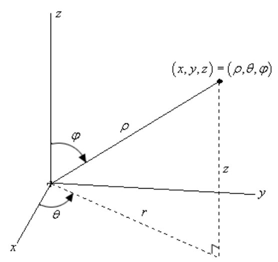

Figure 1: Spherical Coordinates

9 3 Dimensional Schrondinger's equation

Analogous to the 1D case, we have $p \to -i\hbar\nabla$, and

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla\psi + V\psi \tag{9.0.1}$$

We have the **Canonical commutator relations**

$$[r_i, p_j] = -[p_i, r_j] = i\hbar\delta_{ij} \qquad\qquad [r_i, r_j] = [p_i, p_j] = 0$$

In spherical coordinates, the Laplacian becomes

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)$$

Now we perform a separation of variables to berak the Schrodinger equation into the **radial** and **angular** part:

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

This gives

$$\underbrace{\left(\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r)-E)\right)}_{\text{Radial}} + \underbrace{\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right)}_{\text{Angular}} = 0$$

We introduce a constant $l(l+1) =$ Radial, so $-l(l+1) =$ Angular. Only the Radial part includes energy.

Angular Part

For each l, we have $2l+1$ possible constant m's:

$$m = -l, -l+1, \ldots, 0, \ldots, l-1, l$$

The solutions are called **spherical harmonics**, and are given by

$$Y_l^m(\theta,\phi) = Ae^{im\phi}P_l^m(\cos\theta)$$

where P_l^m is the associated Legendre polynomial

$$P_l^m(x) = (-1)^m(1-x^2)^{\frac{m}{2}}\left(\frac{d}{dx}\right)^m P_l(x) \tag{9.0.2}$$

$$P_l^{-m}(x) = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(x) \tag{9.0.3}$$

$$P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l(x^2-1)^l \tag{9.0.4}$$

To perform normalization, we do the following procedure:

$$\int |\psi|^2 d^3r = \int |\psi|^2 r^2 \sin\theta \, dr \, d\theta \, d\phi = \int |R|^2 r^2 dr \int |Y|^2 d\Omega = 1$$

where $d\Omega = sin\theta \, d\theta \, d\phi$. An easy way to do this is to normalize each factor. One could also do it any other way:

$$\int_0^\infty |R|^2 r^2 \, dr = 1 \qquad\qquad \int_0^{2\pi} \int_0^\pi |Y|^2 \sin\theta \, d\theta \, d\phi = 1 \tag{9.0.5}$$

Setting $R(r) = u(r)/r$, the normalization conditions becomes

$$z \int_0^\infty |u|^2 dr = 1 \tag{9.0.6}$$

The normalized spherical harmonics are given by

$$Y_l^m(\theta, \phi) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} e^{im\phi} P_l^m(\cos\theta) \tag{9.0.7}$$

They are Dirac-orthogonal:

$$\iint Y_l^m Y_{l'}^{m'} = \delta_{ll'} \delta_{mm'}$$

Radial Part

Let $u(r) = rR(r)$, we arrive at

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \underbrace{\left(V + \overbrace{\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}}^{\text{centrifugal term}} \right)}_{V_{eff}} u = Eu$$

3D Infinite Square Well

This is a case of **central potential**, where

$$V(r) = \begin{cases} 0 & r \leq a \\ \infty & r > a \end{cases}$$

To solve problems of this kind, note that the spherical harmonics are pre-defined. We just need to solve the Radial part.

$$\frac{d^2u}{dr^2} = \left(\frac{l(l+1)}{r^2} - k^2 \right) u \qquad\qquad k = \frac{\sqrt{2mE}}{\hbar}$$

When $l = 0$ we have

$$\frac{du^2}{d^2r} = -k^2 u \Rightarrow u(r) = A\sin(kr) + B\cos(kr)$$

Using $R(r) = u(r)/r$, we see that $\cos(kr)/r$ blows up as $r \to 0$, so $B = 0$. The boundary conditions require $\sin(ka) = 0 \Rightarrow ka = N\pi$, so we have the energy for $l = 0$

$$E_{N_0} = \frac{N^2\pi^2\hbar^2}{2ma^2} \, , N = 1, 2, 3, \ldots$$

We have for $l = 0$:

$$R(r) = \sqrt{\frac{2}{a}}\frac{1}{r}\sin\left(\frac{N\pi r}{a}\right)$$

and so

$$\psi_{n00} = \sqrt{\frac{1}{2\pi a}}\frac{1}{r}\sin\left(\frac{N\pi r}{a}\right)$$

For general l, we have

$$u(r) = Arj_l(kr) + Brn_l(kr)$$

where j_l is the spherical Bessel function of order l and n_l is the spherical Newman function of order l.

$$j_l(x) = (-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\frac{\sin x}{x}$$
$$n_l(x) = -(-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\frac{\cos x}{x}$$

Similar to $l = 0$, we get $B = 0$, and the corresponding energies are

$$E_{N_l} = \frac{\hbar^2}{2ma^2}\beta_{Nl}^2 \tag{9.0.8}$$

where β_{Nl} is the N-th zero for the lth spherical Bessel function. We now sort the energies and label them by the principle quantum number n. The general solution is written in terms of this index,

$$\psi_{nlm} = A_{nl}j_l(\beta_{Nl}\frac{r}{a})Y_l^m(\theta,\phi) \tag{9.0.9}$$

where A_{nl} is the normalization coefficient. Note that each energy E_n depends on N, l. There are $2l + 1$ possible m's for the spherical harmonic, so energy degeneracy is $2l + 1$. But there are also *extra* degeneracy, not attributed to spherical symmetry alone.

10 The Hydrogen Atom

We solve the radical part for the coulomb potential $V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$. Hence we have

$$-\frac{\hbar^2}{2m_e}\frac{d^2u}{dr^2} + (-\frac{q^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m_e}\frac{l(l+1)}{r^2})u = Eu$$

Define $k = \frac{\sqrt{-2m_eE}}{\hbar}$. We get

$$\frac{1}{k^2}\frac{d^2u}{dr^2} = \left(1 - \frac{m_e e^2}{2\pi\epsilon_0\hbar^2 k}\frac{1}{kr} + \frac{l(l+1)}{(kr)^2}\right)u$$

The energies are given by the **Bohr formula**

$$E_n = -\left[\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2} \tag{10.0.1}$$

Note that the energy *does not* depend on l, meaning that for each n the energies are the same across l. For each n, there are n possible values for l:

$$l = 0, 1, 2, \ldots, n-1$$

and each l has $2l-1$ possible values for m, so each E_n is degenerate with

$$d(n) = \sum_{l=0}^{n-1}(2l+1) = n^2 \tag{10.0.2}$$

Skipping solving steps...
The **Bohr radius** is defined to be

$$a = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = 0.528 \cdot 10^{-10}m \tag{10.0.3}$$

Let

$$\rho = \frac{r}{an} = kr$$

We have

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi),\ R_{nl}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}v(\rho)$$

where $v(\rho)$ is a polynomial of $n-l+1$ in ρ, with coefficients satisfing the recursion formula

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}c_j$$

The ground state energy is

$$E_1 = -13.6eV \tag{10.0.4}$$

corresponding to the ground state

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a} \tag{10.0.5}$$

The general formula is given by Laguerre's polynomials

$$L_p^q(x) = \frac{x^{-p}e^x}{q!}\left(\frac{d}{dx}\right)^q(e^{-x}x^{p+q})$$

with $v(\rho) = L_{n-l-1}^{2l+1}(2\rho)$.

$$\boxed{\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} e^{-r/na} \left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1}(2r/na) Y_l^m(\theta,\phi)} \tag{10.0.6}$$

They are mutually orthogonal: $\langle \psi_{nlm} | \psi_{n'l'm'} \rangle = \delta_{nn'}\delta_{ll'}\delta_{mm'}$.
We can excite a hydrogen state by giving it photons. Such state transitions are called quantum jumps and the difference is given by

$$E_\gamma = E_i - E_f = -13.6eV(\frac{1}{n_i^2} - \frac{1}{n_f^2})$$

Using Planck's formula $E_\gamma = h\nu = \frac{hc}{\lambda}$ we get **Rydberg formula**

$$\frac{1}{\lambda} = \mathcal{R}(\frac{1}{n_f^2} - \frac{1}{n_i^2})$$

with

$$\mathcal{R} = \frac{m_e}{4\pi c\hbar^3}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = 1.907 \cdot 10^7 m^{-1}$$

called **Rydberg constant**. When we hit hydrogen atoms of different states with some ultraviolet light, they collapse to the ground state and these transitions are know as the **Lyman series**. The **Balmer series** and **Paschen series** are to first and second excited state.

11 Angular Momentum

Make the substitution in the formula $L = \mathbf{r} \times \mathbf{p}$ with $p_x \to -i\hbar\partial/\partial x$, etc. to get

$$L_x = yp_z - zp_y = i\hbar(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}) \tag{11.0.1}$$

$$L_y = zp_x - xp_z = i\hbar(x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}) \tag{11.0.2}$$

$$L_z = xp_y - yp_x = i\hbar(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}) \tag{11.0.3}$$

We find the canonical commutator relations

$$[L_x, L_y] = i\hbar L_z,\ [L_y, L_z] = i\hbar L_x,\ [L_z, L_x] = i\hbar L_y \tag{11.0.4}$$

Using Ehrenfest's theorem we see

$$\Delta L_x \Delta L_y \geq \frac{1}{2i}\langle i\hbar L_z\rangle = \frac{\hbar}{2}|\langle L_z\rangle| \tag{11.0.5}$$

We also find

$$[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = 0$$

Define

$$L_\pm = L_x \pm iL_y \tag{11.0.6}$$

Similar to the QHO case, we have

$$L_\pm L_\mp = (L_x \pm iL_y)(L_x \mp iL_y) = L_x^2 + L_y^2 \mp (L_xL_y - L_yL_x) = L^2 - L_z^2 \mp i(i\hbar L_z)$$

$$L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z \tag{11.0.7}$$

We also have

$$[L_z, L_\pm] = [L_z, L_x] \pm i[L_z, L_y] = -i\hbar L_y \pm i(-i\hbar L_x) = \pm\hbar(L_x \pm iL_y)$$

so

$$[L_z, L_\pm] = \pm\hbar L_\pm \tag{11.0.8}$$

along with $[L^2, L_z] = 0$ we can apply Claim 6. (Ladder operation) to get that if f is an eigenfunction of L_z with eigenvalue μ then $L_\pm f$ is an eigenfunction of L_z with new eigenvalue $\mu \pm \hbar$. Hence, each ladder operator boosts the eigenvalue by $\hbar$. Since L^2 and L_z are simultaneously diagonalizable, we can set $L^2 f = \lambda f$.

Call the top runf of the ladder f_t with eigenvalue $\hbar l$ such that $L_+ f_t = 0$. Then

$$\begin{aligned} L^2 f_t &= (L_-L_+ + L_z^2 + \hbar L_z)f_t = (\hbar^2 l^2 + \hbar^2 l)f_t = \hbar^2 l(l+1)f_t \\ &\Rightarrow \lambda = \hbar^2 l(l+1) \end{aligned}$$

Similarly for the bottom rung f_b with eigenvalue $\hbar\bar{l}$ such that $L_- f_b = 0$. Then

$$\begin{aligned} L^2 f_b &= (L_+L_- + L_z^2 + \hbar L_z)f_b = (\hbar^2\bar{l}^2 + \hbar^2\bar{l})f_t = \hbar^2\bar{l}(\bar{l}+1)f_t \\ &\Rightarrow \lambda = \hbar^2\bar{l}(\bar{l}+1) = \hbar^2 l(l+1) \Rightarrow l = -\bar{l} \end{aligned}$$

This means l **is a half integer**. The possible eigenvalues for L_z take the form f^m, where $L_z f^m = \hbar m$ (the rungs on the ladder), with $m = -l, -l+1, \ldots, l$. Hence we have completely categorized our eigenfunctions

$$\boxed{L^2 f_l^m = \hbar^2 l(l+1) f_l^m;\ L_z f_l^m = \hbar m f_l^m} \tag{11.0.9}$$

It turns out that these eigenfunctions f_m^l matches precisely the spherical harmonics, that is they are the simultaneous eigenfunctions of H, L^2, L_z.

$$\boxed{Hf_m^l = Ef_m^l,\ L^2 f_l^m = \hbar^2 l(l+1) f_l^m,\ L_z f_l^m = \hbar m f_l^m} \tag{11.0.10}$$

Interesting that the approach with angular momentum yielded half-integer values, but the approach with spherical harmonics yielded only integer values.

12 Spin

Spin is considered intrinsic angular momentum, in contrast to the orbital angular momentum. We have the same set of canonical commutator relations

$$[S_x, S_y] = i\hbar S_z,\ [S_y, S_z] = i\hbar S_y,\ [S_z, S_x] = i\hbar S_y \tag{12.0.1}$$

More succinctly,

$$\boxed{[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k} \tag{12.0.2}$$

We denoted our eigenfunctions for orbital angular momentum f_l^m, here we denote it $|sm\rangle$ where s is the total spin, and m the spin in the z direction. Similarly,

$$S^2 |sm\rangle = \hbar^2 s(s+1) |sm\rangle\ ,\ S_z |sm\rangle = \hbar m |sm\rangle \tag{12.0.3}$$

$$S_\pm |sm\rangle = \hbar\sqrt{s(s+1) - m(m \pm 1)}\, |s(m \pm 1)\rangle \tag{12.0.4}$$

where

$$s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$$

and

$$m = -s, -s+1, \dots, s\ \ (2s+1 \text{ values})$$

12.1 Spin 1/2, two particles

The eigenstates $\left|\frac{1}{2}, \frac{1}{2}\right\rangle, \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ forms an eigenbasis for the two particle state. Call these two states χ_+, χ_- respectively. A general state is then

$$\chi = a\chi_+ + b\chi_- = \begin{pmatrix} a \\ b \end{pmatrix}$$

$|a|^2, |b|^2$ denote the probability for χ_+, χ_-. Plugging into the formula (12.0.2) we see that

$$S^2\chi_+ = \frac{3}{4}\hbar^2\chi_+,\ S^2\chi_- = \frac{3}{4}\hbar^2\chi_- \tag{12.1.1}$$

We summarize the matrix representations:

$$\sigma_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12.1.2}$$

$$S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\ S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},\ S^2 = \frac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{12.1.3}$$

$$S_x = \frac{1}{2}(S_+ + S_-), S_y = \frac{1}{2i}(S_+ - S_-) \tag{12.1.4}$$

12.1.1 Derivation

Starting from the z-basis, we know that σ_z makes sense. Define

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Take the analogue of equation (11.0.6), we see

$$\sigma_x = \sigma_+ + \sigma_- \qquad \sigma_y = -i(\sigma_+ - \sigma_-)$$

which gives us our desired result.

12.2 Example: x-axis

We find the eigenvectors of S_x to be

$$\frac{\hbar}{2}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}, \frac{\hbar}{2}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix}$$

So

$$x = \frac{a+b}{\sqrt{2}}\chi_+^{(x)} + \frac{a-b}{\sqrt{2}}\chi_-^{(x)}$$

For example $\chi_+^{(z)} = \frac{1}{\sqrt{2}}\chi_+^{(x)} + \frac{1}{\sqrt{2}}\chi_-^{(x)}$. The expectation values can be taken as $\langle\chi|s_x|\chi\rangle$.

12.3 Electrons in a magnetic field

A particle with

$$\vec{\mu} = \gamma\vec{S}$$

γ is called the **gyromagnetic ratio**, given by

$$\gamma = g_e\frac{\mu_B}{\hbar} = g_e\frac{e}{2m_e}$$

Under a magenetic field, the particle experiences potential energy

$$H = -\mu \cdot B$$

and torque $\mu \times B$. We also define a Hamiltonian matrix

$$\mathcal{H} = -\gamma\mathbf{B}\cdot\mathcal{S}$$

where $\mathcal{S} = (S_x, S_y, S_z)$, and hence $\mathcal{H}$ is a superposition of spin matrices.

12.4 Larmor precession

Let our magnetic field be $\mathbf{B} = B_0\hat{k}$. The Hamiltonian is

$$\mathcal{H} = -\gamma B_0 S_z = -\frac{\gamma B_0\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

The eigenstates are the same as S_z, denoted χ_+, χ_-, with energy $E_- = -(\gamma B_0\hbar)/2$ and $E_+ = +(\gamma B_0\hbar)/2$. We can time evolve these states with the Schrodinger equation

$$i\hbar\frac{\partial\chi}{\partial t} = \mathcal{H}\chi$$

Solving,

$$\chi(t) = a\chi_+e^{iE_+t/\hbar} + b\chi_-e^{-iE_t/\hbar}$$

We write

$$\chi(0) = \begin{pmatrix}a\\ b\end{pmatrix} = \begin{pmatrix}\cos\alpha/2\\ \sin\alpha/2\end{pmatrix}$$

Hence

$$\chi(t) = \begin{pmatrix}\cos(\alpha/2)e^{i\gamma B_0 t/\hbar}\\ \sin(\alpha/2)e^{-i\gamma B_0 t/\hbar}\end{pmatrix} \tag{12.4.1}$$

We now calculate $\langle S_x\rangle, \langle S_y\rangle, \langle S_z\rangle$:

$$\langle S_x\rangle = \frac{\hbar}{2}\sin\alpha\cos(\gamma B_0 t)$$
$$\langle S_y\rangle = -\frac{\hbar}{2}\sin\alpha\sin(\gamma B_0 t)$$
$$\langle S_z\rangle = \frac{\hbar}{2}\cos\alpha$$

with Larmor frequency $\omega = \gamma B_0$.

12.5 Stern Gerlach

The force experienced by the particle is (just by definition of potential energy)

$$\mathbf{F} = \nabla(\vec{\mu} \cdot \mathbf{B}) = \gamma(\partial_x S_x B_x + \partial_y S_y B_y + \partial_z S_z B_z)$$

Take our magnetic field to be inhomogeneous

$$B(x, y, z) = -\alpha x \hat{\imath} + (B_0 + \alpha z)\hat{k}$$

where $B_0 \hat{k}$ is a large value and α are small perturbations. So

$$\mathbf{F} = \gamma\alpha(-S_x \hat{\imath} + S_z \hat{k})$$

S_x experiences Larmor precession due to $B_0 \hat{k}$, so its average value is 0. Hence $F_z = \gamma\alpha S_z$. We have $2s + 1$ streams of particles.

13 2 Particles, General spin

Two particles $|s_1 m_1\rangle$ and $|s_2 m_2\rangle$ satisfies

$$S^{(1)^2}|s_1 s_2 m_1 m_2\rangle = s_1(s_1+1)\hbar^2 |s_1 s_2 m_1 m_2\rangle \tag{13.0.1}$$

$$S^{(2)^2}|s_1 s_2 m_1 m_2\rangle = s_2(s_2+1)\hbar^2 |s_1 s_2 m_1 m_2\rangle \tag{13.0.2}$$

$$S_z^{(1)}|s_1 s_2 m_1 m_2\rangle = m_1\hbar |s_1 s_2 m_1 m_2\rangle \tag{13.0.3}$$

$$S_z^{(2)}|s_1 s_2 m_1 m_2\rangle = m_2\hbar |s_1 s_2 m_1 m_2\rangle \tag{13.0.4}$$

The total angular momentum is

$$\vec{S} = S^{(1)} + S^{(2)}$$

We can get the total z-spin of the system easily: it s just the sum

$$\vec{S}_z = S_z^{(1)} + S_z^{(2)} \to (m_1+m_2)\hbar |s_1 s_2 m_1 m_2\rangle$$

But $\vec{S}^2$ is much harder to calculate.

13.1 Example: Two spin 1/2 particles

Denote $|\uparrow\uparrow\rangle = \left|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\right\rangle$ for $m = 1$. Similarly, $|\downarrow\downarrow\rangle = \left|\frac{1}{2}\frac{1}{2} - \frac{1}{2} - \frac{1}{2}\right\rangle$ for $m = -1$.
We can lower the value of total m by 1:

$$\begin{aligned} S_-|\uparrow\uparrow\rangle = (S_{1-}+S_{2-})|\uparrow\uparrow\rangle &= (S_-^{(1)}|\uparrow\rangle)|\uparrow\rangle + |\uparrow\rangle(S_-^{(2)}|\uparrow\rangle) \\ &= (\hbar|\downarrow\rangle)|\uparrow\rangle + |\uparrow\rangle(\hbar|\downarrow\rangle) \\ &= \hbar(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle) \end{aligned}$$

with $m = 0$. This is confirmed by applying the formula (12.0.4), which states

$$S_-|11\rangle = \hbar\sqrt{2}|10\rangle = \hbar(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle) \Rightarrow |10\rangle = \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)$$

Similarly

$$\begin{aligned} S_-|10\rangle &= \frac{1}{\sqrt{2}}(S_-|\downarrow\uparrow\rangle + S_-|\uparrow\downarrow\rangle) \\ &= \sqrt{2}\hbar|\downarrow\downarrow\rangle \end{aligned}$$

$$S_-|10\rangle = \hbar\sqrt{2}|1-1\rangle = \sqrt{2}\hbar|\downarrow\downarrow\rangle \Rightarrow |1-1\rangle = |\downarrow\downarrow\rangle$$

Hence, a two particle spin 1/2 system, we have more or less conclusively exhausted the 3 possible $s = 1$ states, called the **triplet** combination:

$$|11\rangle = |\uparrow\uparrow\rangle \tag{13.1.1}$$

$$|10\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \tag{13.1.2}$$

$$|1-1\rangle = |\downarrow\downarrow\rangle \tag{13.1.3}$$

There is also a $s = 0$ state:

$$|00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \tag{13.1.4}$$

To confirm tthe s values *is* what we claimed, we just check it by applying $\vec{S}^2$, using the identities:

$$\vec{S}^2 = (\mathbf{S}^{(1)} + \mathbf{S}^{(2)})) \cdot (\mathbf{S}^{(1)} + \mathbf{S}^{(2)})) = (S^{(1)})^2 + (S^{(2)})^2 + 2\mathbf{S}^{(1)}\mathbf{S}^{(2)} \tag{13.1.5}$$

$$\mathbf{S}^{(1)}\mathbf{S}^{(2)} = (S_x^{(1)}S_x^{(2)} + S_y^{(1)}S_y^{(2)} + S_z^{(1)}S_z^{(2)}) \tag{13.1.6}$$

The possible spins for a state $|s_1 s_2 m_1 m_2\rangle$ is

$$s = (s_1 + s_2), (s_1 + s_2 - 1), \ldots, |s_1 - s_2| \tag{13.1.7}$$

One could also talk about **total angular momentum (spin + orbital)**. For hydrogen state ψ_{nlm}, the two particle state can have spins $= -1, 0, 1$ and orbital angular momentum l, so it's total momentum can be $l-1, l, l+1$.

13.2 Clebsch-Gordan Table

In general

$$\boxed{|s\, m\rangle = \sum_{m_1+m_2=m} C^{s_1 s_2 s}_{m_1 m_2 m} |s_1\, s_2\, m_1\, m_2\rangle} \tag{13.2.1}$$

each of these Clebsch-Gordan coefficients represents the probability of finding the total state in each of these individual state (i.e. superposition). We can also define an inverse to this process:

$$\boxed{|s_1\, s_2\, m_1\, m_2\rangle = \sum_s C^{s_1 s_2 s}_{m_1 m_2 m} |s\, m\rangle} \tag{13.2.2}$$

14 Minimal Coupling

The Hamiltonian for E&M can written as

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\varphi \tag{14.0.1}$$

where $\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}$ and $\mathbf{B} = \nabla \times \mathbf{A}$. Using the substitution $p \to i\hbar\nabla$, we get

$$\boxed{\hat{H} = \frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})^2 + q\varphi} \tag{14.0.2}$$

Ehrenfest theorem gives

$$\frac{d\langle r\rangle}{dt} = \frac{1}{m}\langle(\mathbf{p} - q\mathbf{A})\rangle \tag{14.0.3}$$

$$m\frac{d\langle v\rangle}{dt} = q(\mathbf{E} + \langle v\rangle \times \mathbf{B}) \tag{14.0.4}$$

The Gauge transformation

$$\varphi' = \varphi - \frac{\partial \Lambda}{\partial t} \qquad\qquad \mathbf{A}' = \mathbf{A} + \nabla\Lambda \tag{14.0.5}$$

does not change $\mathbf{E}, \mathbf{B}$ because

$$\begin{aligned}
\mathbf{E}' &= -\nabla\varphi' - \frac{\partial \mathbf{A}'}{\partial t} \\
&= -\nabla\varphi + \nabla\frac{\partial \Lambda}{\partial t} - \frac{\partial \mathbf{A}}{\partial t} - \nabla\frac{\partial \Lambda}{\partial t} \\
&= \mathbf{E} \\
\mathbf{B}' &= \nabla \times (\mathbf{A} + \nabla\Lambda) = \mathbf{B}
\end{aligned}$$