A Proof of Uncertainty Principle

A.1 Setting Up The Transform

Any physical state will have a probability distribution $\Phi(p)\&\psi(x)$ in momentum and position spcae, respectively. Consider collection of eigen function $\left\{e^{ip\frac{x}{\hbar}}\right\}$ where p in the vector space $\mathbb{R}$

$$\hat{p}e^{ip\frac{x}{\hbar}} = -i\hbar\tfrac{d}{dx}e^{ip\frac{x}{\hbar}}$$

$$= pe^{ip\frac{x}{\hbar}}$$

Realizing this uncountable collection of function forms a complete basis set. If one is interested in representing the same state in position variable x, we need to sum up all of these function with probability density $\Phi(p)$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int \Phi(p)e^{ip\frac{x}{\hbar}}dp \rightarrow \text{position distribution of the same state}$$

We will explain constant later. At this point, consider how to obtain $\Phi(p)$ from $\psi(x)$. This can be achieved by multiplying $\psi(x)$ by $e^{-ip'\frac{x}{\hbar}}$ for some p' followed by integration w.r.t. x.

$$\int \psi(x)e^{-ip'\frac{x}{\hbar}}dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int\int \Phi(p)e^{ip\frac{x}{\hbar}}e^{-ip'\frac{x}{\hbar}}dpdx$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int \Phi(p)\int e^{i(p-p')\frac{x}{\hbar}}dxdp$$

Using Lemma

$$= \frac{1}{\sqrt{2\pi\hbar}}\int \Phi(p)\delta(p-p')2\pi\hbar dp$$

$$= \frac{1}{\sqrt{2\pi\hbar}}2\pi\hbar\Phi(p')$$

By replace p' with p

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int \psi(x)e^{-ip\frac{x}{\hbar}}dx$$

Note that we choose the constant $(\frac{1}{\sqrt{2\pi\hbar}})$ to be symmetric going from $\Phi(p)$ to $\psi(x)$, & from $\psi(x)$ to $\Phi(p)$.

A.2 Lemma: $2\pi\hbar\ \delta(p-p')=\int\ e^{i(p-p')\frac{x}{\hbar}}dx$

Again we use the same transform definition

$$
\begin{aligned}
&\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int \Phi(p)e^{ip\frac{x}{\hbar}}dp \\
&\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int \psi(x)e^{-ip\frac{x}{\hbar}}dx \\
&\text{denote } \hat{\psi}(x) = \Phi(p) \\
&\text{then} \\
&\hat{f}(p') = \frac{1}{\sqrt{2\pi\hbar}}\int f(x)e^{-ip'\frac{x}{\hbar}}dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int \frac{1}{\sqrt{2\pi\hbar}}\int \hat{f}(p)e^{ip\frac{x}{\hbar}}dpe^{-ip'\frac{x}{\hbar}}dx \\
&= \int \hat{f}(p)\left(\frac{1}{2\pi\hbar}\int e^{i(p-p')\frac{x}{\hbar}}dx\right)dp
\end{aligned}
$$

By the definition of the delta function $f(p') = \int \delta(p-p')f(p)dp$ we obtain the desired result

$$\delta(p-p') = \frac{1}{2\pi\hbar}\int e^{i(p-p')\frac{x}{\hbar}}dx$$

A.3 Plancherel Theorem for Position and Momentum Pair

So far we have defined transform

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int \Phi(p) e^{ip\frac{x}{\hbar}} dp$$
$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x) e^{-ip\frac{x}{\hbar}} dx$$
$$\text{denote } \hat{\psi}(x) = \Phi(p)$$

Let $f(x)$ & $g(x)$ be the probability distribution of x
Let us consider the inner product

$$\int f(x) g^*(x) dx$$

using the transform defined above

$$= \int f(x) \frac{1}{\sqrt{2\pi\hbar}} \int \left(\hat{g}(p) e^{ip\frac{x}{\hbar}}\right)^* dp dx$$
$$= \int f(x) \frac{1}{\sqrt{2\pi\hbar}} \int \hat{g^*}(p) e^{-ip\frac{x}{\hbar}} dp dx$$
$$= \int \hat{g^*}(p) \frac{1}{\sqrt{2\pi\hbar}} \int f(x) e^{-ip\frac{x}{\hbar}} dx dp$$
$$= \int \hat{g^*}(p) \hat{f}(p) dp$$

Setting f = g at the beggining

$$\int |f(x)|^2 dx = \int \left|\hat{f}(p)\right|^2 dp$$

A.4 Uncertainty Principle: Distribution Centered at Zero

Consider the case where both $\Phi(p)$ & $\psi(x)$ are centered at zero.

$$1 = \int |\psi(x)|^2 \, dx$$

Perform integration by parts by setting

$$u = |\psi(x)|^2 = \psi^*(x)\psi(x)$$

$$du = \psi^{*'}(x)\psi(x) + \psi^*(x)\psi^{'}(x) = 2Re(\psi^{*'}(x)\psi(x))$$

$$v = x, dv = dx$$

$$= -2Re \int x\psi^{*'}(x)\psi(x)dx$$

$$\leq 2 \left| \int x\psi^{*'}(x)\psi(x)dx \right|$$

By Cauchy-Schwarz inequality

$$\leq 2 \left(\int |x\psi(x)|^2 \, dx \right)^{\frac{1}{2}} \left(\int |\psi'(x)|^2 \, dx \right)^{\frac{1}{2}}$$

$$= 2 \left(\int x^2 \, |\psi(x)|^2 \, dx \right)^{\frac{1}{2}} \left(\int |\psi'(x)|^2 \, dx \right)^{\frac{1}{2}}$$

$$= 2\sigma_x \left(\int |\psi'(x)|^2 \, dx \right)^{\frac{1}{2}} \rightarrow \text{ eq. A1}$$

Also,

$$\psi'(x) = \frac{d}{dx}\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int \Phi(p) \frac{d}{dx} e^{ip\frac{x}{\hbar}} dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int \left(\frac{ip}{\hbar} \Phi(p) \right) \; e^{ip\frac{x}{\hbar}} dp$$

By applying the Plancherel Theorem $\int |f(t)|^2 \, dt = \int \left| \hat{f}(\omega) \right|^2 d\omega$

$$\left(\int |\psi'(x)|^2 \, dx \right)^{\frac{1}{2}} = \left(\int \left| \left(\frac{ip}{\hbar} \Phi(p) \right) \right|^2 dp \right)^{\frac{1}{2}}$$

$$= \frac{1}{\hbar} \left(\int p^2 \, |(\Phi(p))|^2 \, dp \right)^{\frac{1}{2}}$$

$$= \frac{1}{\hbar}\sigma_p$$

from Eq A1

$$1 \leq 2\sigma_x \left(\int |\psi'(x)|^2 \, dx \right)^{\frac{1}{2}} = \frac{2}{\hbar} \sigma_x \sigma_p$$

Hence

$$\frac{\hbar}{2} \leq \sigma_x \sigma_p$$

A.5 Uncertainty Principle: Distribution Centered at Nonzero

Now consider $\psi(x)$ & $\Phi(p)$ which may have nonzero average value
Let $\Psi(x) = e^{-i\frac{mp}{\hbar}x}\psi(x)$

Because $|\Psi(x)| = |\psi(x)|$

$$1 = \int |\Psi(x)|^2 \, dx$$

Perform integration by parts by setting

$$u = |\Psi(x)|^2 = \Psi^*(x)\Psi(x)$$

$$du = \Psi^{*'}(x)\Psi(x) + \Psi^*(x)\Psi'(x) = 2Re(\Psi^{*'}(x)\Psi(x))$$

$$v = x - \mu_x, dv = dx$$

$$= -2Re \int (x - \mu_x) |\Psi(x)|^2 \, dx$$

$$\leq 2 \left(\int \left| (x - \mu_x)^2 \Psi(x) \right|^2 dx \right)^{\frac{1}{2}} \left(\int |\Psi'(x)|^2 \, dx \right)^{\frac{1}{2}}$$

By same approach: Applying the Plancherel Theorem on last parentheses

$$\leq 2\sigma_x \left(\int \left| \frac{i(p - \mu_p)}{\hbar} \hat{\Psi}'(x) \right|^2 dx \right)^{\frac{1}{2}}$$

$$= \frac{2\sigma_x \sigma_p}{\hbar}$$

Therefore $\frac{\hbar}{2} \leq \sigma_x \sigma_p$ as desired

A.6 Uncertainty Principle Proof using Commutator

By the definition of Variance,

$$\sigma_A^2 = \int \Psi^*(x) \left(\hat{A} - \langle A \rangle\right)^2 \Psi(x) dx$$

HW: It is good exercise to get to the next line

$$= \int \Psi^*(x) \hat{A}^2 \Psi(x) dx - \langle A \rangle^2$$

Similarly, you can get $\sigma_B^2 = \int \Psi^*(x) \hat{B}^2 \Psi(x) dx - \langle B \rangle^2$

Let $f(x) = \left(\left(\hat{A} - \langle A \rangle\right) \Psi(x)\right)$ and $g(x) = \left(\left(\hat{B} - \langle B \rangle\right) \Psi(x)\right)$

$$\sigma_A^2 = \int \left(\left(\hat{A} - \langle A \rangle\right) \Psi(x)\right) \left(\left(\hat{A} - \langle A \rangle\right) \Psi(x)\right)^* dx = \int f(x) f^*(x) dx \text{ in } \mathbb{R}$$

$$\sigma_B^2 = \int \left(\left(\hat{B} - \langle B \rangle\right) \Psi(x)\right) \left(\left(\hat{B} - \langle B \rangle\right) \Psi(x)\right)^* dx = \int g(x) g^*(x) dx \text{ in } \mathbb{R}$$

Let us consider quantity $z = x + yi = \int f(x) g^*(x) dx$ which is not necessary in $\mathbb{R}$ but in $\mathbb{C}$

Then, the complex conjugate of z is $z^* = x - yi = \int g(x) f^*(x) dx$

$$z = \int \left(\left(\hat{A} - \langle A \rangle\right) \Psi(x)\right) \left(\left(\hat{B} - \langle B \rangle\right) \Psi(x)\right)^* dx = \int \Psi^*(x) \hat{A}\hat{B} \Psi(x) dx - \langle A \rangle \langle B \rangle$$

Similarly, $z^* = \int \Psi^*(x) \hat{B}\hat{A} \Psi(x) dx - \langle A \rangle \langle B \rangle$

Since $|z|^2 = x^2 + y^2$where x and y are in $\mathbb{R}$. This means that $z^2 \geq y^2 = \left(\frac{z - z^*}{2i}\right)^2$

Therefore, $|z|^2 =\geq y^2 = \left(\frac{\int \Psi^*(x) \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right) \Psi(x) dx}{2i}\right)^2 = \left(\frac{\int \Psi^*(x) \left[\hat{A}, \hat{B}\right] \Psi(x) dx}{2i}\right)^2$

Using Cauchy-Schwarz inequality, $\int f(x) f^*(x) dx \int g(x) g^*(x) dx \geq \left| \int f(x) g^*(x) dx \right|^2$

$\sigma_A^2 \sigma_B^2 \geq z^2 \geq y^2$

for the case the operator does not commute like $[\hat{p_x}, \hat{x}] = \hat{p_x}\hat{x} - \hat{x}\hat{p_x} = i\hbar$

Above inequality will yeild $\frac{\hbar}{2} \leq \sigma_x \sigma_p$ as desired. //

A.7 Average Volume of a State

Now that we have studied uncertainty principle, we are going to think about the average volume occupied by a single state. The volume of single state (h^3) is used in part II of this textbook and it is fundamental to statistical mechanics. Although average volume is sometimes stated as a direct consequence of uncertinty principle, average volume is slightly larger than the minimum volume [cube of the uncertainty bound ($(\hbar/2)^3$)]. We will derive the volume from transform defined in previous page.

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int \Phi(p) e^{ip\frac{x}{\hbar}} dp$$
$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x) e^{-ip\frac{x}{\hbar}} dx$$

Consider 1-D problem. Since we want to avoid a complete specification of p or x, we define converging sequence of function $\tilde{\delta}$ which approaches to δ. We assume ψ is sufficiently smooth. Keep in mind that we can not specify p and x simalteniously. However, we can restrict the domain of x (Ω) so that it represent the single state. Consider $\psi^o(x;p)$ which is identical to ψ within the single state region $\Omega_x \times \Omega_p$ and zero everywhere else. Let momentum $\tilde{p'}$ represent the value approximately close to some momentum p' within this region.

$$\int_{\Omega_x} \psi^o(x;\tilde{p'}) e^{-i\tilde{p'}\frac{x}{\hbar}} dx = \int_{\Omega_x} \left(\frac{1}{\sqrt{2\pi\hbar}} \int_{\Omega_p} \Phi^o(p) e^{ip\frac{x}{\hbar}} \tilde{\delta}\left(p - p'\right) dp \right) e^{-i\tilde{p'}\frac{x}{\hbar}} dx$$
$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{\Omega_x} \Phi^o(\tilde{p'}) e^{i\tilde{p'}\frac{x}{\hbar}} e^{-i\tilde{p'}\frac{x}{\hbar}} dx$$
$$= \frac{1}{2\pi\hbar} \int_{\Omega_x} \left(\int_{\Omega_x} \psi^o(x;\tilde{p'}) e^{-i\tilde{p'}\frac{x}{\hbar}} dx \right) dx$$
$$= \frac{1}{2\pi\hbar} \left(\int_{\Omega_x} \psi^o(x;\tilde{p'}) e^{-i\tilde{p'}\frac{x}{\hbar}} dx \right) \Delta x$$

Rearrange the equation to obtain,

$$2\pi\hbar = h = \Delta x \qquad \text{in 1-D}$$

Average volume of a single state in 3-D (h^3) is simply a cube of the 1-D result.//

A.8 Euler Equation

We have shown that S and V is extensive variables and U is extensive function of these variables. More specifically, all of these are additive (linear relation to size). For this reason, it is obvious that following relation holds

$$U(aS, aV) = aU(S, V)$$

This equation can interprit as "if the new system has twice the volume (a=2) and entropy per volume is unchanged, internal energy is twice as large as original system." Then, it follwos that

$$\begin{aligned}
\frac{dU(aS, aV)}{da} &= U(S, V) \\
&= \left(\frac{\partial U(aS, aV)}{\partial (aS)}\right)_V \frac{d\,(aS)}{da} + \left(\frac{\partial U(aS, aV)}{\partial (aV)}\right)_S \frac{d\,(aV)}{da} \\
&= \left(\frac{\partial U(aS, aV)}{\partial (aS)}\right)_V S + \left(\frac{\partial U(aS, aV)}{\partial (aV)}\right)_S V \\
&\text{by setting a=1} \\
&= \left(\frac{\partial U(S, V)}{\partial S}\right)_V S + \left(\frac{\partial U(S, V)}{\partial V}\right)_S V \\
&\text{from 1st law} \\
&dU(S, T) = \left(\frac{\partial U(S, V)}{\partial S}\right)_V dS + \left(\frac{\partial U(S, V)}{\partial V}\right)_S dV = \delta q + \delta w = Tds - Pdv \\
&\text{ first and second partial derivatives are } T \text{ and } -P\text{, respectively} \\
&U = TS - PV
\end{aligned}$$

It folllows from the argument in the text, U is a state function. This argument can be repeated for $U(S, V, N)$.

A.9 Lagrange Multipliers and Chemical Potential

A.9.1 Single component system

At the beginning of this semester, we used Lagrange multiplier to obtain Boltzmann thermal distribution with 2 constraints:

$$\delta N_i = \sum_i \delta N_i = 0 \cdots ①$$
$$\delta N_i = \sum_i \delta N_i \epsilon_i = 0 \cdots ②$$

When we try to maximize $\ln \Omega$

$$\delta L = \sum_i \underbrace{(1 + \ln N_i + \alpha + \beta\epsilon_i)}_{=0} \delta N_i$$

constraint ① const ②

$$N_i = e^{-(1+\alpha)} e^{-\beta\epsilon_i}$$
$$= e^{-1} e^{-\beta\left(\epsilon_i + \frac{\alpha}{\beta}\right)}$$

chemical potential

$$\frac{\alpha}{\beta} = \mu$$

e^{-1} is going to be cancelled in $Z \Rightarrow$ can be eliminated. From discussion in the text, $\beta = 1/k_B T$. Since alpha is a pure number, the chemical potential has a unit of energy as expected.

A.9.2 Multi-component system

Consider system composed of two chemical components. The constraint we have for such system is

$$\delta N_1 = \sum_i \delta N_{1i} = 0 \cdots \textcircled{1}$$
$$\sum_i N_{2i} = N_2 \cdots \textcircled{2}$$
$$\sum_i N_{1i}\epsilon_i = E_1 \cdots \textcircled{3}$$
$$\sum_j N_{2j}\epsilon_j = E_2 \cdots \textcircled{4}$$

consider Ω

$$\Omega = \frac{N_1}{N_{10}N_{11}N_{12}\cdots N_{1r-1}} \frac{N_2}{N_{20}N_{21}N_{22}\cdots N_{2s-1}}$$

Since constant term disappear in the next step, we can ignore constants

$$\ln \Omega = -\sum_i N_{1i} \ln N_{1i} - \sum_j N_{2j} \ln N_{2j}$$

$$\delta \ln \Omega = -\sum_i \delta N_{1i} \ln N_{1i} - \sum_i \delta N_{1i} - \sum_j \delta N_{2j} \ln N_{2j} - \sum_j \delta N_{2j}$$

Following the similar step as in single component, we introduce the Lagrange multiplier

$$\delta L = \sum_i (1 + \ln N_i + \alpha_1 + \beta_1 \epsilon_i)\delta N_i = 0 = \sum_j (1 + \ln N_j + \alpha_2 + \beta_2 \epsilon_j)\delta N_j$$

Since LHS and RHS is independent, inside the parentheses must be zero.

$$(1 + \ln N_i + \alpha_1 + \beta_1 \epsilon_i) = 0 = -(1 + \ln N_j + \alpha_2 + \beta_2 \epsilon_j)$$

Since each components are thermal equilibrium with thermal bath, namely $\beta_1 = \beta = 1/k_B T = \beta_2$,

$$\ln N_i N_j = -2 - \alpha_1 - \alpha_2 - \beta(\epsilon_i + \epsilon_j)$$

Then,

$$N_{1i}N_{2j} = e^{-2-\alpha_1-\alpha_2-\beta(\epsilon_i+\epsilon_j)} = e^{-2} e^{-\beta([\epsilon_i+\alpha_1/\beta]+[\epsilon_j+\alpha_2/\beta])}$$
$$N_1 N_2 = e^{-2} \sum_{ij} e^{-\beta(\epsilon_i+\epsilon_j+\alpha_1/\beta+\alpha_2/\beta)}$$
$$P(i,j) = \frac{N_{1i}N_{2j}}{N_1 N_2} = \frac{e^{-\beta([\epsilon_i+\alpha_1/\beta]+[\epsilon_j+\alpha_2/\beta])}}{\sum_{ij} e^{-\beta([\epsilon_i+\alpha_1/\beta]+[\epsilon_j+\alpha_2/\beta])}}$$

and chemical potentials for each components are reltate to Lagrange multipliers.