Phys 454: Quantum Theory

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1 Introductions

1.1 Hamiltonian

Definition 1. Hamiltonian equation is some $H(x, p, t)$ that shows the energy of some particle moving with certain momentum p at a certain place x and time t.

Remark. Differential Equations of Motion may be derived by Hamiltonian.

1.2 Poisson algebra

Definition 2. A vector space V over $\mathbb{F}$ has two operations $+, \cdot$ that follows the axioms:

$$\begin{aligned}
&\forall x, y, z \in V, \forall a, b \in \mathbb{F} \\
&(x+y)+z = x+(y+z) \\
&x+y = y+x \\
\exists \mathbf{0} \in V, \forall x \in V, x+\mathbf{0} &= x \\
\exists -x \in M, x+(-x) &= \mathbf{0} \\
(ab)\cdot x &= a\cdot(b\cdot x) \\
1 \in \mathbb{F}, 1\cdot x &= x \\
(a+b)\cdot x &= a\cdot x + b\cdot x \\
a\cdot(x+y) &= a\cdot x + a\cdot y
\end{aligned}$$

Definition 3. The Poisson bracket follows the following axioms (Lie Algebra) on a vector space V over $\mathbb{F}$, s.t. $\forall x, y, z \in V, \forall a, b \in \mathbb{F}$

$$\begin{aligned}
\{x, y\} &= -\{y, x\} \\
\{a\cdot x + b\cdot y, z\} &= a\cdot\{x, z\} + b\cdot\{y, z\} \\
\{x, \{y, z\}\} + \{z, \{x, y\}\} + \{y, \{z, x\}\} &= 0
\end{aligned}$$

Definition 4. Associative Algebra is a ring M as an R-module for a commutative ring R, with three operations $+, \cdot, *$ (addition, scalar multiplication, multiplication), and $\forall a, b \in R, x, y, z \in M$,

$$\begin{aligned}
a \cdot (x * y) = (a \cdot x) * y = x * (a \cdot y) & \\
(x + y) + z = x + (y + z) & \qquad \text{as a ring} \\
x + y = y + x & \qquad \text{as a ring} \\
\exists \mathbf{0} \in M, x + \mathbf{0} = x & \qquad \text{as a ring} \\
\exists -x \in M, x + (-x) = \mathbf{0} & \qquad \text{as a ring} \\
(x * y) * z = x * (y * z) & \qquad \text{as a ring} \\
\exists \mathbf{1} \in M, x * \mathbf{1} = \mathbf{1} * x = x & \qquad \text{as a ring} \\
x * (y + z) = x * y + x * z & \qquad \text{as a ring} \\
(y + z) * x = y * x + z * x & \qquad \text{as a ring} \\
(ab) \cdot x = a \cdot (b \cdot x) & \qquad \text{as an R-module} \\
(a + b) \cdot x = a \cdot x + b \cdot x & \qquad \text{as an R-module} \\
a \cdot (x + y) = a \cdot x + a \cdot y & \qquad \text{as an R-module}
\end{aligned}$$

Definition 5. Poisson Algebra has axioms of

- Lie Algebra (Poisson brackets)
- Associative Algebra
- $\{f, g * h\} = g * \{f, h\} + \{f, g\} * h$

Remark. Neither Lie nor Associative Algebra have $x * y = y * x$.

Remark. $\cdot, *$ are different operations.

Theorem 1.1. *A Poisson bracket for equation of motion should satisfy*

$$\begin{aligned}
\frac{d}{dt} f(\boldsymbol{x}, \boldsymbol{p}, t) &= \{f(\boldsymbol{x}, \boldsymbol{p}, t), H(\boldsymbol{x}, \boldsymbol{p}, t)\} + \frac{\partial}{\partial t} f(\boldsymbol{x}, \boldsymbol{p}, t) \\
\{x_i, p_j\} &= \delta_{ij} \\
\{x_i, x_j\} &= 0 \\
\{p_i, p_j\} &= 0
\end{aligned}$$

Example 1.2.1. $\frac{d}{dt}x_3 = \{x_3, H\} + \cancelto{0}{\frac{\partial}{\partial t}x_3}$

Example 1.2.2. Let $f(x, p, t) = x_2 p_3 - \cos(\omega t) x_1$,
$\frac{d}{dt} f = \{x_2 p_3 - \cos(\omega t) x_1, H\} + \frac{\partial}{\partial t}(x_2 p_3 - \cos(\omega t) x_1) = \{x_2 p_3 - \cos(\omega t) x_1, H\} + \omega \sin(\omega t) x_1$

Example 1.2.3. Conservation laws

1. Want to know if p is conserved for $H = \frac{p^2}{2m}$?
   $\frac{d}{dt}p = \{p, \frac{p^2}{2m}\} + \cancelto{0}{\frac{\partial}{\partial t}p} = \frac{1}{2m}\{p, p * p\} = \frac{1}{2m}(p\cancelto{0}{\{p, p\}} + \cancelto{0}{\{p, p\}}p) = 0$
2. Conservation of energy (H)
   $\frac{d}{dt}H = \cancelto{0}{\{H, H\}} + \cancelto{0}{\frac{\partial}{\partial t}\frac{p^2}{2m}} = 0$
3. For any $f(x, p)$s.t. $\{f, H\} = 0$, then we have $\frac{d}{dt}f = 0$, namely, f is conserved.

Theorem 1.2. $\{f(x_1, \ldots, x_N, p_1, \ldots, p_N), g(x_1, \ldots, x_N, p_1, \ldots, p_N)\} := \sum_{i=1}^{N} \left(\frac{\partial}{\partial x_i} f \frac{\partial}{\partial p_i} g - \frac{\partial}{\partial p_i} f \frac{\partial}{\partial x_i} g\right)$ *is a Poisson bracket given that* $x_i(t), p_i(t) \in \mathbb{R}, f * g = g * f$

Example 1.2.4. $\{x, e^p\} = \cancelto{1}{\frac{\partial}{\partial x}x}\frac{\partial}{\partial p}e^p - \cancelto{0}{\frac{\partial}{\partial p}x\frac{\partial}{\partial x}p} = e^p$

1.3 Quantum Poisson algebra

Definition 6. The ring multiplication is not commutative. Instead, for $k = i\hbar = i\dfrac{h}{2\pi}$,

$$f * g - g * f = k \cdot \{f, g\}$$

Proposition 1.3. *Canonical commutation relation*
$x_i * x_j - x_j * x_i = k \cdot \{x_i, x_j\} = \boldsymbol{0}$
$p_i * p_j - p_j * p_i = k \cdot \{p_i, p_j\} = \boldsymbol{0}$
$x_i * p_j - p_j * x_i = k \cdot \{x_i, p_j\} = i\hbar\delta_{ij} * \boldsymbol{1}$

Definition 7. $[A, B] = A * B - B * A$

Definition 8. Represent x by $\hat{x}, p$ by $\hat{p}$.

Theorem 1.4. *Weinberg*
$\hat{x}, \hat{p}$ cannot be non-linear.

Theorem 1.5. *Stone*
All linear representations of $\hat{x}, \hat{p}$ are the same up to the change of basis.

Proposition 1.6. $\{\hat{x}, \hat{p}^n\} = n \cdot \hat{p}^{n-1}, \{\hat{p}, \hat{x}^n\} = n \cdot \hat{x}^{n-1}$.

Proof. Done by induction on n.
Base case is when $n = 1$, then $\{\hat{x}, \hat{p}\} = \mathbf{1} = 1 \cdot \hat{p}^0$.
Now assume for induction that $\forall 1 \leq m < n, \{\hat{x}, \hat{p}^m\} = n \cdot \hat{p}^{m-1}$, then we have

$$\begin{aligned}
\{\hat{x}, \hat{p}^n\} &= \left\{\hat{x}, \hat{p}^{n-1}\hat{p}\right\} \\
&= \hat{p}^{n-1}\{\hat{x}, \hat{p}\} + \left\{\hat{x}, \hat{p}^{n-1}\right\}\hat{p} \\
&= \hat{p}^{n-1}\cancelto{1}{\{\hat{x}, \hat{p}\}} + (n-1) \cdot \hat{p}^{n-1-1}\hat{p} \\
&= \hat{p}^{n-1} + i\hbar(n-1) \cdot \hat{p}^{n-1} \\
&= n \cdot \hat{p}^{n-1}
\end{aligned}$$

Thus $\{\hat{x}, \hat{p}^n\} = n \cdot \hat{p}^{n-1}$ holds for any n.
Same proof for $\{\hat{p}, \hat{x}^n\} = n \cdot \hat{x}^{n-1}$ □

1.4 Matrix representation

Definition 9. $a = \begin{pmatrix} 0 & \sqrt{1} & 0 & \dots & 0 \\ 0 & 0 & \sqrt{2} & \dots & 0 \\ 0 & \dots & \ddots & \ddots & 0 \\ \vdots & & \dots & & \vdots \end{pmatrix}$

Proposition 1.7. $aa^\dagger = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 2 & 0 & \dots & 0 \\ 0 & \dots & \ddots & \ddots & 0 \\ \vdots & & \dots & & \vdots \end{pmatrix}, a^\dagger a = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 2 & \dots & 0 \\ 0 & \dots & & \ddots & \vdots \\ \vdots & & \dots & & \vdots \end{pmatrix},$

$aa^\dagger - a^\dagger a = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ & 1 & 0 & \dots & 0 \\ \vdots & & 1 & \dots & 0 \\ & & \mathit{0} & \ddots & \vdots \\ \vdots & & \dots & & \vdots \end{pmatrix} = \boldsymbol{1}$

Theorem 1.8. *For position and momentum to be real,* $\forall t, \hat{x}(t)^\dagger = \hat{x}(t), \hat{p}(t)^\dagger = \hat{p}(t)$

Example 1.4.1. For a free particle with $\hat{H}(\hat{x}, \hat{p}) = \frac{\hat{p}^2}{2m} \implies \frac{d}{dy}\hat{x} = \frac{\hat{p}}{m}, \frac{d}{dt}\hat{p} = 0.$
Let $\hat{x}(t_0) = L(a + a^\dagger), \hat{p}(t_0) = i\hbar\frac{1}{2L}(a^\dagger - a)$, then first notice that they are hermitian. In addition,
$[\hat{x}(t_0), \hat{p}(t_0)] = \left[L(a^\dagger + a), \frac{i\hbar}{2L}(a^\dagger - a)\right] = \frac{1}{2}i\hbar\left[a^\dagger + a, a^\dagger - a\right]$
$= \frac{1}{2}i\hbar(\cancelto{0}{[a^\dagger, a^\dagger]} - \cancelto{\mathbf{1}}{[a^\dagger, a]} + \cancelto{\mathbf{1}}{[a, a^\dagger]} - \cancelto{0}{[a, a]}) = i\hbar\mathbf{1}\checkmark$
$\frac{d}{dt}\hat{p} = 0 \implies \forall t > t_0, \hat{p}(t_0) = i\hbar\frac{1}{2L}(a^\dagger - a)$
$\frac{d}{dy}\hat{x} = \frac{\hat{p}}{m} \implies \hat{x}(t) = \hat{x}(t_0) + (t - t_0)\frac{1}{m}\hat{p}(t_0)$
Thus $\hat{x}(t) = L(a + a^\dagger) + (t - t_0)\frac{1}{m}i\hbar\frac{1}{2L}(a^\dagger - a)$

Example 1.4.2. Harmonic oscillator $\hat{H}(\hat{x}, \hat{p}) = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2$
$\frac{d}{dt}\hat{x}(t) = \left\{\hat{x}(t), \hat{H}\right\} = \left\{\hat{x}(t), \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2\right\} = \frac{1}{2m}\left\{\hat{x}(t), \hat{p} * \hat{p}\right\} + \frac{1}{2}k\cancelto{0}{\{\hat{x}, \hat{x} * \hat{x}\}}$
$= \frac{1}{2m}(\hat{p}\cancelto{1}{\{\hat{x}, \hat{p}\}} + \cancelto{1}{\{\hat{x}, \hat{p}\}}\hat{p}) = \frac{1}{m}\hat{p}(t),$
$\frac{d}{dt}\hat{p}(t) = \left\{\hat{p}(t), \hat{H}\right\} = -k\hat{x}(t)$
Notice that $\hat{x}(t_0), \hat{p}(t_0)$ are the same as free particle case.
Now let $\hat{x}(t) = \xi(t)a + \xi^*(t)a^\dagger$, then it's clear that $\hat{x}^\dagger = \hat{x}$
Thus $\hat{p}(t) = \frac{d}{dt}\hat{x}(t) = m(\dot{\xi}a + \dot{\xi}^*a^\dagger)$, and clearly $\hat{p}^\dagger = \hat{p}$
$\frac{d}{dt}\hat{p}(t) = -k\hat{x}(t) \implies m(\ddot{\xi}a + \ddot{\xi}^*a^\dagger) = -k(\xi(t)a + \xi^*(t)a^\dagger) \implies m\ddot{\xi} = -k\xi(t), m\ddot{\xi}^* = -k\xi^*(t)$
Thus $\xi(t) = r\sin(\sqrt{\frac{k}{m}}t) + s\cos(\sqrt{\frac{k}{m}}t)$, and let $\omega = \sqrt{\frac{k}{m}}$
Now solve r, s, s.t. $[\hat{x}, \hat{p}] = i\hbar$, and there is a solution such that $a^2, (a^\dagger)^2$ terms disappear.

1.5 Number Prediction

Want to choose $\{\psi_i\}$ so that we can make number prediction $\bar{f}(t) := \sum_{i,j=1}^{\infty}\psi_i^*\hat{f}_{ij}(t)\psi_j \in \mathbb{R}$

Remark. Notice that the choice of ψ will impact the prediction.

Definition 10. For a random variable Q, $\bar{Q}$ is its mean value (expectation), $Var(Q) = \overline{(Q - \bar{Q})^2}$ is its variance, and $\Delta Q = \sqrt{Var(Q)}$ is its standard deviation.

Proposition 1.9. $Var(Q) = (\bar{Q^2}) - (\bar{Q})^2$

Proof. $Var(Q) = \overline{(Q - \bar{Q})^2} = \overline{Q^2 - Q\bar{Q} - \bar{Q}Q + (\bar{Q})^2} = (\bar{Q^2}) - (\bar{Q})^2 - (\bar{Q})^2 + (\bar{Q})^2$ ☐

Remark. In Classical Mechanics, there are 2 initial conditions $\bar{x}(t_0), \bar{p}(t_0)$, and we always have the expectation (prediction) $\overline{x(t_0)^2} = (\bar{x}(t_0))^2$.
However, in Quantum Mechanics, we have infinite initial conditions ψ_i.
In general, $Var(\hat{f}(t)) = \overline{f(t)^2} - (\bar{f}(t))^2 \neq 0$

Remark. Want $\{\psi_i\}$, s.t. $\sum_i \psi_i^*\psi_i = 1$, so that it is normalized.

Proposition 1.10. *For normalized* $\{\psi_i\}$, *the previous proposition will work for* $Var(\hat{f}(t)) := \overline{\hat{f}(t)^2 - \bar{f}(t)^2 \cdot \mathbf{1}}$,

$$Var(\hat{f}(t)) = \overline{\hat{f}(t)^2} - \bar{f}(t)^2 = \sum_{i,j,k}^{\infty}\psi_i^*\hat{f}_{ij}(t)\hat{f}_{jk}(t)\psi_k - \left(\sum_{i,j=1}^{\infty}\psi_i^*\hat{f}_{ij}(t)\psi_j\right)^2$$

2 Hilbert Space and Bra-Ket Notation

2.1 Motivation

Definition 11. A such $\{\psi_i\}$ give a "ket vector" $|\psi\rangle$, by choosing a basis $\{|b_n\rangle\}_1^\infty$, where

$$|\psi\rangle = \sum_{n=1}^{\infty} \psi_n |b_n\rangle, \psi_n \in \mathbb{C}$$

Remark. $|\psi\rangle$ may be represented in any other basis as well.

Remark. Infinite sums may not commute.
$\sum_{i=1}^\infty \sum_{j=1}^\infty a_{ij} = \sum_{j=1}^\infty \sum_{i=1}^\infty a_{ij}$ is not always true.
However, when the limit converges **absolutely**, the sum commutes.

Remark. In infinite dimensional vector spaces, there can be "continuous" basis where the label is continuous instead of discrete, for instance, $|c_\lambda\rangle_{\lambda\in[a,b]}$

Definition 12. For a continuous basis labeled by $[a, b]$, we take $|\psi\rangle = \int_a^b \psi_\lambda |c_\lambda\rangle d\lambda$, in which case, we can treat $\psi_\lambda = \psi(\lambda), \psi : [a, b] \to \mathbb{C}$

Remark. There can be a mixture of discrete and continuous basis

2.2 Inner Product Space

Definition 13. A set $\mathcal{H}$ is called a complex vector space if it is a vector space2 over $\mathbb{C}$.

Definition 14. Given $\mathcal{H}$, we can define its "dual" vector space $\mathcal{H}^* = \left\{\langle u| : Lin(\mathcal{H}, \mathbb{C}) \cap C^0(\mathcal{H}, \mathbb{C})\right\}$ where the dual vectors $\langle u|$ are continuous linear maps $\mathcal{H} \to \mathbb{C}$

Definition 15. An inner product space is a vector space $\mathcal{H}$ that has an inner product:

$$\begin{aligned}
\langle -, \cdot\rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}, \text{s.t. } \forall |v\rangle, |w\rangle \in \mathcal{H}, a, b \in \mathbb{C}& \\
\langle u, av + bw\rangle &= a\langle u, v\rangle + b\langle u, w\rangle \\
\langle v, w\rangle^* &= \langle w, v\rangle \\
\forall v \neq 0, \langle v, v\rangle &> 0 \\
\langle 0, v\rangle &= 0
\end{aligned}$$

Remark. Note that if we have an inner product space $\mathcal{H}$, we can define $\langle\psi| \in \mathcal{H}^*$ to be $\langle\psi, \cdot\rangle$ and thus $\forall |\phi\rangle \in \mathcal{H}, \langle\psi|(|\phi\rangle) = \langle\psi, \phi\rangle$

Theorem 2.1. *Cauchy-Schwarz: For every inner product space $\mathcal{H}, \forall |\psi\rangle, |\phi\rangle \in \mathcal{H}, |\langle\psi|\phi\rangle| \le ||\psi|| \, ||\phi||$.
In particular, when $V := ||\phi|| \neq 0, ||\psi||^2 \, ||\phi||^2 - |\langle\psi|\phi\rangle|^2 = ||z||^2$, where $z := V|\psi\rangle - \frac{\langle\psi|\phi\rangle}{V}|\phi\rangle$*

Proof. Notice that this is trivially true and equality holds to be zero when $|\phi\rangle = 0$
Now we assume $V \neq 0$, then

$$\begin{aligned}
||z||^2 &= \langle z, z\rangle \\
&= \left\langle V|\psi\rangle - \frac{\langle\psi|\phi\rangle}{V}|\phi\rangle, V|\psi\rangle - \frac{\langle\psi|\phi\rangle}{V}|\phi\rangle\right\rangle \\
&= V^2\langle\psi, \psi\rangle - \langle\psi|\phi\rangle\langle\psi, \phi\rangle - \langle\phi|\psi\rangle\langle\phi, \psi\rangle + \frac{\langle\psi|\phi\rangle\langle\phi|\psi\rangle}{\cancel{V^2}}\cancelto{V^2}{\langle\phi, \phi\rangle} \\
&= V^2||\psi||^2 - |\langle\psi, \phi\rangle|^2 - \cancel{|\langle\psi, \phi\rangle|^2} + \cancel{|\langle\psi, \phi\rangle|^2} \\
&= ||\phi||^2 \, ||\psi||^2 - |\langle\psi, \phi\rangle|^2
\end{aligned}$$

∎

Proposition 2.2. *If* $\forall \psi, \langle \psi, \phi \rangle = 0$*, then* $|\phi\rangle = 0$

Definition 16. A normed vector space is a vector space $\mathcal{V}$ that has an norm (length):

$$
\begin{aligned}
||\cdot|| : \mathcal{V} \to \mathbb{R}, \text{s.t. } \forall x, y \in \mathcal{V}, a \in \mathbb{C}& \\
||a \cdot x|| &= |a| \, ||x|| \\
||x + y|| &\leq ||x|| + ||y|| \\
\forall x \neq 0, ||x|| &> 0 \\
||0|| &= 0
\end{aligned}
$$

Proposition 2.3. *For every inner product space with* $\langle -, \cdot \rangle$*, there is a norm* $||x|| = \sqrt{\langle x, x \rangle}$.

Proof.

$$
\begin{aligned}
||a \cdot x|| &= \sqrt{\langle ax, ax \rangle} = \sqrt{a^* a \langle x, x \rangle} = \sqrt{|a|^2} \sqrt{\langle x, x \rangle} = |a| \, ||x|| \\
||x + y||^2 &= \langle x + y, x + y \rangle = \langle x, x \rangle + \langle y, y \rangle + \langle x, y \rangle + \langle y, x \rangle \\
&\leq ||x||^2 + ||y||^2 + 2 \, ||x|| \, ||y|| \leq (||x|| + ||y||)^2 \\
\forall x \neq 0, ||x|| &= \sqrt{\langle x, x \rangle} > 0 \\
||0|| &= \sqrt{\langle 0, 0 \rangle} = 0
\end{aligned}
$$

Thus $||x|| = \sqrt{\langle x, x \rangle}$ is a norm. □

Definition 17. A metric space is a vector space $\mathcal{V}$ that has a (distance) metric:

$$
\begin{aligned}
d(\cdot, \cdot) : \mathcal{V} \times \mathcal{V} \to \mathbb{R}, \text{s.t. } \forall x, y, z \in \mathcal{V}& \\
d(x, x) &= 0 \\
\forall x \neq y, d(x, y) &> 0 \\
d(x, y) &= d(y, x) \\
d(x, z) &\geq d(x, y) + d(y, z)
\end{aligned}
$$

Proposition 2.4. *For every normed space with* $||\cdot||$*, there is a metric* $d(x, y) = ||x - y||$.

Proof.

$$
\begin{aligned}
d(x, x) &= ||x - x|| = ||0|| = 0 \\
\forall x \neq y, d(x, y) &= ||x - y|| > 0 \\
d(x, y) &= ||x - y|| = ||-(y - x)|| = |-1| \, ||y - x|| = ||y - x|| = d(y, x) \\
d(x, z) &= ||x - z|| = ||x - y + y - z|| \geq ||x - y|| + ||y - z|| = d(x, y) + d(y, z)
\end{aligned}
$$

Thus $d(x, y) = ||x - y||$ is a metric. □

Corollary 2.5. *For every inner product space, there is a metric* $d(x, y) = \sqrt{\langle x - y, x - y \rangle}$

2.3 Completeness and Hilbert Space

Definition 18. Given a metric d, a sequence $(x_i)_1^\infty$ has a limit point $x = \lim\limits_{n \to \infty} x_n$ if $\lim\limits_{n \to \infty} d(x, x_i) = 0$

Proposition 2.6. *For an Inner product space* $\mathcal{H}, \forall y, x = \lim\limits_{i \to \infty} x_i \in \mathcal{H}$*, we have* $\langle x, y \rangle = \lim\limits_{i \to \infty} \langle x_i, y \rangle$.

Proof. Given any $\epsilon > 0$, let $\epsilon_0 = \frac{\epsilon}{||y||}$.
Since $x = \lim_{i \to \infty} x_i$, we can find $N > 0, \text{s.t. } \forall n > N, ||x - x_n|| < \epsilon_0$,
thus $|\langle x, y \rangle - \langle x_n, y \rangle| = |\langle x - x_n, y \rangle| \leq ||x - x_n|| \, ||y|| < \epsilon_0 \, ||y|| = \epsilon$ □

Corollary 2.7. *For an Inner product space $\mathcal{H}, \forall y, x = \lim_{i\to\infty} x_i \in \mathcal{H}$, we have $\langle y, x\rangle = \lim_{i\to\infty} \langle y, x_i\rangle$.*

Definition 19. A sequence $(x_i)_1^\infty$ is a Cauchy sequence in a metric space with metric d if

$$\forall \epsilon > 0, \exists N \in \mathbb{N}^+, \text{s.t. } \forall m, n > N \in \mathbb{N}, d(x_m, x_n) < \epsilon$$

Definition 20. A metric space $\mathcal{V}$ is complete if every Cauchy sequence $(x_i)_1^\infty$ converges to a limit point in $\mathcal{V}$. i.e. $\exists x \in \mathcal{V}, \lim_{i\to\infty} x_i = x$

Definition 21. An inner product space is called a Hilbert space if it is complete.

Definition 22. Bra-ket Notation

$$\begin{aligned}
\langle\psi|\phi\rangle &:= \langle\psi|\left(|\phi\rangle\right) \\
&= \langle\psi, \phi\rangle \\
\langle\psi|\hat{u}\phi\rangle &:= \langle\psi|\hat{u}|\phi\rangle \\
&:= \langle\psi, \hat{u}(|\phi\rangle)\rangle
\end{aligned}$$

Proposition 2.8. *For any inner product space H, we can complete it with respect to the induced metric distance, and the unique completion $\mathcal{H} := \bar{H}$ is a Hilbert space.*

Proof. The completion $(\mathcal{H} := \bar{H}, d_{\mathcal{H}})$ exists and is unique since H is an inner product space, thus a metric space. And we have $\forall x, y \in H, d_{\mathcal{H}}(x, y) = d_H(x, y) = \sqrt{\langle x-y, x-y\rangle_H}$ We now need to show that $\mathcal{H}$ has an inner product, and the induced metric is the same as $d_{\mathcal{H}}$.
Consider the extension of the inner product: $\forall x, y \in \mathcal{H}$, we know that $x = \lim_{n\to\infty} x_n, y = \lim_{n\to\infty} y_n$, for some sequence $x_n, y_n \in H$, define $\langle x, y\rangle_{\mathcal{H}} := \lim_{n\to\infty} \langle x_n, y_n\rangle_H$.
Now suppose there are another two sequences $\lim_{n\to\infty} x'_n = x, \lim_{n\to\infty} y'_n = y$, we must show that $\lim_{n\to\infty} \langle x_n, y_n\rangle_H = \lim_{n\to\infty} \langle x'_n, y'_n\rangle_H$ so that $\langle x, y\rangle_{\mathcal{H}}$ is independent of the choice of converging sequence and thus well defined.
Given any $\epsilon > 0$, we let $\epsilon_0 = \min\left\{\frac{\epsilon}{4(||x||+\epsilon)}, \frac{\epsilon}{4(||y||+\epsilon)}, \epsilon\right\}$.
Pick $N > 0$, s.t. $\forall n > N, d_{\mathcal{H}}(x_n, x), d_{\mathcal{H}}(y_n, y), d_{\mathcal{H}}(x'_n, x), d_{\mathcal{H}}(y'_n, y) < \epsilon_0$, we have

$$\begin{aligned}
||x_n - x'_n|| &= d_H(x_n, x'_n) = d_{\mathcal{H}}(x_n, x'_n) \le d_{\mathcal{H}}(x_n, x) + d_{\mathcal{H}}(x'_n, x) < 2\epsilon_0, \\
||y_n - y'_n|| &= d_H(y_n, y'_n) = d_{\mathcal{H}}(y_n, y'_n) \le d_{\mathcal{H}}(y_n, y) + d_{\mathcal{H}}(y'_n, y) < 2\epsilon_0, \\
||x_n|| &= d_H(x_n, 0) = d_{\mathcal{H}}(x_n, 0) \le d_{\mathcal{H}}(x, 0) + d_{\mathcal{H}}(x_n, x) < d_H(x, 0) + \epsilon_0 \le ||x|| + \epsilon, \\
||y_n|| &= d_H(y_n, 0) = d_{\mathcal{H}}(y_n, 0) \le d_{\mathcal{H}}(y, 0) + d_{\mathcal{H}}(y'_n, y) < d_H(y, 0) + \epsilon_0 \le ||y|| + \epsilon. \\
|\langle x'_n, y'_n\rangle - \langle x_n, y_n\rangle| &= |\langle x'_n, y'_n\rangle - \langle x_n, y'_n\rangle + \langle x_n, y'_n\rangle - \langle x_n, y_n\rangle| \\
&\le |\langle x'_n - x_n, y'_n\rangle| + |\langle x_n, y'_n - y_n\rangle| \\
&\le ||x'_n - x_n||\,||y'_n|| + ||x_n||\,||y'_n - y_n|| \\
&< 2\epsilon_0(||y|| + \epsilon) + (||x|| + \epsilon)2\epsilon_0 \\
&\le \frac{\epsilon}{2} + \frac{\epsilon}{2} \\
&= \epsilon
\end{aligned}$$

Thus we have $\lim_{n\to\infty} \langle x'_n, y'_n\rangle - \langle x_n, y_n\rangle = 0$, and thus $\lim_{n\to\infty} \langle x_n, y_n\rangle_H = \lim_{n\to\infty} \langle x'_n, y'_n\rangle_H$
Notice that if $x, y \in H$, then $\langle x, y\rangle_{\mathcal{H}} := \langle x, y\rangle_H$, thus the inner product and the induced norm and metric are all the same as the ones for H when restricted to H.

In particular, $\forall x, y \in \mathcal{H}$,

$$\begin{aligned}
d_{\mathcal{H}}(x,y) &= \lim_{n\to\infty} d_H(x_n, y_n) \\
&= \lim_{n\to\infty} \sqrt{\langle x_n - y_n, x_n - y_n\rangle_H} \\
&= \lim_{n\to\infty} \sqrt{\langle x_n - y_n, x_n - y_n\rangle_{\mathcal{H}}} \\
&= \sqrt{\lim_{n\to\infty} \langle x_n - y_n, x_n - y_n\rangle_{\mathcal{H}}} \\
&= \sqrt{\langle x, y\rangle_{\mathcal{H}}}
\end{aligned}$$

Thus we have that $\mathcal{H}$ has an inner product and is complete, thus a Hilbert space. □

2.4 Hilbert basis

Definition 23. A basis $\{|b_n\rangle\}_0^\infty$ of Hilbert space $\mathcal{H}$ is called a Hilbert basis, if

$$\forall n, m \in \mathbb{N}, \langle b_n, b_m\rangle = \delta_{nm}$$

$$\forall\, |\psi\rangle \in \mathcal{H}, \exists!\, \{\psi_n\} \in \mathbb{C}, \text{s.t. } |\psi\rangle = \sum_{n=0}^{\infty} \psi_n\, |b_n\rangle$$

Definition 24. A Hilbert space with a countable Hilbert basis is called “separable”.

Remark. All Hilbert spaces in Quantum Physics are separable.

Remark. For a continuous basis $\{|c_\lambda\rangle\}_{\lambda\in\mathbb{R}}$ that gives $|\psi\rangle = \int_a^b \psi_\lambda\, |c_\lambda\rangle\, d\lambda$, it is not a Hilbert basis. In particular, $|c_\lambda \notin \mathcal{H}\rangle, \langle c_\lambda, c_{\lambda'}\rangle \neq \delta_{\lambda\lambda'}$

Remark. In Quantum Mechanics, we only work with a Hilbert space consisting of state $|\psi\rangle$ with finite norm, where $\langle\psi,\psi\rangle < \infty$

Theorem 2.9. *Suppose $\{|b_n\rangle\}_0^\infty$ is a Hilbert basis, then $\forall\, |\psi\rangle = \sum_{n=0}^\infty \psi_n\, |b_n\rangle \in \mathcal{H}$, we have $\langle b_m|\psi\rangle = \psi_m$*

Proof. $\langle b_m|\psi\rangle = \langle b_m|\sum_{n=0}^\infty \psi_n b_n\rangle = \sum_{n=0}^\infty \langle b_m|\psi_n b_n\rangle = \sum_{n=0}^\infty \psi_n \overset{\delta_{mn}}{\cancel{\langle b_m|b_n\rangle}} = \psi_m$ □

Corollary 2.10. *Suppose $\{|b_n\rangle\}_0^\infty$ is a Hilbert basis, then $\mathbf{1} = \sum_{m=1}^\infty |b_m\rangle\langle b_m| \in \mathcal{H}^*$*

Proof. Given any $|\psi\rangle = \sum_{n=0}^\infty \psi_n\, |b_n\rangle \in \mathcal{H}$,
$(\sum_{m=1}^\infty |b_m\rangle\langle b_m|)(|\psi\rangle) = \sum_{m=1}^\infty |b_m\rangle\langle b_m|\psi\rangle = \sum_{m=1}^\infty |b_m\rangle\, \psi_m = |\psi\rangle$ □

Proposition 2.11. *Suppose $\{|b_n\rangle\}_1^\infty$ is a Hilbert basis, then for any $|\psi\rangle = \sum_{n=0}^\infty \psi_n\, |b_n\rangle \in \mathcal{H}$, we have $\||\psi\rangle\|^2 = \sum_{n=1}^\infty \psi_n^*\psi_n$*

Proof. $\||\psi\rangle\|^2 = \langle\psi|\psi\rangle = \langle\psi|\mathbf{1}\psi\rangle = \langle\psi|\sum_{n=1}^\infty |b_n\rangle\langle b_n|\,\psi\rangle = \sum_{n=1}^\infty \langle\psi|b_n\rangle\langle b_n|\psi\rangle = \sum_{n=1}^\infty \psi_n^*\psi_n$ □

2.5 Operators

Definition 25. $\hat{f}(t)_{nm} = \langle b_n|\, \hat{f}(t)\, |b_m\rangle$ given a Hilbert basis $\{|b_n\rangle\}_0^\infty$

Remark. $\hat{f}(t) = \mathbf{1}\hat{f}(t)\mathbf{1} = \sum_{n,m=0}^\infty |b_n\rangle\langle b_n|\, \hat{f}(t)\, |b_m\rangle\langle b_m| = \sum_{n,m=0}^\infty |b_n\rangle\, \hat{f}(t)_{nm}\, \langle b_m| = \sum_{n,m=0}^\infty \hat{f}(t)_{nm}\, |b_n\rangle\langle b_m|$

Proposition 2.12. *If $\{|b_n\rangle\}_0^\infty$ is a Hilbert basis, and $\forall n \in \mathbb{N}, \hat{f}\, |b_n\rangle = 0$, then $\hat{f} = \mathbf{0}$*

Example 2.5.1. Consider $\psi_n = \frac{1}{n}$, we have $\langle\psi,\psi\rangle = \sum_{n=1}^\infty \psi_n^*\psi_n = \sum_{n=1}^\infty \frac{1}{n^2} = \frac{\pi}{6} < \infty$.
Consider $\hat{f}_{mn} = \delta_{nm} n^2$, then if $|\phi\rangle = \hat{f}(|\psi\rangle)$, we have $\phi_n = n$ and thus $\langle\phi,\phi\rangle = \sum_{n=1}^\infty n = \infty$, thus $|\phi\rangle \notin \mathcal{H}$

Remark. we need to consider operators that preserve vectors inside the Hilbert space.

Definition 26. For operator $\hat{f}$, the maximal domain is $D_{\hat{f}} := \left\{ |\psi\rangle \in \mathcal{H} | \hat{f} |\psi\rangle \in \mathcal{H} \right\}$

Definition 27. Change of basis
For Hilbert basis $\{|b_n\rangle\}, \{|c_n\rangle\}$, we can define a change of basis operator $\hat{u} : \mathcal{H} \to \mathcal{H}, \hat{u}(|b_n\rangle) = |c_n\rangle$

Proposition 2.13. $\hat{u}_{nm} = \langle b_n | \hat{u} | b_m \rangle = \langle b_n | c_m \rangle$

Proposition 2.14. $\hat{u} = \sum_{m=0}^{\infty} |c_m\rangle \langle b_m|$

Proof. $\hat{u} = \sum_{n,m=0}^{\infty} \hat{u}_{nm} |b_n\rangle \langle b_m| = \sum_{n,m=0}^{\infty} \langle b_n | c_m \rangle |b_n\rangle \langle b_m| = \sum_{n,m=0}^{\infty} |b_n\rangle \langle b_n| |c_m\rangle \langle b_m| = \sum_{m=0}^{\infty} |c_m\rangle \langle b_m|$ □

Proposition 2.15. *For any two Hilbert basis* $\{|b_n\rangle\}_0^{\infty}, \{|c_m\rangle\}_0^{\infty}$, *and any* $|\psi\rangle = \sum_{n=0}^{\infty} \psi_n |b_n\rangle = \sum_{m=0}^{\infty} \tilde{\psi_m} |c_m\rangle \in \mathcal{H}$, *we have* $\psi_n = \sum_{m=0}^{\infty} \tilde{\psi_m} \langle b_n | c_m \rangle$

Proof. $\psi_n = \langle b_n | \psi \rangle = \langle b_n | \sum_{m=0}^{\infty} \tilde{\psi_m} |c_m\rangle = \sum_{m=0}^{\infty} \tilde{\psi_m} \langle b_n | c_m \rangle$ □

2.6 Adjoint

Definition 28. The Adjoint operator $\hat{f}^{\dagger}$ of $\hat{f}$ is the operator such that

$$\forall |\psi\rangle, |\phi\rangle \in \mathcal{H}, \left\langle \hat{f} |\psi\rangle, \phi \right\rangle = \left\langle \hat{f} |\psi\rangle, |\phi\rangle \right\rangle := \left\langle |\psi\rangle, \hat{f}^{\dagger} |\phi\rangle \right\rangle = \left\langle \psi, \hat{f}^{\dagger} \phi \right\rangle$$

Proposition 2.16. *The Adjoint operator* $\hat{f}^{\dagger}$ *exists and is unique for finite-dimensional Hilbert space.*

Definition 29. The domain for the adjoint $D_{\hat{f}^{\dagger}} := \left\{ |\phi\rangle \in \mathcal{H} | \exists |\rho\rangle \text{ s.t. } \langle \rho | \psi \rangle = \langle \phi | \hat{f} \psi \rangle, \forall |\psi\rangle \in D_{\hat{f}} \right\}$

Proposition 2.17. *On* $D_{\hat{f}^{\dagger}} \cap D_{\hat{f}}$

$$(\hat{f}^{\dagger})^{\dagger} = \hat{f}$$
$$(\hat{f} + \hat{g})^{\dagger} = \hat{f}^{\dagger} + \hat{g}^{\dagger}$$
$$(\hat{f}\hat{g})^{\dagger} = \hat{g}^{\dagger} \hat{f}^{\dagger}$$

Proposition 2.18. *Given any Hilbert basis,* $\hat{f}^{\dagger}_{mn} = \overline{\hat{f}_{nm}}$

Definition 30. $|\psi\rangle^{\dagger}$ is given by $\langle \psi|$

Definition 31. $(|\psi\rangle^{\dagger})^{\dagger} := |\psi\rangle$

Proposition 2.19. *Given any Hilbert basis,* $|\psi\rangle^{\dagger} = \sum_0^{\infty} \overline{\psi_n} \langle b_n|$

Proposition 2.20. *For any* $|\psi\rangle \in \mathcal{H}, \langle \psi | \hat{f}^{\dagger} = \left(\hat{f} |\psi\rangle \right)^{\dagger}$

Proof. Given any $|\phi\rangle \in \mathcal{H}, (\langle \psi | \hat{f}^{\dagger})(|\phi\rangle) = \langle \psi | (\hat{f}^{\dagger} |\phi\rangle) = \left\langle \psi, \hat{f}^{\dagger} |\phi\rangle \right\rangle = \left\langle \hat{f} |\psi\rangle, \phi \right\rangle = \left(\hat{f} |\psi\rangle \right)^{\dagger} |\phi\rangle$ □

Definition 32. $\hat{f}$ is self-adjoint if $D_{\hat{f}} = D_{\hat{f}^{\dagger}} \wedge \forall |\psi\rangle \in D_{\hat{f}}, \hat{f} |\psi\rangle = |\psi\rangle^{\dagger} |\psi\rangle$

2.7 Unitary Operators

Definition 33. An operator $\hat{u}$ is unitary if it obeys $\hat{u}^{\dagger}\hat{u} = \mathbf{1}$

Proposition 2.21. *If an operator* $\hat{u}$ *is a change of basis operator, it is unitary*

Proof. Suppose we have a change of basis $c_m = \hat{u} b_m$.
Then $\langle b_m | \mathbf{1} b_n \rangle = \langle b_m | b_n \rangle = \delta_{nm} = \langle c_m | c_n \rangle = |c_m\rangle^{\dagger} |c_n\rangle = \langle b_m | \hat{u}^{\dagger} \hat{u} |b_n\rangle$
Thus $\langle b_m | (\mathbf{1} - \hat{u}^{\dagger}\hat{u}) b_n \rangle = 0 \implies \mathbf{1} - \hat{u}^{\dagger}\hat{u} = \mathbf{0} \implies \mathbf{1} = \hat{u}^{\dagger}\hat{u}$ □

Proposition 2.22. *For an unitary operator* $\hat{u}, \forall |\psi\rangle \in \mathcal{H}, || |\psi\rangle || = || \hat{u} |\psi\rangle ||$

Proof. $|| \hat{u} |\psi\rangle ||^2 = \langle \psi | \hat{u}^{\dagger} \hat{u} \psi \rangle = \langle \psi | \mathbf{1} \psi \rangle = \langle \psi | \psi \rangle = || |\psi\rangle ||^2$ □

2.8 Eigenbasis and Spectrum

Definition 34. For $\hat{f}$, its eigenvectors $\{|f_n\rangle\}_0^\infty$ are such that $\hat{f}\,|f_n\rangle = f_n\,|f_n\rangle$, where f_n is eigenvalues.

Definition 35. If $\hat{f}$ has a Hilbert basis of eigenvectors $\{|f_n\rangle\}_0^\infty$, they are called the eigenbasis for $\hat{f}$.

Proposition 2.23. *Suppose that $\hat{f}$ has a Hilbert basis, if the initial state is $|\psi\rangle = |f_n\rangle$, then the prediction $\bar{f} = \langle\psi|\hat{f}|\psi\rangle = f_n\langle f_n|f_n\rangle = f_n$, and $(\Delta f)^2 = \overline{(\hat{f}-f)^2} = \langle f_n|(\hat{f}-f_n)^2|f_n\rangle = \langle f_n|(f_n-f_n)^2|f_n\rangle = 0$*

Remark. If the system is in some random state, then after measuring f_n, the new initial state should be $|f_n\rangle$

Definition 36. The spectrum $\mathrm{Spec}(\hat{Q})$ of Operator $\hat{Q}$ is the set of all $\lambda \in \mathbb{C}$ for which $(\hat{Q} - \lambda\mathbf{1})$ does not have an inverse or the inverse $(\hat{Q} - \lambda\mathbf{1})^{-1}$ is not defined on $\mathcal{H}$, i.e. $D_{(\hat{Q}-\lambda\mathbf{1})^{-1}} \neq \mathcal{H}$

Proposition 2.24. *If $\hat{Q}\,|\lambda\rangle = \lambda\,|\lambda\rangle$, then $\lambda \in \mathrm{Spec}(\hat{Q})$*

Proof. $(\hat{Q} - \lambda\mathbf{1})$ does not have an inverse if and only if $(\hat{Q} - \lambda\mathbf{1})\,|\lambda\rangle = 0$ for some $|\lambda\rangle \neq 0$ □

Definition 37. The eigenvalues form the point spectrum $\mathrm{Spec}_{point}(\hat{Q})$

Definition 38. If $D_{(\hat{Q}-\lambda\mathbf{1})^{-1}} \neq \mathcal{H}$ is dense in $\mathcal{H}$, then λ form the continuous spectrum $\mathrm{Spec}_{cont}(\hat{Q})$

Definition 39. If $D_{(\hat{Q}-\lambda\mathbf{1})^{-1}} \neq \mathcal{H}$ is not dense in $\mathcal{H}$, then λ form the residue spectrum $\mathrm{Spec}_{res}(\hat{Q})$.

Proposition 2.25. *If $\lambda \in \mathrm{Spec}_{cont}(\hat{Q}), \forall\epsilon > 0, \exists\,|\psi\rangle \in D_{\hat{Q}}, s.t.\ \ |||\psi\rangle|| = 1, \left|\left|(\hat{Q} - \lambda\boldsymbol{1})\,|\psi\rangle\right|\right| < \epsilon$*

Definition 40. $\lambda \in \mathrm{Spec}_{cont}(\hat{Q})$ are called approximate eigenvalues, and the $|q_\lambda\rangle$ that can be approximated by the above proposition are called approximate eigenvectors.

Remark. Approximate eigenvalues are not eigenvalues, and approximate eigenvectors are thus not vectors.

Proposition 2.26. $\mathrm{Spec}_{cont}(\hat{Q})$ *is always (piece-wise) continuous.*

Definition 41. $\mathrm{Spec}_{\hat{Q}} := \mathrm{Spec}_{point}(\hat{Q}) \cup \mathrm{Spec}_{cont}(\hat{Q}) \cup \mathrm{Spec}_{res}(\hat{Q})$

Remark. Consider the case where $\mathrm{Spec}_{\hat{Q}} = \mathrm{Spec}_{point}(\hat{Q})$, then we have an eigenbasis $\{|q_n\rangle\}_1^\infty$ where $\hat{Q}\,|q_n\rangle = q_n\,|q_n\rangle$. In which case $\mathbf{1} = \sum_{n=1}^\infty |q_n\rangle\langle q_n|$

Definition 42. Partial resolution of the identity is $\hat{E_N} := \sum_{n=1}^N |q_n\rangle\langle q_n|$

Definition 43. $\hat{P} = \hat{P}^\dagger$ is called a Projection if $\hat{P}^2 = \hat{P}$

Proposition 2.27. $(\hat{E_N})^2 = \hat{E_N}$ *and thus a projection.*

2.9 Continuous basis

Remark. If $\mathrm{Spec}_{\hat{Q}} = \mathrm{Spec}_{cont}(\hat{Q}) = J \subseteq \mathbb{R}$, we want to define some continuous eigenbasis $\{|q_\lambda\rangle\}_{\lambda\in J}$, which in shorthand is $\{|q\rangle\}_{q\in J}$, such that $\mathbf{1} = \int_J |q\rangle\langle q|\,dq$ and that $\langle q|q'\rangle = \delta(q-q')$. Now suppose that we have such a continuous eigenbasis, what should be its properties?

Definition 44. Given a continuous eigenbasis $\{|q\rangle\}_{q\in\mathbb{R}}$, define $\hat{E}(\lambda) := \int_{-\infty}^{\lambda} |q\rangle\langle q|\,dq$.

Proposition 2.28. *If $|q\rangle\langle q|$ is well-defined and continuous, then $\frac{d}{dq}\hat{E}(q) = |q\rangle\langle q|$*

Proposition 2.29. *If λ_1, λ_2 satisfies $\hat{Q}\,|\lambda_1\rangle = \lambda_1\,|\lambda_1\rangle, \hat{Q}\,|\lambda_2\rangle = \lambda_2\,|\lambda_2\rangle$, then $(\hat{Q} - \lambda_1\boldsymbol{1})\,|\lambda_2\rangle = (\lambda_2 - \lambda_1)\,|\lambda_2\rangle$. Namely, $\lambda_2 - \lambda_1$ is an eigenvalue of $\hat{Q} - \lambda_1\boldsymbol{1}$.*

Proposition 2.30. *$\forall\lambda \in \mathbb{R}, \hat{E}(\lambda)$ is a valid operator, in fact, the projection onto the null space of $(\hat{Q} - \lambda\boldsymbol{1})^+$, where $A^+ := \frac{1}{2}(\sqrt{A^2} + A)$.*

Proof. Notice that $\sqrt{A^2}$ effectively changes all negative eigenvalue to positive, i.e. if $A|\psi\rangle = \lambda|\psi\rangle$, then $\sqrt{A^2}|\psi\rangle = |\lambda||\psi\rangle$. Now if $\lambda \le 0, \frac{1}{2}(\sqrt{A^2}+A)|\psi\rangle = \frac{1}{2}(-\lambda+\lambda)|\psi\rangle = 0$, and if $\lambda > 0, \frac{1}{2}(\sqrt{A^2}+A)|\psi\rangle = \frac{1}{2}(\lambda+\lambda)|\psi\rangle = \lambda|\psi\rangle$. Thus A^+ eliminates all the negative eigenvalues to zero.
By the previous proposition, if $q < \lambda$ are (approximate) eigenvalues of $\hat{Q}$, then $q - \lambda < 0$ is an eigenvalue of $\hat{Q} - \lambda\mathbf{1}$ with eigenvector $|q\rangle$, thus $(\hat{Q}-\lambda\mathbf{1})^+|q\rangle = 0$.

Now $\forall |\psi\rangle \in \mathcal{H}, (\hat{Q}-\lambda\mathbf{1})\hat{E}_\lambda|\psi\rangle = (\hat{Q}-\lambda\mathbf{1})\int_{-\infty}^{\lambda}|q\rangle\langle q||\psi\rangle\, dq = \int_{-\infty}^{\lambda}\cancelto{0}{(\hat{Q}-\lambda\mathbf{1})|q\rangle}\langle q|\psi\rangle dq = 0$
Thus we have that $\mathrm{Im}(\hat{E}(\lambda)) \subseteq Null((\hat{Q}-\lambda\mathbf{1})^+)$.
In addition, it is a projection, since
$\hat{E}(\lambda)\hat{E}(\lambda) = \int_{-\infty}^{\lambda}|q\rangle\langle q|\, dq \int_{-\infty}^{\lambda}|q'\rangle\langle q'|\, dq' = \int_{-\infty}^{\lambda}\int_{-\infty}^{\lambda}\langle q|\cancelto{\delta(q-q')}{\langle q|q'\rangle}|q'\rangle\, dq'dq = \int_{-\infty}^{\lambda}|q\rangle\langle q|\, dq = \hat{E}(\lambda)$ ☐

Definition 45. Stieltjes integral

$$\int_a^b f(x)dm(x) := \lim_{\epsilon\to 0}\sum_{0}^{n-1} f(\tilde{x_i})(m(x_{i+1}) - m(x_i))$$

where $a = x_0 \le x_1 \le \ldots x_n = b$ is any partition with $|x_{i+1} - x_i| < \epsilon$, and $\tilde{x_i} \in [x_i, x_{i+1}]$

Proposition 2.31. *If $f(x)$ is bounded, $m(x)$ monotonously increases, and $m'(x)$ is Riemann integrable, then $\int_a^b f(x)dm(x) = \int_a^b f(x)m'(x)dx$*

Proposition 2.32. *If $|q\rangle\langle q|$ is well-defined and integrable, then*
$\int_{-\infty}^{\lambda} d\hat{E}(q) = \int_{-\infty}^{\lambda}\frac{d}{dq}\hat{E}(q)dq = \int_{-\infty}^{\lambda}|q\rangle\langle q|\, dq = \hat{E}(\lambda)$*, and* $\mathbf{1} = \int_{\mathbb{R}}|q\rangle\langle q|\, dq = \int_{\mathbb{R}} d\hat{E}(\lambda) = \lim_{\lambda\to\infty}\hat{E}(\lambda)$

Proposition 2.33. $\hat{E}(\lambda)\hat{E}(\lambda') = \int_{-\infty}^{\lambda}\hat{Q}|q\rangle\langle q|\, dq \int_{-\infty}^{\lambda'}\hat{Q}|q'\rangle\langle q'|\, dq' = \int_{-\infty}^{\lambda}\int_{-\infty}^{\lambda'}|q\rangle\cancelto{\delta(q-q')}{\langle q|q'\rangle}\langle q'|\, dq'dq = \int_{-\infty}^{\lambda} H(\lambda'-\lambda)|q\rangle\langle q|\, dq = H(\lambda-\lambda')\hat{E}(\lambda)$

Proposition 2.34. $\hat{Q}\hat{E}(\lambda) = \hat{Q}\int_{-\infty}^{\lambda}|q\rangle\langle q|\, dq = \int_{-\infty}^{\lambda}\hat{Q}|q\rangle\langle q|\, dq = \int_{-\infty}^{\lambda} q|q\rangle\langle q|\, dq = \int_{-\infty}^{\lambda} q d\hat{E}(q)$

Proposition 2.35. $\hat{Q} = \hat{Q}\int_{\mathbb{R}} d\hat{E}(q) = \int_{\mathbb{R}}\hat{Q}d\hat{E}(q) = \int_{\mathbb{R}}\hat{Q}|q\rangle\langle q|\, dq = \int_{\mathbb{R}} q|q\rangle\langle q|\, dq = \int_{\mathbb{R}} q d\hat{E}(q)$

Remark. However, it is not true that $|q\rangle\langle q|$ is well-defined and continuous. Indeed, $|q\rangle \notin \mathcal{H}$. Thus we need to consider reconstructing the previous results with $\hat{E}(\lambda)$ without using $|q\rangle\langle q|$.

Definition 46. Given an operator $\hat{Q}, \forall\lambda \in \mathbb{R}, \hat{E}(\lambda)$ is *defined* to be the projection onto the null space of $(\hat{Q}-\lambda\mathbf{1})^+$

Definition 47. We say that an operator $\hat{Q}$ has a continuous eigenbasis if the following holds:

1. The resolution of the identity: $\mathbf{1} = \int_{\mathbb{R}} d\hat{E}(q) = \lim_{\lambda\to\infty}\hat{E}(\lambda)$
2. The "orthonormality": $\hat{E}(\lambda)\hat{E}(\lambda') = H(\lambda-\lambda')\hat{E}(\lambda)$
3. The "eigenness": $\hat{Q}\hat{E}(\lambda) = \int_{-\infty}^{\lambda} q d\hat{E}(q)$

Remark. Although it is not true that $|q\rangle\langle q|$ is well-defined and continuous, the above definitions are well-defined and correspond to the behavior of an eigenbasis $\{|q\rangle\}_{\mathbb{R}}$ if it exists. Thus we can still use this notation for the sake of simplicity if we adopt the above definitions.

Definition 48. We say that an operator $\hat{Q}$ has a continuous eigenbasis $\{|q\rangle\}_{q\in\mathbb{R}}$ if the above definition47 holds. Notationally, we write $\hat{E}(\lambda)$ as $\int_{-\infty}^{\lambda}|q\rangle\langle q|\, dq$, and we treat $|q\rangle\langle q|$ as $\frac{d}{dq}\hat{E}(q)$, although it may not exists.

2.10 Spectral theorem

Theorem 2.36. *Spectral theorem for self-adjoint operator*
For a self-adjoint operator $\hat{f}, \exists$ *an orthonormal eigenbasis of* $\{|f_n\rangle, |f_\lambda\rangle : n \in \mathbb{N}, \lambda \in J \subseteq \mathbb{R}\}$, *s.t.*
$\hat{f}|f_n\rangle = f_n |f_n\rangle, \hat{f}|f_\lambda\rangle = f(\lambda)|f_\lambda\rangle, \boldsymbol{1} = \sum_{n=1}^{\infty} |f_n\rangle\langle f_n| + \int_J |f_\lambda\rangle\langle f_\lambda| \, d\lambda$, *where* $J = \mathrm{Spec}_{cont}(\hat{f}) \subseteq \mathbb{R}$.

Theorem 2.37. *Spectral theorem for unitary operator*
For a self-adjoint operator $\hat{u}, \exists$ *an orthonormal eigenbasis of* $\{|u_n\rangle, |u_\lambda\rangle : n \in \mathbb{N}, \lambda \in J\}$, *and* $u_n^* = u_n^{-1}$ *and thus are on the unit circle.*

Proof. $1 = \langle u_n|u_n\rangle = \langle u_n|\hat{u}^\dagger\hat{u}|u_n\rangle = \langle \hat{u}|u_n\rangle, \hat{u}|u_n\rangle\rangle = \langle u_n|u_n\rangle, u_n|u_n\rangle\rangle = u_n^* u_n \langle u_n|u_n\rangle = u_n^* u_n$ □

Definition 49. An operator $\hat{Q}$ is normal if $\hat{Q}^\dagger\hat{Q} = \hat{Q}\hat{Q}^\dagger$

Theorem 2.38. *Spectral theorem for self-adjoint operator*
An operator has an orthonormal eigenbasis if and only if its matrix representation is unitarily diagonalizable if and only if it is normal.

Proposition 2.39. *Self-adjoint and unitary operators are normal.*

Corollary 2.40. *The matrix a from def9 is not normal and thus not diagonalizable*

2.11 More Properties

Proposition 2.41. *For any operator f and any $|\psi\rangle \in \mathcal{H}s.t.$ $|\psi\rangle = 1$, we have $\langle\psi|f^\dagger f|\psi\rangle \geq \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$, and $\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle = ||f\,|\psi\rangle - \langle f\psi|\psi\rangle\,|\psi\rangle||^2$.*

Proof. First notice that by definition of the dagger operator, $\langle\psi|f^\dagger f|\psi\rangle = \langle f\,|\psi\rangle\,, f\,|\psi\rangle\rangle = ||f\,|\psi\rangle||\,,$
and $\langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle = \langle f\,|\psi\rangle\,, |\psi\rangle\rangle\,\langle|\psi\rangle\,, f\,|\psi\rangle\rangle = |\,\langle|\psi\rangle\,, f\,|\psi\rangle\rangle\,|^2 = |\langle\psi|f|\psi\rangle|^2$, both in $\mathbb{R}$.

By Cauchy-Schwarz2.1, we have that $\langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle = |\langle\psi|f|\psi\rangle|^2 \leq ||f\,|\psi\rangle||^2\,\cancelto{1}{||\psi||^2} = \langle\psi|f^\dagger f|\psi\rangle$
We have from the last theorem that

$$\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle = ||f\,|\psi\rangle||^2\,||\psi||^2 - |\langle\psi|f|\psi\rangle|^2 = \left|\left|\cancelto{1}{\psi} f\,|\psi\rangle - \frac{\langle f\psi|\psi\rangle}{\cancelto{1}{\psi}}\,|\psi\rangle\right|\right|^2 = ||f\,|\psi\rangle - \langle f\psi|\psi\rangle\,|\psi\rangle||^2$$

□

Lemma 2.42. *For any operator f, if $|\psi\rangle$ is an eigenvector such that $f\,|\psi\rangle = \lambda\,|\psi\rangle\,, |\psi\rangle = 1$, then $\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle = 4\,|\mathrm{Im}(\lambda)|^2$.*

Proof. We have from proposition2.41 that

$$\begin{aligned}
\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle &= ||f\,|\psi\rangle - \langle f\psi|\psi\rangle\,|\psi\rangle||^2 \\
&= ||\lambda\,|\psi\rangle - \langle\lambda\psi|\psi\rangle\,|\psi\rangle||^2 \\
&= \left|\left|\lambda\,|\psi\rangle - \bar{\lambda}\cancelto{1}{\langle\psi|\psi\rangle}\,|\psi\rangle\right|\right|^2 \\
&= \left|\left|\lambda\,|\psi\rangle - \bar{\lambda}\,|\psi\rangle\right|\right|^2 \\
&= ||2i\,\mathrm{Im}(\lambda)\,|\psi\rangle||^2 \\
&= |2i\,\mathrm{Im}(\lambda)|^2\,||\psi||^2 \\
&= 4\,|\mathrm{Im}(\lambda)|^2
\end{aligned}$$

□

Lemma 2.43. *For any operator f and any $|\psi\rangle \in \mathcal{H}s.t.$ $|\psi\rangle = 1$, we have $\langle\psi|f^\dagger f|\psi\rangle = \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$ if and only if $|\psi\rangle$ is an eigenvector with eigenvalue $\langle f\psi|\psi\rangle$*

Proof. Notice that from proposition2.41,
$\langle\psi|f^\dagger f|\psi\rangle = \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle \iff ||f\,|\psi\rangle - \langle f\psi|\psi\rangle\,|\psi\rangle||^2 = 0 \iff f\,|\psi\rangle = \langle f\psi|\psi\rangle\,|\psi\rangle$

□

Proposition 2.44. *For any operator f and any $|\psi\rangle \in \mathcal{H}s.t.$ $|\psi\rangle = 1$, we have $\langle\psi|f^\dagger f|\psi\rangle = \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$ if and only if $|\psi\rangle$ is an eigenvector with eigenvalue $\lambda \in \mathbb{R}$*

Proof. Forward direction: Assume that the equality holds,
By lemma2.43, $|\psi\rangle$ is an eigenvector with eigenvalue $\lambda = \langle f\psi|\psi\rangle$.
By lemma2.42, $4\,|\mathrm{Im}(\lambda)|^2 = 0$, thus $\lambda \in \mathbb{R}$.
Conversely, if $|\psi\rangle$ is an eigenvector with eigenvalue $\lambda \in \mathbb{R}$, by lemma2.42, the equality holds. □

Proposition 2.45. *For any operator f, if $\forall\,|\psi\rangle \in \mathcal{H}s.t.$ $|\psi\rangle = 1$, we have that $\langle\psi|f^\dagger f|\psi\rangle > \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$, then f can not have any real eigenvalues, namely, $\mathrm{Spec}_{point}(f) \cap \mathbb{R} = \emptyset$. The converse is also true.*

Proof. Suppose f has an eigenvalue $\lambda \in \mathbb{R}$ and eigenvector $|\psi\rangle \neq 0$, s.t. $f\,|\psi\rangle = \lambda\,|\psi\rangle$, then we can take $|\phi\rangle := \frac{|\psi\rangle}{||\psi||}$. Notice that $||\phi|| = 1$ and that $f\,|\phi\rangle = f\frac{|\psi\rangle}{||\psi||} = \frac{f|\psi\rangle}{||\psi||} = \frac{\lambda|\psi\rangle}{||\psi||} = \lambda\,|\phi\rangle$ is also an eigenvector with eigenvalue $\lambda \in \mathbb{R}$. By the previous proposition2.44, we have $\langle\psi|f^\dagger f|\psi\rangle = \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$, thus a contradiction.
Now for the Converse, let any $|\psi\rangle \in \mathcal{H}$s.t. $|\psi\rangle = 1$ be given.
From proposition2.41, we have that $\langle\psi|f^\dagger f|\psi\rangle \geq \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$.

Now suppose $\langle\psi|f^\dagger f|\psi\rangle = \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$, then it has a real eigenvalue, thus a contradiction.
Thus we have $\langle\psi|f^\dagger f|\psi\rangle > \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$. $\square$

Corollary 2.46. *For a self-adjoint operator f, and any state $|\psi\rangle \in \mathcal{H}, s.t.\ |\psi\rangle = 1$, we have $\Delta f := \sqrt{\overline{f^2(\psi)} - \overline{f(\psi)}^2} = 0$ if an only if it is an eigenstate $f|\psi\rangle = \lambda|\psi\rangle$.*

Proof. Since f is self-adjoint, we have
$\langle\psi|f^\dagger f|\psi\rangle = \langle\psi|f^2|\psi\rangle = \overline{f^2(\psi)}, \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle = \langle\psi|f|\psi\rangle\langle\psi|f|\psi\rangle = \overline{f(\psi)}^2$.
The forward direction is easy by proposition2.44.
For backward direction, let us assume it is an eigenstate, then we have $\langle\psi|f^2|\psi\rangle = \langle\psi|f\lambda|\psi\rangle = \langle\psi|\lambda^2|\psi\rangle = \lambda^2 = (\langle\psi|\lambda|\psi\rangle)^2 = \langle\psi|f|\psi\rangle^2$. $\square$

Corollary 2.47. *For a self-adjoint operator $f, \mathrm{Spec}_{point}(f) \subseteq \mathbb{R}$.*

Proof. This directly follows from the previous corollary and proposition2.44 $\square$

Lemma 2.48. *For any operator f,if $\lambda \in \mathrm{Spec}_{cont}(f)$, then $\forall|\psi\rangle \in \mathcal{H}, s.t.\ ||\psi|| = 1$, we have $\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle = ||\kappa||^2 + 2Re(2i\,\mathrm{Im}(\lambda)\langle\kappa|\psi\rangle - \langle\kappa|\psi\rangle\langle\kappa|\psi\rangle) + |2i\,\mathrm{Im}(\lambda) - \langle\kappa|\psi\rangle|^2$, where $|\kappa\rangle := (f - \lambda\mathbf{1})|\psi\rangle$.*

Proof.

$$\begin{aligned}
\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle &= ||f|\psi\rangle - \langle f\psi|\psi\rangle|\psi\rangle||^2 \\
&= ||(\lambda|\psi\rangle + |\kappa\rangle) - \langle(\lambda|\psi\rangle + |\kappa\rangle), \psi\rangle|\psi\rangle||^2 \\
&= \left|\left|(\lambda|\psi\rangle + |\kappa\rangle) - \left(\bar{\lambda}\cancelto{1}{\langle\psi,\psi\rangle} + \langle\kappa|\psi\rangle\right)|\psi\rangle\right|\right|^2 \\
&= |||\kappa\rangle + (2i\,\mathrm{Im}(\lambda) - \langle\kappa|\psi\rangle)|\psi\rangle||^2 \\
&= \langle|\kappa\rangle + \alpha|\psi\rangle, |\kappa\rangle + \alpha|\psi\rangle\rangle, \alpha := 2i\,\mathrm{Im}(\lambda) - \langle\kappa|\psi\rangle \\
&= \langle\kappa|\kappa\rangle + \bar{\alpha}\langle\psi|\kappa\rangle + \alpha\langle\kappa|\psi\rangle + \bar{\alpha}\alpha\cancelto{1}{\langle\psi|\psi\rangle} \\
&= ||\kappa||^2 + 2Re(\alpha\langle\kappa|\psi\rangle) + |\alpha|^2 \\
&= ||\kappa||^2 + 2Re(2i\,\mathrm{Im}(\lambda)\langle\kappa|\psi\rangle - \langle\kappa|\psi\rangle\langle\kappa|\psi\rangle) + |2i\,\mathrm{Im}(\lambda) - \langle\kappa|\psi\rangle|^2
\end{aligned}$$

$\square$

Proposition 2.49. *For any operator $f, \forall\lambda \in \mathrm{Spec}_{cont}(f)$, we always have an ϵ approximation, i.e. $\forall\epsilon > 0, \exists|\psi\rangle \in D_f, s.t.\ ||\psi|| = 1, ||(f - \lambda\mathbf{1})|\psi\rangle|| < \epsilon, \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle < \langle\psi|f^\dagger f|\psi\rangle < \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle + \epsilon$, if and only if $\lambda \in \mathbb{R}$.*

Proof. For backward direction, let's assume $\lambda \in \mathbb{R}$.
Take $\epsilon_0 = \min \frac{1}{2}\sqrt{\epsilon}, \epsilon > 0$, then we can find $|\psi\rangle \in D_f$, s.t. $||\psi|| = 1, ||(f - \lambda\mathbf{1})|\psi\rangle|| < \epsilon_0 \le \epsilon$ by proposition2.25
The first inequality is given by proposition2.41, proposition2.44, and the fact that $\lambda \in \mathrm{Spec}_{cont}$ and thus not an eigenvalue.
Now notice that we have $|\langle\kappa|\psi\rangle| \le ||\kappa||\cancelto{1}{||\psi||} = ||\kappa|| < \epsilon_0$. Since $\lambda \in \mathbb{R}$, we have $\mathrm{Im}(\lambda) = 0$, the equation in the previous lemma becomes:

$$\begin{aligned}
\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle &= ||\kappa||^2 + 2Re(2i\,\mathrm{Im}(\lambda)\langle\kappa|\psi\rangle - \langle\kappa|\psi\rangle\langle\kappa|\psi\rangle) + |2i\,\mathrm{Im}(\lambda) - \langle\kappa|\psi\rangle|^2 \\
&= ||\kappa||^2 + 2Re(-\langle\kappa|\psi\rangle\langle\kappa|\psi\rangle) + |-\langle\kappa|\psi\rangle|^2 \\
&\le ||\kappa||^2 + 2\left|\langle\kappa|\psi\rangle^2\right| + |\langle\kappa|\psi\rangle|^2 \\
&< \epsilon_0^2 + 2\epsilon_0^2 + \epsilon_0^2 \\
&= 4\epsilon_0^2 \\
&= \epsilon
\end{aligned}$$

This proves the second inequality and thus the backward direction.
For forward direction, let us assume for contradiction that $\lambda \notin \mathbb{R}, I := |\text{Im}(\lambda)| > 0$, but the ϵ approximation can always be achieved. Now take $\epsilon = \frac{\sqrt{128I^3+1}-1}{16I} > 0$, we have $|\psi\rangle \in D_f$, s.t. $||\psi|| = 1, ||\kappa|| = ||(f - \lambda\mathbf{1})|\psi\rangle|| < \epsilon, \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle < \langle\psi|f^\dagger f|\psi\rangle < \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle + \epsilon$. Then we have

$$
\begin{aligned}
&\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle \\
=&\,||\kappa||^2 + 2Re(\alpha\langle\kappa|\psi\rangle) + |\alpha|^2 \\
=&\,||\kappa||^2 + 2Re(2i\,\text{Im}(\lambda)\langle\kappa|\psi\rangle - \langle\kappa|\psi\rangle\langle\kappa|\psi\rangle) + |2i\,\text{Im}(\lambda) - \langle\kappa|\psi\rangle|^2 \\
\geq&\,||\kappa||^2 - 2\left|2i\,\text{Im}(\lambda)\langle\kappa|\psi\rangle - \langle\kappa|\psi\rangle^2\right| + |2i\,\text{Im}(\lambda) - \langle\kappa|\psi\rangle|^2 \\
\geq&\,||\kappa||^2 - 2\,|2i\,\text{Im}(\lambda)\langle\kappa|\psi\rangle| - 2\left|\langle\kappa|\psi\rangle^2\right| + |\langle\kappa|\psi\rangle|^2 + |2i\,\text{Im}(\lambda)|^2 - 2\,|2i\,\text{Im}(\lambda)\langle\kappa|\psi\rangle| \\
=&\,||\kappa||^2 - 4I\,|\langle\kappa|\psi\rangle| - 2\,|\langle\kappa|\psi\rangle|^2 + |\langle\kappa|\psi\rangle|^2 + 4I^2 - 4I\,|\langle\kappa|\psi\rangle| \\
=&4I^2 + ||\kappa||^2 - |\langle\kappa|\psi\rangle|^2 - 8I\,|\langle\kappa|\psi\rangle| \\
\geq&4I^2 - 8I\,|\langle\kappa|\psi\rangle| \\
\geq&4I^2 - 8I\,||\kappa||^2 \\
>&4I^2 - 8I\epsilon^2 \\
=&4I^2 - 8I\left(\frac{\sqrt{128I^3+1}-1}{16I}\right)^2 \\
=&\epsilon
\end{aligned}
$$

Thus a contradiction with $\langle\psi|f^\dagger f|\psi\rangle < \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle + \epsilon$. □

Remark. Intuitively, we see that $\langle\psi|f^\dagger f|\psi\rangle - \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle$ is bounded below by $4I^2 - 8I\,||\kappa||^2$, thus when $I = |\text{Im}(\lambda)|$ is nontrivial, the approximation of the inequality and the approximation of the eigenvector cannot both be arbitrarily good.

Proposition 2.50. *Given any self-adjoint operator* $f = f^\dagger, \forall\lambda \in \text{Spec}_{cont}(f), \forall\epsilon > 0, \exists\,|\psi\rangle \in D_f$, *s.t.* $||\psi|| = 1, ||(f - \lambda\boldsymbol{1})|\psi\rangle|| < \epsilon, \overline{f(\psi)}^2 < \overline{f^2(\psi)} < \overline{f(\psi)}^2 + \epsilon$

Proof. Let $\epsilon > 0$ be given, can find $|\psi\rangle \in D_f$, s.t. $||\psi|| = 1, ||(f - \lambda\mathbf{1})|\psi\rangle|| < \epsilon$ by proposition2.25
As usual, take $\kappa := (f - \lambda\mathbf{1})|\psi\rangle$
Then $\overline{f(\psi)}^2 = (\langle\psi|f|\psi\rangle)^2 = \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle = \langle\lambda\psi + \kappa, \psi\rangle\,\langle\psi, \lambda\psi + \kappa\rangle = (\bar{\lambda} + \langle\kappa|\psi\rangle)(\lambda + \langle\psi|\kappa\rangle) = |\lambda|^2 + 2Re(\lambda\langle\kappa|\psi\rangle) + |\langle\kappa|\psi\rangle|^2$
And $\overline{f^2(\psi)} = \langle\psi|f^2|\psi\rangle = \langle\psi|f^\dagger f|\psi\rangle = \langle\lambda\psi + \kappa, \lambda\psi + \kappa\rangle = |\lambda|^2 + 2Re(\lambda\langle\kappa|\psi\rangle) + ||\kappa||^2$
Thus $\overline{f^2(\psi)} - \overline{f(\psi)}^2 = ||\kappa||^2 - |\langle\kappa|\psi\rangle|^2 \leq ||\kappa||^2 < \epsilon$
This proves the second inequality.
The first inequality follows from $\lambda \in \text{Spec}_{cont}$ is not an eigenvalue and proposition2.41 and 2.44. □

Remark. In the case where f is self-adjoint, this says that if $\lambda \in \text{Spec}_{cont}(f)$, we can always find some approximate "eigenstate" from which we have Δf arbitrarily small.

Corollary 2.51. *For any operator f, we have* $\forall\lambda \in \text{Spec}_{cont}(f), \forall\epsilon > 0, \exists\,|\psi\rangle \in D_f$, *s.t.* $||\psi|| = 1, ||(f - \lambda\boldsymbol{1})|\psi\rangle|| < \epsilon, \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle < \langle\psi|f^\dagger f|\psi\rangle < \langle\psi|f^\dagger|\psi\rangle\langle\psi|f|\psi\rangle + \epsilon$, *if and only if* $\text{Spec}_{cont}(f) \subseteq \mathbb{R}$

Proof. This directly follows from the previous proposition2.49. If we have any $\lambda \in \text{Spec}_{cont}(f) \setminus \mathbb{R}$, then we do not have an approximation for it. And if we have any $\lambda \in \text{Spec}_{cont}(f) \subseteq \mathbb{R}$, we always have the approximation. □

Corollary 2.52. *For any self-adjoint operator f, we have* $\text{Spec}_{cont}(f) \subseteq \mathbb{R}$

3 Solving quantum problems in different basis

3.1 Position operator

Definition 50. However $a^\dagger a$ is diagonal, and we call the basis that gives this matrix representation $\{|E_n\rangle\}_0^\infty$
We thus have $\hat{a}$, s.t. $\hat{a}_{nm} = \langle E_n|a|E_m\rangle \delta_{n,m-1}\sqrt{m}$

Theorem 3.1. *For position operator $\hat{x}, \mathrm{Spec}(\hat{x}) = \mathbb{R}, \hat{x}\,|x\rangle = x\,|x\rangle\,, \boldsymbol{1} = \int_{-\infty}^{\infty} |x\rangle\,\langle x|\,dx$*

Proposition 3.2. *For $\hat{x} = L(a + a^\dagger)$ in $|E_n\rangle$ basis, $\hat{x}_{nm} = \langle E_n|\hat{x}|E_n\rangle = L(\delta_{n+1,m} + \delta_{n,m+1})\sqrt{\max\{m, n\}}$*
Namely, $[\hat{x}] = L\begin{pmatrix} 0 & \sqrt{1} & 0 & \dots & 0 \\ \sqrt{1} & 0 & \sqrt{2} & \dots & 0 \\ 0 & \sqrt{2} & \ddots & \ddots & 0 \\ \vdots & & \dots & & \vdots \end{pmatrix}$ *in the E_n basis.*
Now since $\hat{x}\,|x\rangle = x\,|x\rangle$, we have
$x\langle E_n|x\rangle = \langle E_n|\hat{x}|x\rangle = \langle E_n|\hat{x}\sum_{m=0}^{\infty}|E_m\rangle\,\langle E_m|\,x\rangle = \sum_{m=0}^{\infty}\langle E_n|\hat{x}\,|E_m\rangle\,\langle E_m|\,x\rangle = \sum_{m=0}^{\infty} x_{nm}\langle E_m|x\rangle$
Solving this equation gives $\langle E_n|x\rangle = \frac{e^{-\frac{x^2}{4L^2}}}{\sqrt{\sqrt{\pi}2^n n!}}H_n(\frac{x}{\sqrt{2}L})$, *where* $H_n(z) := (-1)^n e^{z^2}\frac{d^n}{dz^n}e^{-z^2}$
And notice that $|x\rangle = \sum_{n=0}^{\infty}|E_n\rangle\,\langle E_n|x\rangle = \sum_{n=0}^{\infty}|E_n\rangle\,\overline{\langle x|E_n\rangle}, |E_n\rangle = \int |x\rangle\,\langle x|E_n\rangle dx$

Definition 51. For the position continuous basis $\{|x\rangle\}_{x\in\mathbb{R}}$ and any $|\psi\rangle \in \mathcal{H}, \psi(x) := \langle x|\psi\rangle$ is the wave function.

Proposition 3.3. $|\psi\rangle = \boldsymbol{1}\,|\psi\rangle = \int_{\mathbb{R}}|x\rangle\,\langle x|\,|\psi\rangle\,dx = \int_{\mathbb{R}}\psi(x)\,|x\rangle\,dx$

Corollary 3.4. $\int_{\mathbb{R}}\psi^*(x)\psi(x) = \langle\psi|\psi\rangle < \infty$

Proposition 3.5. *Given some operator $\hat{f}, f(x, x') := \langle x|\hat{f}|x'\rangle$ is its integral kernel.*

Proposition 3.6. $\hat{f} = \boldsymbol{1}\hat{f}\boldsymbol{1} = \int_{\mathbb{R}}\int_{\mathbb{R}} f(x, x')\,|x\rangle\,\langle x'|\,dxdx'$

3.2 Momemtum operator

Proposition 3.7. *Suppose $\hat{p} = i\hbar\frac{1}{2L}(a^\dagger - a)$, then $\langle x|\hat{p}|x'\rangle = \sum_{n,m}\langle x|E_n\rangle\langle E_n|\hat{p}|E_m\rangle\langle E_m|x\rangle = i\hbar\frac{d}{dx'}\delta(x - x')$*

Proposition 3.8. *If $g \in L^2$ is continuous and differentiable, then*
$\int_{-\infty}^{\infty} g(x)\frac{d}{dx}\delta(x - a)dx = \cancelto{0}{g(x)\delta(x - a)|_{-\infty}^{\infty}} - \int_{\mathbb{R}} g'(x)\delta(x - a)dx = -g'(a)$ *since* $g(\pm\infty) = 0$

Proposition 3.9. *Suppose $\hat{p} = i\hbar\frac{1}{2L}(a^\dagger - a)$, consider $|\phi\rangle = \hat{p}\,|\psi\rangle$, then*

$$\begin{aligned}
\phi(x) &= \langle x|\phi\rangle \\
&= \int_{\mathbb{R}}\langle x|\hat{p}|x\rangle\langle x'|\psi\rangle dx' \\
&= \int_{\mathbb{R}} i\hbar\frac{d}{dx'}\delta(x - x')\psi(x)dx' \\
&= -\int_{\mathbb{R}} i\hbar\delta(x - x')\frac{d}{dx'}\psi(x)dx' \\
&= -i\hbar\frac{d}{dx}\psi(x)
\end{aligned}$$

Remark. Notationally, we use the short-hand $\hat{p}\psi(x) = -i\hbar\frac{d}{dx}\psi(x)$. Similarly, we have $\hat{x}\psi(x) = x\psi(x)$

Proposition 3.10. *Suppose $\hat{p} = i\hbar\frac{1}{2L}(a^\dagger - a)$, consider $\hat{p}\,|p\rangle = p\,|p\rangle\,, \psi_p(x) := \langle x|p\rangle$, then*

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{xp}{i\hbar}}$$

. In addition, $\mathrm{Spec}(p) = \mathbb{R}, \boldsymbol{1} = \int_{-\infty}^{\infty}|p\rangle\,\langle p|\,dp$ *gives a continuous eigenbasis.*

Proof.

$$
\begin{aligned}
p\psi_p(x) &= p\langle x|p\rangle \\
&= \langle x|\hat{p}|p\rangle \\
&= \int_{\mathbb{R}} \langle x|\hat{p}|x'\rangle\langle x'|p\rangle dx' \\
&= \int_{\mathbb{R}} i\hbar\frac{d}{dx'}\delta(x-x')\psi_p(x')dx' \\
&= -i\hbar\frac{d}{dx}\psi_p(x) \\
\implies \psi_p(x) &= Ne^{-\frac{xp}{i\hbar}}
\end{aligned}
$$

Take $N = \frac{1}{\sqrt{2\pi\hbar}}$, we have that $\langle p|p'\rangle = \delta(p-p')$ and $\mathrm{Spec}(p) = \mathbb{R}$ $\square$

3.3 Uncertainty relations

Theorem 3.11. *For observables* $\hat{f}, \hat{g}, \Delta f\Delta g \geq \frac{1}{2}\left|\langle\psi|\left[\hat{f},\hat{g}\right]|\psi\rangle\right|$

Proof. Let $|\phi\rangle := ((\hat{f}-\bar{f}\mathbf{1}) + i\alpha(\hat{g}-\bar{g}\mathbf{1}))\,|\psi\rangle\,, \alpha := -\frac{\langle\psi|i\left[\hat{f},\hat{g}\right]|\psi\rangle}{2(\Delta g)^2}$

$$
\begin{aligned}
\langle\phi|\phi\rangle &\geq 0 \\
\text{Thus } \langle\psi|(\hat{f}-\bar{f}\mathbf{1})^2|\psi\rangle + \alpha^2\langle\psi|(\hat{g}-\bar{g}\mathbf{1})^2|\psi\rangle + \alpha\langle\psi|i(\hat{f}\hat{g}-\hat{g}\hat{f})|\psi\rangle &\geq 0 \\
(\Delta f)^2 + \alpha^2(\Delta g)^2 + \langle\psi|i\left[\hat{f},\hat{g}\right]|\psi\rangle &\geq 0 \\
(\Delta f)^2 + (\Delta g)^2\left(\alpha + \frac{\langle\psi|i\left[\hat{f},\hat{g}\right]|\psi\rangle}{2(\Delta g)^2}\right)^2 &\geq \left(\frac{\langle\psi|i\left[\hat{f},\hat{g}\right]|\psi\rangle}{2(\Delta g)^2}\right)^2(\Delta g)^2 \\
(\Delta f)^2 &\geq \left(\frac{\langle\psi|i\left[\hat{f},\hat{g}\right]|\psi\rangle}{2(\Delta g)^2}\right)^2(\Delta g)^2 \\
(\Delta f)^2(\Delta g)^2 &\geq \frac{1}{4}\langle\psi|i\left[\hat{f},\hat{g}\right]|\psi\rangle^2 \\
\Delta f\Delta g &\geq \frac{1}{2}\left|\langle\psi|i\left[\hat{f},\hat{g}\right]|\psi\rangle\right|
\end{aligned}
$$

$\square$

Corollary 3.12. $\Delta x\Delta p \geq \frac{1}{2}\left|\langle\psi|i\hbar\boldsymbol{1}|\psi\rangle\right| = \frac{1}{2}\hbar$

Example 3.3.1. Note that we can determine the angle of a star if we know about its momentum in the x direction. Thus the uncertainty principle implies that the size of the opening restricts the sharpness of that image taken by a telescope.

Definition 52. $\left|\bar{f}\right|$ change observably if $\left|\overline{f(\Delta t + t_0)} - \overline{f(t_0)}\right| \geq \frac{1}{\Delta t}\int_{t_0}^{t_0+\Delta t}\Delta f(t)dt$. Δt is the minimum time that it takes for $\bar{f}(t)$ to change at least by $\overline{\Delta f}$, i.e. this inequality holds true.

Theorem 3.13. $\forall\hat{f}$ *and constant* $\hat{H}, \Delta t\Delta H \geq \frac{\hbar}{2}$

Proof.

$$\begin{aligned}
\Delta f(t)\Delta H &\geq \frac{1}{2}\left|\langle\psi|\left[\hat{f},\hat{H}\right]|\psi\rangle\right| \\
&= \frac{1}{2}\left|\langle\psi|i\hbar\frac{d}{dt}\hat{f}(t)|\psi\rangle\right| \\
&= \frac{\hbar}{2}\left|\frac{d}{dt}\langle\psi|\hat{f}(t)|\psi\rangle\right| \\
&= \frac{\hbar}{2}\left|\frac{d}{dt}\bar{f}(t)\right| \\
\int_{t_0}^{t_0+\Delta t}\Delta f(t)\Delta H dt &\geq \frac{\hbar}{2}\int_{t_0}^{t_0+\Delta t}\left|\frac{d}{dt}\bar{f}(t)\right| \\
&\geq \frac{\hbar}{2}\left|\int_{t_0}^{t_0+\Delta t}\frac{d}{dt}\bar{f}(t)\right| \\
&= \frac{\hbar}{2}\left|\bar{f}(t_0+\Delta t)-\bar{f}(t_0)\right| \\
\Delta H\Delta t = \Delta H\frac{\int_{t_0}^{t_0+\Delta t}\Delta f(t)dt}{\left|\bar{f}(t_0+\Delta t)-\bar{f}(t_0)\right|} &\geq \frac{\hbar}{2}
\end{aligned}$$

□

3.4 Equation of Motions

Proposition 3.14. *When $\hat{H}$ is a polynomial of $\hat{x}_i, \hat{p}_j$ of degree at most 2, then the EOM is of degree at most 1, then quantum predictions are the same as classical EOM. These systems are called "Gaussian".*

Remark. See example of free particle1.4.1

Example 3.4.1. harmonic oscillator1.4.2 $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{\alpha}{2}\hat{x}^2$.
Then the eigenstates are $\hat{H}|E_n\rangle = E_n|E_n\rangle, E_n := \hbar\omega(n+\frac{1}{2})$

3.5 Time Evolution Operator

Proposition 3.15. *Assume we find the solution $\hat{U}(t)$ to $i\hbar\frac{d}{dt}\hat{U}(t) = \hat{U}(t)\hat{H}(t)$ and $\hat{U}(t_0) = \mathbf{1}$, then*
$\hat{x}_i(t) = \hat{U}^\dagger(t)\hat{x}_i(t_0)\hat{U}(t), \hat{p}_j(t) = \hat{U}^\dagger(t)\hat{p}_j(t_0)\hat{U}(t), \hat{f}(t) = \hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)$

Proof. Claim: $i\hbar\frac{d}{dt}\hat{x}(t) = \left[\hat{x}(t),\hat{H}(t)\right], i.e. \frac{d}{dt}\hat{x}(t) = \left\{\hat{x}(t),\hat{H}(t)\right\}$

$$\begin{aligned}
i\hbar\frac{d}{dt}\hat{x}(t) &= i\hbar\frac{d}{dt}\left(\hat{U}^\dagger(t)\hat{x}(t_0)\hat{U}(t)\right) \\
&= i\hbar\left(\frac{d}{dt}\hat{U}^\dagger(t)\hat{x}(t_0)\hat{U}(t) + \hat{U}^\dagger(t)\hat{x}(t_0)\frac{d}{dt}\hat{U}(t)\right) \\
&= -\hat{H}(t)\hat{U}^\dagger(t)\hat{x}(t_0)\hat{U}(t) + \hat{U}^\dagger(t)\hat{x}(t_0)\hat{U}(t)\hat{H}(t) \\
&= -\hat{H}(t)\hat{x}(t) + \hat{x}(t)\hat{H}(t) \\
&= \left[\hat{x}(t),\hat{H}(t)\right]
\end{aligned}$$

Similar proof for $\hat{p}, \hat{f}$ □

Definition 53. The $\hat{U}(t)$ in the above proposition is called the Time Evolution Operator.

Definition 54. For an operator $\hat{f}, e^{\hat{f}} := \sum_{n=0}^{\infty}\frac{\hat{f}^n}{n!}$

Example 3.5.1. If $\hat{H}(t) = \hat{H}$ is constant, then $\hat{U}(t) = e^{\frac{\hat{H}}{i\hbar}(t-t_0)}$

Definition 55. The time-ordering operator $T\hat{H}(t_0)\hat{H}(t_1)\ldots\hat{H}(t_n) := \hat{H}(t_{i0})\hat{H}(t_{i1})\ldots\hat{H}(t_{in})$, s.t. $t_{i0} \leq t_{i1} \leq \ldots t_{in}$ orders $\{t_i\}_0^n$ from left to right.

Proposition 3.16. $T\left(\frac{d}{dt}\left(\int_{t_0}^t \hat{H}(t')dt'\right)^n\right) = nT\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t)$

Proof. Prove by induction on n.
Base case is n=0, then $\frac{d}{dt}\left(\int_{t_0}^t \hat{H}(t')dt'\right) = \hat{H}(t)$ by fundamental theorem of calculus.
Suppose $T\left(\frac{d}{dt}\left(\int_{t_0}^t \hat{H}(t')dt'\right)^m\right) = mT\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{m-1}\hat{H}(t)$ for all $m < n$, then

$$\begin{aligned}
T\left(\frac{d}{dt}\left(\int_{t_0}^t \hat{H}(t')dt'\right)^n\right) &= T\left(\int_{t_0}^t \hat{H}(t')dt'\frac{d}{dt}\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1} + \left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\frac{d}{dt}\int_{t_0}^t \hat{H}(t')dt'\right) \\
&= T\left(\int_{t_0}^t \hat{H}(t')dt' T\left(\frac{d}{dt}\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\right) + \frac{d}{dt}\int_{t_0}^t \hat{H}(t')dt'\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\right) \\
&= T\left(\int_{t_0}^t \hat{H}(t')dt'(n-1)\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1-1}\hat{H}(t) + \hat{H}(t)\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\right) \\
&= T\left(\int_{t_0}^t \hat{H}(t')dt'(n-1)T\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1-1}\hat{H}(t) + \left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t)\right) \\
&= T\left((n-1)\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t) + \left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t)\right) \\
&= nT\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t)
\end{aligned}$$

Thus by induction, this holds for any n. □

Proposition 3.17. *For $\hat{U} = Te^{\frac{1}{i\hbar}\int_{t_0}^t \hat{H}(t')dt'}$, it is the time evolution operator for $\hat{H}(t)$*

Proof.

$$\begin{aligned}
i\hbar\frac{d}{dt}\hat{U}(t) &= i\hbar\frac{d}{dt}\left(Te^{\frac{1}{i\hbar}\int_{t_0}^t \hat{H}(t')dt'}\right) \\
&= i\hbar\frac{d}{dt}\left(T\sum_{n=0}^{\infty}\frac{\left(\frac{1}{i\hbar}\int_{t_0}^t \hat{H}(t')dt'\right)^n}{n!}\right) \\
&= i\hbar\frac{d}{dt}(\mathbf{1}) + i\hbar\sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^n\frac{1}{n!}T\frac{d}{dt}\left(\int_{t_0}^t \hat{H}(t')dt'\right)^n \\
&= \sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^{n-1}\frac{1}{n!}nT\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t) \\
&= \sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^{n-1}\frac{1}{(n-1)!}T\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t) \\
&= \sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^{n-1}\frac{1}{(n-1)!}T\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t) \\
&= \sum_{n=0}^{\infty}\left(\frac{1}{i\hbar}\right)^{n}\frac{1}{n!}T\left(\int_{t_0}^t \hat{H}(t')dt'\right)^{n-1}\hat{H}(t) \\
&= \hat{U}(t)\hat{H}(t)
\end{aligned}$$

$\square$

Proposition 3.18. *The time evolution operator has the following properties:*

1. $\hat{U}(t)^\dagger = \hat{U}(t)^{-1}$ *is unitary.*
2. *If* $\hat{f}(t_0)^\dagger = \hat{f}(t_0)$ *is hermitian, then so is* $\hat{f}(t) = \hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)$.
3. *If* $[\hat{x}(t_0), \hat{p}(t_0)] = i\hbar\mathbf{1}$*, then* $[\hat{x}(t), \hat{p}(t)] = i\hbar\mathbf{1}$

3.6 Schrodinger's equation

Definition 56. The Schrodinger's state is $|\psi(t)\rangle := \hat{U}(t)|\psi\rangle$

Proposition 3.19.

$$\begin{aligned}
\overline{f(t)} &= \langle\psi|\hat{f}(t)|\psi\rangle \\
&= \langle\psi|\hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)|\psi\rangle \\
&= \left(\langle\psi|\,\hat{U}^\dagger(t)\right)\hat{f}(t_0)\left(\hat{U}(t)\,|\psi\rangle\right) \\
&= \langle\psi(t)|\hat{f}(t_0)|\psi(t)\rangle
\end{aligned}$$

Definition 57. $\hat{H}_S(t) := \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t)$

Theorem 3.20. *Schrodinger's Equation:* $i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}_S(t)|\psi(t)\rangle$

Proof.

$$\begin{aligned}
i\hbar\frac{d}{dt}|\psi(t)\rangle &= i\hbar\frac{d}{dt}\hat{U}(t)|\psi\rangle \\
&= \hat{U}(t)\hat{H}(t)|\psi\rangle \\
&= \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t)\hat{U}(t)|\psi\rangle \\
&= \hat{H}_S(t)|\psi(t)\rangle
\end{aligned}$$

$\square$

Proposition 3.21. $\hat{H}_s(\boldsymbol{x}(t), \boldsymbol{p}(t), t) = \hat{H}(\boldsymbol{x}(t_0), \boldsymbol{p}(t_0), t)$

Proof. Observe $\hat{p}(t)^2 = \hat{U}^\dagger(t)\hat{p}(t_0)\cancel{\hat{U}(t)\hat{U}^\dagger(t)}\hat{p}(t_0)\hat{U}(t) = \hat{U}^\dagger(t)\hat{p}(t_0)\hat{p}(t_0)\hat{U}(t) = \hat{U}^\dagger(t)\hat{p}(t_0)^2\hat{U}(t)$.
By induction, it is easy to see that $\hat{p}(t)^n = \left(\hat{U}^\dagger(t)\hat{p}(t_0)\hat{U}(t)\right)^n = \hat{U}^\dagger(t)\hat{p}^n(t_0)\hat{U}(t)$.
Same for $\hat{p}(t)^i\hat{x}(t)^j = \hat{U}^\dagger(t)\hat{p}^i(t_0)\hat{x}^i(t_0)\hat{U}(t)$.
Consider $\hat{H}(\mathbf{x}(t), \mathbf{p}(t), t) = \sum_{i,j=0}^n a(t)\hat{p}(t)^i\hat{x}(t)^j$

$$\begin{aligned}
\hat{H}_s(\mathbf{x}(t), \mathbf{p}(t), t) &= \hat{U}(t)\hat{H}(t)(\mathbf{x}(t), \mathbf{p}(t), t)\hat{U}^\dagger(t) \\
&= \hat{U}(t)\sum_{i,j=0}^n a(t)\hat{p}(t)^i\hat{x}(t)^j\hat{U}^\dagger(t) \\
&= \sum_{i,j=0}^n a(t)\hat{U}(t)\hat{U}^\dagger(t)\hat{p}^i(t_0)\hat{x}^j(t_0)\hat{U}(t)\hat{U}^\dagger(t) \\
&= \sum_{i,j=0}^n a(t)\hat{p}^i(t_0)\hat{x}^j(t_0) \\
&= \hat{H}(\mathbf{x}(t_0), \mathbf{p}(t_0), t)
\end{aligned}$$

$\square$

Definition 58. $\psi(x,t) := \langle x|\psi(t)\rangle$

Proposition 3.22. $i\hbar\frac{d}{dt}\psi(x,t) = \int_{-\infty}^{\infty}\langle x|\hat{H}_s(t)|x'\rangle\psi(x',t)dx'$

Proof. $i\hbar\frac{d}{dt}\psi(x,t) = \langle x|\, i\hbar\frac{d}{dt}\,|\psi(t)\rangle = \langle x|\,\hat{H}_S(t)\,|\psi(t)\rangle = \langle x|\,\hat{H}_S(t)\int_{\mathbb{R}}|x'\rangle\,\langle x'|\,dx'\,|\psi(t)\rangle = \int_{\mathbb{R}}\langle x|\hat{H}_s(t)|x'\rangle\psi(x',t)dx'$ □

Proposition 3.23.

$$i\hbar\frac{d}{dt}\hat{U}(t) = \hat{U}(t)\hat{H}(t) = \hat{U}(t)\hat{U}^{\dagger}(t)\hat{H}(t)\hat{U}(t) = \hat{H}_s(t)\hat{U}(t)$$

Example 3.6.1. Consider Harmonic oscillator1.4.2, with $\hat{H}(\hat{x},\hat{p},t) = \frac{\hat{p}^2(t)}{2m} + \frac{\alpha}{2}\hat{x}^2(t)$. Then we have

$$\begin{aligned}
i\hbar\frac{d}{dt}\psi(x,t) &= \int_{\mathbb{R}}\langle x|\frac{\hat{p}^2}{2m} + \frac{\alpha}{2}\hat{x}^2|x'\rangle\psi(x',t)dx' \\
&= \int_{\mathbb{R}}\langle x|\frac{\hat{p}^2}{2m}|x'\rangle\psi(x',t)dx' + \int_{\mathbb{R}}\frac{\alpha}{2}x'^2\langle x|x'\rangle\psi(x',t)dx' \\
&= \int_{\mathbb{R}}\langle x|\frac{\hat{p}^2}{2m}\int_{\mathbb{R}}|p\rangle\,\langle p|\,dp|x'\rangle\psi(x',t)dx' + \frac{\alpha}{2}\int_{\mathbb{R}}x'^2\langle x|x'\rangle\psi(x',t)dx' \\
&= \int_{\mathbb{R}}\int_{\mathbb{R}}\frac{p^2}{2m}\langle x|\,|p\rangle\,\langle p|\,|x'\rangle\psi(x',t)dx'dp + \frac{\alpha}{2}\int_{\mathbb{R}}x'^2\delta(x-x')\psi(x',t)dx' \\
&= \int_{\mathbb{R}}\frac{p^2}{2m}\langle x|x'\rangle\psi(x',t)dx' + \frac{\alpha}{2}x^2\psi(x,t) \\
&= \frac{p^2}{2m}\psi(x,t) + \frac{\alpha}{2}x^2\psi(x,t) \\
&= \left(\frac{p^2}{2m} + \frac{\alpha}{2}x^2\right)\psi(x,t)
\end{aligned}$$

Example 3.6.2. Consider any Hilbert basis $\{|b_n\rangle\}_{n=0}^{\infty}$, then

$$\begin{aligned}
i\hbar\langle b_n|\frac{d}{dt}|\psi(t)\rangle &= \langle b_n|\,\hat{H}_S(t)\,|\psi(t)\rangle \\
i\hbar\frac{d}{dt}\langle b_n|\psi(t)\rangle &= \sum_{m=0}^{\infty}\langle b_n|\,\hat{H}_S(t)\,|b_m\rangle\,\langle b_m|\,|\psi(t)\rangle \\
i\hbar\frac{d}{dt}\psi_n(t) &= \sum_{m=0}^{\infty}\hat{H}_S(t)_{nm}\psi_m(t)
\end{aligned}$$

Example 3.6.3. Consider $\hat{H}_s(t) = \frac{\hat{p}^2}{2m}$ in the $|p\rangle$ basis.

$$\begin{aligned}
i\hbar\frac{d}{dt}\psi(p,t) &= i\hbar\frac{d}{dt}\langle p|\psi(t)\rangle \\
&= \langle p|i\hbar\frac{d}{dt}|\psi(t)\rangle \\
&= \langle p|\,\hat{H}_S(t)\,|\psi(t)\rangle \\
&= \int_{\mathbb{R}}\langle p|\,\hat{H}_S(t)\,|p'\rangle\,\langle p'|\,|\psi(t)\rangle \\
&= \int_{\mathbb{R}}\langle p|\,\hat{H}_S(t)\,|p'\rangle\,\psi(p',t)dp' \\
&= \int_{\mathbb{R}}\frac{p'^2}{2m}\delta(p-p')\psi(p',t)dp' \\
&= \frac{p^2}{2m}\psi(p,t)
\end{aligned}$$

Proposition 3.24. *As in the previous remark3.2, we write the shorthand*

$$\hat{p}\psi(p,t) = p\psi(p,t); \hat{x}\psi(p,t) = i\hbar\frac{d}{dp}\psi(p,t); \hat{x}\psi(x,t) = x\psi(x,t); \hat{p}\psi(x,t) = -i\hbar\frac{d}{dx}\psi(x,t)$$

3.7 Dirac and interaction

Definition 59. Consider $\hat{H} = \hat{H}^{easy} + \hat{H}^{difficult}$, Dirac model let us apply Heisenberg to the $\hat{H}^e$, and Schrodinger to the $\hat{H}^d$.

Definition 60. $\hat{U}^e(t)$ is the time evolution operator for the easy part: $i\hbar\frac{d}{dt}\hat{U}^e(t) = \hat{H}^e_s(t)\hat{U}^e(t)$.

Definition 61. $\hat{U}'(t) = \hat{U}^{e\dagger}(t)\hat{U}(t)$, then we have $\hat{U}(t) = \hat{U}^e(t)\hat{U}'(t), \hat{U}^\dagger(t) = \hat{U}'^\dagger(t)\hat{U}^{e\dagger}(t)$.

Definition 62. $\hat{f}_D(t) := \hat{U}^{e\dagger}(t)\hat{f}(t_0)\hat{U}^e(t)$, and $|\psi(t)\rangle_D := \hat{U}'(t)\,|\psi\rangle$

Proposition 3.25. $\bar{f}(t) = \langle\psi|\,\hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)\,|\psi\rangle = \langle\psi|\,\hat{U}'^\dagger(t)\hat{U}^{e\dagger}(t)\hat{f}(t_0)\hat{U}^e(t)\hat{U}'(t)\,|\psi\rangle = \langle\psi(t)|_D\,\hat{f}_D(t)\,|\psi(t)\rangle_D$

Proposition 3.26. *$i\hbar\frac{d}{dt}\,|\psi(t)\rangle_D = \hat{H}^d_D(t)\,|\psi(t)\rangle_D$, where in $\hat{H}^d_D(\hat{x}_D(t), \hat{p}_D(t), t) := \hat{U}^{e\dagger}(t)\hat{H}^d_s(t)\hat{U}^e(t)$, we have $\hat{x}_D(t) = \hat{U}^{e\dagger}(t)\hat{x}(t_0)\hat{U}^e(t), \hat{p}_D(t) = \hat{U}^{e\dagger}(t)\hat{p}(t_0)\hat{U}^e(t)$.*

Proof. Start from

$$\begin{aligned}
i\hbar\frac{d}{dt}\hat{U}(t) &= \hat{H}_s(t)\hat{U}(t) \\
i\hbar\frac{d}{dt}\left(\hat{U}^e(t)\hat{U}'(t)\right) &= \hat{H}_s(t)\hat{U}^e(t)\hat{U}'(t) \\
i\hbar(\frac{d}{dt}\hat{U}^e(t)\hat{U}'(t) + \hat{U}^e(t)\frac{d}{dt}\hat{U}'(t)) &= \hat{H}_s(t)\hat{U}^e(t)\hat{U}'(t) \\
\hat{H}^e_s(t)\hat{U}^e(t)\hat{U}'(t) + i\hbar\hat{U}^e(t)\frac{d}{dt}\hat{U}'(t) &= \hat{H}^e_s(t)\hat{U}^e(t)\hat{U}'(t) + \hat{H}^d_s(t)\hat{U}^e(t)\hat{U}'(t) \\
i\hbar\hat{U}^e(t)\frac{d}{dt}\hat{U}'(t) &= \hat{H}^d_s(t)\hat{U}^e(t)\hat{U}'(t) \\
\hat{U}^{e\dagger}(t)i\hbar\hat{U}^e(t)\frac{d}{dt}\hat{U}'(t) &= \hat{U}^{e\dagger}(t)\hat{H}^d_s(t)\hat{U}^e(t)\hat{U}'(t) \\
i\hbar\frac{d}{dt}\hat{U}'(t)) &= \hat{H}^d_D(t)\hat{U}'(t) \\
i\hbar\frac{d}{dt}\hat{U}'(t)\,|\psi\rangle &= \hat{H}^d_D(t)\hat{U}'(t)\,|\psi\rangle \\
i\hbar\frac{d}{dt}\,|\psi(t)\rangle_D &= \hat{H}^d_D(t)\,|\psi(t)\rangle_D
\end{aligned}$$

□

Example 3.7.1. Consider $\hat{H} = \frac{\hat{p}^2(t)}{2m} + \frac{\alpha}{2}\hat{x}^2(t) + \beta\hat{x}^4$, then take $\hat{H}^e = \frac{\hat{p}^2(t)}{2m} + \frac{\alpha}{2}\hat{x}^2(t), \hat{H}^d = \beta\hat{x}^4$

4 Measurement

4.1 Basis measurement

Definition 63. Consider an observable $\hat{f} := \sum_n f_n |f_n\rangle \langle f_n|$, where $\{|f_n\rangle\}$ is the Hilbert basis by spectral theorem. Given a system in state $|\psi\rangle$, the probability of getting $|f_n\rangle$ in a measurement with respect to this basis is $|\langle f_n|\psi\rangle|^2$, and the result state is $\frac{\langle f_n|\psi\rangle}{|\langle f_n|\psi\rangle|} |f_n\rangle =$ normalized $\langle f_n|\psi\rangle |f_n\rangle$

Proposition 4.1. *The observable result of getting $|f_n\rangle$ is $f_n \in \mathbb{R}$*

Proposition 4.2. *For an eigenbasis $\{b_n\}$ for and operator $\hat{f}$, we have $\langle b_m| \hat{f} |b_n\rangle = \delta_{mn} \langle b_m| \hat{f} |b_m\rangle$, ans thus* $\bar{f} = \langle\psi| \hat{f} |\psi\rangle = \sum_m \langle\psi|b_m\rangle \langle b_m| \hat{f} \sum_n \langle b_n|\psi\rangle |b_n\rangle = \sum_m \sum_n \langle\psi|b_m\rangle\langle b_n|\psi\rangle \langle b_m| \hat{f} |b_n\rangle = \sum_m |\langle b_m|\psi\rangle|^2 \langle b_m| \hat{f} |b_m\rangle$

4.2 Projective measurement

Proposition 4.3. *Consider $\hat{f} := \sum_n f_n |f_n\rangle \langle f_n|$, where $\mathrm{Spec}(\hat{f}) = \{f_n\}$ are non-degenerate eigenvalue. Then for the projection $\hat{Q_m} := |f_m\rangle \langle f_m|$, we have $\bar{Q_m} = \langle\psi|\hat{Q_m}|\psi\rangle = \langle\psi|f_m\rangle\langle f_m|\psi\rangle = |\langle f_m|\psi\rangle|^2$ is the probability for finding f_n if the system was prepared in state $|\psi\rangle$*

Theorem 4.4. *Born's Rule*
If the system is in state $|\psi\rangle$, then the probability of finding state $|\phi\rangle$ is $|\langle\phi|\psi\rangle|^2$ by measuring $|\phi\rangle \langle\phi|$

Definition 64. For a (degenerate) eigenvalue f_m, with eigenstates $\{|f_{ma}\rangle\}_{a=1}^N$, then the projection onto the eigenspace of f_m is $\hat{Q_m} := \sum_{a=1}^N |f_{ma}\rangle \langle f_{ma}|$

Proposition 4.5. *The probability of finding $f_m = \bar{Q_m}$*

Proof. $\bar{Q_m} = \langle\psi|\hat{Q_m}|\psi\rangle = \langle\psi| \sum_{a=1}^N |f_{ma}\rangle \langle f_{ma}| \psi\rangle = \sum_{a=1}^N \langle\psi|f_{ma}\rangle\langle f_{ma}|\psi\rangle = \sum_{a=1}^N |\langle f_{ma}|\psi\rangle|^2 = \mathrm{Prob}(f_m)$ ∎

Definition 65. Similarly, we can define the projection $\int_J |c_\lambda\rangle \langle c_\lambda| \, d\lambda$ for a continuous basis. The probability of measuring a result in J is the expectation value of measuring this projection. $\langle\psi| \int_J |c_\lambda\rangle \langle c_\lambda| \, d\lambda \, |\psi\rangle = \int_J ||c_\lambda\rangle \langle c_\lambda| \, \psi|^2 \, d\lambda$

Example 4.2.1. The probability of finding the particle in $[-3, 4] = \int_{-3}^4 |\langle x|\psi\rangle|^2 \, dx = \int_{-3}^4 |\psi(x)|^2 \, dx$

Definition 66. For a projective measurement $\hat{Q}$, the state after the measurement is $|\psi_{after}\rangle = \frac{\hat{Q}}{||\hat{Q}|\psi\rangle||} |\psi\rangle$

Proposition 4.6. *If $\hat{Q} = |f_n\rangle \langle f_n|$, then the resulting state of projective measurement agrees with the basis measurement.*

Proof. $|\psi_{after}\rangle = \frac{|f_n\rangle\langle f_n|}{|||f_n\rangle\langle f_n||\psi\rangle||} |\psi\rangle = \frac{\langle f_n|\psi\rangle}{|\langle f_n|\psi\rangle| \cdot ||f_n||} |f_n\rangle = \frac{\langle f_n|\psi\rangle}{|\langle f_n|\psi\rangle|} |f_n\rangle =$ normalized $\langle f_n|\psi\rangle |f_n\rangle$ ∎

Corollary 4.7. *Projective measurement is a generalization of basis measurement.*

Remark. The measurement $\frac{\hat{Q}}{||\hat{Q}|\psi\rangle||}$ is not linear thus not unitary.

Remark. However, measurement is an outside factor to the system being measured, thus does not violate unitary evolution.

Proposition 4.8. *Two projective measurements are compatible (the order of measuring doe not matter) if and only if they commute.*

Definition 67. A set of commuting observables $\left\{\hat{f}^i\right\}$, i.e. $\forall i, j$, $\left[\hat{f}^i, \hat{f}^j\right] = 0$, is called maximal if every joint eigenspace is 1-dimensional.

4.3 Density Matrix

Definition 68. For a system, where $\{b_n\}$ is an orthonormal basis and the probability of being in $|b_n\rangle$ is μ_n, we define the density matrix to be $\hat{\rho} := \sum_n \mu_n |b_n\rangle \langle b_n|$

Definition 69. The trace of an operator $\hat{f}$ is defined to be $\sum_n \langle b_n| \hat{f} |b_n\rangle$ for any Hilbert basis $\{b_n\}$.

Proposition 4.9. *The trace defined above is basis independent, i.e. given any two Hilbert basis $\{b_n\}, \{c_m\}$, we always have $Tr(\hat{f}) = \sum_n \langle b_n| \hat{f} |b_n\rangle = \sum_m \langle c_m| \hat{f} |c_m\rangle$*

Proof.

$$
\begin{aligned}
Tr(\hat{f}) &= \sum_n \langle b_n| \hat{f} |b_n\rangle \\
&= \sum_n \langle b_n| \sum_m |c_m\rangle \langle c_m| \hat{f} \sum_k |c_k\rangle \langle c_k| |b_n\rangle \\
&= \sum_{n,m,k} \langle c_m| \langle b_n|c_m\rangle \hat{f} \langle c_k|b_n\rangle |c_k\rangle \\
&= \sum_{m,k} \langle c_m| \langle c_k| \sum_n |b_n\rangle \langle b_n|c_m\rangle \hat{f} |c_k\rangle \\
&= \sum_{m,k} \langle c_m| \langle c_k|c_m\rangle \hat{f} |c_k\rangle \\
&= \sum_{m,k} \langle c_m| \hat{f} |c_k\rangle \delta_{km} \\
&= \sum_m \langle c_m| \hat{f} |c_m\rangle
\end{aligned}
$$

□

Proposition 4.10. *$Tr(\hat{\rho}) = 1$ for any density matrix.*

Proof. Pick any basis, $Tr(\hat{\rho}) = \sum_n \langle b_n| \hat{\rho} |b_n\rangle = \sum_n \langle b_n| \sum_m \mu_m |b_m\rangle \langle b_m| |b_n\rangle = \sum_n \mu_n = 1$ □

Proposition 4.11. *If the system is in $|\psi\rangle = \sum_n \langle b_n|\psi\rangle |b_n\rangle$, where $\{b_n\}$ is an orthonormal basis, the density matrix is $\hat{\rho} = \sum_n |\langle b_n|\psi\rangle|^2 |b_n\rangle \langle b_n| = |\psi\rangle \langle\psi|$*

Proposition 4.12. *For a self-adjoint operator, $\bar{f} = Tr(\hat{\rho}\hat{f})$*

Proof. Pick the orthonormal basis $\{b_n\}$ for f_n. Thus,
$Tr(\hat{\rho}\hat{f}) = \sum_m \langle b_m| \hat{\rho}\hat{f} |b_m\rangle = \sum_m \langle b_m| \sum_n |\langle b_n|\psi\rangle|^2 |b_n\rangle \langle b_n| \hat{f} |b_m\rangle = \sum_m |\langle b_m|\psi\rangle|^2 \langle b_m| \hat{f} |b_m\rangle = \bar{f}$ □

Definition 70. If a density matrix $\hat{\rho}$ can be represented as $\hat{\rho} = |\psi\rangle \langle\psi|$, then it is a pure state. Otherwise, it is a mixed state.

Proposition 4.13. *Von Neumann equation*
For $\hat{\rho}(t_0) = \sum_n \rho_n |b_n\rangle \langle b_n|$, we have $i\hbar \frac{d}{dt}\hat{\rho}(t) = \left[\hat{H}_s(t), \hat{\rho}(t)\right]$

Proposition 4.14. *Measuring without reading the result does not change the density matrix.*

Remark. Any interaction with something out of the system might be some kind of measurement.

4.4 Information Theory

Definition 71. The Von Neumann entropy is $S[\hat{\rho}] := -Tr\left(\hat{\rho}\log_a(\hat{\rho})\right) = -\sum_n \rho_n \log_a(\rho_n)$ for any basis where $\hat{\rho} = \sum_n \rho_n |b_n\rangle\langle b_n|$.

Proposition 4.15. *$S[\hat{\rho}] \geq 0$, and the equality holds if and only if $\hat{\rho}$ is a pure state.*

Proposition 4.16. *If A and B are independent systems, and $\hat{\rho}_A \in A, \hat{\rho}_B \in B$, we have*
$S[\hat{\rho}_{AB}] = S[\hat{\rho}_A \otimes \hat{\rho}_B] = S[\hat{\rho}_A] + S[\hat{\rho}_B]$

Remark. If $a = 2$, then $S[\hat{\rho}]$ is the number of binary questions that can be asked to fix this system, and is the number of bits needed to clarify. If $a = d \in \mathbb{N}$, then $S[\hat{\rho}]$ is the number of "dits" needed to clarify. If $a = e$, then $S[\hat{\rho}]$ is the number of "nits" needed to clarify.

Example 4.4.1. Suppose we have a heat box at equilibrium, such that $\frac{d}{dt}\hat{\rho}(t) = 0$, and $\bar{E} = Tr\left(\hat{\rho}, \hat{H}\right) < \infty$.
Then $\hat{\rho}$ is the one that satisfies the two constraints, $Tr(\hat{\rho}) = 1$, and that $S[\hat{\rho}]$ is maximal.
Consider $Q(\rho, \mu, \lambda) := -Tr(\hat{\rho}\ln\hat{\rho}) - \mu(Tr(\hat{\rho}) - 1) - \lambda(Tr(\hat{\rho}\hat{H}) - \bar{E})$
Then $\frac{\partial Q}{\partial \lambda} = 0$ means $Tr(\hat{\rho}\hat{H}) = \bar{E}$, and $\frac{\partial Q}{\partial \mu} = 0$ means $Tr(\hat{\rho}) = 1$.
Notice that $\frac{d}{dt}\hat{\rho}(t) = 0$ means $\left[\hat{\rho}, \hat{H}\right] = 0$, which means $\hat{\rho}$ is diagonal in the energy eigenbasis.
Thus $Tr\left(\hat{\rho}\hat{H}_s\right) = \sum_n \langle b_n|\hat{\rho}\hat{H}_s|b_n\rangle = \sum_n \rho_n E_n$.
Thus $Q(\rho, \mu, \lambda) = -\sum_n \rho_n \log_a(\rho_n) - \mu(\sum_n \rho_n - 1) - \lambda(\sum_n \rho_n E_n - \bar{E})$
Thus $\frac{\partial Q}{\partial \rho_m} = 0 \implies -\ln\rho_m - 1 - \mu - \lambda E_m = 0$
Thus $\sum_m(-\ln\rho_m - 1 - \mu - \lambda E_m)|E_m\rangle\langle E_m| = -\ln(\hat{\rho}) - \mathbf{1} - \mu\mathbf{1} - \lambda\hat{H}_S = 0$
Let $\mu' := \mu + 1$, then $\hat{\rho} = \exp\left(-\lambda\hat{H}_S - \mu'\mathbf{1}\right) = \frac{1}{Tr(e^{-\lambda\hat{H}_s})}e^{-\lambda\hat{H}_S}$ since $Tr(\hat{\rho}) = 1$.
Also, $\hat{E} = Tr(\hat{\rho}\hat{H}_s) = \frac{1}{Tr(e^{-\lambda\hat{H}_s})}Tr(e^{-\lambda\hat{H}_S}\hat{H}_S)$, which makes λ unique. Indeed, $\lambda = \frac{1}{kT}$, where T is the temperature in Kelvin, and k is the Boltzmann constant.
Thus $\hat{\rho} = \frac{1}{Tr(\exp(-\frac{\hat{H}_s}{kT}))}e^{-\frac{\hat{H}_s}{kT}}$

5 Multiple systems

5.1 Tensor Product Space

Definition 72. A Heisenberg Cut separates the system in question and the rest of the universe.

Remark. When a measurement happens, it can be thought of as an interaction between the measured system and the system of the measurement apparatus. The combined system still follows unitary evolution.

Definition 73. Given two vector spaces V, W over $\mathbb{F}$, the free space is the vector space spanned by $V \times W$: $\mathcal{F}(V,W) := \mathbb{F}V \times \mathbb{F}W = \left\{\sum_{v\in V, w\in W} c_{vw}(v,w) : c_{vw} \in \mathbb{F}\right\}$

Definition 74. Let R be the subspace of $\mathcal{F}$, spanned by $\left\{\begin{matrix} (v_1+v_2,w)-(v_1,w)-(v_2,w), \\ (v,w_1+w_2)-(v,w_1)-(v,w_2), \\ (sv,w)-s(v,w), \\ (v,sw)-s(v,w), \end{matrix}\right\}$, then tensor space $V \otimes W$ is the quotient space $\mathcal{F}/R$. We also define $v \otimes w \in V \otimes W$ to be the equivalence class under this quotient equivalence. Namely, the above relations are set to zero.

Proposition 5.1. *The tensor product is bilinear. i.e.* $\forall v_1, v_2 \in V, w_1, w_2 \in W, s \in \mathbb{F}$,

$$\begin{aligned} (v_1+v_2)\otimes w &= v_1 \otimes w + v_2 \otimes w, \\ v \otimes (w_1+w_2) &= v \otimes w_1 + v \otimes w_2, \\ (sv)\otimes w &= s(v\otimes w), \\ v\otimes(sw) &= s(v\otimes w) \end{aligned}$$

Proposition 5.2. *Given two vector spaces V, W, then the tensor space $V \otimes W$ is spanned by $v \otimes w, v \in V, w \in W$.*

Definition 75. Consider $\langle -, \cdot \rangle_{AB} : (\mathcal{H}^A \otimes \mathcal{H}^B) \times (\mathcal{H}^A \otimes \mathcal{H}^B) \to \mathbb{C}$ by linearly extending $\langle |\psi_1\rangle \otimes |\phi_1\rangle, |\psi_2\rangle \otimes |\phi_2\rangle \rangle_{AB} := \langle \psi_1, \psi_2 \rangle_A \langle \phi_1, \phi_2 \rangle_B$

Proposition 5.3. $\langle -, \cdot \rangle_{AB}$ *is an inner product for $\mathcal{H}^A \otimes \mathcal{H}^B$, thus it is an inner product space.*

Definition 76. The Hilbert space $\mathcal{H}^{AB}$ is $\mathcal{H}^A \otimes \mathcal{H}^B$, completed under the induced distance $d_{AB}(v,w) := \sqrt{\langle v-w, v-w\rangle_{AB}}$

Proposition 5.4. $V \otimes W \cong W \otimes V$ *for any vector spaces V, W.*

Proposition 5.5. $V \otimes (W \otimes U) \cong (V \otimes W) \otimes U$ *for any vector spaces V, W.*

Proposition 5.6. $\mathbb{C} \otimes V \cong V$ *for any vector spaces V over $\mathbb{C}$.*

Definition 77. If $|\omega\rangle \in \mathcal{H}^{AB}$ can be written as $|\psi\rangle \otimes |\phi\rangle, |\psi\rangle \in \mathcal{H}^A, |\phi\rangle \in \mathcal{H}^B$, then it is an unentangled product state. Otherwise, it is called entangled.

5.2 Tensor Product of Operators

Definition 78. Consider two separate systems A, and B, where A is described by $\mathcal{H}^A$ with Hamiltonian $\hat{H}^A$, and B by $\mathcal{H}^B$ with Hamiltonian $\hat{H}^B$, each with their own observables. The combined system is described by $\mathcal{H}^{AB}$.

Definition 79. For $\hat{f} : \mathcal{H}^A \to \mathcal{H}^{A\prime}$, $\hat{g} : \mathcal{H}^B \to \mathcal{H}^{B\prime}$, then $\hat{f} \otimes \hat{g} : \mathcal{H}^{AB} \to \mathcal{H}^{AB\prime}$ is defined by $(\hat{f} \otimes \hat{g})(v \otimes w) := \hat{f}(v) \otimes \hat{g}(w)$

Proposition 5.7. $\forall \psi, \phi \in \mathcal{H}^A, \eta, \xi \in \mathcal{H}^B, (\langle\psi| \otimes \langle\eta|)(|\phi\rangle \otimes |\xi\rangle) = \langle\psi|\phi\rangle \otimes \langle\eta|\xi\rangle = \langle \psi \otimes \eta, \phi \otimes \xi \rangle_{AB}$

Proposition 5.8. *For any observable $\hat{f}^A$ of system A, then the same observable is in system AB, and is $\hat{f}^A \otimes \mathbf{1}$.*

Proof. Assume system A is in $|\psi\rangle$, and system B is in $|\phi\rangle$.
Then the system AB is in $|\psi\rangle \otimes |\phi\rangle$, then
$\overline{f^A \otimes \mathbf{1}} = \langle\psi| \otimes \langle\phi| \left(f^A \otimes \mathbf{1}\right) |\psi\rangle \otimes |\phi\rangle = \langle\psi| \otimes \langle\phi| \left((f^A |\psi\rangle) \otimes |\phi\rangle\right) = \langle\psi| f^A |\psi\rangle \langle\phi|\phi\rangle = \bar{f^A}$ ☐

Corollary 5.9. *For Hamiltonian $\hat{H}^A$ of system A, the Hamiltonian in system AB is $\hat{H}^A \otimes \mathbf{1}$. For Hamiltonian $\hat{H}^B$ of system B, the Hamiltonian in system AB is $\mathbf{1} \otimes \hat{H}^B$.*

Proposition 5.10. *$\forall \psi, \phi \in \mathcal{H}^A, \eta, \xi \in \mathcal{H}^B$, we have that $\langle \psi, (\mathbf{1}_A \otimes \langle\eta|) (|\phi\rangle \otimes |\xi\rangle)\rangle_A = (\langle\psi| \otimes \langle\eta|)(|\phi\rangle \otimes |\xi\rangle)$*

Proof.

$$
\begin{aligned}
(\langle\psi| \otimes \langle\eta|)(|\phi\rangle \otimes |\xi\rangle) &= \langle\psi|\phi\rangle\langle\eta|\xi\rangle \\
&= \langle\psi| \left(|\phi\rangle \langle\eta|\xi\rangle\right) \\
&= \langle\psi| \left((\mathbf{1}_A |\phi\rangle) \otimes \langle\eta| (|\xi\rangle)\right) \\
&= \langle\psi| \left((\mathbf{1}_A \otimes \langle\xi|) (|\phi\rangle \otimes |\xi\rangle)\right) \\
&= \langle\psi, (\mathbf{1}_A \otimes \langle\eta|) (|\phi\rangle \otimes |\xi\rangle)\rangle_A
\end{aligned}
$$

☐

Definition 80. The total Hamiltonian of the system AB is $\hat{H}^A \otimes \mathbf{1} + \mathbf{1} \otimes \hat{H}^B + \hat{H}_{interaction}$

5.3 Partial Trace and entanglement

Definition 81. Partial Trace
For $\hat{Q} : \mathcal{H}^{AB} \to \mathcal{H}^{AB}$, then $Tr_B(\hat{Q}) := \sum_n \langle b_n| \hat{Q} |b_n\rangle := \sum_n (\mathbf{1}_A \otimes \langle b_n|)\hat{Q}(\mathbf{1}_A \otimes |b_n\rangle) : \mathcal{H}^A \to \mathcal{H}^A$, for any Hilbert basis $\{b_n\}$ of $\mathcal{H}^B$. In other words, $\forall |\psi\rangle \in \mathcal{H}^A, Tr_B(\hat{Q}) |\psi\rangle := \sum_n \langle b_n| \hat{Q} |\psi\rangle |b_n\rangle := \sum_n (\mathbf{1}_A \otimes \langle b_n|) \hat{Q} (|\psi\rangle \otimes |b_n\rangle) \in \mathcal{H}^A$

Theorem 5.11. *Given $\hat{\rho}^{AB}$, we have $\hat{\rho}^A = Tr_B(\hat{\rho}^{AB}), \hat{\rho}^B = Tr_A(\hat{\rho}^{AB})$*

Proof. Consider any observable $\hat{f} : \mathcal{H}^A \to \mathcal{H}^A$

$$
\begin{aligned}
\overline{\hat{f}^A \otimes \mathbf{1}} &= \bar{f}^A \\
&= Tr(\hat{f}^A \hat{\rho}^A) \\
\overline{\hat{f}^A \otimes \mathbf{1}} &= Tr\left((\hat{f}^A \otimes \mathbf{1})\hat{\rho}^{AB}\right) \\
&= \sum_{n,m} \langle a_n| \langle b_m| \left((\hat{f}^A \otimes \mathbf{1})\hat{\rho}^{AB}\right) |a_n\rangle |b_m\rangle \\
&= \sum_{n,m} \left(\langle a_n| \langle b_m| (\hat{f}^A \otimes \mathbf{1})^\dagger\right) \left(\hat{\rho}^{AB} |a_n\rangle |b_m\rangle\right) \\
&= \sum_{n,m} \left(\langle a_n| (\hat{f}^A)^\dagger\right) \langle b_m| \hat{\rho}^{AB} |a_n\rangle |b_m\rangle \\
&= \sum_{n} \langle a_n| \hat{f}^A \sum_m \langle b_m| \hat{\rho}^{AB} |a_n\rangle |b_m\rangle \\
&= \sum_{n} \langle a_n| \hat{f}^A Tr_B(\hat{\rho}^{AB}) |a_n\rangle \\
&= Tr(\hat{f}^A Tr_B(\hat{\rho}^{AB}))
\end{aligned}
$$

☐

Proposition 5.12. *For any $|\Omega\rangle = \sum_n \Omega_n |\psi_n\rangle \otimes |\phi_n\rangle \in \mathcal{H}^{AB}$, if the total system AB is in pure state $\hat{\rho} = |\Omega\rangle \langle\Omega|$, then we have $\hat{\rho}^A = \sum_n \sum_{n'} \Omega_n \Omega^*_{n'} \langle\phi_{n'}|\phi_n\rangle |\psi_n\rangle \langle\psi_{n'}|$.*

Proof.

$$
\begin{aligned}
\hat{\rho}^A &= Tr_B(|\Omega\rangle\langle\Omega|) \\
&= Tr_B(\sum_n \Omega_n |\psi_n\rangle \otimes |\phi_n\rangle \sum_{n'} \Omega^*_{n'} \langle\psi_{n'}| \otimes \langle\phi_{n'}|) \\
&= \sum_m \langle b_m| \sum_n \Omega_n |\psi_n\rangle \otimes |\phi_n\rangle \sum_{n'} \Omega^*_{n'} \langle\psi_{n'}| \otimes \langle\phi_{n'}| \, |b_m\rangle \\
&= \sum_m \sum_n \sum_{n'} \Omega_n \Omega^*_{n'} |\psi_n\rangle \langle\psi_{n'}| \otimes (\langle b_m| \, |\phi_n\rangle \langle\phi_{n'}| \, |b_m\rangle) \\
&= \sum_n \sum_{n'} \Omega_n \Omega^*_{n'} |\psi_n\rangle \langle\psi_{n'}| \otimes (\langle\phi_{n'}| \cancelto{\mathbf{1}}{\sum_m |b_m\rangle\langle b_m|} \, |\phi_n\rangle) \\
&= \sum_n \sum_{n'} \Omega_n \Omega^*_{n'} \langle\phi_{n'}|\phi_n\rangle |\psi_n\rangle \langle\psi_{n'}|
\end{aligned}
$$

□

Theorem 5.13. *Assume that $\hat{\rho}^{AB} = |\Omega\rangle\langle\Omega|$ is pure, then the following are equal:*

$$|\Omega\rangle \text{ is unentangled} \tag{1}$$
$$\hat{\rho}^A \text{ is pure} \tag{2}$$
$$\mathcal{S}[\hat{\rho}^A] = 0 \tag{3}$$
$$\hat{\rho}^B \text{ is pure} \tag{4}$$
$$\mathcal{S}[\hat{\rho}^B] = 0 \tag{5}$$

Proof. We will show that (1) and (2) are equivalent.
Assume (1) is true, i.e. $|\Omega\rangle = |\psi\rangle \otimes |\phi\rangle \in \mathcal{H}^{AB}$ is pure, then $\hat{\rho}^A = \langle\phi|\phi\rangle |\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|$ is not entangled.
Assume (2) is true, i.e. $\hat{\rho}^A = |\psi\rangle\langle\psi|$ is not entangled. Now if we pick a Hilbert basis $\{\phi_n\}$ for $\mathcal{H}^B$, we will have $|\psi\rangle\langle\psi| = \sum_n \sum_{n'} \Omega_n \Omega^*_{n'} \langle\phi_{n'}|\phi_n\rangle |\psi_n\rangle\langle\psi_{n'}| = \sum_n |\Omega_n|^2 |\psi_n\rangle\langle\psi_n|$. Thus we must have one and only one of $\Omega_n = 1$, and the others zero. Without loss of generality, $|\psi_1\rangle = |\psi\rangle, \Omega_1 = 1$, and $|\Omega\rangle = |\psi\rangle \otimes |\phi_1\rangle$ is pure. □

Theorem 5.14. *Assume that $\hat{\rho}^{AB} = |\Omega\rangle\langle\Omega|$ is pure, then $\mathcal{S}[\hat{\rho}^A] = \mathcal{S}[\hat{\rho}^B]$*

Theorem 5.15. *Assume that $\hat{\rho}^{AB} = |\Omega\rangle\langle\Omega|$ is pure, then the eigenvalues of $\hat{\rho}^A$ and $\hat{\rho}^B$ are the same.*

Definition 82. The Purity of a state $\hat{\rho}$ is $\mathcal{P}[\hat{\rho}] := Tr(\hat{\rho}^2)$.

Proposition 5.16. $0 < \mathcal{P}[\hat{\rho}] \leq 1$

Proof. Let $\hat{\rho} = \sum_n p_n |e_n\rangle\langle e_n|, \sum_n p_n = 1$.
Then $\hat{\rho}^2 = \sum_n p_n^2 |e_n\rangle\langle e_n|$, and $\mathcal{P}[\hat{\rho}] = \sum_n p_n^2$.
Notice that $\forall n, 0 \leq p_n \leq 1$, thus $0 < \max(p_n)^2 \leq \sum_n p_n^2 \leq \sum_n p_n = 1$, and the equality holds only when exactly one of them is 1, and the others are all 0. □

Corollary 5.17. $\mathcal{P}[\hat{\rho}] = 1 \iff \hat{\rho}$ *is pure.*

Corollary 5.18. *The larger $\mathcal{S}[\hat{\rho}^A] = \mathcal{S}[\hat{\rho}^B]$, the smaller $\mathcal{P}[\hat{\rho}^A] = \mathcal{P}[\hat{\rho}^B]$, the more mixed are $\hat{\rho}^A, \hat{\rho}^B$, the more entangled is $\hat{\rho}^{AB}$*

6 Feynman's Picture

Suppose that at time t_0, a particle can be at any of a_i, and at time t_1, it can be at any of b_j. Notice that by classical statistic, $\mathcal{P}(b_j) = \sum_i \mathcal{P}(a_i \wedge b_j) = \sum_i \mathcal{P}(b_j|a_i)\mathcal{P}(a_i)$.
Consider a measurement $\hat{A}$ at t_1, where $\hat{A}\,|a_n\rangle = a_n\,|a_n\rangle$, and another measurement $\hat{A}$ at t_2, where $\hat{B}\,|b_m\rangle = b_m\,|b_m\rangle$. Notice that $\mathcal{P}(a_n) = |\langle a_n|\psi(t_1)\rangle|^2 = \left|\langle a_n|\hat{U}(t_1)|\psi_0\rangle\right|^2$. In addition, $\mathcal{P}(b_m|a_n) = \left|\langle b_m|\,\hat{U}(t_1,t_2)\,|a_n\rangle\right|^2$
Thus, $\mathcal{P}(a_n \wedge b_m) = \mathcal{P}(b_j|a_i)\mathcal{P}(a_i) = \left|\langle b_m|\,\hat{U}(t_1,t_2)\,|a_n\rangle\right|^2 \left|\langle a_n|\hat{U}(t_1)|\psi_0\rangle\right|^2 = \left|\langle b_m|\,\hat{U}(t_1,t_2)\,|a_n\rangle\,\langle a_n|\,\hat{U}(t_1)\,|\psi_0\rangle\right|^2$.
Thus $\mathcal{P}(b_m) = \sum_n \left|\langle b_m|\,\hat{U}(t_1,t_2)\,|a_n\rangle\,\langle a_n|\,\hat{U}(t_1)\,|\psi_0\rangle\right|^2$ if we don't care about the measurement $\hat{A}$.
On the other hand, if we did not perform $\hat{A}$, we have $\mathcal{P}(b_m) = \left|\langle b_m|\hat{U}(t_2)|\psi_0\rangle\right|^2 = \left|\langle b_m|\hat{U}(t_2,t_1)\hat{U}(t_1)|\psi_0\rangle\right|^2 = \left|\langle b_m|\hat{U}(t_2,t_1)\sum_n |a_n\rangle\,\langle a_n|\,\hat{U}(t_1)|\psi_0\rangle\right|^2$ which is different.

Definition 83. If the system is in state $|\psi\rangle$, the probability amplitude of finding state $|\phi\rangle$ is $\langle\phi|\psi\rangle \in \mathbb{C}$

Proposition 6.1. *The probability is the norm square of the probability amplitude.*

Theorem 6.2. *When there is no measurement, the probability amplitude should follow the same rules as classical probability.*