3.1.4 Density Matrices

$\psi \in \mathcal{H} := L^2(\mathbb{R}^{3N}; \mathbb{C}^{q^N}) \cong \bigotimes^N L^2(\mathbb{R}^3; \mathbb{C}^q)$

with $\|\psi\|_2^2 = \int |\psi(\underline{z})|^2 d\underline{z} = 1$ unit norm

Q orthogonal projection on $\mathcal{H}$

$$\Gamma_\psi : \mathcal{H} \to \mathcal{H}$$
$$\phi \mapsto \Gamma_\psi \phi$$

$$(\Gamma_\psi \phi)(\underline{z}) = (\psi, \phi)\, \psi(\underline{z})$$

where $(\psi, \phi) = \int \overline{\psi(\underline{z})}\, \phi(\underline{z})\, d\underline{z}$

Properties of $\Gamma_{\tilde\psi}$

- $\Gamma_{\tilde\psi}\Gamma_{\tilde\psi} = \Gamma_{\tilde\psi}$

$\because)$ $\Gamma_{\tilde\psi}\Gamma_{\tilde\psi}\phi = \Gamma((\tilde\psi, \phi)\tilde\psi)$

$= (\tilde\psi, (\tilde\psi, \phi)\tilde\psi)\tilde\psi$

$= (\tilde\psi, \phi)(\tilde\psi, \tilde\psi)\tilde\psi$ $\quad \|\tilde\psi\|_2 = 1$

$= (\tilde\psi, \phi)\tilde\psi = \Gamma_{\tilde\psi}\phi$ //

- $\Gamma_{\tilde\psi}^* = \Gamma_{\tilde\psi}$ (self-adjoint)

$\because)$ $(\phi', \Gamma_{\tilde\psi}\phi) = (\phi', (\tilde\psi, \phi)\tilde\psi)$

$= (\tilde\psi, \phi)(\phi', \tilde\psi)$

$= (\overline{(\phi', \tilde\psi)}\tilde\psi, \phi)$

$= ((\tilde\psi, \phi')\tilde\psi, \phi)$

$= (\Gamma_{\tilde\psi}\phi', \phi)$

$\forall \phi, \phi' \in \mathcal{H}$ //

- $(\phi, \Gamma_\psi \phi) \geq 0$ (positive semidefinite)

$\because)$ $(\phi, \Gamma_\psi \phi) = (\phi, (\psi, \phi)\psi)$

$= (\psi, \phi)(\phi, \psi)$

$= \overline{(\phi, \psi)}(\phi, \psi)$

$= |(\phi, \psi)|^2 \geq 0$

$\forall \phi \in \mathcal{H}$ //

- $\mathrm{Tr}\,\Gamma_\psi = 1$ (unit trace)

$\because)$ $\mathrm{Tr}\,\Gamma_\psi = \sum_\alpha (\phi_\alpha, \Gamma_\psi \phi_\alpha)$

$\forall \{\phi_\alpha\} \subseteq \mathcal{H}$ ONB

Here, $\phi_1 = \psi$, $(\psi, \phi_\alpha) = 0$ for $\alpha = 2, 3, \ldots$

$\Rightarrow \mathrm{Tr}\,\Gamma_\psi = (\psi, \Gamma_\psi \psi) + \sum_{\alpha \geq 2} (\phi_\alpha, \Gamma_\psi \phi_\alpha)$

$$\left(\begin{array}{l} \Gamma_\psi \psi = (\psi, \psi)\psi = \psi \\ \Gamma_\psi \phi_\alpha = (\psi, \phi_\alpha)\psi = 0 \end{array}\right.$$

$\therefore \mathrm{Tr}\,\Gamma_\psi = 1$ //

- $\Gamma_\psi \psi = 1\psi$ (eigenvalue 1)

$\because$) $\Gamma_\psi \psi = (\psi, \psi)\psi = \psi$ //

as previous property

Conversely,

Γ : pure state density matrix

$$\underset{\text{def}}{\Longleftrightarrow} \begin{cases} \Gamma(c\phi + c'\phi') = c\Gamma(\phi) + c'\Gamma(\phi') & \text{linear} \\ \Gamma^* = \Gamma & \text{self-adjoint} \\ (\phi, \Gamma\phi) \geq 0 & \text{positive semidifinite} \\ \mathrm{Tr}\,\Gamma = 1 & \text{unit trace} \\ \Gamma\psi = \psi & \text{one eigenvalue} = 1 \end{cases}$$

$$\Longrightarrow (\Gamma\phi)(z) = (\psi, \phi)\psi(\underline{z})$$

with $\Gamma\psi = \psi$.

Proof. $\{\phi_\alpha\} = \{\psi\} \cup \{\phi_1, \phi_2, \ldots\}$ ONB

$$1 = \operatorname{Tr}\Gamma = (\psi, \boxed{\Gamma\psi}) + \sum_j (\phi_j, \Gamma\phi_j)$$

($\Gamma\psi = \psi$)

$$= 1 + \sum_j (\phi_j, \Gamma\phi_j)$$

$$\therefore \sum_j (\phi_j, \Gamma\phi_j) = 0$$

$$(\phi_j, \Gamma\phi_j) \geq 0 \Rightarrow (\phi_j, \Gamma\phi_j) = 0$$

$$\therefore \Gamma\phi \in \operatorname{Span}\{\psi\}$$

$$\Rightarrow \exists c \in \mathbb{C}$$

$$\text{s.t. } (\Gamma\phi)(z) = c_\phi \psi(z)$$

($c_\phi = c_0(\psi, \phi)$)

$$(\Gamma\phi', \phi) = (\phi', \Gamma\phi)$$

$$\Rightarrow \frac{\overline{c_{\phi'}}}{\overline{(\psi, \phi')}} = \frac{c_\phi}{(\psi, \phi)} = c_0 \in \mathbb{C}$$

Constant

$$\phi' = \phi \Rightarrow \overline{c_0} = c_0 \Rightarrow c_0 \in \mathbb{R}$$

$$\Gamma\psi = c_\psi \psi = c_0(\psi, \psi)\psi = c_0\psi$$

$$= \psi$$

$$\therefore c_0 = 1$$

OK.

(general) density matrix ← wavefunction

✗ one eigenvalue $= 1$ dropped

$$0 \leq \Gamma \leq I, \quad \mathrm{Tr}\,\Gamma = 1$$

where $I : \psi \mapsto \psi$

i.e. $I\psi = \psi$

stronger than Γ : bdd $\Leftrightarrow \|\Gamma\psi\| \leq C\|\psi\|$

$\mathrm{Tr}\,\Gamma = 1$ & $\Gamma \geq 0$

$\Rightarrow \quad \Gamma \leq I$ i.e. $(\psi, \Gamma\psi) \leq (\psi, \psi)$

$\because$) $\forall \phi \in \mathcal{H}$ with $\|\phi\|_2 = 1$

$$1 = \mathrm{Tr}\,\Gamma = (\phi, \Gamma\phi) + \sum_j (\phi_j, \Gamma\phi_j)$$

$(\phi_j, \Gamma\phi_j) \geq 0$

$$\Rightarrow (\phi, \Gamma\phi) \leq 1 = (\phi, \phi)$$

$$\therefore \Gamma \leq I \quad //$$

In fact,

$$\begin{cases} \Gamma\psi_j = \lambda_j \psi_j, & \lambda_1 \geq \lambda_2 \geq \cdots \geq 0 \\ \{\psi_j\} : \text{ONB} & \sum_{j=1}^{\infty} \lambda_j = 1 \quad (= \mathrm{Tr}\,\Gamma) \\ \Gamma = \sum_{j=1}^{\infty} \lambda_j \Gamma_{\psi_j} & \end{cases}$$

eigenfunction expansion

Spectral theorem for <u>compact</u> self-adjoint operators

<u>Γ is compact</u>

$\because$) $\Gamma\phi = (\psi, \phi)\psi$

$\{\phi_n\} \subseteq \mathcal{H}$

$$\|\Gamma\phi_n - \Gamma\phi_m\|_2$$

$$= \|(\psi, \phi_n)\psi - (\psi, \phi_m)\psi\|$$

$$= \|((\psi, \phi_n) - (\psi, \phi_m))\psi\|$$

$$\leq |(\psi, \phi_n) - (\psi, \phi_m)| \cdot \|\psi\|_2$$

$$\longrightarrow 0 \quad \text{as Cauchy} \quad //$$