Γ : H^1 density matrix

$\overset{\text{def}}{\Longleftrightarrow}$ $\displaystyle\sum_{j=1}^{\infty} \lambda_j \|\nabla \psi_j\|_2^2 < \infty$

where $\psi_j \in H^1(\mathbb{R}^{3N}; \mathbb{C}^{2N})$

$\Gamma \psi_j = \lambda_j \psi_j \quad \forall j = 1, 2, \ldots$

$(\psi_j, \psi_k) = \delta_{jk}$

$\underset{\text{Condition}}{\overset{\text{stronger}}{\Longleftarrow}}$ $\left(\displaystyle\sum_{j=1}^{\infty} \lambda_j^2 \|\nabla \psi_j\|_2^2 < \infty \right)$

since $\lambda_j^2 \leq \lambda_j$

so $\displaystyle\sum_{j=1}^{\infty} \lambda_j^2 \|\nabla \psi_j\|_2^2 \leq \sum_{j=1}^{\infty} \lambda_j \|\nabla \psi_j\|_2^2$

$$\Gamma : L^2(\mathbb{R}^{3N}; \mathbb{C}^{2N}) \longrightarrow H^1(\mathbb{R}^{3N}; \mathbb{C}^{2N})$$

$$\phi \longmapsto \Gamma\phi$$

$$\Gamma\phi = \sum_{j=1}^{\infty} \lambda_j \Gamma_{\psi_j}\phi = \sum_{j=1}^{\infty} \lambda_j (\psi_j, \phi)\psi_j$$

Parseval's identity

$$\|f\|^2 = \sum_k |(f, \phi_k)|^2 \quad \text{for } \{\phi_k\} \text{ ONB}$$

$$\nabla(\Gamma\phi)(\underline{z}) = \sum_{j=1}^{\infty} \lambda_j (\psi_j, \phi) \nabla\psi_j(\underline{z})$$

$$\begin{aligned}
&\|\nabla(\Gamma\phi)\|^2 \\
&= \sum_k \Big| \sum_j \lambda_j (\psi_j, \phi)(\nabla\psi_j, \phi_k)\Big|^2 \\
&\le \sum_k \sum_j \lambda_j^2 |(\nabla\psi_j, \phi_k)|^2 \underbrace{\sum_j |(\psi_j, \phi)|^2}_{\|\phi\|^2} \\
&= \|\phi\|^2 \sum_j \lambda_j^2 \underbrace{\sum_k |(\nabla\psi_j, \phi_k)|^2}_{\|\nabla\psi_j\|^2} \\
&= \|\phi\|^2 \sum_j \lambda_j^2 \|\nabla\psi_j\|^2
\end{aligned}$$

$$\therefore \sum_j \lambda_j^2 \|\nabla\psi_j\|^2 < \infty \Rightarrow \Gamma\phi \in H^1 \quad //$$

c.f. $H^{1/2}$ density matrix

$$\underset{\text{def}}{\iff} \sum_{j=1}^{\infty} \lambda_j \| |\nabla|^{1/2} \psi_j \|_2^2 < \infty$$

$$\| |k|^{1/2} \hat{\psi}_j \|_2^2$$

$$\Gamma = \sum_{j=1}^{\infty} \lambda_j \Gamma_{\psi_j}$$

$$(\Gamma\psi)(\underline{z}) = \int \underbrace{\Gamma(\underline{z}, \underline{z}')}_{\text{kernel function}} \psi(\underline{z}')\, d\underline{z}'$$

(iii) Γ : self-adjoint $\Longrightarrow$ $\overline{\Gamma(\underline{z}, \underline{z}')} = \Gamma(\underline{z}', \underline{z})$

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

$$= \int_{\underline{z}} \left(\int_{\underline{z}'} \overline{\Gamma(\underline{z}, \underline{z}') \phi'(\underline{z}')\, d\underline{z}'} \right) \phi(\underline{z})\, d\underline{z}$$

$$= \iint \overline{\Gamma(\underline{z}, \underline{z}')}\ \overline{\phi'(\underline{z}')}\ \phi(\underline{z})\, d\underline{z}'\, d\underline{z}$$

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

$$= \int_{\underline{z}} \overline{\phi'(\underline{z})} \left(\int_{\underline{z}'} \Gamma(\underline{z}, \underline{z}') \phi(\underline{z}')\, d\underline{z}' \right) d\underline{z}$$

$$= \iint \Gamma(\underline{z}', \underline{z})\ \overline{\phi'(\underline{z}')}\ \phi(\underline{z})\, d\underline{z}\, d\underline{z}'$$

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

$$\Longrightarrow \quad \overline{\Gamma(\underline{z}, \underline{z}')} = \Gamma(\underline{z}', \underline{z}) \quad //$$

$\Gamma = \Gamma_\psi$: pure state

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

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

$$= \int \underbrace{\psi(\underline{z})\overline{\psi(\underline{z}')}}_{=\ \Gamma(\underline{z}, \underline{z}')} \phi(\underline{z}')\, d\underline{z}'$$

In general, $\Gamma = \sum_{j=1}^{\infty} \lambda_j \Gamma_{\psi_j}$

$$\sum_{j=1}^{N} \lambda_j \Gamma_{\psi_j} \phi(\underline{z})$$

$$= \int \sum_{j=1}^{N} \lambda_j \psi_j(\underline{z}) \overline{\psi_j(\underline{z}')} \cdot \phi(\underline{z}')\, d\underline{z}'$$

Exchange limits and integrals
(using the dominated convergence theorem)

$$(\Gamma\phi)(\underline{z}) = \lim_{N\to\infty} \sum_{j=1}^{N} \lambda_j (\psi_j, \phi)\, \psi_j(\underline{z})$$

$$= \lim_{N\to\infty} \sum_{j=1}^{N} \lambda_j \int \overline{\psi_j(\underline{z}')}\, \psi_j(\underline{z})\, \phi(\underline{z}')\, d\underline{z}'$$

$$= \lim_{N\to\infty} \int \sum_{j=1}^{N} \lambda_j \overline{\psi_j(\underline{z}')}\, \psi_j(\underline{z})\, \phi(\underline{z}')\, d\underline{z}'$$

$$\left| \sum_j \lambda_j \overline{\psi_j(\underline{z}')}\, \psi_j(\underline{z})\, \phi(\underline{z}') \right|$$

$$\leq \sum_j \lambda_j \left| \overline{\psi_j(\underline{z}')}\, \psi_j(\underline{z})\, \phi(\underline{z}') \right|$$

$$\leq \sum_j \lambda_j |\psi_j(\underline{z})| \cdot \frac{1}{2}\left(|\psi_j(\underline{z}')|^2 + |\phi(\underline{z}')|^2\right)$$

$$\therefore \int \left| \sum_{j=1}^{N} \lambda_j \overline{\psi_j(\underline{z}')}\, \psi_j(\underline{z})\, \phi(\underline{z}') \right| d\underline{z}'$$

$$\leq \frac{1}{2} \sum_{j=1}^{N} \lambda_j |\psi_j(\underline{z})| \int \left(|\psi_j(\underline{z}')|^2 + |\phi(\underline{z}')|^2\right) d\underline{z}'$$

$$= \frac{1}{2}\left(1 + \|\phi\|_2^2\right) \sum_{j=1}^{N} \lambda_j |\psi_j(\underline{z})|$$

$$\left| \sum_{j=1}^{N} \lambda_j |\psi_j(\underline{z})| \right|^2$$

$$= \left| \sum_{j=1}^{N} \lambda_j^{1/2} \cdot \lambda_j^{1/2} |\psi_j(\underline{z})| \right|^2$$

$$\leq \underbrace{\left(\sum_j \lambda_j \right)}_{=1} \sum_j \lambda_j |\psi_j(\underline{z})|^2$$

$$\therefore \int \left| \sum_{j=1}^{N} \lambda_j |\psi_j(\underline{z})| \right|^2 d\underline{z}$$

$$\leq \sum_j \lambda_j \underbrace{\int |\psi_j(\underline{z})|^2 d\underline{z}}_{=1}$$

$$= \sum_j \lambda_j = 1 \qquad \forall N$$

$$\therefore \sum_{j=1}^{N} \lambda_j \overline{\psi_j(\underline{z}')} \psi_j(\underline{z}) \phi(z') \in L^1$$

$$(\Gamma \phi)(\underline{z}) = \lim_{N \to \infty} \int \sum_{j=1}^{N} \lambda_j \overline{\psi_j(\underline{z}')} \psi_j(\underline{z}) \phi(\underline{z}') d\underline{z}'$$

$$= \int \underbrace{\lim_{N \to \infty} \sum_{j=1}^{N} \lambda_j \overline{\psi_j(z')} \psi_j(\underline{z})}_{= \Gamma(z, z') \text{ kernel}} \phi(\underline{z}') d\underline{z}'$$

$$\mathrm{Tr}\,\Gamma = \int \Gamma(\underline{z}, \underline{z})\, d\underline{z}$$

$$(\Gamma\psi)(\underline{z}) = \int \Gamma(\underline{z}, \underline{z}')\, \psi(\underline{z}')\, d\underline{z}'$$

$\Gamma(\underline{z}, \underline{z})$ is undefined for all $\underline{z} = (\underline{X}, \underline{\sigma})$

$(\underline{X}, \underline{X}) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N}$

Lebesgue measure zero in $\mathbb{R}^{6N}$

$\times$

$$\bigcirc \quad \Gamma(\underline{z}, \underline{z}) = \sum_{j=1}^{\infty} \lambda_j |\psi_j(\underline{z})|^2$$

diagonal part of Γ

In fact,

$$\mathrm{Tr}\,\Gamma = \int \sum_j \lambda_j |\psi_j(\underline{z})|^2\, d\underline{z}$$

$$= \sum_j \lambda_j \underbrace{\int |\psi_j(\underline{z})|^2\, d\underline{z}}_{= 1}$$

$$= \sum_j \lambda_j = 1$$

$$\operatorname{Tr} H\Gamma = \operatorname{Tr} \Gamma H$$
$$:= \sum_{j=1}^{\infty} \lambda_j \mathcal{E}(\psi_j)$$

where $\mathcal{E}(\psi) = (\psi, H\psi)$

for $\psi \in H^1(\mathbb{R}^{3N}; \mathbb{C}^{2^N})$

H: unbounded $\Longrightarrow$ $\operatorname{Tr} H$?

$$\sum_j \lambda_j |\mathcal{E}(\psi_j)| < \infty$$
$$\Longrightarrow \sum_j \lambda_j \mathcal{E}(\psi_j) \longrightarrow \operatorname{Tr} H\Gamma = \operatorname{Tr} \Gamma H$$

$$\inf \{ \mathcal{E}(\psi) ; (\psi, \psi) = 1 \}$$
$$= \inf \{ \mathcal{E}(\Gamma) = \sum_j \lambda_j \mathcal{E}(\psi_j) ; \Gamma : \text{density matrix} \}$$

$$\psi \mapsto \mathcal{E}(\psi) = (\psi, H\psi)$$

$\Gamma = \Gamma_\psi$: pure state

$$\mathcal{E}(\Gamma) = \sum_j \lambda_j \mathcal{E}(\psi_j) = 1 \cdot \mathcal{E}(\psi)$$ //

$$\mathcal{E}(\Gamma) = \sum_j \lambda_j \, \mathcal{E}(\Gamma_{\psi_j})$$

$$\geq \sum_j \lambda_j \cdot \inf\{\mathcal{E}(\psi) \mid (\psi, \psi) = 1\}$$

$$= \inf\{\mathcal{E}(\psi) \mid (\psi, \psi) = 1\}$$