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Last time we defined the orthogonal projectors $p^\varphi : L^2 \to L^2, \chi \mapsto \langle \varphi, \chi \rangle \varphi$ and $q^\varphi = \mathbb{1} - p^\varphi$.
p_j^φ and q_j^φ denote the projections in the j-th coordinate only.

Note that in "bra-ket" notation, we write $p^\varphi |\chi\rangle = |\varphi\rangle\langle\varphi|\chi\rangle$, i.e., $p^\varphi = |\varphi\rangle\langle\varphi|$.

p^φ tells us "how much" of the wave function is in the state φ. E.g., if $\varphi^\perp$ is orthogonal to φ, i.e., $\langle\varphi^\perp, \varphi\rangle = 0$, and $\chi := \frac{a}{\sqrt{a^2+b^2}}\varphi + \frac{b}{\sqrt{a^2+b^2}}\varphi^\perp$ s.t. $\|\chi\|^2 = \frac{a^2+b^2}{a^2+b^2} = 1$, then $\|p^\varphi \chi\| = \frac{a}{\sqrt{a^2+b^2}}$.

Next, we define a projection that measures "how much" of the N-body wave function is not in the state φ.

<u>Definition 4.3:</u> For $\varphi \in L^2$, $\|\varphi\| = 1$, we def. for any $0 \le k \le N$ the bounded operator

$$P_{N,k}^\varphi : L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N}), \quad P_{N,k} := \sum_{\vec{a} \in A_k} \prod_{j=1}^{N} (p_j^\varphi)^{1-a_j} (q_j^\varphi)^{a_j}, \text{ where}$$

$$A_k := \left\{ \vec{a} \in \{0,1\}^N : \sum_{j=1}^{N} a_j = k \right\}.$$

Example:
- $P_{N,0}^\varphi = p_1^\varphi \cdots p_N^\varphi$
- $P_{N,1}^\varphi = q_1^\varphi p_2^\varphi \cdots p_N^\varphi + p_1^\varphi q_2^\varphi p_3^\varphi \cdots p_N^\varphi + \ldots + p_1^\varphi \cdots p_{N-1}^\varphi q_N^\varphi = \sum_{m=1}^{N} q_m^\varphi \prod_{\substack{j=1 \\ j \neq m}}^{N} p_j^\varphi$
- $P_{N,N}^\varphi = q_1^\varphi \cdots q_N^\varphi$

Note: $P_{N,k}$ contains in each summand k q's and $(N-k)$ p's

Lemma 4.4: We have (i) $P^\varphi_{N,k}$ is an orthogonal projector for all $0 \le k \le N$,

(ii) $P^\varphi_{N,k} P^\varphi_{N,j} = 0$ for all $j \neq k$,

(iii) $\sum_{k=0}^{N} P^\varphi_{N,k} = \mathbb{1}$

(iv) $\sum_{k=0}^{N} \frac{k}{N} P^\varphi_{N,k} = \frac{1}{N} \sum_{j=1}^{N} q^\varphi_j$

Proof: HW 10.

We can now decompose the wave function as $\Psi_N = \sum_{k=0}^{N} P^\varphi_{N,k} \Psi_N$.

Then $\|P^\varphi_{N,k} \Psi_N\|^2$ is the probability for k particles not being in the state φ.

Thus, we define:

Definition 4.5: The expected relative number of particles not in the state φ is given by $\alpha(\Psi_N,\varphi) := \sum_{k=0}^{N} \frac{k}{N} \|P^\varphi_{N,k} \Psi_N\|^2$.

Corollary 4.6: For all symmetric $\Psi_N \in L^2(\mathbb{R}^{3N})$ and for all $\varphi \in L^2(\mathbb{R}^3)$,

$$\alpha(\Psi_N,\varphi) = \sum_{k=0}^{N} \frac{k}{N} \langle \Psi_N, P^\varphi_{N,k} \Psi_N \rangle = \frac{1}{N} \sum_{j=1}^{N} \langle \Psi_N, q^\varphi_j \Psi_N \rangle = \langle \Psi_N, q^\varphi_1 \Psi_N \rangle = \|q^\varphi_1 \Psi_N\|^2.$$

Proof: First equality follows directly from Lemma 4.4 (i), second from (iv) and third from Ψ_N symmetric.

Note:
- For $\Psi_N = \prod_{i=1}^{N} \varphi$, we have $\alpha(\Psi_N,\varphi) = \|q^\varphi_1 \prod_{i=1}^{N} \varphi\|^2 = 0$.
- For $\varphi^\perp$ with $\langle \varphi^\perp, \varphi \rangle = 0$, $\Psi_N = \prod_{i=1}^{N} \varphi^\perp$, we have $\alpha(\Psi_N,\varphi) = 1$.
- $0 \le \alpha(\Psi_N,\varphi) \le 1$ for $\|\Psi_N\| = 1 = \|\varphi\|$
- For $\Psi_N = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \prod_{\substack{i=1 \\ i\neq j}}^{N} \varphi(x_i) \varphi_\perp(x_j)$, we have $\alpha(\Psi_N,\varphi) = \frac{1}{N}$ (but $\|\Psi_N - \prod_{i=1}^{N} \varphi(x_i)\|_{L^2(\mathbb{R}^{3N})} = 2$).

Next, let us look at expressions of the type $\langle \Psi_N, A_1 \Psi_N \rangle$ more closely, where $A \in \mathcal{L}_\infty(L^2(\mathbb{R}^3))$, and A_1 denotes the action of A on variable x_1 only. We call A_1 a one-body operator. We want to ask the question: Can we approximate $\langle \Psi_N(t), A_1 \Psi_N(t) \rangle$ by its BEC mean value $\langle \varphi(t), A \varphi(t) \rangle$? E.g., for $A = \mathbb{1}_\Lambda$ ($\Lambda \subset \mathbb{R}^3$), $\langle \Psi_N(t), A_1 \Psi_N(t) \rangle$ is the probability for finding particle one (or any one of the particles by symmetry) in the region $\Lambda \subset \mathbb{R}^3$.

Definition 4.7.: For $\Psi_N \in L^2(\mathbb{R}^{3N})$, we define the reduced one-particle density matrix $\gamma_{\Psi_N}(x,y) := \int dx_2 \dots dx_N \, \overline{\Psi_N(y, x_2, \dots, x_N)} \, \Psi_N(x, x_2, \dots, x_N)$.

E.g., $\gamma_{\prod_{i=1}^N \varphi}(x,y) = \int dx_2 \dots dx_N \, \overline{\varphi(y)\varphi(x_2)\dots\varphi(x_N)} \, \varphi(x)\varphi(x_2)\dots\varphi(x_N) = \overline{\varphi(y)}\varphi(x)$.

Definition 4.8: For any $K \in \mathcal{S}'(\mathbb{R}^6)$, we define the integral operator

$A: \mathcal{S}(\mathbb{R}^3) \to \mathcal{S}'(\mathbb{R}^3)$, $f(x) \mapsto (Af)(x) := \int dy \, K(x,y) f(y)$. We call K the integral kernel of A.

E.g., the identity has integral kernel $K_{\mathbb{1}}(x,y) = \delta(x-y)$ (since $\int dy \, \delta(x-y) f(y) = f(x)$).

Thus, we can define γ_{Ψ_N} as the operator with integral kernel $\gamma_{\Psi_N}(x,y)$.

Lemma 4.9: γ_{Ψ_N} has the following properties:

(i) $\gamma_{\Psi_N} \in \mathcal{L}_\infty(L^2(\mathbb{R}^3))$, $\|\gamma_{\Psi_N}\|_\infty \leq 1$, $\gamma_{\Psi_N}^* = \gamma_{\Psi_N}$

(ii) γ_{Ψ_N} is non-negative, i.e., $\langle \chi, \gamma_{\Psi_N} \chi \rangle \geq 0 \quad \forall \chi \in L^2(\mathbb{R}^3)$

Proof of lemma 4.9:

(i) $\left|\int dy\, \gamma_{\psi_N}(x,y)\, \chi(y)\right| = \left|\int dx_2 \dots dx_N \int dy\, \chi(y)\, \overline{\psi_N(y,x_2,\dots,x_N)}\, \psi_N(x,x_2,\dots,x_N)\right|$

$$\leq \int dx_2 \dots dx_N\, dy\, |\psi_N(y,x_2,\dots,x_N)|\, |\chi(y)|\, |\psi_N(x,x_2,\dots,x_N)|$$

Cauchy-Schwarz
$$\leq \left(\int dy\, dx_2 \dots dx_N\, |\psi_N(y,x_2,\dots,x_N)|^2\right)^{\frac{1}{2}} \left(\int dy\, dx_2 \dots dx_N\, |\chi(y)|^2 |\psi_N(x,x_2,\dots,x_N)|^2\right)^{\frac{1}{2}}$$

$$= \|\psi_N\|\, \|\chi\| \underbrace{\left(\int dx_2 \dots dx_N\, |\psi_N(x,x_2,\dots,x_N)|^2\right)^{\frac{1}{2}}}_{\in L^2(\mathbb{R}^3)}$$

$\Rightarrow \|\gamma_{\psi_N}\chi\|_{L^2} \leq \|\chi\|$ $(\|\psi_N\| = 1)$, so $\|\gamma_{\psi_N}\|_{\mathcal{L}} \leq 1$.

$\gamma_{\psi_N}^* = \gamma_{\psi_N}$ clear from def.

(ii) $\langle \chi, \gamma_{\psi_N}\chi\rangle = \int dy\, \overline{\psi_N(y,x_2,\dots,x_N)}\, \chi(y) \int dx\, \overline{\chi(x)}\, \psi_N(x,x_2,\dots,x_N) = \langle \psi_N, p_1^\chi \psi_N\rangle$

$$= \|p_1^\chi \psi_N\|^2 \geq 0.$$

$\square$

Finally, we establish a relation between $\gamma_{\psi_N} - \overbrace{\gamma_{\prod_{i=1}^N \varphi}}^{=p^\varphi}$ and $\alpha(\psi_N,\varphi)$:

Lemma 4.10: For any symmetric $\psi_N \in L^2(\mathbb{R}^{3N})$, $\varphi \in L^2(\mathbb{R}^3)$ with $\|\psi_N\| = 1 = \|\varphi\|$, we have

$$\alpha(\psi_N,\varphi) \leq \|\gamma_{\psi_N} - p^\varphi\|_{\mathcal{L}} \leq 4\sqrt{\alpha(\psi_N,\varphi)}.$$

Proof: Note that $p^\varphi + q^\varphi = \mathbb{1}$ by def., so we can decompose

$$\gamma_{\psi_N} = (p^\varphi + q^\varphi)\, \gamma_{\psi_N} (p^\varphi + q^\varphi)$$

$$= \underbrace{p^\varphi \gamma_{\psi_N} p^\varphi}_{\substack{= p^\varphi \langle \varphi, \gamma_{\psi_N}\varphi\rangle \\ = p^\varphi \langle \psi_N, p_1^\varphi \psi_N\rangle = p^\varphi - p^\varphi \langle \psi_N, q_1^\varphi \psi_N\rangle}} + p^\varphi \gamma_{\psi_N} q^\varphi + q^\varphi \gamma_{\psi_N} p^\varphi + q^\varphi \gamma_{\psi_N} q^\varphi$$

$$\Rightarrow \|\gamma_{\psi_N} - p^\varphi\|_{\mathcal{L}} = \| -p^\varphi \langle \psi_N, q_1^\varphi \psi_N\rangle + p^\varphi \gamma_{\psi_N} q^\varphi + q^\varphi \gamma_{\psi_N} p^\varphi + q^\varphi \gamma_{\psi_N} q^\varphi \|_{\mathcal{L}}$$

$$\leq \underbrace{\|p^\varphi\|_{\mathcal{L}}}_{\leq 1} \underbrace{\langle \psi_N, q_1^\varphi \psi_N\rangle}_{\substack{= \|q_1^\varphi \psi_N\|^2 \\ = \alpha(\psi_N, \varphi)}} + \underbrace{\|p^\varphi \gamma_{\psi_N} q^\varphi\|_{\mathcal{L}}}_{\leq \underbrace{\|p^\varphi \psi_N\|}_{\leq 1} \underbrace{\|q^\varphi \psi_N\|}_{= \sqrt{\alpha(\psi_N, \varphi)}} \text{ as in proof of Lemma 4.9}} + \|q^\varphi \gamma_{\psi_N} p^\varphi\|_{\mathcal{L}} + \|q^\varphi \gamma_{\psi_N} q^\varphi\|_{\mathcal{L}}$$

$$\leq 2 \underbrace{\alpha(\psi_N, \varphi)}_{\leq \sqrt{\alpha(\psi_N, \varphi)} \text{ since } 0 \leq \alpha(\psi_N, \varphi) \leq 1} + 2\sqrt{\alpha(\psi_N, \varphi)}$$

$$\leq 4\sqrt{\alpha(\psi_N, \varphi)}$$

Also:

$$\alpha(\psi_N, \varphi) = \|q_1^\varphi \psi_N\|^2 = 1 - \|p_1^\varphi \psi_N\|^2 = 1 - \langle \varphi, \gamma_{\psi_N} \varphi\rangle = \langle \varphi, (p^\varphi - \gamma_{\psi_N})\varphi\rangle \leq \|p^\varphi - \gamma_{\psi_N}\|_{\mathcal{L}}.$$

$\square$

So in particular: $\alpha(\psi_N, \varphi) \xrightarrow{N\to\infty} 0 \iff \|\gamma_{\psi_N} - p^\varphi\|_{\mathcal{L}} \xrightarrow{N\to\infty} 0$.

Next time we will prove that indeed $\alpha(\psi_N(t), \varphi(t)) \xrightarrow{N\to\infty} 0 \quad \forall t \in \mathbb{R}$.