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M. Manybody QM

11. Many-body quantum mechanics

•) We will consider quantum systems that consist of many (say, N) quantum particles which are described by a N-body wave function

$$\varphi_N(x_1, x_2, \dots, x_N), \quad x_i \in \mathbb{R}^d$$

$\varphi_N \in L^2(\mathbb{R}^{dN})$.

•) total energy — Self-adjoint Hamiltonian H_N

$$H_N = \sum_{i=1}^{N} h_i + \sum_{1 \le i < j \le N} W_{ij}$$

Here h_i is the copy of the operator h on $L^2(\mathbb{R}^d)$ acting on the i-th variable $x_i \in \mathbb{R}^d$, namely

$$h_i = \mathbb{1} \otimes \dots \otimes \mathbb{1} \otimes \underbrace{h}_{i\text{-th variable}} \otimes \mathbb{1} \dots \otimes \mathbb{1}$$

Similarly for the two-body interaction W_{ij}.

•) ground state energy

$$E_N = \inf_{\|\varphi\| = 1} \langle \varphi, H_N \varphi \rangle$$

•) If ground state exists it satisfies $H_N \varphi = E_N \varphi$

Bosons and fermions:

- •) bosonic wave function is symmetric:

$\forall i \neq j \quad \varphi(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = \varphi(x_1, \dots, x_j, \dots, x_i, \dots, x_N)$

- •) fermionic wave function is antisymmetric:

$\forall i \neq j \quad \varphi(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = - \varphi(x_1, \dots, x_j, \dots, x_i, \dots, x_N)$

Examples:

- •) If $\varphi \in L^2(\mathbb{R}^d)$, then

$$\psi(x_1, \dots, x_N) = \varphi(x_1) \dots \varphi(x_N) \text{ is a bosonic}$$

N-particle wave function (product state or Hartree state)

- •) Slater determinants

For any functions $\{u_i\}_{i=1}^N$ in $L^2(\mathbb{R}^d)$, define

$$(u_1 \wedge u_2 \wedge \dots \wedge u_N)(x_1, \dots, x_N) := \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \operatorname{sign}(\sigma) u_1(x_{\sigma(1)}) \dots u_N(x_{\sigma(N)})$$

$$= \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \operatorname{sign}(\sigma) u_{\sigma(1)}(x_1) \dots u_{\sigma(N)}(x_N)$$

$$= \frac{1}{\sqrt{N!}} \det \left[(u_i(x_j))_{1 \leq i,j \leq N} \right].$$

Clearly, this is an antisymmetric function in $L^2(\mathbb{R}^{dN})$.

In fact, it is an orthonormal basis for $L^2_a(\mathbb{R}^{dN})$ the subspace of antisymmetric functions in $L^2(\mathbb{R}^{dN})$.

Thm Let $\{u_i\}_{i=1}^{\infty}$ be an orthonormal basis of $L^2(\mathbb{R}^d)$. Then the Slater determinants

$$S(\{u_i\}) \equiv \{u_{i_1} \wedge \dots \wedge u_{i_N} : i_1, \dots, i_N \in \mathbb{N},\ i_1 < \dots < i_N\}$$

form an orthonormal basis of $L^2_a(\mathbb{R}^{dN})$.

Proof: •) Step 1

First we check that $S(\{u_i\})$ are orthonormal functions in $L^2_a(\mathbb{R}^{dN})$. For $i_1 < \dots < i_N$ and $j_1 < \dots < j_N$ we can write

$$\langle u_{i_1} \wedge \dots \wedge u_{i_N} | u_{j_1} \wedge \dots \wedge u_{j_N} \rangle =$$

$$= \langle (N!)^{-\frac{1}{2}} \sum_{\sigma \in S_N} \mathrm{sign}(\sigma)\, u_{i_{\sigma(1)}}(x_1) \dots u_{i_{\sigma(N)}}(x_N) | (N!)^{-\frac{1}{2}} \sum_{\tau \in S_N} \mathrm{sign}(\tau)\, u_{j_{\tau(1)}}(x_1) \dots u_{j_{\tau(N)}}(x_N) \rangle$$

$$= \frac{1}{N!} \sum_{\sigma, \tau \in S_N} \mathrm{sign}(\sigma)\, \mathrm{sign}(\tau) \langle u_{i_{\sigma(1)}}, u_{j_{\tau(1)}} \rangle \dots \langle u_{i_{\sigma(N)}}, u_{j_{\tau(N)}} \rangle$$

$$= \frac{1}{N!} \sum_{\sigma, \tau \in S_N} \mathrm{sign}(\sigma)\, \mathrm{sign}(\tau)\, \delta_{i_{\sigma(1)}, j_{\tau(1)}} \dots \delta_{i_{\sigma(N)}, j_{\tau(N)}}$$

It is clear that if $(i_1, \dots, i_N) \neq (j_1, \dots, j_N)$ then this expression is 0. When $(i_1, \dots, i_N) = (j_1, \dots, j_N)$, then the delta's are non-zero iff $\sigma = \tau$. Then we sum over $N!$ σ's $\Rightarrow 1$.

•) <u>step 2</u> We prove that if Ω_1 and Ω_2 are two measure spaces, then

$$L^2(\Omega_1 \times \Omega_2) \cong L^2(\Omega_1) \otimes L^2(\Omega_2) =: \overline{\mathrm{Span}\{u \otimes v \mid u \in L^2(\Omega_1), v \in L^2(\Omega_2)\}}$$

where we used the usual notation of tensor product:

$$(u \otimes v)(x,y) = u(x)\, v(y).$$

More precisely, we prove that if $\{u_i\}$ is ONB for $L^2(\Omega_1)$ and $\{v_j\}$ ONB for $L^2(\Omega_2)$, then $\{u_i \otimes v_j\}_{i,j}$ is ONB for $L^2(\Omega_1 \times \Omega_2)$. Indeed:

•) $\{u_i \otimes v_j\}$ are orthonormal fcts in $L^2(\Omega_1 \times \Omega_2)$ as

$$\langle u_i \otimes v_j , u_l \otimes v_k \rangle = \langle u_i , u_l \rangle \cdot \langle v_j , v_k \rangle = \delta_{il}\, \delta_{jk}$$

•) $\{u_i \otimes v_j\}$ is complete. Assume $f \in L^2(\Omega_1 \times \Omega_2)$ and $f \perp u_i \otimes v_j \ \forall i,j$. Then

$$0 = \langle f , u_i \otimes v_j \rangle = \iint_{\Omega_1 \times \Omega_2} \overline{f(x,y)}\, u_i(x)\, v_j(y)\, d\mu_1(x)\, d\mu_2(y)$$

$$= \int_{\Omega_1} u_i(x) \underbrace{\int_{\Omega_2} \overline{f(x,y)}\, v_j(y)\, d\mu_2(y)}_{g_j(x)}\, d\mu_1(x)$$

Since $\{u_i\}$ is ONB for $L^2(\Omega_1)$ we must have $g_j \equiv 0$ namely for a.e. $x \in \Omega_1$

$$\int_{\Omega_2} \overline{f(x,y)}\, v_j(y)\, d\mu_2(y) = 0.$$

This holds for any $j \in \mathbb{N}$ and since $\{v_j\}$ is ONB for the space $L^2(\Omega_2)$ we find that for a.e. $x \in \Omega_1$ and a.e. $y \in \Omega_2$: $f(x,y) = 0$. Thus $f \equiv 0$ in $L^2(\Omega_1 \times \Omega_2)$.

With these two facts we have (by induction)

$$L^2(\mathbb{R}^{dN}) = L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d) \otimes \cdots \otimes L^2(\mathbb{R}^d) = L^2(\mathbb{R}^d)^{\otimes N}$$

and if $\{e_i\}$ is ONB for $L^2(\mathbb{R}^d)$, then

$$\{e_{i_1} \otimes \cdots \otimes e_{i_N} \mid i_1, \ldots, i_N \in \mathbb{N}\}$$

is an ONB for $L^2(\mathbb{R}^{dN})$.

•) Step 3

We define the operator P_N on $L^2(\mathbb{R}^{dN})$ by

$$(P_N \psi_N)(x_1, \ldots, x_N) = \frac{1}{N!} \sum_{\sigma \in S_N} \operatorname{sign}(\sigma)\, \psi_N(x_{\sigma(1)}, \ldots, x_{\sigma(N)})$$

→ Then P_N is a projection $(P_N)^2 = P_N$:

$$(P_N)^2 \psi_N(x_1, \ldots, x_N) = P_N \frac{1}{N!} \sum_{\sigma \in S_N} \operatorname{sign}(\sigma)\, \psi_N(x_{\sigma(1)}, \ldots, x_{\sigma(N)}) =$$

$$= \frac{1}{N!} \sum_{\sigma \in S_N} \operatorname{sign}(\sigma) \frac{1}{N!} \sum_{\tau \in S_N} \operatorname{sign}(\tau)\, \psi_N(x_{\tau\circ\sigma(1)}, \ldots, x_{\tau\circ\sigma(N)}) =$$

$$= \frac{1}{N!} \sum_{\sigma \in S_N} \underbrace{\frac{1}{N!} \sum_{\tau \in S_N} \operatorname{sign}(\tau\circ\sigma)\, \psi_N(x_{\tau\circ\sigma(1)}, \ldots, x_{\tau\circ\sigma(N)})}_{\text{independent of } \sigma}$$

$$= \frac{1}{N!} \sum_{\tau \in S_N} \operatorname{sign}(\tau)\, \psi_N(x_{\tau(1)}, \ldots, x_{\tau(N)}) = P_N \psi_N(x_1, \ldots, x_N)$$

→ Moreover, $P_N \psi_N \in L^2_a(\mathbb{R}^{dN}) \;\forall \psi_N \in L^2(\mathbb{R}^{dN})$:

$$P_N \varphi_N (x_{\tau(1)}, \dots, x_{\tau(N)}) = \frac{1}{N!} \sum_{\sigma \in S_N} \text{sign}(\sigma) \varphi_N (x_{\sigma\circ\tau(1)}, \dots, x_{\sigma\circ\tau(N)})$$

$$= \text{sign}(\tau) \frac{1}{N!} \sum_{\sigma \in S_N} \text{sign}(\sigma\circ\tau) \varphi_N (x_{\sigma\circ\tau(1)}, \dots, x_{\sigma\circ\tau(N)})$$

$$= \text{sign}(\tau) \; P_N \varphi_N (x_1, \dots, x_N).$$

Furthermore $P_N \varphi_N = \varphi_N$ if $\varphi_N \in L^2_a(\mathbb{R}^{dN})$:

$$P_N \varphi_N (x_1, \dots, x_N) = \frac{1}{N!} \sum_{\sigma \in S_N} \text{sign}(\sigma) \varphi_N (x_{\sigma(1)}, \dots, x_{\sigma(N)})$$

$$= \frac{1}{N!} \sum_{\sigma \in S_N} \underbrace{(\text{sign}(\sigma))^2}_{=1} \varphi_N (x_1, \dots, x_N) = \varphi_N (x_1, \dots, x_N)$$

Thus

$$L^2_a(\mathbb{R}^{dN}) = P_N L^2(\mathbb{R}^{dN})$$

•) <u>Step 4</u> From steps 2 and 3, we obtain

$$L^2_a(\mathbb{R}^{dN}) = \overline{\text{Span} \{ P_N (u_{i_1} \otimes \dots \otimes u_{i_N}) \mid i_1, \dots, i_N \in \mathbb{N} \}}$$

It remains to compute

$$P_N (u_{i_1} \otimes \dots \otimes u_{i_N})(x_1, \dots, x_N) = P_N (u_{i_1}(x_1) \dots u_{i_N}(x_N))$$

$$= \frac{1}{N!} \sum_{\sigma \in S_N} \text{sign}(\sigma) u_{i_1}(x_{\sigma(1)}) \dots u_{i_N}(x_{\sigma(N)})$$

$$= \frac{1}{N!} \det \left[(u_{i_k}(x_\ell))_{1 \le k, \ell \le N} \right]$$

$$\Longrightarrow \quad P_N (u_{i_1} \otimes \dots \otimes u_{i_N}) = \frac{1}{\sqrt{N!}} u_{i_1} \wedge \dots \wedge u_{i_N}$$

Consequently, if $i_k = i_l$ for some $k \neq l$ $\Rightarrow$

$$\Rightarrow P_N(u_{i_1} \otimes \dots \otimes u_{i_N}) = 0 \text{. Also}$$

$$P_N(u_{i_{\sigma(1)}} \otimes \dots \otimes u_{i_{\sigma(N)}}) = \operatorname{sgn}(\sigma) \, P_N(u_{i_1} \otimes \dots \otimes u_{i_N})$$

Hence

$$L^2_a(\mathbb{R}^{dN}) = \operatorname{Span}\{P_N(u_{i_1} \otimes \dots \otimes u_{i_N}) \mid i_1, \dots, i_N \in \mathbb{N}\}$$

$$= \operatorname{Span}\{u_{i_1} \wedge \dots \wedge u_{i_N} \mid i_1, \dots, i_N \in \mathbb{N},\ i_1 < i_2 < \dots < i_N\}.$$

Thus Slater determinants form ONB of $L^2_a(\mathbb{R}^{dN})$ $\boxtimes$

Reduced density matrices

For most applications, the wave function in $L^2_a(\mathbb{R}^{dN})$ has too many variables for practical computations. Therefore, it is often useful to consider reduced density matrices

Def Let Ψ_N be a normalized wave function in $L^2_a(\mathbb{R}^{dN})$. The one-body density matrix $\gamma^{(1)}_{\Psi_N}$ of Ψ_N is a trace class operator on $L^2(\mathbb{R}^d)$ with kernel

$$\gamma^{(1)}_{\Psi_N}(x,y) = N \int_{\mathbb{R}^{d(N-1)}} \Psi_N(x, x_2, \dots, x_N) \overline{\Psi_N(y, x_2, \dots, x_N)} \, dx_2 \dots dx_N$$

We call the diagonal part of $\gamma^{(1)}_{\Psi_N}$ the one-body density and denote $\rho_{\Psi_N}(x)$.

Exercise

Check that: •) $\gamma^{(1)}_{\varphi_N} \geq 0$ ••) $\mathrm{Tr}\, \gamma^{(1)}_{\varphi_N} = N$

Solution:

•)

$$\langle f, \gamma^{(1)}_{\varphi_N} f \rangle = \int_{\mathbb{R}^d} \bar{f}(x) \iint_{\mathbb{R}^{d(N-1)}} \varphi_N(x, x_2, \dots, x_N) \overline{\varphi_N(y, x_2, \dots, x_N)}\, dx_2 \dots dx_N\, f(y)\, dy\, dx$$

$$= \int_{\mathbb{R}^{d(N-1)}} dx_2 \dots dx_N \underbrace{\int_{\mathbb{R}^d} dx\, \bar{f}(x) \varphi_N(x, x_2, \dots, x_N)}_{\stackrel{!!}{g_N}(x_2, \dots, x_N)} \underbrace{\int_{\mathbb{R}^d} f(y) \overline{\varphi_N(y, x_2, \dots, x_N)}\, dy}_{\overline{g_N(x_2 \dots x_N)}}$$

$$= \int_{\mathbb{R}^{d(N-1)}} |g_N(x_2, \dots, x_N)|^2\, dx_2 \dots dx_N \geq 0.$$

••) For a trace class operator we know that the trace is given by integral of diagonal of the kernel. Here immediately $\mathrm{Tr}\, \gamma^{(1)}_{\varphi_N} = N$ (c.f. $\rho_{\varphi_N}(x)$).

□

The following exercise shows why $\gamma^{(1)}_{\varphi_N}$ is useful.

Exercise

Show that

$$\langle \varphi_N, \sum_{i=1}^{N} h_i \varphi_N \rangle = \mathrm{Tr}\,(h\, \gamma^{(1)}_{\varphi_N}).$$

LHS:

$$\langle \varphi_N, h_1 \varphi_N \rangle = \int dx_1 \dots dx_N \overline{\varphi_N(x_1, \dots, x_N)} \int h(x_1, y) \varphi_N(y, x_2, \dots, x_N) \, dy$$

$$= \int dx \int dy \, \frac{1}{N} h(x, y) \, \gamma^{(1)}_{\varphi_N}(x, y) = \frac{1}{N} \operatorname{Tr}(h \gamma^{(1)}_{\varphi_N})$$

Now we do it $h_2, \dots, h_N \rightsquigarrow$ factor N, by permutations (in both sides of scalar product $\rightsquigarrow \operatorname{sgn}(\sigma)^2 = 1$)

Digression: trace class operators

without too many details: for a positive operator we define

$$\operatorname{Tr} A = \sum_i \langle u_i | A u_i \rangle \quad , \quad \{u_i\} \text{ - ONB}$$

This is independent of the choice of basis.

Trace class operators are a subset of Hilbert-Schmidt operators. They are compact. For positive, trace class operators one has the decomposition

$$A = \sum \lambda_i |u_i\rangle\langle u_i| \quad \text{for a ONB } \{u_i\}$$

with $\operatorname{Tr} A = \sum_i \lambda_i$

This implies in particular $A(x,y) = \sum_i \lambda_i \, u_i(x) \overline{u_i(y)}$

and

$$\operatorname{Tr} A = \int A(x,x) \, dx .$$

$$AB(x,y) = \int A(x,z) B(z,y) \, dz \Rightarrow \operatorname{Tr} AB = \iint A(x,z) B(z,x)$$

Exercise Let V be a multiplication operator on $L^2(\mathbb{R}^d)$. Then

$$\langle \varphi_N , \sum_{i=1}^N V(x_i) \varphi_N \rangle = \int_{\mathbb{R}^d} V(x) \rho_{\varphi_N}(x) dx$$

Solution:

$$\int \cdots \int dx_1 \ldots dx_N \, V(x_1) \overline{\varphi_N} \varphi_N = \frac{1}{N} \int dx_1 \, V(x_1) \gamma^{(1)}_{\varphi_N}(x_1, x_1) =$$

$$= \frac{1}{N} \int dx \quad V(x) \rho_{\varphi_N}(x)$$

Exercise

Let $\{u_i\}_{i=1}^N$ be orthonormal in $L^2(\mathbb{R}^d)$ and consider the Slater determinant $\varphi_N = u_1 \wedge \cdots \wedge u_N$. Show that the one-body density matrix of φ_N is $\gamma^{(1)}_{\varphi_N} = \sum_{i=1}^N |u_i\rangle\langle u_i|$.

Solution

$$\int dx_2 \ldots dx_N \, \varphi_N(x, x_2, \ldots, x_N) \overline{\varphi_N(y, x_2, \ldots, x_N)} =$$

$$= \frac{\int dx_2 \cdots dx_N}{N!} \sum_{\substack{\sigma \in S_N \\ \tau \in S_N}} \operatorname{sign}(\sigma \tau) \, u_{\sigma(1)}(x) u_{\sigma(2)}(x_2) \cdots u_{\sigma(N)}(x_N) \overline{u_{\tau(1)}(y)} \, \overline{u_{\tau(2)}(x_2)} \cdots \overline{u_{\tau(N)}(x_N)}$$

$$= \frac{1}{N!} \sum_{\sigma, \tau \in S_N} \operatorname{sign}(\sigma) \operatorname{sign}(\tau) \, u_{\sigma(1)}(x) \overline{u_{\tau(1)}(y)} \quad \delta_{\sigma(2), \tau(2)} \cdots \delta_{\tau(N), \sigma(N)}$$

$$= \frac{1}{N!} \sum_{\sigma \in S_N} u_{\sigma(1)}(x) \overline{u_{\sigma(1)}(y)} = \frac{1}{N} \sum_{i=1}^N u_i(x) \overline{u_i(y)}$$

$\boxtimes$