Foundations of Mathematical Physics, Jacobs University, Fall 2021 — Session 27

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Last time: We introduced the unitary map

$$U_{N,\varphi}: L^2(\mathbb{R}^{3N}) \longrightarrow \mathcal{F}_\varphi^{\leq N}, \quad \Psi_N \longmapsto \left(\chi_{\leq N}^{(k)}\right)_{k=0,\dots,N} \equiv \chi_{\leq N}, \quad \text{where}$$

$$\chi_{\leq N}^{(k)}(x_1,\dots,x_k) = \binom{N}{k}^{\frac{1}{2}} q_1^\varphi \cdots q_k^\varphi \int dx_{k+1}\dots dx_N\, \overline{\varphi(x_{k+1})} \cdots \overline{\varphi(x_N)}\, \Psi_N(x_1,\dots,x_N).$$

Inverse: $$\Psi_N(x_1,\dots,x_N) = \sum_{k=0}^{N} \Big[\varphi(x_{k+1})\dots\varphi(x_N)\, \chi^{(k)}(x_1,\dots,x_k)\Big]_{\text{sym}}$$ symmetrization as in Lemma 4.13.

Next: We would like to approximate the fluctuation dynamics $U_{N,\varphi(t)}\Psi_N(t)$, where $\varphi(t)$ solves the Hartree eq., and $i\frac{d}{dt}\Psi_N(t) = H_N \Psi_N(t)$.

We find: $$i\frac{d}{dt}\left(U_{N,\varphi(t)}\Psi_N(t)\right) = i\,\frac{dU_{N,\varphi(t)}}{dt}\Psi_N(t) + U_{N,\varphi(t)}\underbrace{i\frac{d\Psi_N(t)}{dt}}_{= H_N\Psi_N(t) = H_N U^*_{N,\varphi(t)} U_{N,\varphi(t)}\Psi_N(t)}$$

$$= \underbrace{\left[i\,\frac{dU_{N,\varphi(t)}}{dt} U^*_{N,\varphi(t)} + U_{N,\varphi(t)} H_N U^*_{N,\varphi(t)}\right]}_{:= \mathbb{H}^{\leq N}_{\varphi(t)}} U_{N,\varphi(t)}\Psi_N(t).$$

Thus, setting $\chi_{\leq N}(t) := U_{N,\varphi(t)}\Psi_N(t)$, it satisfies the excitation Schrödinger equation

$$\boxed{i\frac{d}{dt}\chi_{\leq N}(t) = \mathbb{H}^{\leq N}_{\varphi(t)}\,\chi_{\leq N}(t)}.$$

Computing $\mathbb{H}^{\leq N}_{\varphi(t)}$ is rather lengthy. It will contain terms that relate $i\frac{d}{dt}\chi^{(k)}_{\leq N}(t)$ to $\chi^{(k\pm 1)}_{\leq N}(t)$ or $\chi^{(k\pm 2)}_{\leq N}(t)$ due to the pair interaction. So next, we should introduce operators that describe such mappings.

Definition 4.17: On Fock space $\mathcal{F}$ we define, for any $f \in L^2(\mathbb{R}^3)$:

- The creation operator $a(f): \mathcal{F} \to \mathcal{F}$, def. by

$$\left(a(f)\chi\right)^{(k)}(x_1,\dots,x_k) = \sqrt{k+1}\int dx\, \overline{f(x)}\, \chi^{(k+1)}(x_1,\dots,x_k,x) \quad \forall k \in \mathbb{N}_0 .$$

- The annihilation operator $a^+(f): \mathcal{F} \to \mathcal{F}$, def. by

$$\left(a^+(f)\chi\right)^{(k)}(x_1,\dots,x_k) = \frac{1}{\sqrt{k}} \sum_{j=1}^{k} f(x_j)\, \chi^{(k-1)}(x_1,\dots,x_{j-1},x_{j+1},\dots,x_k) \quad \forall k \in \mathbb{N}_0 .$$

We find:

Lemma 4.18: (i) $a^+(f) = a^*(f) \quad \forall f \in L^2(\mathbb{R}^3)$.

(ii) The canonical commutation relations (CCR) hold: $[a(f), a^+(g)] = \langle f, g\rangle$,

$[a(f), a(g)] = 0 = [a^+(f), a^+(g)] \quad \forall f,g \in L^2(\mathbb{R}^3)$.

Proof:

(i)
$$\langle a^+(f)\chi, \tilde{\chi}\rangle = \sum_{k=1}^{\infty} \int dx_1 \dots dx_k \frac{1}{\sqrt{k}} \sum_{j=1}^{k} \overline{f(x_j)}\, \overline{\chi^{(k-1)}(x_1,\dots,x_{j-1},x_{j+1},\dots,x_k)}\, \tilde{\chi}^{(k)}(x_1,\dots,x_k)$$

$$= \sum_{k=1}^{\infty} \frac{1}{\sqrt{k}} \sum_{j=1}^{k} \int dx_1 \dots dx_{j-1} dx_{j+1} \dots dx_k\, \overline{\chi^{(k-1)}(x_1,\dots,x_{j-1},x_{j+1},\dots,x_k)}\, \underbrace{\int dx_j\, \overline{f(x_j)}\, \tilde{\chi}^{(k)}(x_1,\dots,x_k)}_{= \int dx\, \overline{f(x)}\, \tilde{\chi}^{(k)}(x_1,\dots,x_{j-1},x,x_{j+1},\dots,x_k)}$$

$k-1 := m$

renaming integration variables

$\chi, \tilde{\chi}$ symmetric

$$= \sum_{m=0}^{\infty} \underbrace{\frac{1}{\sqrt{m+1}} \sum_{j=1}^{m+1}}_{= \sqrt{m+1}} \int dx_1 \dots dx_m\, \overline{\chi^{(k-1)}(x_1,\dots,x_m)} \int dx\, \overline{f(x)}\, \tilde{\chi}(x_1,\dots,x_m,x)$$

$$= \langle \chi, a(f)\tilde{\chi}\rangle .$$

(ii) $\left(a(f)a^+(g)\chi\right)^{(k)}(x_1,\dots,x_k)$

$$= \sqrt{k+1}\int dx_{k+1}\,\overline{f(x_{k+1})}\left(a^+(g)\chi\right)^{(k+1)}(x_1,\dots,x_k,x_{k+1})$$

$$= \sqrt{k+1}\int dx_{k+1}\,\overline{f(x_{k+1})}\,\frac{1}{\sqrt{k+1}}\sum_{j=1}^{k+1} g(x_j)\,\chi^{(k)}(x_1,\dots,x_{j-1},x_{j+1},\dots,x_{k+1})$$

$\left(a^+(g)a(f)\chi\right)^{(k)}(x_1,\dots,x_k)$

$$= \frac{1}{\sqrt{k}}\sum_{j=1}^{k} g(x_j)\,\left(a(f)\chi\right)^{(k-1)}(x_1,\dots,x_{j-1},x_{j+1},\dots,x_k)$$

$$= \frac{1}{\sqrt{k}}\sum_{j=1}^{k} g(x_j)\,\sqrt{k}\int dx_{k+1}\,\overline{f(x_{k+1})}\,\chi^{(k)}(x_1,\dots,x_{j-1},x_{j+1},\dots,x_{k+1})$$

$$\Rightarrow \left(a(f)a^+(g)\chi\right)^{(k)}(x_1,\dots,x_k) - \left(a^+(g)a(f)\chi\right)^{(k)}(x_1,\dots,x_k)$$

$$= \underbrace{\int dx\,\overline{f(x)}\,g(x)}_{=\langle f,g\rangle}\,\chi^{(k)}(x_1,\dots,x_k)$$

Also: $[a(f),a(g)] = 0 = [a^+(f),a^+(g)]$ can be checked by direct computation. $\square$

Definition 4.19:

For an ONB $(\varphi_n)_n$, we call $\mathcal{N} := \sum_n a^+(\varphi_n)a(\varphi_n)$ the number operator.

Lemma 4.20: $\mathcal{N}$ is independent of the ONB (from its definition), and

$(\mathcal{N}\chi)^{(k)}(x_1,\dots,x_k) = k\,\chi^{(k)}(x_1,\dots,x_k)$. Thus $\mathcal{N}:\mathcal{F}\to\mathcal{F}$ is an unbounded symmetric operator with domain $D(\mathcal{N}) = \{\chi\in\mathcal{F} : \sum_{k=0}^{\infty} k^2\|\chi^{(k)}\|^2 < \infty\}$.

Proof: $(\mathcal{N}\chi)^{(k)}(x_1,\dots,x_k) = \sum_n \left(a^\dagger(\varphi_n)a(\varphi_n)\chi\right)^{(k)}(x_1,\dots,x_k)$

Def. of ONB:

$\psi = \sum_n \langle\varphi_n,\psi\rangle\varphi_n$

$\Rightarrow \psi(x) = \sum_n \int dy\, \overline{\varphi_n(y)}\psi(y)\varphi_n(x)$

$$= \sum_n \sum_{j=1}^{k} \varphi_n(x_j) \int dx\, \overline{\varphi_n(x)}\, \chi^{(k)}(x_1,\dots,x_{j-1},x_{j+1},\dots,x_k,x)$$

$$= \sum_{j=1}^{k} \int dx\, \delta(x_j - x)\, \chi^{(k)}(x_1,\dots,x_{j-1},x_{j+1},\dots,x_k,x)$$

$\chi^{(k)}$ symmetric

$$= k\, \chi^{(k)}(x_1,\dots,x_k). \qquad \square$$

Sketch for how to continue:

Since $\left(\mathbb{H}^{\le N}_{\varphi(t)}\chi\right)^{(k)}$ equals some expression involving $\chi^{(k\pm1)}$ and $\chi^{(k\pm2)}$, we can write it in terms of terms of the type:

- $a^\dagger a$ ← no change in excitation number
- aa, $a^\dagger a^\dagger$ ← pair excitations
- $a^\dagger aa$, $a^\dagger a^\dagger a$ ← comes with $\frac{1}{\sqrt{N}}$
- $a^\dagger a^\dagger aa$ ← comes with $\frac{1}{N}$
- it turns out that all other combinations vanish

The approximation where we keep only $a^\dagger a$ and $aa, a^\dagger a^\dagger$ terms is called Bogoliubov approximation; let us denote it by $\mathbb{H}^{\mathrm{Bog}}_{\varphi(t)}$.

Then one can show that $\left\|\left(\mathbb{H}^{\le N}_{\varphi(t)} - \mathbb{H}^{\mathrm{Bog}}_{\varphi(t)}\right)\chi\right\| \le \frac{1}{\sqrt{N}}\, \mathrm{const}\, \left\|(\mathcal{N}+1)^{\frac{3}{2}}\chi\right\|.$

This would allow us to prove that $\|\chi_{\le N}(t) - \chi_{\mathrm{Bog}}(t)\| \le e^{\mathrm{const}\cdot t}\left(\|\chi_{\le N}(0) - \chi_{\mathrm{Bog}}(0)\| + \frac{1}{\sqrt{N}}\right)$

by a Gronwall argument, where $\chi_{\mathrm{Bog}}(t)$ solves the Bogoliubov equation

$$i\frac{d}{dt}\chi_{\mathrm{Bog}}(t) = \mathbb{H}^{\mathrm{Bog}}_{\varphi(t)}\chi_{\mathrm{Bog}}(t).$$