Bogoliubov dymamics of mean-field Bose gases

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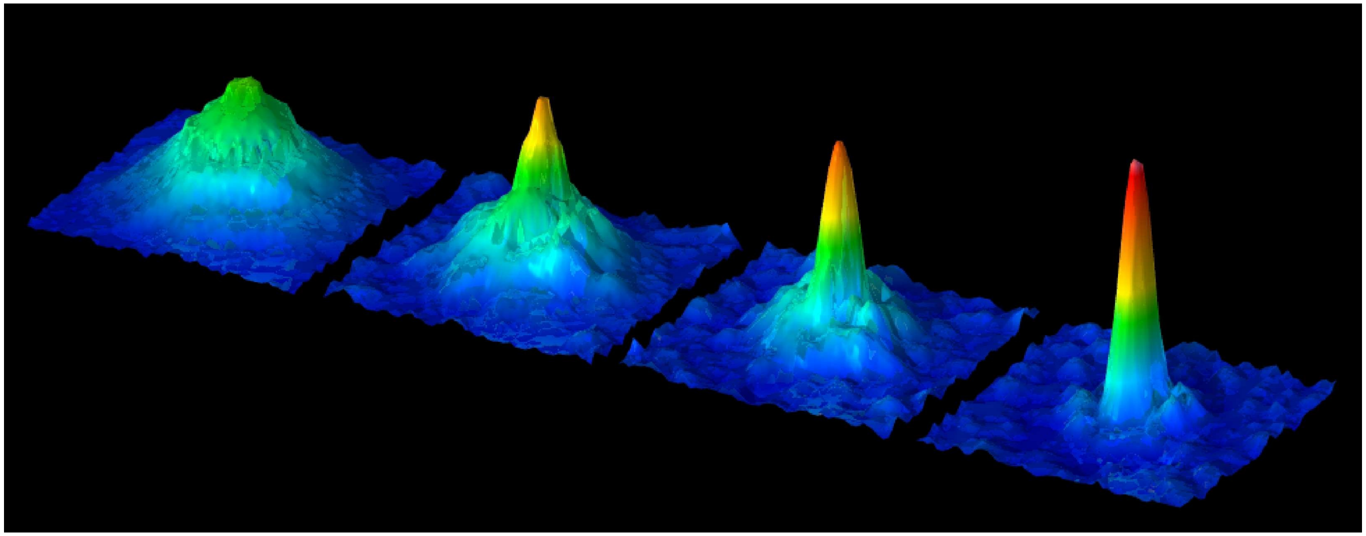
Bose-Einstein condensation

▶ Bose and Einstein 1924-25: non-interacting particles at low temperature. Many particles in the same quantum state.

▶ Cornell and Wieman 1995 (2001 Nobel with Ketterle): experiment with cold dilute atomic gases.



▶ Bosons at 0 temperature with very weak interactions: condensation and fluctuations around the condensate state.

Model

- N interacting bosons in $\mathbb{R}^d$

$$H_N = \sum_{j=1}^{N}(-\Delta_{x_j} + V(x_j)) + \frac{1}{N-1}\sum_{1\le j<k\le N} w(x_j - x_k)$$

on $\mathfrak{H}^N = \bigotimes_{\text{sym}}^N L^2(\mathbb{R}^d) = \{\Psi(x_1, ..., x_N) \in L^2((\mathbb{R}^d)^N) \text{ symmetric}\}$ with real-valued, regular potentials:

$$w(x) = w(-x), w^2 \le C(1-\Delta), V \in L^{d/2}_{\text{loc}}, |V_-|^2 \le C(1-\Delta).$$

Remark. We can deal with confined/unconfined systems, or fractional Laplacians, or magnetic fields ...

- **Goal:** understand the asymptotic structure of the time evolution

$$\Psi_N(t) = e^{-itH_N}\Psi_{N,0}, \quad \Psi_{N,0} \approx u_0^{\otimes N},$$

as $N \to \infty$.

BEC of approximate ground states

▶ **Hartree's theory:** $\Psi_N \approx u^{\otimes N}$. Hartree functional

$$\frac{\langle u^{\otimes N}, H_N u^{\otimes N}\rangle}{N} = \langle u, \big(-\Delta + V + |u|^2 * w/2\big)u\rangle := \mathcal{E}_{\rm H}(u).$$

Hartree energy $\quad e_{\rm H}(\lambda) = \inf\big\{\mathcal{E}_{\rm H}(u), \|u\|^2 = \lambda\big\}.$

Binding inequality $\quad e_{\rm H}(1) < e_{\rm H}(1-\lambda) + e_{\rm H}^\infty(\lambda)$ for all $0 < \lambda \le 1$.

▶ **Theorem** (Lewin-N-Rougerie 2013) *If $e_{\rm H}(1)$ has a unique bound state u_0 and $\langle \Psi_N, H_N \Psi_N\rangle = \inf \sigma(H_N) + o(N)$, then there exists a subsequence Ψ_{N_j} such that we have the complete BEC*

$$\boxed{\lim_{j\to\infty} {\rm Tr}_{2\to N_j} |\Psi_{N_j}\rangle\langle \Psi_{N_j}| = |u_0\rangle\langle u_0|.}$$

- Benguria-Lieb 1983, Lieb-Yau 1987 (boson stars, no BEC)
- Raggio-Werner & Petz-Raggio-Verbeure 1989 (trapped system)
- Lieb-Seiringer-Yngvason 2000-03 (GP).

Hartree dynamics

- Mean-field approximation: $\Psi_N(t) \approx u(t)^{\otimes N}$.
- The potential experienced by each particle $\approx V + |u(t)|^2 * w$.
- The nonlinear Hartree equation

$$i\,\partial_t u(t) = \big(-\Delta + V + |u(t)|^2 * w - \mu(t)\big)u(t), \quad u(0) = u_0.$$

- The gauge parameter $\mu(t) \in \mathbb{R}$ is the phase of $u(t)$.

We can choose $\mu(t)$ to keep the compatibility of the energy

$$\begin{aligned}\langle u(t)^{\otimes N}, H_N(u(t)^{\otimes N})\rangle &\approx \langle \Psi_N(t), H_N\Psi_N(t)\rangle \\ &= \Psi_N(t), i\partial_t\Psi_N(t)\rangle \approx \langle u(t)^{\otimes N}, i\partial_t(u(t)^{\otimes N})\rangle.\end{aligned}$$

That is

$$\mu(t) := \frac{1}{2}\iint |u(t,x)|^2 w(x-y)|u(t,y)|^2\,dx\,dy,$$

for which the H-energy $\big\langle u(t), \big(-\Delta + |u(t)|^2 * w/2\big)\,u(t)\big\rangle$ is constant.

Convergence towards Hartree dynamics

▶ **Theorem** (Convergence towards Hartree dynamics). *Let $u(t)$ be the Hartree dynamics with initial datum $u_0 \in H^1(\mathbb{R}^d)$, $\|u_0\|_{L^2} = 1$, and let $\Psi_N(t) = e^{-itH_N} u_0^{\otimes N}$. Then for every $t > 0$ fixed,*

$$\boxed{\lim_{N\to\infty} \mathrm{Tr}_{2\to N} |\Psi_N(t)\rangle\langle\Psi_N(t)| = |u(t)\rangle\langle u(t)|.}$$

- Spohn 1980, Erdös-Yau 2001, Rodnianski-Schlein 2009 & Chen-Lee-Schlein 2011 (quantitative estimate)
- Hepp 1974, Ginibre-Velo 1979 (coherent states approach)
- Erdös-Schlein-Yau 2006-10 & Benedikter-Oliveira-Schlein 2012 (GP)

▶ **Remark:** when $t > 0$, $\Psi_N(t)$ is *never* close to $u(t)^{\otimes N}$ in norm!

Beyond Hartree approximation: static problem

- If u_0 is a Hartree minimizer for $e_{\mathrm{H}}(1) = e_{\mathrm{H}}$, then

$$\mathcal{E}_{\mathrm{H}}\Big(\frac{u_0 + v}{\sqrt{1 + \|v\|^2}}\Big) = \mathcal{E}_{\mathrm{H}}(u_0) + \frac{1}{2}\mathrm{Hess}\ \mathcal{E}_{\mathrm{H}}(u_0)(v, v) + o(\|v\|^2_{H^1})$$

for $v \in \mathfrak{H}_+ = \{u_0\}^\perp$.

- Bogoliubov's theory (1947)

$$\boxed{H_N - N e_{\mathrm{H}} \approx \mathbb{H}}$$

with $\mathbb{H}$ the second quantization of $\frac{1}{2}\mathrm{Hess}\ \mathcal{E}_{\mathrm{H}}(u_0)$.

- **Remark:** $H_N - N e_{\mathrm{H}}$ acts on $\mathfrak{H}^N$, while the Bogoliubov Hamiltonian $\mathbb{H}$ acts on Fock space $\mathcal{F}_+ = \mathbb{C} \oplus \mathfrak{H}_+ \oplus \mathfrak{H}_+^2 \oplus ...$

  - $\mathbb{H}$ is not a particle-conserving Hamiltonian.
  - $\mathbb{H}$ describes the fluctuations around the Hartree state $u_0^{\otimes N}$.

Fluctuations around Hartree states

- Symmetric tensor: for $\Psi_k \in \mathfrak{H}^k$ and $\Psi_\ell \in \mathfrak{H}^\ell$, denote

$$\Psi_k \otimes_s \Psi_\ell(x_1, ..., x_{k+\ell})$$
$$= \frac{1}{\sqrt{k!\ell!(k+\ell)!}} \sum_{\sigma \in \mathfrak{S}_{k+\ell}} \Psi_k(x_{\sigma(1)}, ..., x_{\sigma(k)}) \Psi_\ell(x_{\sigma(k+1)}, ..., x_{\sigma(k+\ell)}).$$

Remark: $a^*(f)\Psi = f \otimes_s \Psi = \Psi \otimes_s f$ for every $f \in \mathfrak{H}$.

- For any wave function $\Psi \in \mathfrak{H}^N$, we can write

$$\Psi = \varphi_0 \, u_0^{\otimes N} + \varphi_1 \otimes_s u_0^{\otimes(N-1)} + \varphi_2 \otimes_s u_0^{\otimes(N-2)} + \cdots + \varphi_N$$

where $\varphi_n \in \mathfrak{H}_+^n$.

- The unitary mapping $U_N : \mathfrak{H}^N \to \mathcal{F}_+^{\leq N} = \mathbb{C} \oplus \mathfrak{H}_+ \oplus ... \oplus \mathfrak{H}_+^N$,

$$\Psi \mapsto \varphi_0 \oplus \varphi_1 \oplus \cdots \oplus \varphi_N,$$

extends to a partial unitary $\mathfrak{H}^N \to \mathcal{F}_+$ with $U_N^* \equiv 0$ outside $\mathcal{F}_+^{\leq N}$.

Bogoliubov Hamiltonian

- Second quantization: for an ONB $\{u_n\}_{n=0}^{\infty}$ for $\mathfrak{H}$,

$$\mathbb{H}_N = \sum_{m,n\geq 0} T_{mn} a_m^* a_n + \frac{1}{2(N-1)} \sum_{m,n,p,q\geq 0} W_{mnpq} a_m^* a_n^* a_p a_q$$

where $T_{mn} = \langle u_m, (-\Delta + V) u_n \rangle$ and $W_{mnpq} = \langle u_m \otimes u_n, w u_p \otimes u_q \rangle$.

- Actions of $U_N(\cdot)U_N^*$: $a_0^\# \to \sqrt{N - \mathcal{N}_+}$ and $a_n^\# \to a_n^\#$ for $n \neq 0$.
- $U_N(H_N - Ne_{\mathrm{H}})U_N^* = \mathbb{H} + \text{error where}$

$$\begin{aligned}\mathbb{H} &= \sum_{m,n\geq 1} \langle u_m, (h + K_1) u_n \rangle \, a_m^* a_n + \frac{1}{2}\Big(\langle u_m \otimes u_n, K_2 \rangle \; a_m^* a_n^* + c.c. \Big) \\ &= d\Gamma(h + K_1) + \frac{1}{2} \iint \Big(K_2(x,y) a^\dagger(x) a^\dagger(y) + c.c. \Big),\end{aligned}$$

$h = -\Delta + V + |u_0|^2 * w - \mu_{\mathrm{H}}$, $K_1 = P^\perp \Big(u_0(x) w(x-y) \overline{u_0(y)} \Big) P^\perp$

and $K_2 = P^\perp \otimes P^\perp \Big(u_0(x) w(x-y) u_0(y) \Big)$. Here $P^\perp = 1 - |u_0\rangle\langle u_0|$.

Convergence of eigenstates

▶ **Theorem** (Lewin-N-Serfaty-Solovej 2012) *If* $e_{\rm H}(1)$ *has a unique, non-degenerate minimizer* u_0*, then*

$$U_N(H_N - Ne_{\rm H})U_N^* \to \mathbb{H}$$

weakly on the quadratic form domain of $\mathbb{H}$ *on* $\mathcal{F}_+$*. Moreover, if the (complete) BEC occurs, then we have the convergence of the corresponding eigenvalues and eigenstates. In particular, the ground state* Ψ_N *of* H_N *and the ground state* $\varphi_0 \oplus \varphi_1 \oplus \dots$ *of* $\mathbb{H}$ *satisfy*

$$\lim_{N\to\infty} \left\| \Psi_N - \sum_{n=0}^{N} u_0^{\otimes(N-n)} \otimes_s \varphi_n \right\|_{\mathfrak{H}^N} = 0.$$

- Seiringer 2011, Grech-Seiringer 2012, Derezínski-Napiórkowski 2013 (confined systems with positive-type interactions)
- Other models: Lieb-Liniger 1963, Lieb-Solovej 2001-04, Giuliani-Seiringer 2009 & Yau-Yin 2009 (LHY formula)

Convergence of Schrödinger dynamics

- Let $u(t)$ be the Hartree dynamics with an arbitrary initial datum $u_0 \in H^1$. Let $\mathfrak{H}_+(t) = u(t)^\perp$ and let Φ_0 in q.f. domain of $\mathbb{H}$,

$$\Phi_0 = (\varphi_n)_{n=0}^\infty \in \mathcal{F}_+(t) = \mathbb{C} \oplus \mathfrak{H}_+(t) \oplus \mathfrak{H}_+(t)^2 \oplus \dots$$

- **Theorem** (Lewin-N-Schlein 2013) *If*

$$\Psi_{N,0} = \sum_{n=0}^{N} u_0^{\otimes(N-n)} \otimes_s \varphi_n,$$

then the Schrödinger dynamics $\Psi_N(t) = e^{-itH_N}\Psi_{N,0}$ *satisfies*

$$\boxed{\lim_{N\to\infty} \left\| \Psi_N(t) - \sum_{n=0}^{N} u(t)^{\otimes(N-n)} \otimes_s \varphi_n(t) \right\|_{\mathfrak{H}^N} = 0}$$

for every $t > 0$ *fixed, with* $\Phi(t) = (\varphi_n(t))_{n=0}^\infty \in \mathcal{F}_+(t)$ *determined by*

$$i\partial_t \Phi(t) = \mathbb{H}(t)\Phi(t), \quad \Phi(0) = \Phi_0.$$

Comparison of convergences

▶ The norm convergence

$$\lim_{N\to\infty}\left\|\Psi_N(t)-\sum_{n=0}^{N}u(t)^{\otimes(N-n)}\otimes_s\varphi_n(t)\right\|_{\mathfrak{H}^N}=0$$

implies the convergence of density matrices

$$\lim_{N\to\infty}\gamma^{(1)}_{\Psi_N(t)}=|u(t)\rangle\langle u(t)|.$$

Proof. For two wave functions Ψ and Ψ' in $\mathfrak{H}^N$,

$$\operatorname{Tr}\left|\gamma^{(1)}_{\Psi}-\gamma^{(1)}_{\Psi'}\right|\le 2\|\Psi-\Psi'\|_{\mathfrak{H}^N}.$$

▶ Optimal convergence rate on norm: $O(N^{-1/2})$.

Remark: Optimal rate for density matrices: $O(N^{-1})$.

▶ **Remark:** in general, $\Psi_N(t)$ is *never* close to $u(t)^{\otimes N}$ in norm for every $t>0$, even if $\Psi_N(0)=u(0)^{\otimes N}$.

Bogoliubov dynamics

- Time-dependent Bogoliubov Hamiltonian

$$
\begin{aligned}
\mathbb{H}(t) &= d\Gamma\big(h(t)+K_1(t)\big)+\frac{1}{2}\iint\Big(K_2(t,x,y)a^\dagger(x)a^\dagger(y)+c.c.\Big)\\
h(t) &= -\Delta+V+|u(t)|^2*w-\mu(t),\ \ P^\perp(t)=1-|u(t)\rangle\langle u(t)|,\\
K_1(t) &= P^\perp(t)\Big(u(t,x)w(x-y)\overline{u(t,y)}\Big)P^\perp(t),\\
K_2(t) &= (P^\perp(t)\otimes P^\perp(t))\Big(u(t,x)w(x-y)u(t,y)\Big).
\end{aligned}
$$

  - $\mathbb{H}(t)$ is *not* necessarily bounded from below.
  - $\mathbb{H}(t)$ does *not* preserve $\mathcal{F}_+(t)$.

- The time-dependent Bogoliubov equation

$$
i\partial_t\Phi(t)=\mathbb{H}(t)\Phi(t),\quad \Phi(0)=\Phi_0
$$

is well-posed on the quadratic form domain of $d\Gamma(1-\Delta+|V|)$. Moreover, $\Phi(t)\in\mathcal{F}_+(t)$ for all $t>0$ provided $\Phi_0\in\mathcal{F}_+(0)$.

Paring

- The equation $i\dot{\Phi}(t) = \mathbb{H}(t)\Phi(t)$ with $\Phi(t) = (\varphi_k(t))_{k\geq 0}$ means

$$\begin{cases} i\dot{\varphi}_0(t) &= \sqrt{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \overline{K_2(t,x_1,x_2)}\varphi_2(t,x_1,x_2)\,dx_1\,dx_2 \\ i\dot{\varphi}_1(t,x_1) &= (h(t)+K_1(t))\varphi_1(t,x_1) \\ & \quad +\sqrt{6}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \overline{K_2(t,x_2,x_3)}\varphi_3(t,x_1,x_2,x_3)dx_2\,dx_3 \\ i\dot{\varphi}_2(t,x_1,x_2) &= \big((h(t)+K_1(t))_{x_1}+(h(t)+K_1(t))_{x_2}\big)\varphi_2(t,x_1,x_2) \\ & \quad +\sqrt{2}\,K_2(t,x_1,x_2)\varphi_0(t) \\ & \quad +\sqrt{12}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \overline{K_2(t,x_3,x_4)}\varphi_4(t,x_1,x_2,x_3,x_4)dx_3\,dx_4 \\ & \dots \end{cases}$$

- If $\Phi(0) = \Omega = 1 \oplus 0 \oplus ...$, then $\varphi_{2j+1}(t) \equiv 0$ but $\varphi_{2j}(t) \neq 0$ (since e.g. $\dot{\varphi}_2(0) = -(i/2)K_2(0) \neq 0$).

Thus $\Psi_N(0) = u(0)^{\otimes N} \Rightarrow \Psi_N(t)$ is *not* close to $u(t)^{\otimes N}$ when $t > 0$.

Coherent states approach

- Weyl operator $W(f) = \exp\big(a^*(f) - a(f)\big)$ satisfies

$$W(f)^* a^\dagger(g) W(f) = a^\dagger(g) + \langle f, g\rangle, \quad W(f)^* a(g) W(f) = a(g) + \langle g, f\rangle.$$

- Coherent state

$$W(f)\Omega = e^{-\|f\|^2/2} \sum_{n\geq 0} \frac{1}{\sqrt{n!}} f^{\otimes n}.$$

- The fluctuations around the coherent states: Hepp 1974, Ginibre-Velo 1979 and Grillakis-Machedon-Margetis 2010-12.

Theorem. *If* $\Psi_{N,0} = W(\sqrt{N} u_0)\widetilde{\Phi}_0$, *then*

$$\boxed{\lim_{N\to\infty} \left\| e^{-it\mathbb{H}_N} \Psi_{N,0} - W(\sqrt{N} u(t))\widetilde{\Phi}(t) \right\|_{\mathcal{F}} = 0}$$

where $u(t)$ *is the Hartree state (as before) and* $\widetilde{\Phi}(t)$ *determined by*

$$i\partial_t \widetilde{\Phi}(t) = \widetilde{\mathbb{H}}(t)\widetilde{\Phi}(t), \quad \widetilde{\Phi}(0) = \widetilde{\Phi}_0.$$

Comparison to coherent states

- $\widetilde{\mathbb{H}}(t)$ is *different* from $\mathbb{H}(t)$.

$$\widetilde{\mathbb{H}}(t) := d\Gamma\big(h(t) + \widetilde{K}_1\big) + \frac{1}{2}\iint \Big(\widetilde{K}_2(x,y)a^*(x)a^*(y) + c.c.\Big)dx\,dy$$

with $\widetilde{K}_1(t) = u(t,x)w(x-y)\overline{u(t,y)}$, $\widetilde{K}_2(t) = u(t,x)w(x-y)u(t,y)$.

- If $\Psi_{N,0} = W(\sqrt{N}u_0)\Omega$, the coherent state approach says that

$$\Big\| e^{-it\mathbb{H}_N} W(\sqrt{N}u_0)\Omega - W(\sqrt{N}u(t))\widetilde{\Phi}(t)\Big\|_{\mathcal{F}} \sim O(N^{-1/2}).$$

Projecting onto $\mathfrak{H}^N$ gives

$$\Big\| \frac{(N/e)^{N/2}}{\sqrt{N!}} e^{-itH_N} u_0^{\otimes N} - \mathbb{1}_{\mathfrak{H}^N} W(\sqrt{N}u(t))\widetilde{\Phi}(t)\Big\|_{\mathfrak{H}^N} \sim O(N^{-1/2}).$$

By Stirling's formula

$$\boxed{\Big\| e^{-itH_N} u_0^{\otimes N} - (2\pi N)^{1/4}\mathbb{1}_{\mathfrak{H}^N} W(\sqrt{N}u(t))\widetilde{\Phi}(t)\Big\|_{\mathfrak{H}^N} \sim O(N^{-1/4}).}$$

Comparison to coherent states (cont.)

▶ If the initial datum is $u_0^{\otimes N}$, the coherent state approach says that

$$\left\| e^{-itH_N} u_0^{\otimes N} - (2\pi N)^{1/4} \mathbb{1}_{\mathfrak{H}^N} W(\sqrt{N} u(t)) \widetilde{\Phi}(t) \right\|_{\mathfrak{H}^N} \sim O(N^{-1/4}).$$

Remark: the effective dynamics

$$(2\pi N)^{1/4} \mathbb{1}_{\mathfrak{H}^N} W(\sqrt{N} u(t)) \widetilde{\Phi}(t)$$

agrees with our fluctuations $\sum_{n=0}^{N} u(t)^{\otimes (N-n)} \otimes_s \varphi_n(t)$ to the leading order, but it is not easy to see directly.

▶ In general, if the initial datum is not a Hartree state, the comparison between the two dynamics is much less clear.

- Getting information in $\mathfrak{H}^N$ using the coherent state method requires good convergence rates, and hence further assumptions on the initial datum.
- Our direct method on $\mathfrak{H}^N$: more general form of initial datum.

Heuristic derivation of Bogoliubov dynamics

- Let $u(t)$ be the Hartree dynamics and $U_N(t) : \mathfrak{H}^N \to \mathcal{F}_+(t)^{\leq N}$

$$\sum_{n=0}^{N} \varphi_n \otimes_s u(t)^{\otimes(N-n)} \mapsto \bigoplus_{n=0}^{N} \varphi_n.$$

- Consider the transformed evolution $\Phi_N(t) = U_N(t)\Psi_N(t)$.

Using $i\partial_t \Psi_N(t) = H_N \Psi_N(t)$ and

$$i\dot{U}_N(t) = \Big(a^\dagger(u(t))a(P^\perp(t)i\dot{u}(t)) - \sqrt{N - \mathcal{N}_+(t)}\, a(P^\perp(t)i\dot{u}(t)) \\ - a^\dagger(P^\perp(t)i\dot{u}(t))\sqrt{N - \mathcal{N}_+(t)} - \langle i\dot{u}(t), u(t)\rangle (N - \mathcal{N}_+(t)) \Big) U_N(t)$$

we find $\boxed{i\partial_t \Phi_N(t) = \Big(\mathbb{H}(t) + R_N(t)\Big)\Phi_N(t), \quad \Phi_N(0) = \mathbb{1}_{\mathcal{F}^{\leq N}} \Phi_0.}$

- Since $R_N(t) \approx 0$, we have $\Phi_N(t) \approx \Phi(t)$ where

$$\boxed{i\partial_t \Phi(t) = \mathbb{H}(t)\Phi(t), \quad \Phi(0) = \Phi_0.}$$

Ingredients of proof

- Using the equations of $\Phi_N(t)$ and $\Phi(t)$,

$$\begin{aligned} \frac{d}{dt}\|\Phi_N(t)-\Phi(t)\|^2 &= 2\Re\Big\langle \Phi_N(t)-\Phi(t), \dot{\Phi}_N(t)-\dot{\Phi}(t)\Big\rangle \\ &= -2\mathrm{Im}\Big\langle \Phi_N(t), R_N(t)\Phi(t)\Big\rangle \end{aligned}$$

- Control energy of $\Phi(t)$

$$\langle \Phi(t), d\Gamma(1-\Delta+|V|)\Phi(t)\rangle \le Ce^{Ct}\langle \Phi_0, d\Gamma(1-\Delta+|V|)\Phi_0\rangle.$$

- Control number of particle of $\Phi_N(t)$

$$\langle \Phi_N(t), (\mathcal{N}+1)\Phi_N(t)\rangle \le Ce^{Ct}\langle \Phi_N(0), (\mathcal{N}+1)\Phi_N(0)\rangle.$$

- Conclusion

$$\lim_{N\to\infty}\frac{d}{dt}\|\Phi_N(t)-\Phi(t)\|^2 = 0 \quad \text{and} \quad \lim_{N\to\infty}\|\Phi_N(0)-\Phi(0)\|^2 = 0$$

implies $\quad \lim_{N\to\infty}\|\Phi_N(t)-\Phi(t)\|^2 = 0.$

Thank you !