# Effective Evolution Equations from Many-Body Quantum Mechanics


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- For one-particle observables, i. e. self-adjoint operators $O$ on $L^2(\mathbb{R}^3)$: Expectation value: $\operatorname{tr} O\gamma_{\psi_N}$ with

$$\gamma_{\psi_N} := \operatorname{tr}_{2,\ldots,N} |\psi_N\rangle\langle\psi_N|$$

the one-particle reduced density, a trace-class operator on $L^2(\mathbb{R}^3)$.

# Time Evolution

- Exact evolution: Schrödinger equation

$$i\partial_t \psi_t = H\psi_t, \qquad \psi_0 = \psi \in L^2(\mathbb{R}^{3N}),$$

with Hamilton operator

$$H = \sum_{j=1}^{N} -\Delta_j + \lambda \sum_{1 \le i < j \le N} V(x_i - x_j).$$

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- E. g. by Kato-Rellich: $H$ self-adjoint, $D(H) = H^2(\mathbb{R}^{3N})$.
- But: In physical systems $N$ is huge. How to make predictions?

Goal: Approximate $\gamma_{\psi_t}$ by effective equation. Estimate error for $N \gg 1$.

# Physical Regimes

Simplest:

- Bosonic mean-field regime

Studied in my thesis:

- Bosons in Gross-Pitaevskii regime: Strong interaction and strong correlations.
- Fermionic mean-field regime: Semiclassical parameter and semiclassical structure.
- Fermionic mean-field regime with relativistic dispersion.

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$$\psi_0 \simeq \varphi \otimes \cdots \otimes \varphi, \qquad \varphi \in L^2(\mathbb{R}^3).$$

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$$\psi_0 \simeq \varphi \otimes \cdots \otimes \varphi, \qquad \varphi \in L^2(\mathbb{R}^3).$$

- We expect:

$$\psi_t \simeq \varphi_t \otimes \cdots \otimes \varphi_t,$$

where $\varphi_t$ solves Hartree equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + \left( V * |\varphi_t|^2 \right) \varphi_t, \qquad \varphi_0 = \varphi.$$

# Proofs of Validity

Spohn '80, Erdős-Yau '01, Pickl '11, Fröhlich-Knowles-Schwarz '09, Knowles-Pickl '10, Hepp '74, Ginibre-Velo '79, ...

**Theorem (Rodnianski-Schlein '09, Chen-Lee-Schlein '11)**

*Let* $V^2 \leq C(1-\Delta)$. *Let*

$\psi_t$: *solution of Schrödinger equation with* $\psi_0 = \varphi \otimes \cdots \otimes \varphi$,

$\varphi_t$: *solution of Hartree equation with* $\varphi_0 = \varphi$.

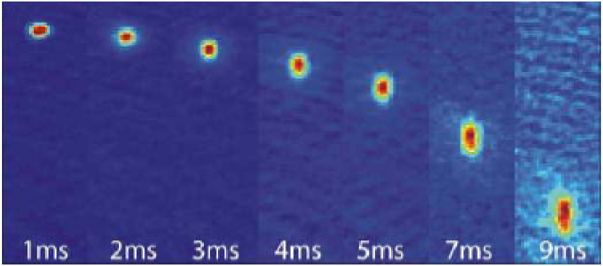
*Then*

$$\| \gamma_{\psi_t} - |\varphi_t\rangle\langle\varphi_t| \|_{\mathrm{tr}} \leq \frac{C}{N} e^{c|t|}.$$

*Remark:* $|\varphi_t\rangle\langle\varphi_t|$ = *one-particle reduced density of* $\varphi_t \otimes \cdots \otimes \varphi_t$.

# Bosons in the Gross-Pitaevskii regime

# Releasing a Bose-Einstein Condensate from a Trap




A. Griesmaier *et al*, Phys. Rev. Lett. '05

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$$H = \sum_{j=1}^{N} -\Delta_j + N^2 \sum_{i<j}^{N} V(N(x_i - x_j)).$$

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- interaction is repulsive, $V \geq 0$
- Bose-Einstein condensation in trap (Lieb-Seiringer '02):

  Let $\varphi_{\mathrm{GP}} \in L^2(\mathbb{R}^3)$ minimize

$$\mathcal{E}_{\mathrm{GP}}(\varphi) := \int \left( |\nabla\varphi|^2 + V_{\mathrm{trap}}|\varphi|^2 + 4\pi a_0 |\varphi|^4 \right) \mathrm{d}x, \qquad \|\varphi\|_2 = 1,$$

  where $a_0$: scattering length of $V$.

  The ground state $\psi$ of $H_{\mathrm{trapped}}$ satisfies

$$\gamma_\psi \longrightarrow |\varphi_{\mathrm{GP}}\rangle\langle\varphi_{\mathrm{GP}}| \qquad (N \to \infty).$$

# Effective Evolution Equation

- Erdős-Schlein-Yau '06–'08, Pickl '10:

  Let $\psi_t$ solve the Schrödinger equation; assume $\gamma_{\psi_0} \to |\varphi\rangle\langle\varphi|$ and bounded energy per particle in $\psi_0$.
  Then
  $$\gamma_{\psi_t} \longrightarrow |\varphi_t\rangle\langle\varphi_t| \qquad (N \to \infty),$$
  where $\varphi_t \in L^2(\mathbb{R}^3)$ solves the Gross-Pitaevskii equation
  $$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t, \qquad \varphi_0 = \varphi.$$

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- C. f. mean-field:

  $$i\partial_t\varphi_t = -\Delta\varphi_t + \left(N^3 V(N.) * |\varphi_t|^2\right)\varphi_t \quad \to \quad -\Delta\varphi_t + b|\varphi_t|^2\varphi_t.$$

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- Error bounds? Need new methods without BBGKY hierarchy/compactness.

# Second Quantization

- Bosonic Fock space

$$\mathcal{F} = \mathbb{C} \oplus L^2(\mathbb{R}^3) \oplus \cdots \oplus L^2_{\mathsf{symm}}(\mathbb{R}^{3N}) \oplus \cdots$$

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- $a_x^*$, $a_x$: create/annihilate delta distribution at $x \in \mathbb{R}^3$.

  Canonical commutation relations:

$$[a_x, a_y^*] = \delta(x - y), \qquad [a_x, a_y] = [a_x^*, a_y^*] = 0$$

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- Hamiltonian extended to Fock space:

$$\mathcal{H} := \int \nabla_x a_x^* \nabla_x a_x \, \mathrm{d}x + \frac{1}{2} \int N^2 V(N(x-y)) a_x^* a_y^* a_y a_x \, \mathrm{d}x\mathrm{d}y$$

# Construction of Initial Data

- Weyl operator: for $f \in L^2(\mathbb{R}^3)$

$$W(f) = \exp\left(\int a_x^* f(x)\mathrm{d}x - \text{h.c.}\right) : \quad \mathcal{F} \to \mathcal{F}$$

- Coherent states:

$$W(f)\Omega = e^{-\|f\|_2^2/2}\{1, f, \frac{f \otimes f}{\sqrt{2!}}, \ldots, \frac{f \otimes \ldots \otimes f}{\sqrt{N!}}, \ldots\} \in \mathcal{F}.$$

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**Modeling correlations by a Bogoliubov transformation**

$$T(k_t) = \exp\left(\int k_t(x;y) a_x^* a_y^* \,\mathrm{d}x\mathrm{d}y - \text{h.c.}\right),$$

$$k_t(x;y) = N(f(N(x-y)) - 1)\,\varphi_t(x)\varphi_t(y),$$

where $\left(-\Delta + \frac{1}{2}V\right) f = 0, \qquad f(x) \to 1 \text{ for } |x| \to \infty.$

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- Squeezed Coherent States: $W(\sqrt{N}\varphi_t)T(k_t)\Omega \in \mathcal{F}$.

# Error Bound

**Theorem (B-Oliveira-Schlein '12, to appear in *CPAM*)**

*Let* $V \in L^1 \cap L^3(\mathbb{R}^3, (1+|x|^6)dx)$.

*Let* $\psi_t$ *solve the Schrödinger equation with initial data*

$$\psi_0 = W(\sqrt{N}\varphi)T(k_0)\Omega, \quad \textit{with } \varphi \in H^4(\mathbb{R}^3), \quad \|\varphi\|_2 = 1.$$

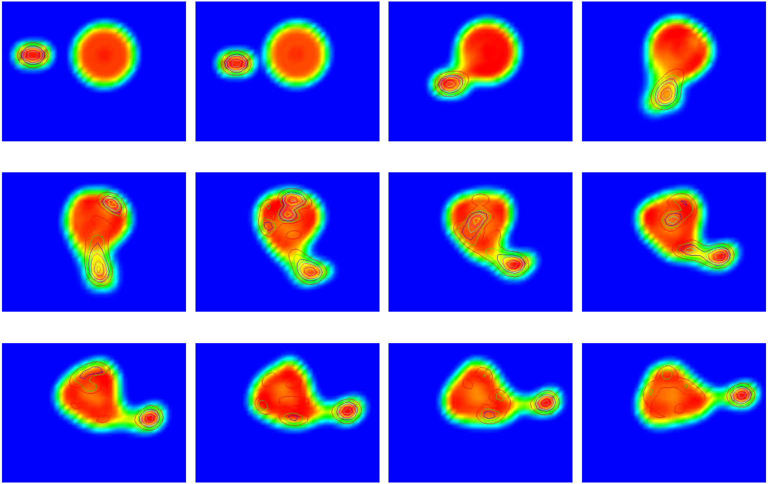
*Let* $\varphi_t$ *solve the Gross-Pitaevskii equation with initial data* $\varphi_0 = \varphi$.

*Then*

$$\|\gamma_{\psi_t} - |\varphi_t\rangle\langle\varphi_t|\|_{\mathrm{tr}} \leq \frac{C}{N^{1/2}} e^{ce^{c|t|}}.$$

# Fermionic Mean-Field Regime

# Collision of Nuclei



J. A. Maruhn, private communication

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Example: $H = \sum_{j=1}^{N} -\Delta_j$ in box $[0,1]^3$. Ground state:

$\psi_0 = \mathcal{A}(\varphi_1 \otimes \cdots \otimes \varphi_N)$ with $\varphi_j(x) = e^{ik_j x},\ k_j \in 2\pi\mathbb{Z}^3,$ up to $|k_N| \simeq N^{1/3}$.

$$\Rightarrow \text{ Large kinetic energy: } \quad \sum_{j=1}^{N} -\Delta_j = \sum_{j=1}^{N} k_j^2 \simeq N^{5/3}.$$

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- Non-trivial scaling:

$$i\partial_t \psi_t = \left[ \sum_{j=1}^{N} -\Delta_j + \frac{1}{N^{1/3}} \sum_{i<j}^{N} V(x_i - x_j) \right] \psi_t.$$

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- Rescaling time with $\varepsilon := N^{-1/3}$ exposes semi-classical regime:

$$i\varepsilon\partial_t\psi_t = \left[\sum_{j=1}^{N} -\varepsilon^2\Delta_j + \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j)\right]\psi_t.$$

# Hartree-Fock Approximation

Restrict to simplest fermionic states, i. e. $\mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N)$, and optimize the choice of the $\varphi_j \in L^2(\mathbb{R}^3)$.

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- Approximate time-evolution

$$e^{-iHt/\varepsilon}\mathcal{A}(\varphi_{1,0} \otimes \ldots \otimes \varphi_{N,0}) \simeq \mathcal{A}(\varphi_{1,t} \otimes \ldots \otimes \varphi_{N,t}).$$

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- Hartree-Fock equation for $\gamma_t^{\mathrm{HF}} = \frac{1}{N}\sum_{j=1}^{N}|\varphi_{j,t}\rangle\langle\varphi_{j,t}|$:

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- Narnhofer-Sewell '81, Spohn '81: $\rightarrow$ Vlasov equation.
  Erdős-Elgart-Schlein-Yau '04: HF for $t < t_0$, analytic potential.

# Validity and Error Bound

**Theorem (B-Porta-Schlein '13, *CMP* 329)**

*Let* $\int |\hat{V}(p)|(1+|p|)^2 dp < \infty$. *Let* $\{\varphi_j\}_{j=1}^\infty$ *be orthonormal in* $L^2(\mathbb{R}^3)$.

*Let* $\psi_0 = \mathcal{A}(\varphi_1 \otimes \ldots \otimes \varphi_N)$. *Assume 'semiclassical structure'*

$$\|[x, \gamma_{\psi_0}]\|_{\mathrm{tr}} \leq \varepsilon C, \qquad \|[\varepsilon\nabla, \gamma_{\psi_0}]\|_{\mathrm{tr}} \leq \varepsilon C.$$

*Let* $\psi_t$ *solve the Schrödinger equation with initial data* $\psi_0$, *and* $\gamma_t^{HF}$ *the Hartree-Fock equation with initial data* $\gamma_{\psi_0}$.
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**Theorem (B-Porta-Schlein '13, *JMP* 55)**

*Similar result for relativistic dispersion* $\sqrt{-\varepsilon^2\Delta + m^2}$.

# Justification of the Semiclassical Structure

- Initial data: e. g. ground state of non-interacting fermions in a box,

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Then:

$$\gamma_{\psi_0}(x;y) = \frac{1}{N}\sum_{j=1}^{N} \varphi_j(x)\overline{\varphi_j}(y) = \frac{1}{N}\sum_{|k|\leq cN^{1/3}} e^{ik(x-y)}$$
$$\simeq \int_{|q|\leq 1} e^{iq(x-y)/\varepsilon}\mathrm{d}q = \varphi\left(\frac{x-y}{\varepsilon}\right).$$

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  Then:

$$\begin{aligned}\gamma_{\psi_0}(x;y) = \frac{1}{N}\sum_{j=1}^{N} \varphi_j(x)\overline{\varphi_j}(y) &= \frac{1}{N}\sum_{|k|\leq cN^{1/3}} e^{ik(x-y)} \\ &\simeq \int_{|q|\leq 1} e^{iq(x-y)/\varepsilon}\mathrm{d}q = \varphi\left(\frac{x-y}{\varepsilon}\right).\end{aligned}$$

- In general trap:

$$\gamma_{\psi_0}(x;y) \simeq \varphi\left(\frac{x-y}{\varepsilon}\right)\chi\left(\frac{x+y}{2}\right).$$

Trace-norm heuristically:

- Integral kernel

$$[x, \gamma_{\psi_0}](x; y) \simeq (x - y)\varphi\left(\frac{x-y}{\varepsilon}\right)\chi\left(\frac{x+y}{2}\right) \simeq \varepsilon\varphi\left(\frac{x-y}{\varepsilon}\right)\chi\left(\frac{x+y}{2}\right).$$

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- We have $\varepsilon\nabla_x\gamma_{\psi_0}(x; y) = \nabla\varphi\left(\frac{x-y}{\varepsilon}\right)\chi\left(\frac{x+y}{2}\right) + \ldots$, but

$$[\varepsilon\nabla, \gamma_{\psi_0}](x; y) = \varepsilon(\nabla_x + \nabla_y)\gamma_{\psi_0}(x; y) \simeq \varepsilon\varphi\left(\frac{x-y}{\varepsilon}\right)\nabla\chi\left(\frac{x+y}{2}\right).$$

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- Semiclassical structure is stable w. r. t. Hartree-Fock evolution:
  If satisfied by $\gamma_{\psi_0}$, then for all times $t$:

$$\|[x, \gamma_t^{\mathrm{HF}}]\|_{\mathrm{tr}} \leq \varepsilon C e^{c|t|}, \qquad \|[\varepsilon\nabla, \gamma_t^{\mathrm{HF}}]\|_{\mathrm{tr}} \leq \varepsilon C e^{c|t|}.$$

# Proof: Bosonic Gross-Pitaevskii Regime

# Recalling the Rodnianski-Schlein Method

- If factorization was preserved:

$$e^{-i\mathcal{H}t}W(\sqrt{N}\varphi)\Omega \simeq W(\sqrt{N}\varphi_t)\Omega$$

$$\Updownarrow$$

$$\underbrace{W^*(\sqrt{N}\varphi_t)e^{-i\mathcal{H}t}W(\sqrt{N}\varphi)}_{=:\,U(t)}\Omega \simeq \Omega,$$

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$$\underbrace{W^*(\sqrt{N}\varphi_t)e^{-i\mathcal{H}t}W(\sqrt{N}\varphi)}_{=:\,U(t)}\Omega \simeq \Omega,$$

- Basic estimate:

$$\|\gamma_{\psi_t} - |\varphi_t\rangle\langle\varphi_t|\|_{\mathrm{tr}} \leq \frac{C}{N^{1/2}}\langle\Omega, U^*(t)\mathcal{N}U(t)\Omega\rangle.$$

- But r. h. s. can not be controlled in Gross-Pitaevskii regime because $W(\sqrt{N}\varphi_t)\Omega$ does not describe the correlations!

# Bogoliubov Transformation Approach

- For initial data $W(\sqrt{N}\varphi)T(k_0)\Omega$, we get

$$\tilde{U}(t) = T^*(k_t)W^*(\sqrt{N}\varphi_t)e^{-i\mathcal{H}t}W(\sqrt{N}\varphi)T(k_0).$$

- Need to show

$$\langle\Omega, \tilde{U}^*(t)\mathcal{N}\tilde{U}(t)\Omega\rangle \leq \tilde{C}(t).$$

  By Gronwall's lemma it is sufficient to show

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega, \tilde{U}^*(t)\mathcal{N}\tilde{U}(t)\Omega\rangle \leq C(t)\langle\Omega, \tilde{U}^*(t)\mathcal{N}\tilde{U}(t)\Omega\rangle.$$

- Key step: identify cancellations between Schrödinger evolution and Gross-Pitaevskii evolution.

# Coherent Part Cancellation

We have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{U}(t)\Omega, \mathcal{N}\tilde{U}(t)\Omega\rangle = \langle \tilde{U}(t)\Omega, [i\mathcal{L}(t), \mathcal{N}]\tilde{U}(t)\Omega\rangle$$

with

$$\begin{aligned}\mathcal{L}(t) &= \cancel{i\frac{dT_t^*}{\mathrm{d}t}} T_t + T_t^* \left[ i\frac{\mathrm{d}W_t^*}{\mathrm{d}t} W_t + W_t^* \mathcal{H} W_t \right] T_t \\ &\simeq T_t^* \left[ a^\sharp (\sqrt{N} i \partial_t \varphi_t) + \sqrt{N} a^\sharp + a^\sharp a^\sharp + \frac{1}{\sqrt{N}} a^\sharp a^\sharp a^\sharp + \frac{1}{N} a^\sharp a^\sharp a^\sharp a^\sharp \right] T_t .\end{aligned}$$

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Use approximate Gross-Pitaevskii equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + (N^3 f(N.)V(N.) * |\varphi_t|^2)\varphi_t$$

to get partial cancellation

$$a^\sharp(\sqrt{N}i\partial_t\varphi_t) + \sqrt{N}a^\sharp = \sqrt{N}a^\sharp\Big(N^3(1-f(N.))V(N.) * |\varphi_t|^2\varphi_t\Big).$$

# Bogoliubov Part Cancellation

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{U}(t)\Omega, \mathcal{N}\tilde{U}(t)\Omega\rangle \simeq$$

$$\langle \tilde{U}(t)\Omega, T_t^* \underbrace{\left[\sqrt{N} a^\sharp(..) + a^\sharp a^\sharp + \frac{1}{\sqrt{N}} a^\sharp a^\sharp a^\sharp + \frac{1}{N} a^\sharp a^\sharp a^\sharp a^\sharp\right]}_{\text{normalordered}} T_t \tilde{U}(t)\Omega\rangle$$

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Bogoliubov transformation

$$T_t^* a_x T_t \simeq a_x + a^*(k_t(\cdot, x))$$

destroys normalorder.

$$T_t^*\left(\sqrt{N}a^\sharp(..) + \frac{1}{\sqrt{N}}a^\sharp a^\sharp a^\sharp\right) T_t = \text{linear} + \text{cubic,not normalordered}$$
$$= \cancel{\text{linear} - \text{linear}} + \text{cubic,normalordered.}$$

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Normalordering of quartic terms creates quadratic terms.
Cancellations among quadratics due to $(-\Delta + \frac{1}{2}V)f = 0$. □

# Proof: Fermionic Mean-Field Regime

# Particle-Hole Transformation

Redefine 'particle' as excitation over Slater determinant, through a unitary $R : \mathcal{F} \to \mathcal{F}$.

Let $\{\varphi_j\}_{j\in\mathbb{N}}$ orthonormal basis of $L^2(\mathbb{R}^3)$.

- Transformed vacuum:

$$R\Omega := \{0, \dots, 0, \underbrace{\mathcal{A}(\varphi_1 \otimes \dots \otimes \varphi_N)}_{= \psi_0}, 0, \dots\} \in \mathcal{F}.$$

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- Transformed operators (create "excitations"):

$$Ra^*(\varphi_i)R^* := \begin{cases} a(\varphi_i) & \text{for } i \leq N \quad \text{(creates hole)} \\ a^*(\varphi_i) & \text{for } i > N \quad \text{(creates particle).} \end{cases}$$

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- Write as Bogoliubov transformation:

$$R\, a_x\, R^* = a(u_x) + a^*(v_x).$$

# Analogy to Rodnianski-Schlein

- If HF approximation is good:

$$e^{-i\mathcal{H}t/\varepsilon} R_0 \Omega \simeq R_t \Omega,$$

with $R_t$ the particle-hole transf. with $R_t\Omega = \mathcal{A}(\varphi_{1,t} \otimes \ldots \otimes \varphi_{N,t})$.

$$\Leftrightarrow \qquad \underbrace{R_t^* e^{-i\mathcal{H}t/\varepsilon} R_0}_{=:\ U(t)} \Omega \simeq \Omega.$$

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- More precisely

$$\|\gamma_{\psi_t} - \gamma_t^{\mathrm{HF}}\|_{\mathrm{tr}} \leq \frac{C}{N^{1/2}} \langle U(t)\Omega, \mathcal{N} U(t)\Omega \rangle.$$

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- By Gronwall, it is sufficient to prove

$$\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \langle U(t)\Omega, \mathcal{N} U(t)\Omega \rangle \leq \varepsilon \tilde{C}(t) \langle U(t)\Omega, \mathcal{N} U(t)\Omega \rangle.$$

# Cancellations

- with $\mathrm{d}\Gamma(O) := \int \mathrm{d}x \, O(x;y) a_x^* a_y$:

$$i\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} U^*(t) \mathcal{N} U(t) = U^*(t) R_t^* \Big( \mathrm{d}\Gamma(i\varepsilon \partial_t \gamma_t^{\mathsf{HF}}) - [\mathcal{H}, \mathrm{d}\Gamma(\gamma_t^{\mathsf{HF}})] \Big) R_t U(t).$$

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- Normal-ordering $R_t^*[\mathcal{H}, \mathrm{d}\Gamma(\gamma_t^{\mathsf{HF}})] R_t$
  $\rightsquigarrow$ quadratic + quartic terms.
- Use Hartree-Fock equation for $\mathrm{d}\Gamma(i\varepsilon\partial_t \gamma_t^{\mathsf{HF}})$
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- Use Hartree-Fock equation for $\mathrm{d}\Gamma(i\varepsilon\partial_t\gamma_t^{\mathsf{HF}})$
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- Remaining:

$$\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \langle U(t)\Omega, \mathcal{N} U(t)\Omega\rangle$$
$$\simeq \frac{1}{N} \int V(x-y) \langle U(t)\Omega, a^*(u_{t,y}) a(u_{t,y}) a(v_{t,x}) a(u_{t,x}) U(t)\Omega\rangle \,\mathrm{d}x\mathrm{d}y.$$

  Have to extract a factor $\varepsilon$ from r. h. s.

# Using the Semiclassical Structure

- Notice

$$\frac{1}{N}\int V(x-y)\langle U(t)\Omega, a^*(u_{t,y})a(u_{t,y})a(v_{t,x})a(u_{t,x})U(t)\Omega\rangle \,\mathrm{d}x\mathrm{d}y,$$

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$$\int v_{t,x}u_{t,x}\,\mathrm{d}x = 0.$$

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- Use Fourier:

$$\int v_{t,x}e^{ipx}u_{t,x}\,\mathrm{d}x = \int v_{t,x}[e^{ipx}, u_t](.,x)\,\mathrm{d}x = \int v_{t,x}\underbrace{[e^{ipx}, N\gamma_t^{\mathrm{HF}}](.,x)}_{\text{gain }\varepsilon}\,\mathrm{d}x.$$

□