Bosonic mean field limit and discrete Schrödinger equation

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WeConMApp

Mean field dynamics, a typical example

- n-body quantum Schrödinger equation: $\Psi(x_1, \ldots, x_n; t) \in L^2(\mathbb{R}^{dn})$

$$i\partial_t \Psi = \sum_{i=1}^{n} -\Delta_{x_i} \Psi + \frac{1}{n} \sum_{1 \le i < j \le n} V(x_i - x_j)\Psi \ ,$$

- Bosons : $\Psi(x_1, ..., x_n) = \Psi(x_{\sigma(1)}, ..., x_{\sigma(n)})$ for all permutation σ.
- Bosonic mean-field 1-body dynamics: $\varphi(x; t) \in L^2(\mathbb{R}^d)$

$$i\partial_t \varphi = -\Delta\varphi + (V * |\varphi|^2)\varphi$$

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$$i\frac{1}{n}\partial_t \Psi = \frac{1}{n}\sum_{i=1}^{n} -\Delta_{x_i}\Psi + \frac{1}{n^2}\sum_{1\le i<j\le n} V(x_i - x_j)\Psi ,$$

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$$\varepsilon = \frac{1}{n} \qquad H_\varepsilon = \varepsilon\sum_{i=1}^{n} -\Delta_{x_i} + \varepsilon^2 \sum_{1\le i<j\le n} V(x_i - x_j)$$

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Bosonic Fock space

- Phase space: $\mathcal{Z}$ separable Hilbert space
- Projection on $\mathcal{Z}^{\otimes n}$:

$$\mathcal{S}_n(\xi_1 \otimes \ldots \otimes \xi_n) = \frac{1}{n!} \sum_{\sigma \in \Sigma_n} \xi_{\sigma(1)} \otimes \ldots \otimes \xi_{\sigma(n)}.$$

$\bigvee^n \mathcal{Z} := \mathcal{S}_n(\mathcal{Z}^{\otimes n})$

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$\Gamma_s(\mathcal{Z}) = \bigoplus_{n \geq 0} \bigvee^n \mathcal{Z}$

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Annihilation and creation operators

$\forall z\,,\Phi \in \mathscr{Z}\,,\, \varepsilon > 0$, we define the annihilation and creation operators:

$$a(z)\Phi^{\otimes n} = \sqrt{\varepsilon n}\langle z\,,\,\Phi\rangle\Phi^{\otimes n-1}\,,$$
$$a^*(z)\Phi^{\otimes n} = \sqrt{\varepsilon(n+1)}\mathcal{S}_{n+1}(z\otimes\Phi^{\otimes n})\,.$$

Canonical commutation relations (CCR):

$$[a(z_1), a^*(z_2)] = \varepsilon\langle z_1, z_2\rangle \mathrm{Id}\,,$$
$$[a(z_1), a(z_2)] = [a^*(z_1), a^*(z_2)] = 0\,.$$

Notations:

$$\mathbb{C} \to \mathcal{Z}$$
$$|z\rangle : \lambda \mapsto \lambda z$$

linear map

$$\mathcal{Z} \to \mathbb{C}$$
$$\langle z| : z_1 \mapsto \langle z\,,\, z_1\rangle$$

The corresponding quantum Liouville equation for the state $\varrho_\varepsilon(t) = |\Psi_N(t)\rangle\langle\Psi_N(t)|$ is

$$\mathrm{i}\varepsilon\partial_t\varrho_\varepsilon(t) = [H_\varepsilon\,,\, \varrho_\varepsilon(t)]$$

Field and Weyl operators, second quantization

- $\forall f \in \mathcal{Z}$, field operator:

$$\Phi(f) = \frac{1}{\sqrt{2}}(a^*(f) + a(f)) \text{ ess s.a. on } \Gamma_{fin}(\mathcal{Z}) = \bigoplus_{n\in\mathbb{N}}^{alg} \bigvee^n \mathcal{Z}\,.$$

- Weyl operator:

$$W(f) = e^{i\Phi(f)}\,.$$

- Second quantization of A operator on $\mathcal{Z}$:

$$\mathrm{d}\Gamma(A)_{|\vee^{n,alg} D(A)} = \varepsilon \sum_{i=1}^{n} \mathrm{Id}^{\otimes i-1} \otimes A \otimes \mathrm{Id}^{\otimes n-i}\,.$$

Number operator:

$$\mathbf{N}_{|\vee^n \mathcal{Z}} := \mathrm{d}\Gamma(\mathrm{Id}) = \varepsilon n \mathrm{Id}_{\vee^n \mathcal{Z}}\,.$$

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Normal states and Wigner measures

Definition

Let $(\varrho_\varepsilon)_{\varepsilon \in \mathcal{E}}$ *be a family of normal states on* $\Gamma_s(\mathcal{Z})$ *with* $\mathcal{E} \subset (0, +\infty)$ *,* $0 \in \overline{\mathcal{E}}$ *.*
μ *is a Wigner measure for this family,* $\mu \in \mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E})$ *, if there exists* $\mathcal{E}' \subset \mathcal{E}$ *,* $0 \in \overline{\mathcal{E}'}$ *such that*

$$\forall f \in \mathcal{Z}\,, \lim_{\varepsilon \in \mathcal{E}', \varepsilon \to 0} \mathrm{Tr}\left[\varrho_\varepsilon W(\sqrt{2}\pi f)\right] = \int_{\mathcal{Z}} e^{2i\pi Re\, \langle f, z \rangle}\, d\mu(z)$$

Theorem [a]

[a] Ammari-Nier Ann. Henri-Poincaré 2008

If $(\varrho_\varepsilon)_{\varepsilon \in \mathcal{E}}$ *satisfies the uniform estimate* $\mathrm{Tr}\left[\varrho_\varepsilon \mathbf{N}^\delta\right] \leq C_\delta < +\infty$ *for some* $\delta > 0$ *fixed,* $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E})$ *is not empty and made of Borel probability measures (*$\mathcal{Z}$ *separable) such that* $\int_{\mathcal{Z}} |z|^{2\delta} d\mu(z) \leq C_\delta$ *.*

Wick symbols and operators

- Symbol class: $\mathcal{Z} \ni z \mapsto b(z) = \langle z^{\otimes q} \, , \, \tilde{b} z^{\otimes p} \rangle$

$$(b \in \mathcal{P}_{p,q}) \Leftrightarrow \left(\tilde{b} = \frac{1}{p!q!} \partial_{\bar{z}}^{q} \partial_{z}^{p} b(z) \in \mathcal{L}(\vee^{p} \mathcal{Z}, \vee^{q} \mathcal{Z}) \right)$$

- Wick quantization

$$b^{Wick}{}_{|\vee^{n}\mathcal{Z}} = 1_{[p,+\infty)}(n) \frac{\sqrt{n!(n+q-p)!}}{(n-p)!} \, \varepsilon^{\frac{p+q}{2}} \, \mathcal{S}_{n-p+q} \left(\tilde{b} \otimes 1^{\otimes(n-p)} \right) .$$

- $$H_{\varepsilon} = \mathrm{d}\Gamma(A) + Q^{Wick} = h^{Wick}$$

  with A self-adjoint and the symbol

$$h(z, \bar{z}) = \langle z \, , \, Az \rangle + Q(z, \bar{z})$$

- Mean field equation

$$\mathrm{i}\partial_{t} z_{t} = \partial_{\bar{z}} h(z_{t} \, , \bar{z}_{t}) = A z_{t} + \partial_{\bar{z}} Q(z_{t}, \bar{z}_{t})$$

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Reduced density matrices

Reduced density matrix:
$\varrho_\varepsilon^{(p)} \in \mathcal{L}^1(\bigvee^p \mathcal{Z})$, $p \in \mathbb{N}$,
unique non-negative trace class operator $\varrho_\varepsilon^{(p)}$ satisfying

$$\mathrm{Tr}\,[\varrho_\varepsilon\,(A \otimes 1^{\otimes(n-p)})] = \mathrm{Tr}\,[\varrho_\varepsilon^{(p)}\,A]\,,$$

$\forall A \in \mathcal{L}(\bigvee^p \mathcal{Z})$.
For instance for Hermite states $\varrho_\varepsilon = |\phi^{\otimes n}\rangle\langle\phi^{\otimes n}|$

$$\begin{aligned}\mathrm{Tr}\,[\varrho_\varepsilon\,(A \otimes 1^{\otimes(n-p)})] = \langle\phi^{\otimes n}\,, A\phi^{\otimes p} \otimes \phi^{\otimes n-p}\rangle = \langle\phi^{\otimes p}\,, A\phi^{\otimes p}\rangle \\ = \mathrm{Tr}\,[|\phi^{\otimes p}\rangle\langle\phi^{\otimes p}|A]\,.\end{aligned}$$

So $\varrho_\varepsilon^{(p)} = |\phi^{\otimes p}\rangle\langle\phi^{\otimes p}|$.

Convergence of reduced density matrices

Theorem[a]

[a] Ammari-Nier JMPA 2011

If the family $(\varrho_\varepsilon)_{\varepsilon\in\mathcal{E}}$ *satisfies* $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E}) = \{\mu\}$ *with the* (PI)*-condition:*

$$\forall p \in \mathbb{N}, \lim_{\varepsilon\in\mathcal{E}, \varepsilon\to 0} \mathrm{Tr}\,[\varrho_\varepsilon \mathbf{N}^p] = \int_{\mathcal{Z}} |z|^{2p}\, d\mu(z)\,;$$

then $\mathrm{Tr}\,\left[\varrho_\varepsilon b^{Wick}\right]$ *converges to* $\int_{\mathcal{Z}} b(z)\, d\mu(z)$ *for all polynomial* $b(z)$ *and*

$$\lim_{\varepsilon\in\mathcal{E}, \varepsilon\to 0} \|\varrho_\varepsilon^{(p)} - \varrho_0^{(p)}\|_{\mathcal{L}^1} = 0$$

for all $p \in \mathbb{N}$, $\varrho_0^{(p)} := \dfrac{\int_{\mathcal{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}| d\mu(z)}{\int_{\mathcal{Z}} |z|^{2p} d\mu(z)}$.

Propagation of the Wigner measures

Theorem[a]

[a] Ammari-Nier

Assume $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in (0, \bar{\varepsilon})) = \{\mu_0\}$ *and the (PI) condition.*
Then $\mathcal{M}(e^{-i\frac{t}{\varepsilon}H_\varepsilon}\rho_\varepsilon e^{i\frac{t}{\varepsilon}H_\varepsilon}, \varepsilon \in (0, \bar{\varepsilon})) = \{\mu_t\}$ *.*
The measure $\mu_t = \Phi(t,0)_*\mu_0$ *is the push-forward measure of the initial measure* μ_0 *where* $\Phi(t,0)$ *is the hamiltonian flow associated with the Hartree equation:*

$$\begin{cases} i\partial_t\varphi_t = -\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t \,, \\ \varphi_{t=0} = \varphi \,. \end{cases} \tag{1.1}$$

Hamiltonian with compact kernel interaction

Hamiltonian:

$$H_\varepsilon = \mathrm{d}\Gamma(A) + \sum_{\ell=2}^{r} \langle z^{\otimes \ell}\,,\ \tilde{Q}_\ell z^{\otimes \ell} \rangle^{Wick}\,.$$

$\tilde{Q}_\ell$ compact bounded symmetric operators on $\bigvee^\ell \mathcal{Z}$, A self-adjoint.
$Q(z) = \sum_{\ell=2}^{r} \langle z^{\otimes \ell}\,,\ \tilde{Q}_\ell z^{\otimes \ell} \rangle$

Propagation of the Wigner measure

Under these conditions, we get the following theorem:

Theorem

Let $(\varrho_\varepsilon)_{\varepsilon\in(0,\bar{\varepsilon})}$ be a family of trace class operators on $\Gamma_s(\mathcal{Z})$ such that

$$\exists\delta>0\,,\exists C_\delta>0\,,\forall\varepsilon\in(0,\bar{\varepsilon})\,,\quad \mathrm{Tr}\,[\varrho_\varepsilon \mathbf{N}^\delta]\leq C_\delta<\infty\,, \tag{2.1}$$

and which admits a unique Wigner measure μ_0 . The family $(\varrho_\varepsilon(t)=e^{-\mathrm{i}\frac{t}{\varepsilon}H_\varepsilon}\varrho_\varepsilon e^{i\frac{t}{\varepsilon}H_\varepsilon})_{\varepsilon\in(0,\bar{\varepsilon})}$ admits for every $t\in\mathbb{R}$ a unique Wigner measure μ_t , which is the push-forward $\Phi(t,0)_*\mu_0$ of the initial measure μ_0 by the flow associated with

$$\begin{cases} i\partial_t z_t = Az_t+\partial_{\bar{z}}Q(z_t), \\ z_{t=0}=z_0. \end{cases} \tag{2.2}$$

Rate of convergence

Theorem

Let $(\alpha(n))_{n\in\mathbb{N}^*}$ *be a sequence of positive numbers with* $\lim \alpha(n) = \infty$, $\frac{\alpha(n)}{n} \leq C$. $\varrho_\varepsilon \in \mathcal{L}^1(\bigvee^n \mathcal{Z})$ *and* $\varrho_0^{(p)} \in \mathcal{L}^1(\bigvee^p \mathcal{Z})$. *If there exists* $C_0 > 0$,*and* $\gamma \geq 1$ *such that for all* $n, p \in \mathbb{N}^*$ *with* $n \geq \gamma p$ $\left\| \varrho_\varepsilon^{(p)} - \varrho_0^{(p)} \right\|_1 \leq C_0 \frac{C^p}{\alpha(n)}$.
Then for any $T > 0$ *there exists* $C_T > 0$ *such that for all* $t \in [-T, T]$ *and all* $n, p \in \mathbb{N}^*$ *with* $n \geq \gamma p$,

$$\left\| \varrho_\varepsilon^{(p)}(t) - \varrho_0^{(p)}(t) \right\|_1 \leq C_T \frac{C^p}{\alpha(n)}.$$

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Typical case: $\alpha(n) = n$

Rate of convergence

Theorem

Let $(\alpha(n))_{n\in\mathbb{N}^*}$ be a sequence of positive numbers with $\lim \alpha(n) = \infty$, $\frac{\alpha(n)}{n} \leq C$. $\varrho_\varepsilon \in \mathcal{L}^1(\bigvee^n \mathcal{Z})$ and $\varrho_0^{(p)} \in \mathcal{L}^1(\bigvee^p \mathcal{Z})$. If there exists $C_0 > 0$,and $\gamma \geq 1$ such that for all $n, p \in \mathbb{N}^*$ with $n \geq \gamma p$ $\left\|\varrho_\varepsilon^{(p)} - \varrho_0^{(p)}\right\|_1 \leq C_0 \frac{C^p}{\alpha(n)}$.
Then for any $T > 0$ there exists $C_T > 0$ such that for all $t \in [-T, T]$ and all $n, p \in \mathbb{N}^*$ with $n \geq \gamma p$,

$$\left\|\varrho_\varepsilon^{(p)}(t) - \varrho_0^{(p)}(t)\right\|_1 \leq C_T \frac{C^p}{\alpha(n)} .$$

Typical case: $\alpha(n) = n$...but e.g. $\alpha(n) = n^{1/2}$ can be done at $t = 0$

Mean field expansion

Idea of the proof:

$$e^{i\frac{t}{\varepsilon}H_\varepsilon}\; D^{Wick} e^{-i\frac{t}{\varepsilon}H_\varepsilon} = D(t)^{Wick} + R(\varepsilon),$$

with $R(\varepsilon) \to 0$ when $\varepsilon \to 0$ and $D(t)^{Wick}$ is an infinite sum of Wick operators .

The strategy: an iterated integral formula the Dyson-Schwinger expansion (elaborated in the works by Frölich,Graffi,Schwarz,Knowles and Pizzo) is used with the Wick calculus to expand commutators of Wick operators according to ε.

Numerical discrete model of the bosonic mean field - Framework

$\mathcal{Z} = \mathbb{C}^K$. Discrete Laplacian operator: Δ_K

$$\forall z \in \mathbb{C}^K \quad \forall i \in \mathbb{Z}/K\mathbb{Z}, \quad (\Delta_K z)_i = z_{i+1} + z_{i-1} \,.$$

Hamiltonian: $H_\varepsilon = \mathrm{d}\Gamma(-\Delta_K) + \mathcal{V}$.

$$\mathbb{Z}_K := \mathbb{Z}/K\mathbb{Z}$$

$$\alpha := (\alpha_1, \cdots, \alpha_K) \in \mathbb{N}^K \,, \quad |\alpha| := \alpha_1 + \cdots + \alpha_K \,, \quad \alpha! := \alpha_1! \cdots \alpha_K! \,.$$

Orthogonal basis of the N-fold sector

$(e_1, \cdots, e_K)$: orthonormal basis of $\mathbb{C}^K$.
Orthonormal basis of $\bigvee^N \mathcal{Z}$ labelled by the multi-indices α such that $|\alpha| = N$:

$$\frac{a^*(e)^\alpha}{\sqrt{\varepsilon^{|\alpha|}\alpha!}}|\Omega\rangle := \frac{1}{\sqrt{\varepsilon^{|\alpha|}\alpha!}} a^*(e_1)^{\alpha_1} \cdots a^*(e_K)^{\alpha_K}|\Omega\rangle \,,$$

$|\Omega\rangle = (1, 0, 0, 0, \dots)$: vacuum of the Fock space.
Then the dimension of $\bigvee^N \mathcal{Z}$ is

$$\sharp\{\alpha \in \mathbb{N}^K / |\alpha| = N\} = C_{N+K-1}^{K-1} \,,$$

Discrete Hartree equation

$$H_\varepsilon = H(z,\bar{z})^{Wick}$$

Energy of the Hamiltonian:

$$H(z,\bar{z}) = \langle z, -\Delta_K z\rangle + \frac{1}{2}\sum_{i,j} V_{ij}|z_i|^2|z_j|^2$$

Hartree equation $\forall k \in \mathbb{Z}_K$:

$$\begin{aligned} \mathrm{i}\partial_t z_k &= \partial_{\overline{z_k}} H = -(\Delta_K z)_k + \sum_j V_{kj} z_k |z_j|^2 \\ &= -(\Delta_K z)_k + (V * |z|^2)_k z_k \quad \text{if} \quad V_{ij} = V(i-j)\,. \end{aligned}$$

Wick operator finite dimensional

In finite dimensional framework

$$b^{Wick} = a^*(e)^\alpha a(e)^\beta, \quad b(z) = \overline{z}^\alpha z^\beta \text{, and } \tilde{b} = |\frac{a^*(e)^\alpha}{\sqrt{\varepsilon^{|\alpha|}\alpha!}}\Omega\rangle\langle\frac{a^*(e)^\beta}{\sqrt{\varepsilon^{|\beta|}\beta!}}\Omega|$$

Quantum reduced density matrices $\varrho_\varepsilon^{(p)} \in \mathcal{L}^1(\bigvee^p \mathcal{Z})$ (trace class operators) defined by
the linear form on $\mathcal{L}^\infty(\bigvee^p \mathcal{Z})$ (compact operators)

$$\tilde{b} \mapsto \frac{\mathrm{Tr}\left[\varrho_\varepsilon b^{Wick}\right]}{\mathrm{Tr}\left[\varrho_\varepsilon (|z|^{2p})^{Wick}\right]} =: \mathrm{Tr}\left[\varrho_\varepsilon^{(p)} \tilde{b}\right]$$

by using $\left(\mathcal{L}^\infty(\bigvee^p \mathcal{Z})\right)' = \mathcal{L}^1(\bigvee^p \mathcal{Z})$

Propagation of Wigner measures

Wigner measure associated with a Hermite state $\frac{a^*(z)^N}{\sqrt{\varepsilon^N N!}}|\Omega\rangle$:
$\delta_z^{S^1} = \frac{1}{2\pi}\int_0^{2\pi} \delta_{e^{i\theta}z} d\theta$.
Wigner measures of states $\varrho_\varepsilon \in \mathcal{L}^1(\bigvee^N \mathcal{Z})$
gauge invariant probability measures $\mu = " \sum_{k=1}^m t_k \delta_{z_k}^{S^1} "$,
$" \sum_{k=1}^m t_k " = 1$.
After mean field propagation

$$Tr(\rho_\varepsilon(t) b^{Wick}) \longrightarrow_{\varepsilon \longrightarrow 0} \int_{\mathcal{Z}} b(z) d\mu_t(z)$$
$$\simeq \sum_{k=1}^m t_k \frac{1}{2\pi} \int_0^{2\pi} b(e^{i\theta} z_k(t)) d\theta$$

$z_k(t)$: solution to the Hartree equation.

Convergence of reduced density matrices

For any $p \in \mathbb{N}$, the following quantity is numerically evaluated:

$$\left\| \varrho_{\varepsilon}^{(p)}(t) - \frac{\int_{\mathcal{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}| d\mu_t(z)}{\int_{\mathcal{Z}} |z|^{2p} d\mu_0(z)} \right\|_{\mathcal{L}^1},$$

the matrix element of

$$\varrho_{\varepsilon}^{(p)}(t) - \frac{\int_{\mathcal{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}| d\mu_t(z)}{\int_{\mathcal{Z}} |z|^{2p} d\mu_0(z)}$$

is

$$\frac{p!}{\sqrt{\alpha!\beta!}} \left(\frac{\mathrm{Tr}\,\left(\varrho_{\varepsilon}(t) a^*(e)^{\alpha} a(e)^{\beta}\right)}{\varepsilon^p N(N-1)\dots(N-p+1)} - \frac{\sum_{k=1}^m t_k \bar{z}_k(t)^{\alpha} z_k(t)^{\beta}}{\sum_{k=1}^m t_k |z_k|^{2p}} \right).$$

Composition method

Numerical computation of $e^{-i\frac{t}{\varepsilon}H_\varepsilon}\Psi_0$ on $\bigvee^N \mathcal{Z}$ for $N \in \mathbb{N} - \{0\}$.
Computation of $e^{-i\frac{t}{\varepsilon}H_\varepsilon}\Psi_0$ by a composition method based on the Strang splitting method:

$$e^{-i\frac{t}{\varepsilon}H_\varepsilon} = \lim_{p\to\infty}\left(e^{-i\frac{t}{2\varepsilon p}\mathcal{V}}e^{-i\frac{t}{\varepsilon p}H_0}e^{-i\frac{t}{2\varepsilon p}\mathcal{V}}\right)^p \quad .$$

Order 4 composition method:

$$\begin{aligned}&e^{-i\frac{t}{\varepsilon}H_\varepsilon}\\ &= \lim_{p\to\infty}\Big(e^{-i\frac{a_3 t}{2\varepsilon p}\mathcal{V}}e^{-i\frac{a_3 t}{\varepsilon p}H_0}e^{-i\frac{a_3 t}{2\varepsilon p}\mathcal{V}}e^{-i\frac{a_2 t}{2\varepsilon p}\mathcal{V}}e^{-i\frac{a_2 t}{\varepsilon p}H_0}e^{-i\frac{a_2 t}{2\varepsilon p}\mathcal{V}}\\ &e^{-i\frac{a_1 t}{2\varepsilon p}\mathcal{V}}e^{-i\frac{a_1 t}{\varepsilon p}H_0}e^{-i\frac{a_1 t}{2\varepsilon p}\mathcal{V}}\Big)^p \ ,\end{aligned}$$

Coefficients

The coefficients of the method are satisfying the both equations:

$$a_1 + a_2 + a_3 = 1$$
$$a_1^3 + a_2^3 + a_3^3 = 0$$

and are given by[1]:

$$a_1 = a_3 = \frac{1}{2 - 2^{1/3}} \,, \qquad a_2 = -\frac{2^{1/3}}{2 - 2^{1/3}} \,.$$

[1] Hairer,E.,Lubich,C.,Wanner,G. Geometric numerical integration. Structure preserving algorithms for ordinary differential equations, Springer-Verlag 2002

Complexity

Dimension of $\bigvee^{20} \mathcal{Z}$ when $K = 10$: $10015005 \simeq 10^7$.
Sparse matrix of $\mathrm{d}\Gamma(-\Delta_K)$ on the basis of the bosons space containing only $2KC_{N+K-2}^{K-2}$ elements.
A full matrix contains $(C_{N+K-1}^{K-1})^2$ elements.
Computation of $e^{-i\frac{\Delta t}{\varepsilon}\mathrm{d}\Gamma(-\Delta_K)}$ at each time step by an order 4 Taylor expansion.
This expansion is replaced in the composition method.

Error estimate in the approximation of the composition method

Proposition

Let A and B be two anti-adjoint matrices and J an integer such that $\frac{\Delta t}{\varepsilon}(|a_1 - a_2|\|A\| + \frac{3|a_2|}{2}\|B\|) \leq 5$ *and* $J \geq \frac{t}{5\varepsilon}(|a_1 - a_2|\|A\| + \frac{3|a_2|}{2}\|B\|)$. *Then*

$$\|e^{\frac{t}{\varepsilon}(A+B)}u - (\tilde{\Psi}_{\frac{\Delta t}{\varepsilon}A,\frac{\Delta t}{\varepsilon}B})^J u\| \leq \left(2(\frac{e}{5})^5\left((a_1 - a_2)\|A\| - \frac{3a_2}{2}\|B\|\right)^5 + \frac{3}{4}\|A\|^5\right) t\frac{\Delta t^4}{\varepsilon^5}\|u\|,$$

with

$$\tilde{\Psi}_{A,B} = e^{\frac{a_1 B}{2}}\tilde{T}L(e^{a_1 A})e^{\frac{a_1 B}{2}}e^{\frac{a_2 B}{2}}\tilde{T}L(e^{a_2 A})e^{\frac{a_2 B}{2}}e^{\frac{a_1 B}{2}}\tilde{T}L(e^{a_1 A})e^{\frac{a_1 B}{2}}.$$

Constant independent on ε

$$\tilde{T}L(e^A)u = \frac{\|u\|}{\|TL(e^A)u\|} TL(e^A)u \text{ if } \|TL(e^A)u\| \neq 0$$

to preserve the norm.
$TL(e^A)$: order 4 Taylor expansion of e^A.

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to preserve the norm.
$TL(e^A)$: order 4 Taylor expansion of e^A.

Application: $A = -i\mathrm{d}\Gamma(-\Delta_K)$ $B = -i\mathcal{V}$ with
$\|\mathrm{d}\Gamma(-\Delta_K)\| + \| - i\mathcal{V}\| \leq C$ independent of $\varepsilon = \frac{1}{N}$.
Constant in the error estimate independent of ε or N
$\rightarrow$ Rule to adapt the time-step according to ε: $\Delta t = O(\varepsilon^{5/4})$

Examples of states

Twin states:
$\Psi_N = \frac{a^*(\psi_1)^{n_1} a^*(\psi_2)^{n_2}}{\sqrt{\varepsilon^{n_1+n_2} n_1! n_2!}} |\Omega\rangle$, $n_1 = n_2 = \frac{N}{2}$.
Wq states:
$\Psi_N = \frac{a^*(\psi_1)^{n_1} a^*(\psi_2)^{n_2}}{\sqrt{\varepsilon^{n_1+n_2} n_1! n_2!}} |\Omega\rangle$, $n_1 = N - q$ and $n_2 = q$ fixed.
With $\psi_1 = \frac{1}{\sqrt{2}}(e_1 + \mathrm{i} e_3)$ and $\psi_2 = e_2$.

Order of convergence of reduced density matrices

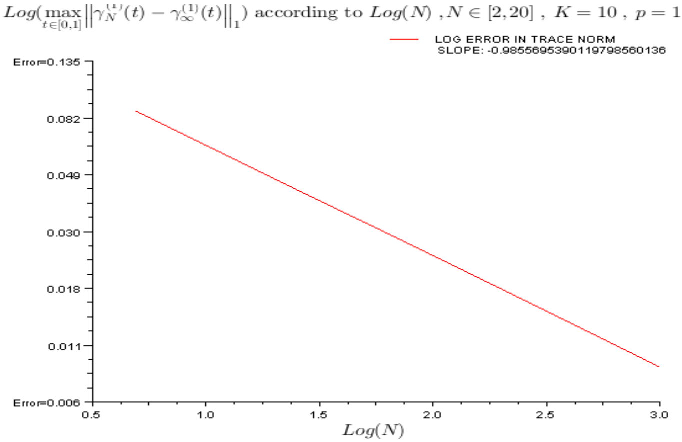

Figure: Order of convergence of reduced density matrices for mixed states. Numerical slope : $-0,9855$. $Log(\max_{t\in[0,1]} \|\varrho_\varepsilon^{(1)}(t) - \varrho_0^{(1)}(t)\|_1)$

Time-evolved densities of particles

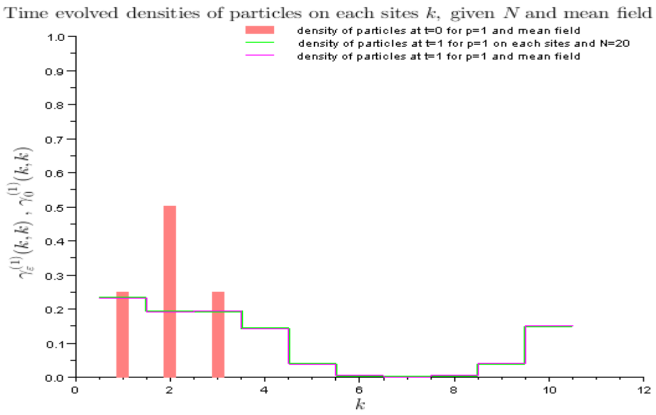

Figure: Time-evolved densities of particles for $K = 10$, $p = 1, N = 20$ and mean field limit for mixed states. $\varrho_\varepsilon^{(1)}(k,k)$, $\varrho_0^{(1)}(k,k)$

Correlations for twin states

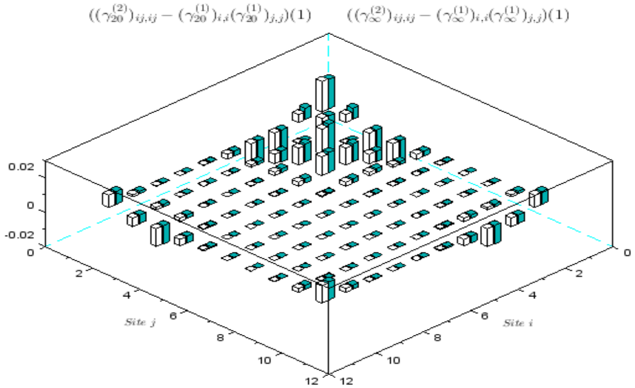

Figure: Correlations for $K = 10$, $N = 20$ and mean field limit for mixed states.

Orders of convergence for Wq states

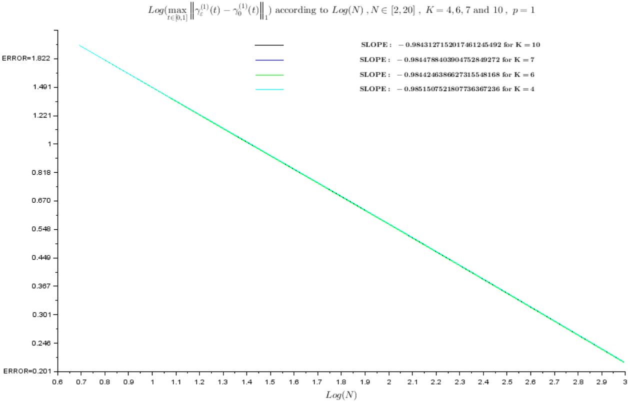

Figure: Orders for $K = 4{,}6{,}7{,}10$, $N = 20$, $p = 1$. Numerical slopes: $K = 10$: -0.98431, $K = 7$: -0.98447, $K = 6$: -0.98442, $K = 4$: -0.98515

Error estimate in trace norm I

Estimate the error trace norm at $t = 0$. We have:

$$\Psi_N = \frac{a^*(\psi_1)^{N-2} a^*(\psi_2)^2}{\sqrt{\varepsilon^N (N-2)!2!}} \Omega = \sqrt{\frac{\varepsilon^N N!}{2\varepsilon^N (N-2)!}} \mathcal{S}_N(\psi_1^{\otimes N-2} \otimes \psi_2^{\otimes 2})$$

$$= \sqrt{\frac{2}{N(N-1)}} \sum_{i,j} \psi_1 \otimes \ldots \otimes \underbrace{\psi_2}_{i} \otimes \ldots \otimes \underbrace{\psi_2}_{j} \otimes \psi_1 \ldots \psi_1 \, .$$

Consider $A \in \mathcal{L}(\mathcal{Z})$ defined by $A\psi_1 = \psi_1$, $A\psi_2 = -\psi_2$ and $A_{\{\psi_1,\psi_2\}^\perp} = 0$, we have $\|A\| = 1$.
$d\Gamma(A)\Psi_N = \varepsilon(1 \times (N-2) + 2 \times (-1))\Psi_N = \frac{N-4}{N}\Psi_N$.
Hence

$$\mathrm{Tr}\,(\gamma_\varepsilon^{(1)} A) = \frac{\mathrm{Tr}\,(\varrho_\varepsilon d\Gamma(A))}{\mathrm{Tr}\,(\varrho_\varepsilon(|z|^2)^{Wick})} = \frac{\langle \Psi_N \, , \, d\Gamma(A)\Psi_N \rangle}{\varepsilon N} = \frac{N-4}{N} \, .$$

Error estimate in trace norm II

$$\mathrm{Tr}\,(\gamma_0^{(1)}A) = \mathrm{Tr}\,(A\int_{\mathcal{Z}}|z\rangle\langle z|\mathrm{d}\delta_{\psi_1}^{S^1}) = \mathrm{Tr}\,(A|\psi_1\rangle\langle\psi_1|) = \langle\psi_1\,,\,A\psi_1\rangle = 1\,.$$

Therefore

$$\|\gamma_\varepsilon^{(1)} - \gamma_0^{(1)}\|_1 \geq |\,\mathrm{Tr}\,((\gamma_\varepsilon^{(1)} - \gamma_0^{(1)})A)| = 1 - \frac{N-4}{N} = \frac{4}{N}\,.$$

So at the initial time, for $N = 20$, the error is greater than 0.2.

Correlations for Wq states

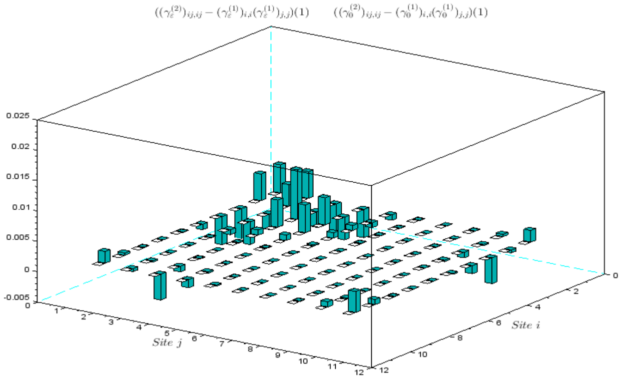

Figure: Mean field(white) and 20-body quantum(blue) correlations for Wq states at $t = 1$

References:

- 2016, On the rate of convergence for the mean field approximation of bosonic many-body quantum dynamics.Communications in Mathematical Sciences volume 14 nunber 5, p.1417 1442. Joint work with Zied Ammari and Marco Falconi
- 2014, Mean field limit for Bosons with compact kernels interactions by Wigner measures transportation. Journal of Mathematical Physics 55, 092304 . Joint work with Quentin Liard

Thanks for your attention