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Mean field approximation of many-body quantum dynamics for
Bosons in a discrete numerical model

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Abstract

The mean field approximation is numerically validated in the bosonic case by considering the time evolution of quantum states and their associated reduced density matrices by many-body Schrödinger dynamics. The model phase-space is finite-dimensional. The results are illustrated with numerical simulations of the evolution of quantum states according to the time, the number of the particles, and the dimension of the phase-space.

Mathematics subject classification: 81S30, 81S05, 81T10, 35Q55, 81P40

Keywords: mean field limit, reduced density matrices, Wigner measures, bosons Fock space, second quantization.

1 Introduction

The mean field approximation is known to be a good way to approximate the many-body Schrödinger dynamics when the number of particles is large enough (see [2, 6, 9, 10, 15, 19, 20, 21, 24, 25, 26, 32, 37, 43, 46, 29, 30, 33, 50]).

It consists in looking for the solutions to the non-linear Schrödinger equation for one particle called the Hartree equation. We are interested in the density matrix associated with the wave function, this matrix satisfies the quantum Liouville equation dual to the Von Neumann equation. The partial trace operators of this matrix, called the reduced density matrices, satisfy a hierarchy of equations. For instance, by considering the case where the initial state for the Schrödinger equation is a Hartree ansatz (a product state) which is suitable for a bosons condensate, the limit, when the number of particles \(N\) goes to the infinity of these matrices converge in trace norm to the product of the density matrix associated with the solution to the Hartree equation. And this asymptotic density matrix satisfies the time dependent Hartree equation [8].

When the particles are bosons, the suitable space for the bosons is the symmetric Fock space on the phase-space. Moreover for the sake of numerical computations, a finite-dimensional phase-space will be used instead of an usual phase-space of type \(L^2(\mathbb{R}^d)\). So here the phase-space will be \(\mathcal{Z} = l^2(\{0, \cdots, K\}) \simeq \mathbb{C}^K\) where \(K\) is a given integer representing the number of sites. Each particle can live in one of the \(K\) sites.

For the numerical implementation, an explicit basis of the \(N\)-fold sector of the Fock bosonic spaces is specified. This basis allows the numerical computation of the full \(N\)-body quantum problem for \(N\) large enough to validate various mean field regimes, in spite of a rapidly increasing complexity.

The resolution of the \(N\)-particles Schrödinger equation will rely on a splitting method, one part for the free Hamiltonian and the other one for the two particles interaction term.

For the simulations, the considered real bounded potential associated with the interaction term will be \(V\) defined on \(\mathbb{Z}/K\mathbb{Z}\) by \(V(i) = \frac{1}{|i|}\) if \(i \neq 0\) and \(V(0) = 0\).

According to previous results related to the propagation of the Wigner measures [3, 4, 5, 6] knowing the Wigner measure at time \(t = 0\) determines the Wigner measure at time \(t\) and all asymptotic reduced density matrices. For many examples, like Hermite states, twin Fock states or states studied in quantum information theory (see [1]) their Wigner measure as well as the order of convergence of reduced density matrices is known explicitly. The evolution of the Wigner measure, and consequently of the asymptotic density matrices, is evaluated after integrating numerically the mean field non linear Hartree time-dependent equation. In order

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These operators are then extended by linearity and density to a discretization of a time interval \([0,t_{\text{max}}]\) is considered, in the examples \(t_{\text{max}} = 1\) is chosen, then the quantity \(\max_{t \in [0,t_{\text{max}}]} \| \gamma_{N}^{(p)}(t) - \gamma_{\infty}^{(p)}(t) \|_1\) is observed. Here \(\gamma_{N}^{(p)}(t)\) denotes the time-evolved \(p\) particles reduced density matrix for \(N\) bosons, while \(\gamma_{\infty}^{(p)}(t)\) is its theoretical limit when \(N\) goes to the infinity, and \(\| . \|_1\) denoting the trace norm.

For the evaluation of the order of convergence, the logarithm of the previous error estimate is drawn according to \(\log(N)\). This gives a straight line whose the slope is the order of convergence in \(1/N\).

These numerical results agree very well and illustrate the theoretical analysis carried out in [1].

By increasing \(K\), we wish to approach a continuous model. The complexity of the computations increase in the same time that \(K\) and \(N\) increase because of the dimension of the \(N\)-particles bosons Fock space on \(\mathbb{C}^K\) which is a binomial coefficient.

\section{Framework}

The bosons Fock space on an Hilbert space \(\mathcal{Z}\) is defined as \(\Gamma_{\times}(\mathcal{Z}) = \bigoplus_{n \geq 0} \mathcal{V}^n \mathcal{Z}\) where \(\mathcal{V}^n \mathcal{Z}\) is the symmetric \(n\)-fold Hilbertian tensor product of \(\mathcal{Z}\) which is the range of the projection defined on the Hilbert tensor product \(\mathcal{Z}^\otimes n\), by:

\[
S_n(\xi_1 \otimes \xi_2 \otimes \ldots \otimes \xi_n) = \frac{1}{n!} \sum_{\sigma \in \Sigma_n} \xi_{\sigma(1)} \otimes \xi_{\sigma(2)} \otimes \ldots \otimes \xi_{\sigma(n)},
\]

where \(\xi_i\) is in \(\mathcal{Z}\) for each \(i\) in \([1,n]\) and \(\Sigma_n\) is the set of the permutations of \(n\) elements.

For \(z\) in \(\mathcal{Z}\) and \(\varepsilon\) positive, the \(\varepsilon\)-scaled annihilation and creation operators are defined for all \(\Phi\) in \(\mathcal{Z}\) and \(n\) in \(\mathbb{N}\) by:

\[
a(z)\Phi^{\otimes n} = \sqrt{\varepsilon n}(\varepsilon | \Phi\Phi^{\otimes n-1},
\]

\[
a^\ast(z)\Phi^{\otimes n} = \sqrt{\varepsilon(n+1)}S_{n+1}(|z\rangle \otimes \Phi^{\otimes n}).
\]

These operators are then extended by linearity and density to \(\mathcal{V}^n \mathcal{Z}\).

These operators satisfy the canonical commutation relations (CCR):

\[
[a(z_1), a^\ast(z_2)] = \varepsilon(z_1, z_2) I d,
\]

\[
[a(z_1), a(z_2)] = 0,
\]

\[
[a^\ast(z_1), a^\ast(z_2)] = 0.
\]

The second quantization of an operator \(A \in \mathcal{L}(\mathcal{Z})\) or a self-adjoint operator \((A, D(A))\) in \(\mathcal{Z}\) is defined by:

\[
d\Gamma(A)_{\mathcal{V}^n, \mathcal{V}^n, A, D(A)} = \varepsilon \sum_{i=1}^{n} I d^{\otimes i-1} \otimes A \otimes I d^{\otimes n-i}.
\]

The second quantization of \(Id_{\mathcal{Z}}\) is the number operator:

\[
\mathcal{N}_{\mathcal{V}^n, \mathcal{Z}} = \varepsilon n Id_{\mathcal{V}^n, \mathcal{Z}}.
\]

\subsection{Orthogonal basis of the \(N\)-fold sector}

Use the following notations: \(\mathbb{Z}_K = \mathbb{Z}/K\mathbb{Z}\).

For \(\alpha = (\alpha_1, \ldots, \alpha_K)\) in \(\mathbb{N}^K\), the length of \(\alpha\) is written \(|\alpha| = \alpha_1 + \cdots + \alpha_K\) and the factorial of \(\alpha\)

\(\alpha! = \alpha_1! \cdots \alpha_K!\).

Let \((\epsilon_1, \cdots, \epsilon_K)\) be an orthonormal basis of \(\mathbb{C}^K\).

Set \(\mathcal{Z} = \mathbb{C}^K\). Then an orthonormal basis of \(\mathcal{V}^N \mathcal{Z}\) can be built from this basis which is labelled by the
multi-indices $\alpha$ in $\mathbb{N}^K$ such that $|\alpha| = N$.

With the creation operators, an orthonormal basis can be written as:

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

where $|\Omega\rangle = (1, 0, 0, \ldots)$ is the vacuum of the Fock space.

Then the dimension of $\bigvee_{N} Z$ is

$$\text{card}(\{\alpha \in \mathbb{N}^K / |\alpha| = N\}) = (N + K - 1)^K.$$

And $\text{card}(\{\alpha \in \mathbb{N}^K / |\alpha| \leq N\}) = (N + K)^K$ is the dimension of $\bigvee_{n=0}^{N} \bigvee^n Z$.

### 2.2 Hamiltonian

As a binomial number, the dimension of the $N$ particles bosonic sector increases rapidly but not too much, as $N$ increases (see Table 6.4 for numerical values). The complexity has to be handled carefully if we want to approach the mean field limit by taking $N$ large or the continuous model by taking $K$ large.

Define $\Delta_K$ the discrete Laplacian operator on $\mathbb{C}^K$ by:

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

And let $H_0 = d\Gamma(-\Delta_K)$ be the free Hamiltonian.

The interaction term denoted by $V$ equals:

$$V = \frac{1}{2} \sum_{(i,j) \in \mathbb{Z}_K^2} V_{ij} a^*(e_i)a^*(e_j)a(e_i)a(e_j),$$

where $V_{ij} = V_{ji} = V(i-j)$. In this framework changing the value of $V(0)$ add an irrelevant phase factor in the time evolved wave function. In the sequel $V(0) = 0$ is assumed.

Or as a Wick quantized operator (14):

$$V = \langle z^\otimes 2, \left(\frac{1}{2} \sum_{(i,j) \in \mathbb{Z}_K^2} V_{ij} |e_i \otimes e_j\rangle |e_i \otimes e_j| z^\otimes 2\rangle\rangle_{\text{Wick}}.$$

The considered linear Schrödinger equation is:

$$i\varepsilon \partial_t \Psi = H_\varepsilon \Psi,$$

where the complete Hamiltonian is defined on the bosonic Fock space by:

$$H_\varepsilon = d\Gamma(-\Delta_K) + V.$$

### 3 Finite dimensional mean field equation

#### 3.1 Energy of the Hamiltonian

The energy of the Hamiltonian corresponds to the symbol of the complete Hamiltonian:

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

while recalling our convention $V_{ii} = V(0) = 0$ for all $i$ in $\mathbb{Z}_K$. 
3.2 Hartree equation

The mean field equation in $\mathcal{Z}$ is written as:

$$i\partial_t z = \partial_z H(z, \bar{z}).$$

For each component in $\mathbb{C}^K$ we obtain:

$$i\partial_t \overset{k}{z} = \partial_{\overset{k}{z}} (\sum_{i'} |z_{i'} - z_{i'-1}|^2 - 2|z_i|^2 + \frac{1}{2} \sum_{i' \neq j} V_{ij} |z_{i'}|^2 |z_j|^2)$$

$$= \partial_{\overset{k}{z}} (\sum_{i'} (z_{i'} - z_{i'-1})(z_{i'} - z_{i'-1}) - 2z_i z_i + \frac{1}{2} \sum_{i' \neq j} V_{ij} |z_{i'}|^2 z_j z_j)$$

$$= z_i - z_{i-1} - (z_{i+1} - z_i) - 2z_i + \sum_{j \neq i} V_{ij} |z_j|^2 z_i$$

$$= -(z_{i+1} - z_{i-1}) + (\sum_{j \neq i} V_{ij} |z_j|^2) z_i$$

$$\dot{z}_i = -i[-(\Delta_K z)_i + (\sum_{j \neq i} V_{ij} |z_j|^2) z_i]$$

By writing $z = q + ip$ where $q$ and $p$ belong to $\mathbb{R}^K$, it becomes:

$$\dot{q}_i = -(p_{i+1} + p_{i-1}) + \sum_{j \neq i} V_{ij} (q_j^2 + p_j^2) p_i$$

$$\dot{p}_i = -(q_{i+1} + q_{i-1}) + \sum_{j \neq i} V_{ij} (q_j^2 + p_j^2) q_i$$

A $4^{th}$ or $6^{th}$ order Gauss RK method is used by using the coefficients given in [35] to solve the Hartree equation.

A symplectic method is used to preserve the quadratic part of the energy, the symplectic form and the phase space volume.

3.3 Wigner measures

For $f \in \mathcal{Z}$ the field operator is defined by $\Phi(f) = \frac{1}{\sqrt{2}} (a^*(f) + a(f))$ which is essentially self-adjoint on $\Gamma_{fin}(\mathcal{Z}) = \oplus_{n \in \mathbb{N}} \mathcal{V}^n \mathcal{Z}$

The Weyl operator is defined by $W(f) = e^{i\Phi(f)}$.

Let $(\varrho_\varepsilon)_{\varepsilon \in \mathcal{E}}$ be a family of normal states on $\Gamma_\varepsilon(\mathcal{Z})$ with $\mathcal{E} \subset (0, +\infty)$, $0 \in \mathcal{E}$.

A measure $\mu$ is a Wigner measure for this family, $\mu \in \mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E})$, if there exists $\mathcal{E}' \subset \mathcal{E}, 0 \in \mathcal{E}'$ such that

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

see [42].

The following result valid for separable Hilbert spaces $\mathcal{Z}$, apply to our finite dimensional $\mathcal{Z} \simeq \mathbb{C}^K$.

**Theorem 3.1 [3].** If $(\varrho_\varepsilon)_{\varepsilon \in \mathcal{E}}$ satisfies the uniform estimate $\text{Tr}[\varrho_\varepsilon N^\delta] \leq C_\delta < +\infty$ 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 $\int_{\mathcal{Z}} |z|^{2\delta} d\mu(z) \leq C_\delta$.

For each $p$ in $\mathbb{N}$, the reduced density matrix associated with a state $\varrho_\varepsilon$ is a trace class operator in $\mathcal{L}^1(\mathcal{V}^p \mathcal{Z})$ defined by the duality relation:

$$\text{Tr} [\gamma^p \varrho_\varepsilon] = \frac{\text{Tr} [\varrho_\varepsilon b^{\text{Wick}}]}{\text{Tr} [\varrho_\varepsilon (|z|^{2p})^{\text{Wick}}]} \quad (5)$$
where $\tilde{b} \in \mathcal{L}(\mathbb{V}^p)$. The asymptotic reduced density matrix associated with the Wigner measure $\mu$ equals:

$$\gamma_0^p = \frac{\int_{\mathbb{E}} |z|^p \langle z^p \rangle d\mu(z)}{\int_{\mathbb{E}} |z|^{2p} d\mu(z)}. \quad (6)$$

In finite dimension, if the family $(\varrho_{\varepsilon})_{\varepsilon \in \varepsilon}$ satisfies $\mathcal{M}(\varrho_{\varepsilon}, \varepsilon \in \varepsilon) = \{\mu\}$ then the (PI)-condition (see [3]):

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

is always satisfied.

### 3.4 Reduced density matrices

**Theorem 3.2** [5]. If the family $(\varrho_{\varepsilon})_{\varepsilon \in \varepsilon}$ satisfies $\mathcal{M}(\varrho_{\varepsilon}, \varepsilon \in \varepsilon) = \{\mu\}$ with the (PI)-condition:

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

then $\text{Tr}[\varrho_{\varepsilon} b_{\text{Wick}}]$ converges to $\int_{\mathbb{E}} b(z) d\mu(z)$ for all polynomial $b(z)$ and

$$\lim_{\varepsilon \to 0} \|\gamma_\varepsilon^p - \gamma_0^p\|_{L^1} = 0$$

for all $p \in \mathbb{N}$.

**Theorem 3.3** [5, 6, 42]. Assume $\mathcal{M}(\varrho_{\varepsilon}, \varepsilon \in (0, \varepsilon)) = \{\mu_0\}$ and the condition (PI). Then $\mathcal{M}(e^{-iH_{\varepsilon}t}, \varrho_{\varepsilon} e^{iH_{\varepsilon}t}, \varepsilon \in (0, \varepsilon)) = \{\mu_t\}$. The measure $\mu_t = \Phi(t, 0) \mu_0$ is the push-forward measure of the initial measure $\mu_0$ where $\Phi(t, 0)$ is the hamiltonian flow associated with the equation

$$i\partial_t z_k(t) = -\Delta_K z_k(t) + \sum_j V_{kj} j^2 z_k. \quad (7)$$

After propagation of the Wigner measures, for any $p \in \mathbb{N}$, the convergence of the reduced density matrices is obtained at any time $t$:

$$\left\|\gamma^p(t) - \frac{\int_{\mathbb{E}} |z|^p \langle z^p \rangle d\mu(z)}{\int_{\mathbb{E}} |z|^{2p} d\mu(z)}\right\|_{L^1} \to 0.$$

**Theorem 3.4** [1]. Let $(\alpha(n))_{n \in \mathbb{N}^*}$ be a sequence of positive numbers with $\lim \alpha(n) = \infty$ and such that $(\frac{\alpha(n)}{n})_{n \in \mathbb{N}^*}$ is bounded. Let $(\varrho_n)_{n \in \mathbb{N}^*}$ and $(\gamma_{\infty}^p)_{p \in \mathbb{N}^*}$ be two sequences of density matrices with $\varrho_n \in \mathcal{L}^1(\mathbb{V}^n \mathbb{E})$ and $\gamma_{\infty}^p \in \mathcal{L}^1(\mathbb{V}^p \mathbb{E})$ for each $n, p \in \mathbb{N}^*$. Assume that there exist $C_0 > 0$, $C > 2$ and $\gamma \geq 1$ such that for all $n, p \in \mathbb{N}^*$ with $n \geq \gamma p$:

$$\left\|\gamma_{\infty}^p - \gamma_{\infty}^p\right\|_1 \leq C_0 \frac{Cp}{\alpha(n)}. \quad (8)$$

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 $n \geq \gamma p$,

$$\left\|\gamma_{n}^p(t) - \gamma_{n}^p(t)\right\|_1 \leq C_T \frac{Cp}{\alpha(n)}, \quad (9)$$

where

$$\gamma_{\infty}^p(t) = \int_{\mathbb{E}} |z|^p \langle z^p \rangle d\mu_0(z),$$

with $\mu_i = (\Phi_i)_t \mu_0$ is the push-forward of the initial measure $\mu_0$ by the well defined and continuous Hartree flow $\Phi_i$ on $\mathbb{E}$. 

5
4 Numerical methods

4.1 Method to solve the Hartree equation

To solve the mean field equation (7), a Runge-Kutta method is used.

Let $b_i, a_{ij} \ (i,j = 1,\ldots,s)$ be real numbers and $c_i = \sum_{j=1}^s a_{ij}$.

An s-stage Runge-Kutta method with a time step $h$ to solve a first-order ordinary equation $y' = f(t, y)$, $y(t_0) = y_0$ is given by:

$\begin{align*}
k_i &= f(t_0 + c_i h, y_0 + h \sum_{j=1}^s a_{ij} k_j), \ i = 1,\ldots,s \\
y_1 &= y_0 + h \sum_{i=1}^s b_i k_i
\end{align*}$

represented as:

$\begin{array}{ccc|cccccc}
c_1 & a_{11} & \ldots & a_{1s} \\
\vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & \ldots & a_{ss} \\
\hline
b_1 & \ldots & b_s
\end{array}$

Here the system is autonomous, and according to [35] the coefficients used for the Gauss RK method are:

$\begin{array}{cccc|cccc}
0 & 1/2 & 1/2 & 0 & 1/3 & 1/3 & 1/2 - \sqrt{3}/6 & 1/4 & 1/4 - \sqrt{3}/6 \\
1/2 & 0 & 1/2 & , & 2/3 & -1/3 & 1 & or & 1/2 + \sqrt{3}/6 & 1/4 + \sqrt{3}/6 & 1/4 \\
1 & 0 & 0 & 1 & 1 & 1 & 1 & & 1/2 & 1/2 & \\
\hline
1/6 & 2/6 & 2/6 & 1/6 & 1/8 & 3/8 & 3/8 & 1/8
\end{array}$

In our case, the function $f$ corresponds to $f(z) = -i \left( -\Delta z + \sum_j V_{kj}[z_j]^2 z_k \right)$.

As a function in $\mathbb{R}^{2K}$ by replacing $z$ by $q + ip$,

$\begin{align*}
f(q, p) &= f_{q}(q, p) + i f_{p}(q, p) \\
f_{q}(q, p) &= -(p_{i+1} + p_{i-1}) + \sum_{j \neq i} V_{ij} (q_{j}^2 + p_{j}^2) p_i \\
f_{p}(q, p) &= q_{i+1} + q_{i-1} - \sum_{j \neq i} V_{ij} (q_{j}^2 + p_{j}^2) q_i
\end{align*}$

For an implicit Runge-Kutta method, a Newton method is applied to find the coefficients $k_i$ for each step of the RK method to the function $g_{y_0} : (k_i)_{i=1,\ldots,s} \mapsto \left( k_i - f(y_0 + h \sum_{j=1}^s a_{ij} k_j) \right)_{i=1,\ldots,s}$.

Given the time step $h$ small enough, the starting point of the Newton method is chosen by setting $k_i = f(y_0)$ for all $i$.

To apply the Newton’s method the differential of $f$ is computed by using the following partial derivatives of $f$:

$\begin{align*}
\frac{\partial f_{q_i}}{\partial q_k} &= (1 - \delta_{i,k}) 2 V_{ik} q_k p_i \\
\frac{\partial f_{q_i}}{\partial q_k} &= \delta_{i+1,k} + \delta_{i-1,k} + (\delta_{i,k} - 1) 2 V_{ik} q_k q_i - \delta_{i,k} \sum_{j \neq i} V_{ij} (q_{j}^2 + p_{j}^2) \\
\frac{\partial f_{q_i}}{\partial p_k} &= -(\delta_{i+1,k} + \delta_{i-1,k}) + (1 - \delta_{i,k}) 2 V_{ik} p_k p_i + \delta_{i,k} \sum_{j \neq i} V_{ij} (q_{j}^2 + p_{j}^2) \\
\frac{\partial f_{q_i}}{\partial p_k} &= (1 - \delta_{i,k}) 2 V_{ik} p_k q_i
\end{align*}$
Then the differential of $g_{y_0}$ is:

$$Dg_{y_0}((k_i)_{i=1,\ldots,s}) \equiv \left( Id_{2K} - ha_d Df(y_0 + h \sum_{j=1}^s a_{ij} k_j) \right)_{i,d=1,\ldots,s}$$

where $g_{y_0}$ is considered as a function from $\mathbb{R}^{2Ks}$.

### 4.2 Resolution of the Schrödinger equation in $\mathcal{V}^N \mathcal{Z}$

#### 4.2.1 Composition method

For a given $\Psi$ in $\mathcal{V}^N \mathcal{Z}$, the full $N$-body evolved state $e^{-i \frac{t}{2}} H \Psi$ is computed in the basis $(e_\alpha)_{|\alpha|=N}$. After writing $\Psi = \sum_{|\alpha|=N} \Psi_\alpha e_\alpha$ a modified splitting method for which the numerical error is carefully controlled (see 5), involves only multiplications by the diagonal matrix $e^{-i \frac{t}{2}} V$ and the sparse matrix $d\Gamma(-\Delta_K)$.

In order to handle the high complexity of the problem (see table 6.4) no matrix, but only vectors or the sparse matrices $d\Gamma(-\Delta_K)$ and the matrix $(V_{ij})_{i,j}$ are stored.

The complete evolution $e^{-i \frac{t}{2}} H$ is computed by a composition method based on the Strang splitting method:

$$e^{-i \frac{t}{2}} H = \lim_{p \to \infty} (e^{-i \frac{2}{2^p}} V e^{-i \frac{2}{2^p} H_0} e^{-i \frac{2}{2^p} V})^p.$$

The 4th order composition method is given by:

$$e^{-i \frac{t}{2}} H = \lim_{p \to \infty} (e^{-i \frac{2}{2^p}} V e^{-i \frac{2}{2^p} H_0} e^{-i \frac{2}{2^p} V} e^{-i \frac{2}{2^p} H_0} e^{-i \frac{2}{2^p} V} e^{-i \frac{2}{2^p} H_0} e^{-i \frac{2}{2^p} V})^p,$$

where the coefficients of the method are satisfying the two equations (see [35]):

$$a_1 + a_2 + a_3 = 1 \quad (10)$$

$$a_3^1 + a_3^2 + a_3^3 = 0 \quad (11)$$

and are given by:

$$a_1 = a_3 = \frac{1}{2 - 2^{1/3}}, \quad a_2 = \frac{2^{1/3}}{2 - 2^{1/3}}. \quad (12)$$

#### 4.2.2 Computation of the free evolution $e^{-i \frac{t}{2}} d\Gamma(-\Delta_K)$

The numerical computation of $e^{-i \frac{t}{2}} d\Gamma(-\Delta_K) = \Gamma(e^{it\Delta_K})$, relies on the following two remarks:

- the dimension of the $N$-fold sectors $(\frac{N+K-1}{K-1})$ prevents the storage of any square matrix.
- the matrix of $\Gamma(e^{it\Delta_K})$ is actually non trivial sparse matrix in the basis $(e_\alpha)$.

The matrix of $\Delta_K$ is given by:

$$\Delta_K = \begin{pmatrix}
0 & 1 & 0 & \cdots & 0 & 1 \\
1 & \ddots & \ddots & \ddots & 0 \\
0 & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \ddots & \ddots & \ddots & 0 & 1 \\
1 & 0 & \cdots & 0 & 1 & 0
\end{pmatrix}.$$
We are interested in the matrix of the second quantization of the discrete Laplacian on the basis of the bosons space to implement it numerically as a sparse matrix containing only $2K \binom{N+K-2}{K-1}$ elements whereas a full matrix contains $\binom{N+K-1}{K-1}$

Then $e^{-i\frac{\Delta t}{\hbar}\Delta K}$ will be computed at each time step by a 4th order Taylor expansion. This expansion is then replaced in the composition method.

For an operator $A : \mathbb{C}^K \rightarrow \mathbb{C}^K$, $A = (A_{i,j})_{i,j}$,

\[d\Gamma(A)\big|_{\mathbb{C}^K} = \sum_{i,j=1}^{K} A_{i,j}a^*(e_i)a(e_j).\]

This yields:

\[d\Gamma(-\Delta_K) = -\sum_{j=1}^{K} a^*(e_{j+1})a(e_j) + a^*(e_j)a(e_{j+1}). \tag{13}\]

**Lemma 4.1** For all multi-indices $\gamma$ and $\alpha$ the following equality holds:

\[a(e)^{\gamma}a^*(e)^{\alpha}|\Omega\rangle = \delta_{\gamma \leq \alpha}e^{[\gamma]}\frac{\alpha!}{(\alpha - \gamma)!}a^*(e)^{\alpha - \gamma}|\Omega\rangle.\]

**Proof.**

\[
a(e)^{\gamma}a^*(e)^{\alpha} = a(e_1)^{\gamma_1} \ldots a(e_K)^{\gamma_K} a^*(e_1)^{\alpha_1} \ldots a^*(e_K)^{\alpha_K} = \prod_{i=1}^{K} a(e_i)^{\gamma_i}a^*(e_i)^{\alpha_i} \text{ which is a commutative product because of CCR (1)}
\]

\[
= \bigotimes_{i=1}^{K} a(e_i)^{\gamma_i}a^*(e_i)^{\alpha_i}
\]

by using the following separation of the variables: $\Gamma(Z) = \Gamma(\mathbb{C}e_1) \otimes \ldots \otimes \Gamma(\mathbb{C}e_K)$.

In this space let $|\Omega\rangle$ be $|\Omega_1\rangle \otimes \ldots \otimes |\Omega_K\rangle$.

Let us consider $\gamma_i \geq 1$ and $\alpha_i \geq 1$,

\[
a(e_i)^{\gamma_i}a^*(e_i)^{\alpha_i}|\Omega_i\rangle = a(e_i)^{\gamma_i-1}a(e_i)a^*(e_i)^{\alpha_i}|\Omega_i\rangle = a(e_i)^{\gamma_i-1}a^*(e_i)^{\alpha_i}a(e_i)|\Omega_i\rangle + a(e_i)^{\gamma_i-1}|\alpha_i\rangle a^*(e_i)^{\alpha_i}|\Omega_i\rangle
\]

\[
= \varepsilon a_i a(e_i)^{\gamma_i-1}a^*(e_i)^{\alpha_i-1}|\Omega_i\rangle.
\]

By induction, we obtain

\[
a(e_i)^{\gamma_i}a^*(e_i)^{\alpha_i}|\Omega_i\rangle = \alpha_i \varepsilon \times (\alpha_i - 1) \varepsilon \times \ldots \times 2 \varepsilon \times \varepsilon a(e_i)^{\gamma_i-\alpha_i}|\Omega_i\rangle = 0, \text{ when } \alpha_i < \gamma_i
\]

and

\[
a(e_i)^{\gamma_i}a^*(e_i)^{\alpha_i}|\Omega_i\rangle = \alpha_i \varepsilon \times (\alpha_i - 1) \varepsilon \times \ldots \times (\alpha_i - (\gamma_i - 1)) \varepsilon a^*(e_i)^{\alpha_i-\gamma_i}|\Omega_i\rangle
\]

\[
= \varepsilon^{\gamma_i - \alpha_i} \frac{\alpha_i!}{(\alpha_i - \gamma_i)!} a^*(e_i)^{\alpha_i-\gamma_i}|\Omega_i\rangle, \text{ when } \gamma_i \leq \alpha_i.
\]
The above separation of variables leads under the condition $\gamma \leq \alpha$ to:
\[
a(e)^\gamma a^*(e)^\alpha |\Omega\rangle = \bigotimes_{i=1}^{K} a(e_i)^{\gamma_i} a^*(e_i)^{\alpha_i} |\Omega_i\rangle
\]
\[
= \left( \prod_{i=1}^{K} \epsilon^{\gamma_i} a_i^! \right) \bigotimes_{i=1}^{K} a^*(e_i)^{\alpha_i-\gamma_i} |\Omega_i\rangle
\]
\[
= \epsilon^{\gamma_1} \frac{\alpha_1!}{(\alpha - \gamma_1)!} \left( \prod_{i=1}^{K} a^*(e_i)^{\alpha_i-\gamma_i} \right) (|\Omega_1\rangle \otimes \ldots \otimes |\Omega_K\rangle)
\]
\[
= \epsilon^{\gamma_1} \frac{\alpha_1!}{(\alpha - \gamma_1)!} a^*(e)^{\alpha-\gamma} |\Omega\rangle.
\]

\[\square\]

**Proposition 4.2** For all multi-indices $\alpha$ and $\beta$, the matrix elements of $d\Gamma(-\Delta_K)$ are given by:
\[
d\Gamma(-\Delta_K)_{\alpha,\beta} = -\epsilon \sum_i (\delta_{\beta-e_i, \alpha-e_i} \sqrt{\beta_i (\beta_i+1)} + \delta_{\beta-e_i, \alpha-e_i} \sqrt{\beta_i+1 (\beta_i+1)})
\]
where $\delta_{\alpha,\beta} = \delta_{\alpha,\beta} 1_{\mathbb{N}^K}(\alpha)$ for $\alpha$ and $\beta$ multi-indices in $\mathbb{Z}^K$.

**Proof.**
According to (13) and to Lemma 4.1, we obtain:
\[
a^*(e_{i+1})a(e_i)a^*(e)^\alpha |\Omega\rangle = \delta_{e_i \leq \alpha} \epsilon \frac{\alpha!}{(\alpha - e_i)!} a^*(e)^{e_i+1+\alpha-e_i} |\Omega\rangle
\]
\[
= \delta_{1 \leq \alpha} \epsilon \alpha_i a^*(e)^{e_i+1+\alpha-e_i} |\Omega\rangle,
\]
and
\[
a^*(e_i)a(e_{i+1})a^*(e)^\alpha |\Omega\rangle = \delta_{e_{i+1} \leq \alpha} \epsilon \frac{\alpha!}{(\alpha - e_{i+1})!} a^*(e)^{e_{i+1}+\alpha-e_{i+1}} |\Omega\rangle
\]
\[
= \delta_{1 \leq \alpha} \epsilon \alpha_{i+1} a^*(e)^{e_{i+1}+\alpha-e_{i+1}} |\Omega\rangle.
\]

Then
\[
\langle e_\alpha, d\Gamma(-\Delta_K) e_\beta \rangle = -\left( e_\alpha, \sum_{i=1}^{K} a^*(e_{i+1})a(e_i) + a^*(e_i)a(e_{i+1}) \right) e_\beta \]
\[
= -\epsilon \sum_i (a^*(e)^\alpha |\Omega\rangle \left( \delta_{\beta_i \leq \alpha} \beta_i a^*(e)^{\beta_i+e_i+1} + \delta_{1 \leq \beta_i \leq \alpha} \beta_i a^*(e)^{\beta_i+e_i+1} \right) |\Omega\rangle)
\]
\[
= \epsilon \sum_i (\delta_{\beta_i \leq \alpha} \beta_i a^*(e)^{\beta_i+e_i+1} \sqrt{\alpha! (\beta-e_i+e_{i+1})!} + \delta_{1 \leq \beta_i \leq \alpha} \beta_i a^*(e)^{\beta_i+e_i+1} \sqrt{\alpha! (\beta-e_i+1+e_{i+1})!})
\]
\[
= -\epsilon \sum_i (\delta_{\beta_i \leq \alpha} \beta_i a^*(e)^{\beta_i+e_i+1} \sqrt{\beta_i+1 \beta_i+1} + \delta_{1 \leq \beta_i \leq \alpha} \beta_i a^*(e)^{\beta_i+e_i+1} \sqrt{\beta_i+1 \beta_i+1})
\]
\[
d\Gamma(-\Delta_K)_{\alpha,\beta} = -\epsilon \sum_i (\delta_{\beta_i \leq \alpha} \sqrt{\beta_i+1 \beta_i+1} + \delta_{1 \leq \beta_i \leq \alpha} \sqrt{\beta_i+1 \beta_i+1})
\]

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Numerically only the indices of the multi-indices $\alpha$ and $\beta$ corresponding to the nonzero components of $d\Gamma(-\Delta_K)$ with their values, are stored in an array. In the algorithm instead of running over the multi-indices $\alpha$ or $\beta$ with a length $N$, the multi-indices $\beta'$ with a length $N-1$ are run over. And for each $i$ in $[1,K]$, the changes of multi-indices $\beta' = \beta - e_i$ or $\beta' = \beta - e_{i+1}$ are used, then the indices of the corresponding multi-indices $\alpha$ and $\beta$ with length $N$ are looked for. Therefore an array composed of $2K(\binom{N+K-2}{K-2})$ triplets of elements is numerically stored.

4.2.3 Computation of the interaction factor $e^{-i\frac{z}{\hbar}\mathcal{V}}$

Denote $a_j^\# = a^\#(e_j)$ and $N_i = a_i^*a_i$.

By using the relations CCR (1):

$$a_i^*a_j^*a_i a_j = a_i^*(a_ja_j^* - \varepsilon\delta_{ij})a_j = a_i^*a_i a_j^*a_j - \varepsilon\delta_{ij}a_i^*a_j$$

$$= N_iN_j - \varepsilon\delta_{ij}N_i = N_i(N_j - \varepsilon\delta_{ij}).$$

Then $\mathcal{V}$ can be rewritten as:

$$\mathcal{V} = \frac{1}{2} \sum_{(i,j)\in\mathbb{Z}_K^2} V_{ij}N_i(N_j - \varepsilon\delta_{ij}).$$

And since $N_ie_\alpha = \varepsilon a_ie_\alpha$ then $\mathcal{V}$ is diagonal in the basis $(e_\alpha)_\alpha$:

$$\mathcal{V}e_\alpha = \left( \frac{1}{2} \sum_{(i,j)\in\mathbb{Z}_K^2} V_{ij}\varepsilon\alpha_i(\varepsilon\alpha_j - \varepsilon\delta_{ij}) \right) e_\alpha = \left( \frac{\varepsilon^2}{2} \sum_{(i,j)\in\mathbb{Z}_K^2} V_{ij}\alpha_i(\alpha_j - \delta_{ij}) \right) e_\alpha$$

and

$$e^{-i\frac{z}{\hbar}\mathcal{V}}e_\alpha = e^{-i\frac{z}{\hbar}\left( \frac{\varepsilon^2}{2} \sum_{(i,j)\in\mathbb{Z}_K^2} V_{ij}\alpha_i(\alpha_j - \delta_{ij}) \right) e_\alpha} = e^{-i\frac{z}{\hbar}\left( \sum_{i\neq j} V_{ij}\alpha_i\alpha_j + \sum_{i\in\mathbb{Z}_K} V_{i\alpha_i(\alpha_i-1)} \right) e_\alpha}.$$

4.3 Numerical computation of the reduced density matrices

Consider $b_{\text{Wick}} = a^*(e)^\delta a(e)^\gamma$ with $|\delta| = |\gamma|$ and its associated homogeneous polynomial:

$$b(z) = z^\delta z^\gamma = z_1^{\delta_1} \cdots z_K^{\delta_K} z_1^{\gamma_1} \cdots z_K^{\gamma_K}.$$

Let us compute the quantity $\text{Tr}(\rho_zb_{\text{Wick}})$ when $\rho_z$ is a normal state. Using an orthonormal basis of the $N$-fold sector $\mathcal{V}^N\mathbb{Z}$, $\rho_z$ is a linear combination of operators $|\Phi\rangle \langle \Psi|$. It suffices to compute $\text{Tr}(|\Phi\rangle \langle \Psi|b_{\text{Wick}}) = \langle \Phi, b_{\text{Wick}}\Phi \rangle$.

**Lemma 4.3** Set $b_{\text{Wick}} = a^*(e)^\delta a(e)^\gamma$ with $|\delta| = |\gamma|$ and let $\Phi$ and $\Psi$ be in $\mathcal{V}^N\mathbb{Z}$ then:

$$\langle \Psi, b_{\text{Wick}}\Phi \rangle = \varepsilon^{|\gamma|} \sum_{|\alpha'|=N-|\delta|} \tilde{\Psi}_{\alpha'+\delta} \Phi_{\alpha'+\gamma} \sqrt{(\alpha'+\delta)! (\alpha'+\gamma)!} \frac{1}{\alpha'!}$$

in the orthonormal basis $\left( \frac{a^*_\alpha(z)^\gamma}{\sqrt{z^N\alpha!}} \right)_{|\alpha|=N}$ of $\mathcal{V}^N\mathbb{Z}$. 

\[10\]
Proof. Given $\Psi$ and $\Phi$ in the N-particles bosons space and the formula 4.1

$$a^*(e)^\delta a(e)^\gamma a^*(e)^\alpha |\Omega\rangle = \delta_{\gamma,\alpha} e^{\alpha |} \frac{\alpha!}{(\alpha - \gamma)!} a^*(e)^{\delta + \alpha - \gamma} |\Omega\rangle,$$

we can write:

$$\langle \Psi, b^{Wick}\Phi \rangle = \left\{ \sum_{|\alpha| = N} \frac{\Psi_{\alpha} a^*(e)^\alpha}{\sqrt{\varepsilon^N \alpha!}} \Omega, e^{\alpha |} \right\} \sum_{|\beta| = N, \beta \geq \gamma} \frac{\Phi_{\beta} \varepsilon^{N/2} (\beta - \gamma)!}{\sqrt{\alpha!}} a^*(e)^{\delta + \beta - \gamma} |\Omega\rangle$$

$$= e^{\alpha |} \sum_{|\alpha| = N, \alpha \geq \delta} \frac{\bar{\Psi}_{\alpha} \bar{\Phi}_{\alpha + \gamma - \delta}}{\sqrt{\alpha!}} (a^*(e)^\alpha \Omega, a^*(e)^{\delta + \beta - \gamma} |\Omega\rangle)$$

$$= e^{\alpha |} \sum_{|\alpha| = N, \alpha \geq \delta} \frac{\bar{\Psi}_{\alpha} \bar{\Phi}_{\alpha + \gamma - \delta}}{\sqrt{\alpha!}} (a^*(e)^\alpha \Omega, a^*(e)^{\delta + \beta - \gamma} |\Omega\rangle)$$

$$= e^{\alpha |} \sum_{|\alpha'| = N - |\delta|} \bar{\Psi}_{\alpha' + \delta} \bar{\Phi}_{\alpha' + \gamma} \frac{(\alpha' + \delta)! (\alpha' + \gamma)!}{\alpha!}.$$ 

because

$$\langle a^*(e)^\alpha, a^*(e)^{\delta + \beta - \gamma} |\Omega\rangle \neq 0$$

if and only if $\alpha = \delta + \beta - \gamma$ so $\beta = \alpha + \gamma - \delta$ and $\beta \geq \gamma$ means $\alpha - \delta \geq 0$.

The last line is obtained by a change of multi-indices by setting for each $\alpha$, $\alpha' = \alpha - \delta$ because $\alpha \geq \delta$, and then $|\alpha'| = |\alpha| - |\delta| = N - |\delta|$.

Numerically, all multi-indices of $N^K$ with length not larger than a given $N_{max}$ are stored in the lexicographic order.

For our algorithms, we pay attention to preserve this lexicographic order (or reverse).

For a given $N \leq N_{max}$, the list of relevant multi-indices (with length $N$) is extracted and handled in the lexicographic order.

For a given $\delta$, numerically the above summation is performed over multi-indices $\alpha'$ such that $|\alpha'| = N - |\delta|$ in the lexicographic order.

Then for each $\alpha'$, the multi-indices of length $N$ written as $\alpha = \alpha' + \delta$ are looked for. These $\alpha$ are exactly the multi-indices such that $\alpha \geq \delta$ and $|\alpha| = N$.

Note in particular that the mapping $\alpha' \rightarrow \alpha' + \delta$ preserves the lexicographic order.

First let us compute the matrix elements of $\gamma_p^p$ in the orthonormal basis $(e_\alpha)_\alpha$.

The matrix element corresponding to the line $\beta$ and column $\alpha$ is:

$$\langle a^*(e)^\beta |\gamma_p^p a^*(e)^\alpha |\Omega\rangle = \text{Tr} \left( \gamma_p^p(t) e^{\alpha |} \mathcal{D}a^*(e)^\alpha \Omega, e^\beta | \right)$$

$$= \text{Tr} \left( \gamma_p^p(t) b^{Wick} \right)$$

according to the duality relation (5) of the reduced density matrices with $\tilde{b} = \left[ \frac{a^*(e)^\alpha}{\sqrt{\varepsilon^p \alpha!}} \Omega, a^*(e)^{\delta} \right]$, and $b(z) = \langle z^\otimes p, b^\otimes p | \rangle \in \mathcal{P}_{p,p}$.

If $\tilde{b} = \left[ \frac{a^*(e)^\alpha}{\sqrt{\varepsilon^p \alpha!}} \Omega, a^*(e)^{\delta} \right]$, its Wick quantized is:

$$\tilde{b}^{Wick} = \frac{p!}{\sqrt{\alpha! \beta!}} a^*(e)^\alpha a(e)^\beta.$$
And then
\[ \gamma_t^p(t)(\beta, \alpha) = \frac{1}{\sqrt{\alpha!\beta!}} \frac{\text{Tr}(\varrho(t)a^*(e)^\alpha a(e)^\beta)}{\varepsilon^pN(N-1)\ldots(N-p+1)}. \]

Then owing to Lemma 4.3, all the elements of the matrices \( \gamma_t^p \) can be numerically computed.

In the case where the initial state is a twin state, the following lemma is used to obtain an expansion in the orthonormal basis \((e_\alpha)\) which is given by the following lemma.

**Lemma 4.4** For all \( p \in \mathbb{N} \), and \( z \in \mathcal{Z} \), we obtain in the basis \((e_\alpha)_\alpha\):

\[ z^\otimes p = \sum_{|\alpha|=p} \sqrt{\frac{p!}{\alpha!}} z^\alpha e_\alpha. \]

**Proof.**

\[ a^*(z)^p|\Omega\rangle = a^*(z_1e_1 + \ldots + z_K e_K)^p|\Omega\rangle = (z_1 a^*(e_1) + \ldots + z_K a^*(e_K))^p|\Omega\rangle = \sum_{|\alpha|=p} \frac{p!}{\alpha!} z^\alpha a^*(e)^\alpha|\Omega\rangle. \]

And then
\[ z^\otimes p = \frac{a^*(z)^p}{\sqrt{\varepsilon^p p!}}|\Omega\rangle = \sum_{|\alpha|=p} \sqrt{\frac{p!}{\alpha!}} z^\alpha e_\alpha. \]

In the case where the initial state is a twin state, the following lemma is used to obtain an expansion in the basis \((e_\alpha)\).

**Lemma 4.5** Let \( \phi, \psi \) be in \( \mathcal{Z} \) and \( z \) the state

\[ \frac{a^*(\phi)^n a^*(\psi)^m}{\sqrt{\varepsilon^{n+m} n! m!}}|\Omega\rangle \]

such that \( n + m = N \).

Then we obtain

\[ z = \sqrt{n!m!} \sum_{|\gamma|=N} \left( \sum_{|\alpha|=n, \alpha \leq \gamma} \frac{\sqrt{\gamma!}}{\alpha! (\gamma-\alpha)!} \phi^\alpha \psi^{\gamma-\alpha} \right) \frac{a^*(e)^\gamma}{\sqrt{\varepsilon^N \gamma!}}|\Omega\rangle. \]

**Proof.**

\[ a^*(\phi)^n = \sum_{|\alpha|=n} \frac{n!}{\alpha!} \phi^\alpha a^*(e)^\alpha \]

\[ a^*(\psi)^m = \sum_{|\beta|=m} \frac{m!}{\beta!} \psi^\beta a^*(e)^\beta \]

\[ a^*(\phi)^n a^*(\psi)^m = \sum_{|\alpha|=n, |\beta|=m} \frac{n! m!}{\alpha! \beta!} \phi^\alpha \psi^\beta a^*(e)^\alpha a^*(e)^\beta = \sum_{|\alpha|=n, |\beta|=m} \frac{n! m!}{\alpha! \beta!} \phi^\alpha \psi^\beta a^*(e)^{\alpha+\beta} \]

because of the CCR relations (1).

\[ \frac{a^*(\phi)^n a^*(\psi)^m}{\sqrt{n!m!}}|\Omega\rangle = \sum_{|\alpha|=n, |\beta|=m} \frac{\sqrt{\gamma!}}{\alpha! \beta!} \frac{a^*(e)^{\alpha+\beta}}{\sqrt{(\alpha+\beta)!}}|\Omega\rangle \]

\[ = \sqrt{n!m!} \sum_{|\gamma|=N, |\alpha|=n, |\beta|=m} \frac{\sqrt{\gamma!}}{\alpha! (\gamma-\alpha)!} \phi^\alpha \psi^{\gamma-\alpha} a^*(e)^\gamma|\Omega\rangle. \]
By setting $\gamma = \alpha + \beta$, 

$$ z = \sqrt{n!m!} \sum_{|\gamma| = N} \sum_{|\alpha| = n, \alpha \leq \gamma} \frac{\sqrt{\gamma!}}{\alpha!(\gamma - \alpha)!} \phi^\alpha \psi^{\gamma - \alpha} a^*(e)^\gamma \sqrt{\epsilon^{N\gamma!}} |\Omega| . $$

Further the limit reduced density matrices (6) have to be computed numerically. In order to do this, the integration over $\mathcal{Z}$ of the Wigner measure is discretized. The problem is then reduced to the computation of the matrix elements of $|z \otimes p \rangle \langle z \otimes p |$ in the basis $(e_\alpha)_{|\alpha| = p}$.

Compute the matrix elements of $|z \otimes p \rangle \langle z \otimes p |$, according to Lemma 4.4:

$$ (z \otimes p | a^*(e)^\alpha | \overline{z}^\alpha \overline{p} \alpha! | \Omega) = \sqrt{\frac{pl!}{\alpha!}} z^\alpha $$

Then

$$ (|z \otimes p \rangle \langle z \otimes p |) e_\alpha = \sqrt{\frac{pl!}{\alpha!}} z^\alpha \sum_{|\beta| = p} \sqrt{\frac{pl!}{\beta!}} z^\beta e_\beta $$

$$ = \sum_{|\beta| = p} \frac{pl!}{\alpha! \beta!} z^\alpha z^\beta e_\beta . $$

For the computation of the integral $\int_\mathcal{Z} |z \otimes p \rangle \langle z \otimes p | d\mu(z)$, the Wigner measure is approximated by a convex combination of gauge invariant delta functions $\delta_z^{S^1}$, where $\delta_z^{S^1} = \frac{1}{2\pi} \int_0^{2\pi} \delta_{e^{i\theta}} z d\theta$.

For the Wigner measure associated with the Hermite states, $\mu = \delta_z^{S^1}$, and the discretization is trivial and exact. It is not needed to be approximated because of the gauge invariance. In the case of the twin states given by $\Psi_N = a^*(\psi_1) a^*(\psi_2) \sqrt{\epsilon^{n_1 n_2 n_1 n_2!}} |\Omega|$, where $\psi_1, \psi_2 \in \mathcal{Z}$, $\|\psi_1\| = \|\psi_2\| = 1$, and $n_1 = n_2 = \frac{N}{2}$, the Wigner measure is $\mu_0 = \frac{1}{2\pi} \int_0^{2\pi} \delta_{\psi_0}^{S^1} \delta_{\psi_0}^{S^1} d\phi$ according to [6], with:

$$ \psi_0 = \cos(\phi)\psi_0 + \sin(\phi)\psi_1, $$

$$ \psi_0 = \frac{\sqrt{2}}{2}(\psi_1 + \psi_2), \quad \psi_1 = \frac{\sqrt{2}}{2}(\psi_1 - \psi_2). $$

Numerically the interval $[0, 2\pi]$ is discretized and $\mu_0$ is approximated by $\frac{1}{m} \sum_{k=1}^m \delta_{\psi_0}^{S^1} \delta_{\psi_0}^{S^1}$. The Wigner measure $\mu_t$ propagated at the time $t$ of the twin states is given by:

$$ \mu_t = \frac{1}{2\pi} \int_0^{2\pi} \delta_{\psi_0(t)}^{S^1} \delta_{\psi_0(t)}^{S^1} d\phi, $$

where $\psi_0(t)$ is solution to the Hartree equation at the time $t$ with initial condition $\psi_0$.

Numerically it is now approximated by $\frac{1}{m} \sum_{k=1}^m \delta_{\psi_0(t)}^{S^1} \delta_{\psi_0(t)}^{S^1}$ where $z_k(t)$ solves the Hartree equation (7).

Thus the matrix elements of $\int_\mathcal{Z} |z \otimes p \rangle \langle z \otimes p | d\mu_0(z)$ are given by the formula:

$$ \frac{1}{m} \sum_{k=1}^m \frac{pl!}{\alpha! \beta!} z_k(t)^\alpha z_k(t)^\beta. $$

And the approximation of the scalar $\int_\mathcal{Z} |z|^{2p} d\mu_0(z)$ is given by the formula $\frac{1}{m} \sum_{k=1}^m |z_k|^{2p}$.

The matrix of $\gamma^p_\ell(t) - \int_\mathcal{Z} |z \otimes p \rangle \langle z \otimes p | d\mu_0(z)$ can then be computed at any time $t$ numerically with a good approximation.
5 Error estimates

5.1 Error estimate of the composition method

The Baker-Campbell-Hausdorff formula (see [35]) allows to find the order of the composition method which is 4. Then the Taylor’s formula with 4th order integral remainder and the Cauchy inequalities are used to estimate the error.

The following proposition gives an estimate of the composition method.

Proposition 5.1 Let $R > 0$, $A$ and $B$ be two anti-adjoint matrices such that $(a_1 - a_2)\|A\| - \frac{3a_2}{2} \|B\| \leq R$. Then

$$\|e^{A+B} - \Psi_{A,B}\| \leq \frac{2eR}{R^5} \left( (a_1 - a_2)\|A\| - \frac{3a_2}{2} \|B\| \right)^5$$

where $\Psi_{A,B} = e^{\frac{a_1}{2}}B e^{\frac{a_2}{2}}A e^{\frac{a_1}{2}}B e^{\frac{a_2}{2}}A e^{\frac{a_1}{2}}B e^{\frac{a_2}{2}}A e^{\frac{a_1}{2}}B$ is the composition method.

Proof.

$$e^{A+B} - \Psi_{A,B} = e^{A+B} - e^{\frac{a_1}{2}}B e^{\frac{a_2}{2}}A e^{\frac{a_1}{2}}B e^{\frac{a_2}{2}}A e^{\frac{a_1}{2}}B e^{\frac{a_2}{2}}A e^{\frac{a_1}{2}}B$$

Then for $z \in \mathbb{C}$

$$\|e^{z(A+B)} - \Psi_{zA,zB}\| \leq e^{-\frac{a_1 + a_2}{2} |\Re(z)||B|} e^{\frac{a_1}{2} |\Re(z)||A|} (e^{\frac{a_1}{2} |\Re(z)||B|} e^{-a_1 |\Re(z)||A|})$$

Since the composition method is of 4th order then for $\lambda \in \mathbb{R}$, the Taylor’s formula with integral remainder yields:

$$f_{A,B}(z) = e^{z(A+B)} - \Psi_{zA,zB}.$$
By the Cauchy’s integral formula, we know for each $t \in [0, 1]$:

$$\left\| \frac{f^{(5)}_{A,B}(t)}{5!} \right\| = \left\| \frac{1}{2\pi} \int_{|z-t|=1} \frac{f_{A,B}(z)}{(z-t)^6} dz \right\| \leq \frac{1}{2\pi} \int_0^{2\pi} \|f_{A,B}(t + e^{i\theta})\| \, d\theta$$

$$\leq \sup_{|Im(z)| \leq 1} \|f_{A,B}(z)\| \leq 2e^{\|Im(z)\|((a_1-a_2)\|A\| - \frac{3a_2}{2} \|B\|)}$$

Hence for all $A_R$ and $B_R$ such that $(a_1 - a_2)\|A\| - \frac{3a_2}{2} \|B\| \leq R$ we obtain:

$$\|f_{A_R,B_R}(\lambda)\| \leq 2\lambda^5 e^R, \text{ if } \lambda \leq 1.$$  

Let $A$ and $B$ be such that $(a_1 - a_2)\|A\| - \frac{3a_2}{2} \|B\| \leq R$. 

By setting $A_R = \frac{RA}{(a_1-a_2)\|A\| - \frac{3a_2}{2} \|B\|}$ and $B_R = \frac{RB}{(a_1-a_2)\|A\| - \frac{3a_2}{2} \|B\|}$, we obtain

$$A = \frac{(a_1 - a_2)\|A\| - \frac{3a_2}{2} \|B\|}{R} A_R, \quad B = \frac{(a_1 - a_2)\|A\| - \frac{3a_2}{2} \|B\|}{R} B_R$$

and $(a_1 - a_2)\|A_R\| - \frac{3a_2}{2} \|B_R\| = R$.

Then

$$f_{A,B}(1) = f_{A_R,B_R} \left( \frac{(a_1 - a_2)\|A\| - \frac{3a_2}{2} \|B\|}{R} \right)$$

$$\|f_{A,B}(1)\| \leq 2e^{R \left( \frac{(a_1 - a_2)\|A\| - \frac{3a_2}{2} \|B\|}{R} \right)^5}$$

5.2 Error estimate of the approximated composition method

The composition method is approximated by replacing $e^{-i \Delta \tau} dR(-\Delta \kappa)$ by its $4^{th}$ order Taylor expansion, with some normalization factor.

Errors estimates for this modified composition method rely on the two following lemmas.

**Lemma 5.2** Let $E$ be a normed vector space, $J \in \mathbb{N}^*$, $(f_j)_j$ and $(g_j)_j$ two maps sequences from $E$ to $E$ such that for all $j \in \{1, \ldots, J\}$:

- $f_j$ is linear.
- $\|f_j(u)\| = \|g_j(u)\| = \|u\|$ for all $u \in E$.
- $\forall u \in E \quad \|u\| \leq \varepsilon \Rightarrow \|f_j(u) - g_j(u)\| \leq \delta$

For $u_0 \in E$, $\|u_0\| \leq \varepsilon$ set $u_j = f_j(u_{j-1})$ and $v_j = g_j(v_{j-1})$ with $v_0 = u_0$. Then we deduce $\|u_j - v_j\| \leq J\delta$. 

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Proof. Let us proceed by induction on $J$.

For $J = 0$, \( \|u_0 - v_0\| = 0 \leq 0\delta \).

Let us assume \( \|u_j - v_j\| \leq J\delta \) with the hypotheses fulfilled for \( j \in \{1, \ldots, J + 1\} \).

\[
\begin{align*}
    u_{J+1} - v_{J+1} &= f_{J+1}(u_J) - g_{J+1}(v_J) \\
    &= f_{J+1}(u_J) - f_{J+1}(v_J) + f_{J+1}(v_J) - g_{J+1}(v_J).
\end{align*}
\]

Since \( f_{J+1} \) is linear and unitary we obtain:

\[
\|f_{J+1}(u_J) - f_{J+1}(v_J)\| = \|f_{J+1}(u_J) - v_J\| \leq J\delta.
\]

Moreover \( \|v_J\| = \|g_J \circ g_{J-1} \circ \ldots \circ g_1(u_0)\| = \|u_0\| \leq \varrho \),

then

\[
\|f_{J+1}(v_J) - g_{J+1}(v_J)\| \leq \delta,
\]

we obtain

\[
\|u_{J+1} - v_{J+1}\| \leq (J + 1)\delta.
\]

\[\square\]

Let \( TL(e^A) \) denote the 4th order Taylor expansion of \( e^A \) around 0.

Let \( A \) be in \( B(0, c_R) \), \( c_R > 0 \).

Lemma 5.3 Let \( u \) be a vector in a normed vector space \( E \) and let \( A \) be an anti-adjoint operator on \( E \). Define the application \( TL(e^A) \) on \( E \) which is non linear by:

\[
\tilde{TL}(e^A)u = \frac{\|u\|}{\|TL(e^A)u\|} TL(e^A)u \text{ if } \|TL(e^A)u\| \neq 0,
\]

it preserves the norm.

Then \( \|(TL(e^A) - \tilde{TL}(e^A))u\| \leq \|TL(e^A) - e^A\|\|u\| \).

Proof.

\[
\begin{align*}
    TL(e^A)u - \tilde{TL}(e^A)u &= TL(e^A)u - \frac{\|u\|}{\|TL(e^A)u\|} TL(e^A)u \\
    &= \left(1 - \frac{\|u\|}{\|TL(e^A)u\|}\right) TL(e^A)u.
\end{align*}
\]

\[
\begin{align*}
    \|TL(e^A)u - \tilde{TL}(e^A)u\| &= \left\|\left(1 - \frac{\|u\|}{\|TL(e^A)u\|}\right) TL(e^A)u\right\| \\
    &= \|TL(e^A)u\| - \|u\| \\
    &= \|TL(e^A)u\| - \|e^A u\| \\
    &\leq \|TL(e^A)u - e^A u\| \\
    \|TL(e^A) - \tilde{TL}(e^A))u\| &\leq \|TL(e^A) - e^A\|\|u\|.
\end{align*}
\]

\[\square\]
The 4\textsuperscript{th} order error of the Taylor expansion gives:

\[ \| e^A - TL(e^A) \| = \left\| \sum_{i=5}^{\infty} \frac{A^i}{i!} \right\| \leq \| A \|^5 \int_0^1 \frac{(1 - t)^4}{4!} \| e^{tA} \| dt \leq \| A \|^5 \frac{1}{5!}. \]

The following proposition gives an estimate of the approximation of the composition method.

\textbf{Proposition 5.4} \ Let \( A \) and \( B \) be two anti-adjoint matrices and \( J \) an integer such that

\[ \frac{\Delta t}{\varepsilon} ( (a_1 - a_2) \| A \| - \frac{3a_2}{2} \| B \| ) \leq 5 \]

and

\[ J \geq \frac{t}{5\varepsilon} ( (a_1 - a_2) \| A \| - \frac{3a_2}{2} \| B \| ). \]

Then

\[ \| e^{\frac{t}{\varepsilon} (A+B)} u - (\widetilde{\Psi}_{A,B} u) \| \leq \frac{3}{4} \| A \|^5. \]

for all vector \( u \), where

\[ \widetilde{\Psi}_{A,B} = e^{\frac{a_1 B}{2}} TL(e^{a_1 A}) e^{\frac{a_2 B}{2}} TL(e^{a_2 A}) e^{\frac{a_1 B}{2}} TL(e^{a_1 A}) e^{-\frac{a_1 B}{2}}. \]

\textbf{Proof.}

Let \( u \) be a normed vector.

First for \( i = 1, 2, 3 \) let us estimate the error:

\[ \| e^{\frac{a_i B}{2}} e^{\frac{a_i A}{2}} e^{\frac{a_i B}{2}} u - e^{\frac{a_i B}{2}} TL(e^{a_i A}) e^{\frac{a_i B}{2}} u \| \]

by using the fact \( e^{\frac{a_i B}{2}} \) is an unitary operator and Lemma 5.3:

\[ \| e^{\frac{a_i B}{2}} e^{\frac{a_i A}{2}} e^{\frac{a_i B}{2}} u - e^{\frac{a_i B}{2}} TL(e^{a_i A}) e^{\frac{a_i B}{2}} u \| = \| (e^{a_i A} - TL(e^{a_i A})) e^{\frac{a_i B}{2}} u \| \leq \frac{\| a_i A \|^5}{60} \leq \| A \|^5 \frac{4}{4}. \]

like in the previous proof.

Now Lemma 5.2 can be applied with \( f_i = e^{\frac{a_i B}{2}} e^{\frac{a_i A}{2}} e^{\frac{a_i B}{2}} \), \( g_i = e^{\frac{a_i B}{2}} TL(e^{a_i A}) e^{\frac{a_i B}{2}} \) and \( J = 3 \).

Then

\[ \| \Psi_{A,B} u - \widetilde{\Psi}_{A,B} u \| \leq \frac{3}{4} \| A \|^5. \]

Secondly let us estimate the error:

\[ \| e^{A+B} - \widetilde{\Psi}_{A,B} u \| \]

By using Proposition 5.1 with its hypotheses and the previous estimates:

\[ \| e^{A+B} - \widetilde{\Psi}_{A,B} u \| \leq \| e^{A+B} - \Psi_{A,B} u \| + \| (\Psi_{A,B} - \widetilde{\Psi}_{A,B}) u \| \]

\[ \leq 2e^{R} \left( (a_1 - a_2) \| A \| - \frac{3a_2}{2} \| B \| \right)^{\frac{5}{2}} + \frac{3}{4} \| A \|^5. \]
By applying that to $\frac{\Delta t}{\varepsilon}A$ and $\frac{\Delta t}{\varepsilon}B$ where $\Delta t = \frac{t}{J}$ with $J$ positive integer, we obtain:

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

Then by applying Lemma 5.2 with $f_j = e^{\frac{\Delta t}{\varepsilon}(A^{B})}$ and $g_j = \Psi A, \Psi B$, we obtain:

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

By knowing that for all positive integer $\tau$ and positive real $a$, $R \mapsto \frac{eR}{R^r}$ is minimal in $R_{min} = \frac{\varepsilon}{\tau}$ and $\min_{R > 0} \frac{eR}{R^r} = \left( \frac{\varepsilon}{\tau} \right)^r$, the condition

$$\frac{\Delta t}{\varepsilon} \left( (a_1 - a_2)\|A\| - \frac{3a_2}{2}\|B\| \right) \leq 5,$$

that is

$$J \geq \frac{t}{5\varepsilon} \left( (a_1 - a_2)\|A\| - \frac{3a_2}{2}\|B\| \right),$$

implies

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

For $Q \in \mathcal{L}(\mathbb{V} \mathcal{Z})$, we know according to (15):

$$Q_{\mathcal{W}ick}^{N} = \sqrt{n!(n+2-2)!} \frac{e^{2a}}{2} S_{n-2+2}(Q \otimes I_{d^n-2}) = \varepsilon^2 n(n-1) S_{n} (Q \otimes I_{d^n-2}),$$

then

$$\|Q_{\mathcal{W}ick}^{N} \| \leq \varepsilon^2 N (N-1)\|S_{N}\|\|Q\| \leq \varepsilon^2 N^2 \|Q\| = \|\tilde{Q}\|.$$ 

When $Q_{\mathcal{W}ick} = \mathcal{V}$ with

$$\tilde{\mathcal{V}}(e_i \lor e_j) = \frac{1}{2} V_{ij} e_i \lor e_j,$$

the norm $\|\mathcal{V}\|$ is bounded from above by $\|\tilde{\mathcal{V}}\| = \frac{1}{2} \max |V_{ij}|$ independently of the number $N = \lfloor \frac{t}{\varepsilon} \rfloor$ of particles.

Moreover $\|d\Gamma(A)\|_{\mathcal{W}ick} \leq \varepsilon N \|A\| = \|A\|$, therefore $\|d\Gamma(-\Delta K)\| \leq \|\Delta K\| = 2$.

Finally by applying the last proposition with $A = -d\Gamma(-\Delta K)$ and $B = -i\mathcal{V}$, an error estimate is obtained for the complete evolution:

$$\|e^{-\frac{\Delta H_{\varepsilon}}{2}}u - (\Psi A, i\Gamma(-\Delta_{K}), -\frac{\Delta t}{\varepsilon}i\mathcal{V})^J u\| \leq \left( 2 \left( \frac{e}{5} \right)^5 \left( (-a_1 - a_2)\|\Delta_{K}\| - \frac{3a_2}{2}\|\tilde{\mathcal{V}}\| \right)^5 + \frac{3}{4}\|\Delta_{K}\|^5 \right) t \frac{\Delta t^4}{\varepsilon^5}.$$ 

Practically, the time step is chosen according to $N$ and $t$ so that the above error is negligible.
6 Numerical simulations

For all the numerical simulations the final time is chosen to be $t_{\text{max}} = 1$, the number of time steps for the 4th order Runge-Kutta method applied to solve the mean field equation is 100. The loop of the number of particles is performed numerically from $N_{\text{min}} = 2$ to $N_{\text{max}} = 20$ particles, and only for an even number of particles. In the Fortran program the computations were performed by parallelizing the loop in the computation of the product sparse matrix-vector $d F(−\Delta K)u$ with Openmp on 8 threads.

Results and orders of convergence for $\gamma_c^{(1)}$ and $\gamma_c^{(2)}$

For each type of states, the following graphics show for the reduced density matrices and for $K = 10$ sites:

1) The logarithm of the error in trace norm $\log(\max_{t\in[0,1]} \| \gamma_N^{(p)}(t) - \gamma^{(p)}_{\infty}(t) \|_1)$ according to the logarithm of the number of particles $N$ in the cases $p = 1$ and 2.
   A straight line is obtained whose the slope is the order of the error in $1/N$.
   These numerical experiments also validate the idea that for rather smooth but non trivial $N$-body bosonic system, the mean field asymptotics start to be relevant at $N = 4$. The numerical plot agree perfectly with the theoretical results of [1].

2) In the case $p = 1$ the density of particles on each site $k \in \{1, \ldots, K\}$ given by $\gamma_{kk}^{(1)}(t)$ for $N = 20$ particles and for the mean field limit at the same times $t = 0$ and $t = 1$.

3) The correlations in terms of the 1 and 2 particles reduced density matrices, for $N = 20$ particles and the mean field at the time $t = 1$. Depending on the case, this plot shows with which accuracy the mean field also catches some quantum correlations.

6.1 Hermite states

For the Hermite states $z \otimes N$ the vector $z$ is given by $z = \frac{1}{\sqrt{3}}((1 + i)e_1 + ie_3)$.

Log-log plot for Hermite states. $p=1$, $K=10$.

(a) Log-log plot for Hermite states. $p=1$, $K=10$. Numerical slope -0.9804

(b) Compared densities of particles at times $t=0$ and $t=1$
6.2 Twin states

For the twin states $\Psi_N = \frac{a^*(\psi_1)^n + a^*(\psi_2)^n}{\sqrt{e^{n_1} + e^{n_2}}}|\Omega\rangle$, $\psi_1 = \frac{1}{\sqrt{2}}(e_1 + ie_3)$ and $\psi_2 = e_2$.

Log-log plot for twin states. $p=1$, $K=10$. Numerical slope -0.9855

(f) Compared densities of particles at times $t=0$ and $t=1$
6.3 Wq states

For the Wq states \( \Psi_N = \frac{\alpha^*(\psi_1)^{n_1} \alpha^*(\psi_2)^{n_2}}{\sqrt{n_1!n_2!}} \left| \Omega \right> \), \( \psi_1 = \frac{1}{\sqrt{2}}(e_1 + i e_3) \) and \( \psi_2 = e_2 \).

In this case the state is given by \( S_N(\psi_1^{\otimes n_1} \otimes \psi_2^{\otimes n_2}) \), with \( n_1 + n_2 = N \), \( n_1 = N - q \) and \( n_2 = q \) fixed for the mean field.

The associated Wigner measure is \( \delta_{\psi_1}^{n_1} \).

In these simulations \( q = 2 \).
6.4 Other states

A case when the order of convergence is equal to $1/2$, (see [1])

In this case $\varrho_\varepsilon = |\phi^\otimes N_1(\phi^\otimes N_1) |$ with $\phi_1 = \frac{1}{N^1}\sqrt{e_1 + \sqrt{1 - \frac{1}{N^2}e_2}}$.

The associated Wigner measure is $\delta^N_{\varrho_\varepsilon}$.

$$\text{Log}[\text{trace}(\|e^\otimes N(t) - \gamma^\otimes N(t)\|_1)] \quad \text{according to Log}(N) , N \in [2, 200] , K = 10 , p = 1$$

(m) Log-log plot, p=1, K=10, Numerical slope -0.4711

(n) Compared densities of particles at times t=0 and t=1
\[ \log(\max_{i,j} |\gamma^p_i(t) - \gamma^p_j(t)|) \] according to \( \log(N) \), \( N \in [2,20] \), \( K = 10 \), \( p = 2 \)

(a) Log-log plot. \( p=2 \), \( K=10 \). Numerical slope -0.4524

(p) Mean field (white) and 20-body quantum (blue) correlations at time \( t = 1 \)
Appendix

Class of symbols \([3, 4, 5, 6]\). For any \(p,q \in \mathbb{N}\), define \(\mathcal{P}_{p,q}\) to be the space of homogeneous complex-valued polynomials on \(\mathcal{Z}\) such that \(b \in \mathcal{P}_{p,q}\) if and only if there exists a (unique) bounded operator \(\tilde{b} \in \mathcal{L}(\vee^p \mathcal{Z}, \vee^q \mathcal{Z})\) such that for all \(z \in \mathcal{Z}\):

\[
b(z) = \langle z^\otimes q, \tilde{b} z^\otimes p \rangle.
\] (14)

\[
b_{\text{Wick}}|_{\vee^n \mathcal{Z}} = 1_{[p, +\infty)}(n) \sqrt{n!(n + q - p)!} \frac{\varepsilon^{n+p}}{(n-p)!} \, S_{n-p+q} \left( \tilde{b} \otimes 1^\otimes (n-p) \right)
\] (15)

where \(\tilde{b}\) denotes the operator associated with the symbol \(b\) according to (14).

The composition method based on the Strang splitting with the coefficients (12) is of 4th order (see [35]).

Dimension of \(\sqrt{N} \mathcal{C}^K: \binom{N+K-1}{K-1}\) for \(K\) in \([1, 10]\) and \(N\) in \([1, 20]\):

| \(|K = 1\) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| \(N = 1\) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 2 | 1 | 3 | 6 | 10 | 15 | 21 | 28 | 36 | 45 | 55 |
| 3 | 1 | 4 | 10 | 20 | 35 | 56 | 84 | 120 | 165 | 220 |
| 4 | 1 | 5 | 15 | 35 | 70 | 126 | 210 | 330 | 495 | 715 |
| 5 | 1 | 6 | 21 | 56 | 126 | 252 | 462 | 792 | 1287 | 2002 |
| 6 | 1 | 7 | 28 | 84 | 210 | 462 | 924 | 1716 | 3003 | 5005 |
| 7 | 1 | 8 | 36 | 120 | 330 | 792 | 1716 | 3432 | 6435 | 11440 |
| 8 | 1 | 9 | 45 | 165 | 495 | 1287 | 3003 | 6435 | 12870 | 24310 |
| 9 | 1 | 10 | 55 | 220 | 715 | 2002 | 5005 | 11440 | 24310 | 48620 |
| 10 | 1 | 11 | 66 | 286 | 1001 | 3003 | 8008 | 19448 | 43758 | 92378 |
| 11 | 1 | 12 | 78 | 364 | 1365 | 4368 | 12376 | 31824 | 75582 | 167960 |
| 12 | 1 | 13 | 91 | 455 | 1820 | 6188 | 18564 | 50388 | 125970 | 293930 |
| 13 | 1 | 14 | 105 | 560 | 2380 | 8568 | 27132 | 77520 | 203490 | 497420 |
| 14 | 1 | 15 | 120 | 680 | 3060 | 11628 | 38760 | 116280 | 319770 | 817900 |
| 15 | 1 | 16 | 136 | 816 | 3876 | 15504 | 54264 | 170544 | 490314 | 1307504 |
| 16 | 1 | 17 | 153 | 969 | 4845 | 18288 | 61884 | 203490 | 594027 | 1679600 |
| 17 | 1 | 18 | 171 | 1140 | 5985 | 26334 | 94264 | 314596 | 942640 | 2734800 |
| 18 | 1 | 19 | 190 | 1330 | 7315 | 33649 | 124596 | 429000 | 1378500 | 4032000 |
| 19 | 1 | 20 | 210 | 1540 | 8855 | 42504 | 177100 | 637800 | 2220075 | 6906900 |
| 20 | 1 | 21 | 231 | 1771 | 10626 | 53130 | 230230 | 888030 | 3108105 | 10015005 |
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References

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