Insights on the Many-Body Physics of Tunneling from Numerically Exact Solutions of the Time-Dependent Schrödinger Equation for Ultracold Bosons

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See also: PNAS 2012 **109** (34) 13521-13525

http://MCTDHB.org

http://OpenMCTDHB.uni-hd.de

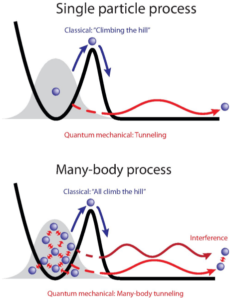
Quantum Technologies III, Warsaw 13/09/12

Outline

Many-Body Tunneling

Why tunneling?!

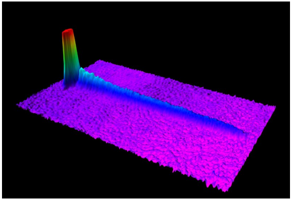
- Tunneling is omnipresent
- Characterizes a lot of processes
  - α-decay
  - fusion
  - fission
  - photo dissosiciation
  - photo association



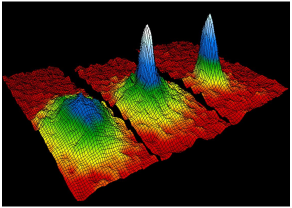
- Processes take place in *many-particle* systems
- In principle *all* systems are correlated and open.

Intro: Why Bosons?

- Interparticle interactions + Trapping potential are tunable.
- A rich variety of phenomena can be modelled.
- "Simple" (linear) governing equation: $\hat{H}\Psi = i\partial_t\Psi$ (TDSE).
- Reduced dimensional Ψ often fails to describe the physics



Atom lasers



BECs[1]

[1] Cornell E.A. and Wieman C.E. Rev.Mod.Phys. **74**, 875, (2002); Ketterle W. Rev.Mod.Phys. **74**, 1131, (2002)

How to approach Many-Body Quantum Mechanics?

How to approach the multidimensional/many-body TDSE?

- Schrödinger equation: $\hat{H}\Psi = i\partial_t \Psi$
- Simple, **but** $\Psi = \Psi(x_1, ..., x_N, t)$ and $N \sim 10$ or more
- The Hamiltonian is well-known:

$$\begin{aligned}\hat{H} &= \sum_{i=1}^{N}\left(\hat{T}_i + V(\hat{x}_i)\right) + \lambda_0 \sum_{i<j}^{N} \delta(x_i - x_j) \\ &= \sum_{i=1}^{N} \hat{h}_i + \lambda_0 \sum_{i<j}^{N} \delta(x_i - x_j)\end{aligned}$$

How to approach Many-Body Quantum Mechanics?

- To solve the TDSE we need to deal with the high dimensionality of many-body wavefunctions
- Variational approaches:
  - Gross-Pitaevskii (1961)[2]
  - Best Mean Field (BMF) / Time-Dependent Multi-Orbital Mean-Field (TDMF) (2003/2007)[3]
  - The **M**ulti**C**onfigurational **T**ime-**D**ependent **H**artree (for **B**osons) Method (2007/2008)[4]

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[2] Gross E.P., Il Nuovo Cimento **20** (3): 454 (1961); Pitaevskii, L., Sov. Phys. JETP **13** (2): 451-454 (1961).

[3] Cederbaum, L. S. and Streltsov, A. I., Phys. Lett. A **318**, 564 (2003); Alon,O. E., Streltsov, A. I. and Cederbaum, L. S., Phys. Lett. A **362**, 453 (2007).

[4] Meyer H.-D., Manthe U. and Cederbaum L.S., Chem.Phys.Lett. **165**, 73 (1990); Manthe U., Meyer H.-D. and Cederbaum L.S., J.Chem.Phys., **97**, 3199 (1992); Streltsov A.I., Alon O.E. and Cederbaum L.S., Phys.Rev.Lett. **99**, 030402, (2007); Alon O.E., Streltsov A.I. and Cederbaum L.S., Phys.Rev.A **77**, 033613, (2008)

MCTDHB method: Theory.

The Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \hat{h}(x_i) + \sum_{i<j=1} \hat{W}(x_i - x_j)$$

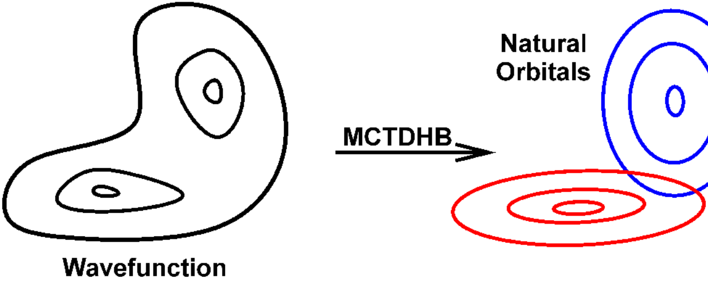
Ansatz for the wavefunction:

$$\begin{aligned} \Psi(x_1, ..., x_N, t) &= \sum_{\vec{n}} C_{\vec{n}}(t) |\vec{n}; t\rangle; \\ |\vec{n}; t\rangle &= \frac{1}{\sqrt{n_1! \cdots n_M!}} \left(\hat{b}_1^\dagger(t)\right)^{n_1} \cdots \left(\hat{b}_M^\dagger(t)\right)^{n_M} |vac\rangle \end{aligned}$$

Dirac-Frenkel Variational Principle with respect to Coefficients **and** Orbitals:

$$\langle \delta\Psi | H - i\partial_t | \Psi \rangle = 0$$

MCTDH(B): Theory.



[5]

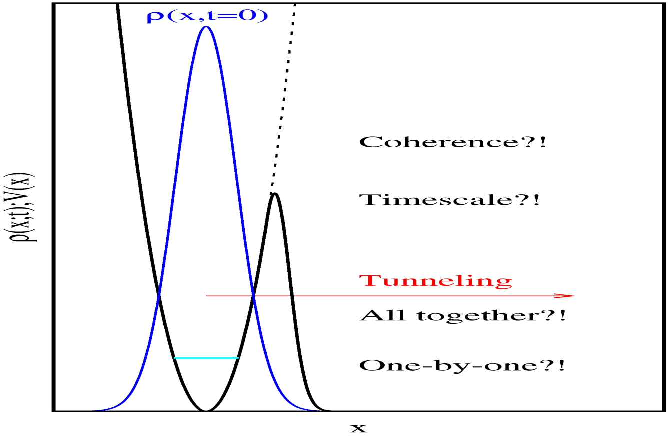
Ansatz: $|\Psi(t)\rangle = \sum_{\{\vec{n}\}} C_{\vec{n}}(t)|\vec{n},t\rangle$

TDVP:

$$\frac{\delta S[\{\Phi_i(x,t)\}\{C_{\vec{n}}(t)\}]}{\delta\Phi_i^*(x,t)\delta C_{\vec{n}}^*(t)} = \frac{\int dt \left(\langle\delta\Psi|\hat{H} - i\partial_t|\Psi\rangle - \sum_{kj}\mu_{kj}(t)\left[\langle\Phi_k|\Phi_j\rangle - \delta_{kj}^M\right]\right)}{\delta\Phi_i^*(x,t)\delta C_{\vec{n}}^*(t)}$$

[5] Image: Courtesy of Markus Schröder.

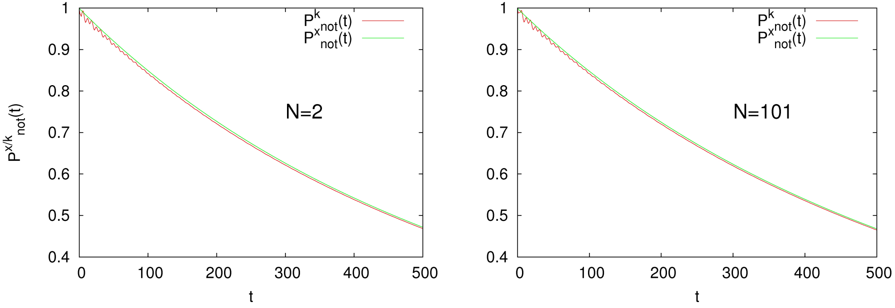
Tunneling Many-Body Systems



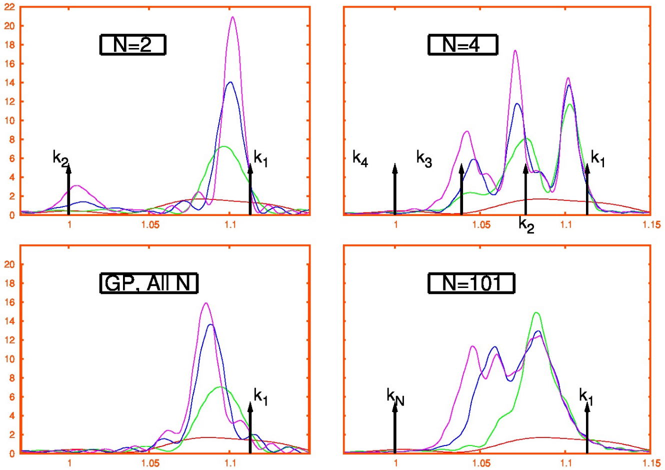
This talk: $\lambda = \lambda_0(N-1) = 0.3; N = 2, 4, 101.$

Integrals of Densities

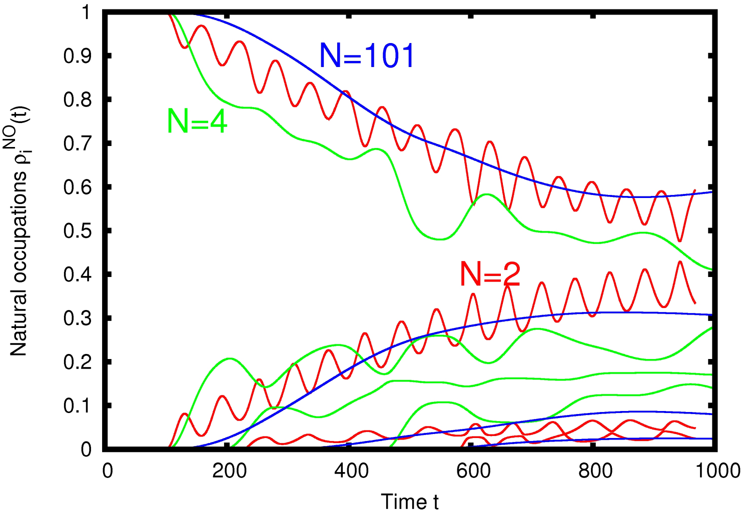
$P_{not}(t) = \int_{-\infty}^{C} \rho(x)dx$
Movie of $\rho(x, t$ and $\phi_k(x, t)$; $k = 1, ..., 4$.
Movie of $\rho(k, t)$ and $\rho(k, t)-$gaussian fit(k).



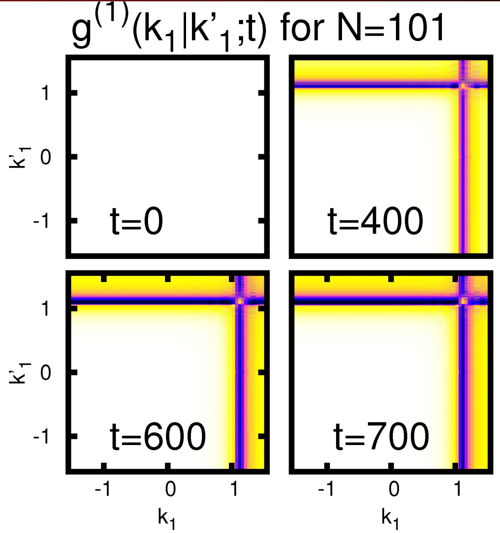
Densities of the Emitted Bosons in Momentum Space



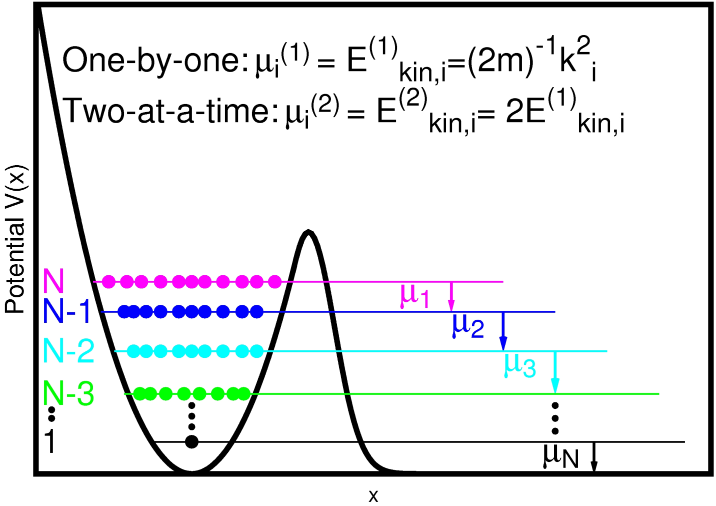
Natural Occupations



Correlation Functions



A Model of the Process

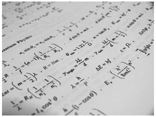


Conclusions

- The tunneling process in open systems is characterized by different coherence properties in distinct spatial regions or momentum domains.
- The involved momenta are defined by the chemical potentials of systems with different particle numbers, $N, N-1, \ldots, 2, 1$.
- The many-body tunneling process is a superposition of *one-by-one* processes.

Outlook

- Different potentials, e.g. with a threshold.
- Define coherence properties of quantum systems locally.
- Measures and analytical models for quantum many body dynamics in general.

:

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Alexej Streltsov

Computations: bwGRiD

CRAY THE SUPERCOMPUTER COMPANY XE6 (Hermit) @ HLRS Stuttgart

$$$: HGS MathComp

Center for Quantum Dynamics

MAX-PLANCK-GESELLSCHAFT

Minerva Foundation

Thank you for your attention!

Supplementary - Analysis programs

A solution, $\Psi(x_1, ..., x_N; t) = \sum_{\vec{n}} C_{\vec{n}}(t)|\vec{n}; t\rangle$, was obtained. What next?

- Specially adapted analysis tools necessary.
- Sampling and FFT methods are essential (full grid representations cost $>$ Terabytes for a single point in time).
- Efficient I/O is crucial.
- Demonstration: Sampled (reduced grid density and space) $g^{(1)}(x_1|x_1', t)$, with $n_g = 2^{16}$; $M = 4$; $n_{conf} = 10$. Full time slice would require $(2^{16}) \cdot (2^{16}) \cdot 4 \cdot 10 \cdot 16\text{bytes} = 2.74 \cdot 10^{12}\text{bytes}$.

Supplementary – MCTDHB: Equations of Motion.

- Equations of Motion (EOM):
  Coupled —— Non-linear —— Integro-Differential.

$$M \quad \text{Orbitals:} \qquad i\partial_t|\phi_j\rangle = \hat{\mathbf{P}}\left[\hat{h}|\phi_j\rangle + \sum_{k,s,q,l=1}^{M} \{\rho(t)\}^{-1}_{jk}\rho_{ksql}\hat{W}_{sl}|\phi_q\rangle\right]$$

$$\binom{N+M-1}{N} \quad \text{Coefficients:} \qquad i\partial_t C_{\vec{n}}(t) = \sum_{\vec{n}'}\langle\vec{n};t|\hat{H}|\vec{n}';t\rangle C_{\vec{n}'}$$

- MCTDHB package: Solve the EOM, efficiently.
  Use Adams-Bashforth-Moulton (ABM) for Orbital EOM (recently: also BS,RK,ZVODE).
  Use Short Iterative Lanczos (SIL) for Coefficients' EOM.

Supplementary – The current MCTDHB integration scheme

SIL Propagate $C(0) \mapsto C(\frac{\tau}{2})$ using $h_{kq}(0), W_{kqsl}(0)$, obtain $\rho_{kq}(\frac{\tau}{2}), \rho_{kqsl}(\frac{\tau}{2})$;

ABM/RK/ZVODE Propagate $\Phi(0) \mapsto \Phi(\frac{\tau}{2})$ using $\rho_{kq}(\frac{\tau}{2}), \rho_{kqsl}(\frac{\tau}{2})$.

ABM/RK/ZVODE Propagate $\Phi(0) \mapsto \Phi'(\frac{\tau}{2})$ using $\rho_{kq}(0), \rho_{kqsl}(0)$, obtain error estimate.

ABM/RK/ZVODE Propagate $\Phi(\frac{\tau}{2}) \mapsto \Phi(\tau)$ using $\rho_{kq}(\frac{\tau}{2}), \rho_{kqsl}(\frac{\tau}{2})$, obtain $h_{kq}(\tau), W_{ksql}(\tau)$ using $\Phi(\tau)$.

SIL Propagate $C(\frac{\tau}{2}) \mapsto C(\tau)$ using $h_{kq}(\tau), W_{kqsl}(\tau)$, obtain $\rho_{kq}(\tau), \rho_{kqsl}(\tau)$.

SIL Backwards Propagate $C(\frac{\tau}{2}) \mapsto C'(0)$ using $h_{kq}(\tau), W_{kqsl}(\tau)$ obtain error estimate.

Supplementary - MCTDHB method: Reduced Density Matrices

- The one-body reduced density Matrix (RDM):

$$\begin{aligned}\rho(x_1|x_1';t) &= \langle\Psi|\hat{\Psi}^\dagger(x_1')\hat{\Psi}(x_1)|\Psi\rangle \\ &= N\int \Psi^*(x_1',x_2,...,x_N)\Psi(x_1,...,x_N)dx_2\cdots dx_N \\ &= \sum_{a,b}\rho_{ab}(t)\phi_a^*(x_1')\phi_b(x_1)\end{aligned}$$

- The two-body RDM:

$$\begin{aligned}\rho(x_1,x_2|x_1',x_2';t) &= \langle\Psi|\hat{\Psi}^\dagger(x_1')\hat{\Psi}^\dagger(x_2')\hat{\Psi}(x_1)\hat{\Psi}(x_2)|\Psi\rangle \\ &= N(N-1)\int \Psi^*(x_1',x_2',x_3,...,x_N)dx_3\cdots dx_N \\ &= \sum_{a,b,c,d}\rho_{abcd}\phi_a^*(x_1')\phi_b^*(x_2')\phi_c(x_1)\phi_d(x_2)\end{aligned}$$

Supplementary - Normalized Correlation Functions

- The first order correlation function:

$$g^{(1)}(x_1|x_1';t) = \frac{\rho^{(1)}(x_1|x_1')}{\sqrt{\rho^{(1)}(x_1|x_1)\rho^{(1)}(x_1'|x_1')}}$$

- The p-th order correlation function:

$$g^{(p)}(x_1,...,x_p|x_1',...,x_p;t) = \frac{\rho^{(p)}(x_1,...,x_p|x_1',...,x_p)}{\sqrt{\prod_{\mu=1}^{p}\rho^{(1)}(x_\mu|x_\mu)\rho^{(1)}(x_\mu'|x_\mu')}}$$

Supplementary – MCTDH vs MCTDHB

- Numerical effort for N bosons and M orbitals:

	MCTDH	**MCTDHB**
Configurations	(M^N)	$\binom{M+N-1}{N}$
$N = 4, M = 10$	10^4	715
$N = 5, M = 10$	10^5	2002
$N = 25, M = 6$	$> 10^{19}$	142506
$N = 100, M = 5$	$> 10^{69}$	4598126

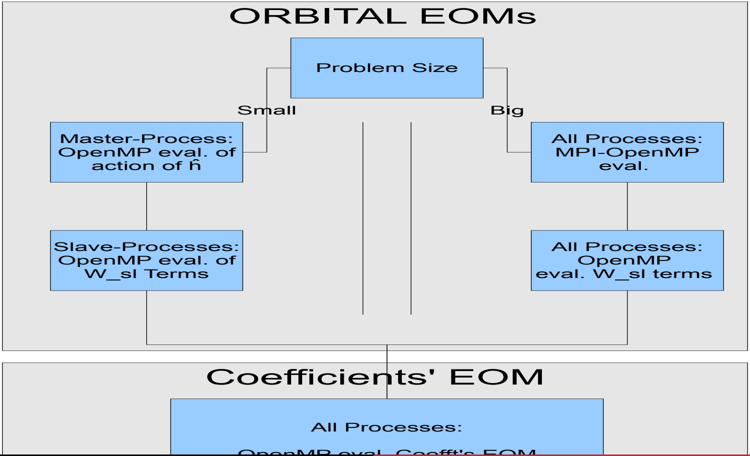
- System consists of
  - *few* bosons $\Rightarrow$ symmetrization of **MCTDH** algorithm
  - *many* bosons $\Rightarrow$ exploit symmetry by using the **MCTDHB**[6]

[6] Streltsov A.I., Alon O.E. and Cederbaum L.S., Phys.Rev.Lett. **99**, 030402 (2007); Alon O.E., Streltsov A.I. and Cederbaum L.S., Phys.Rev.A **77**, 033613 (2008)

Supplementary – MCTDHB package: Key Developments

- Huge grids necessary: Fast Fourier transform (FFT) collocation to circumvent expensive DVR-matrix-vector operations.
- Analysis tools: Sampling and FFT methods.
- Efficiency: Parallelization of integrators, hybridly and problem-size adapted parallel evaluation of the right-hand sides of the EOM.

Supplementary – The Problem Size Adaptive Hybrid Parallelization



Supplementary – MCTDH(B) package: Software Development

Four golden rules:

1. COORDINATION: *Version management* — Subversion (svn), Mercurial (Hg) or Git.
2. BIG STEPS WITH SMALL TESTS: Scientific software's development is best done *test-driven*: Implement a test suite (i.e. automated tests for consistency after building for instant feedback).
3. CODE VISUALIZATION FOR OPTIMIZATIONS: Use *performance analysis software* (Scalasca, Tau, Periscope [all free]) for code visualization.
4. DOCUMENTATION: Use doxygen for automatic (online) user manual and code description.

Supplementary – Example: Typical Problem Sizes

- Number of particles: $N \sim 2, ..., \sim 10^7$.
- Number of gridpoints/basis functions: $n_g = 2, ..., 2^{21}$
- Spatial dimensionality: $D = 1, 2, 3$
- Demonstration with
  $D = 2; n_g = 2^{16} = 64k; N = 101; M = 4; n_{conf} = 182104.$
  Computation time $\sim$ hours, $\sim$ 100s CPU hours.
  Primitive grid size for this
  example:$2^{16 \cdot 101} = 2^{1616} = 2.914 \cdot 10^{486}$(!!!)

Supplementary – Some History: TDGP

The GP ansatz for the wavefunction:

$$|\Psi\rangle = |N;t\rangle = \frac{1}{\sqrt{N!}} \prod_{i=1}^{N} \Phi(x_i,t)$$

Time-Dependent Variational Principle (TDVP):

$$\frac{\delta S[\Phi(x,t)]}{\delta \Phi^*(x,t)} \stackrel{!}{=} 0 = \frac{\int dt \left(\langle \delta\Psi | \hat{H} - i\partial_t | \Psi \rangle - \mu(t) \left[\langle \Phi | \Phi \rangle - 1 \right] \right)}{\delta \Phi^*(x,t)}$$

The equation of motion / the TDGP:

$$i\dot{\Phi}(x,t) = \left[\hat{h} + \lambda_0 (N-1) |\Phi(x,t)|^2 \right] \Phi(x,t)$$

Supplementary – Some more recent History: BMF/TDMF

The TDMF ansatz for the wavefunction:

$$|\Psi\rangle = |n_1, n_2, \dots, n_M; t\rangle = \hat{\mathcal{S}}\left[\prod_{i=1}^{n_1} \Phi_1(x_i, t) \cdots \prod_{i=N-n_M+1}^{n_M} \Phi_M(x_i, t)\right]$$

TDVP:

$$\frac{\delta S[\{\Phi_i(x,t)\}]}{\delta \Phi_q^*(x,t)} \overset{!}{=} 0 = \frac{\int dt \left(\langle \delta\Psi | \hat{H} - i\partial_t | \Psi\rangle - \sum_{kj} \mu_{kj}(t) \left[\langle \Phi_k | \Phi_j \rangle - \delta_{kj}^M\right]\right)}{\delta \Phi_q^*(x,t)}$$

The M equations of motion:

$$i|\dot{\Phi}_k\rangle = \hat{\mathbf{P}}\left[\hat{h} + \lambda_0(n_k - 1)|\Phi_k|^2 \sum_{l \neq k}^{M} 2\lambda_0 n_l |\Phi_l|^2\right] |\Phi_k\rangle$$

$$\hat{\mathbf{P}} = 1 - \sum^{M} |\Phi_l\rangle\langle\Phi_l|$$

Supplementary – Orbital EOM in Detail

$$i\partial_t \underbrace{|\phi_j\rangle}_{\text{ABM}} = \hat{\mathbf{P}}\left[\underbrace{\hat{h}|\phi_j\rangle}_{\mathcal{O}(n_g \log n_g)} + \underbrace{\sum_{k,s,q,l=1}^{M} \{\rho(t)\}^{-1}_{jk} \rho_{ksql} \hat{W}_{sl} |\phi_q\rangle}_{\mathcal{O}(M^4);\#\{k,s,q,l\}+\mathcal{O}(M^2)\hat{W}_{sl}\text{–integrals}} \right]$$

$$\hat{W}_{sl}(x) = \int \phi_s^*(x')\hat{W}(x-x')\phi_l(x')dx'$$

- A problem-size-adaptive hybrid parallelization.
- OpenMP-parallelized ABM.

Supplementary – Coefficients' EOM in Detail

$$\underbrace{i\partial_t C_{\vec{n}}(t)}_{\text{SIL}} = \underbrace{\sum_{\vec{n}'} \langle \vec{n}; t | \hat{H} | \vec{n}'; t \rangle C_{\vec{n}'}}_{\binom{N+M-1}{N}}$$

- SIL is a Krylov-Method $\Rightarrow$ Needs $\{\hat{H}|\Psi\rangle, \hat{H}^2|\Psi\rangle, ..., \hat{H}^K|\Psi\rangle\}$.
- An efficient mapping/re-addressing[7] scheme allowed to hybridly parallelize the evaluation of $\hat{H}$ and its powers.

[7] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. A **81**, 022124 (2010)