Solving the Kadanoff-Baym equations with grid-based methodologies.

I. Computational concepts, and II. application to atomic model systems

Karsten Balzer

ITAP, Christian-Albrechts-Universität Kiel

C A U
Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

KBE 2010 "Solving the Two-time Kadanoff-Baym Equations. Status and Open Problems"

Thursday 25th March, 2010—(2:00 p.m)

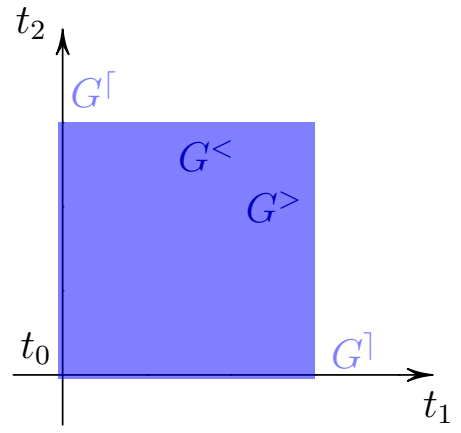
Outline

Outline

Solution of the 2-time Kadanoff-Baym equations

Spatially homogeneous systems

- nuclear matter, Danielewicz, Köhler, Bożek, Greiner etc.
- correlated electron gas, Kwong, Bonitz
- dense plasmas, Bonitz, Semkat, Kremp
- electron-hole plasma/semiconductors
  Schäfer, Binder, Kwong, Banyai, Gartner, Jahnke, Haug, Jauho



Spatially **in**homogeneous (localized) systems

- few/multi-electron atoms and small molecules[1]
- few-electron quantum dots[2]
- lattice models[3]

[1] N.E. Dahlen et al, PRL **98**, 153004 (2007), A. Stan et al, EPL **76**, 298 (2006)

[2] K. Balzer et al, PRB **79**, 245306 (2009) *and* J. Phys. A **42**, 214020 (2009)

[3] M. Puig von Friesen et al, PRL **103**, 176404 (2009); P. Myöhänen et al, EPL **84**, 67001 (2008)

Outline

NEGF approach to inhomogeneous systems

Consider Ne^- Hamiltonian [in a.u.]:

$$\hat{H}(t) = \hat{T} + \hat{V}(t) + \hat{U} \,,$$

$$\hat{T} = \sum_{i=1}^{N} -\frac{1}{2}\nabla_i^2 \,, \qquad \hat{V}(t) = \sum_{i=1}^{N} V(x_i, t) \,, \qquad \hat{U} = \sum_{i<j}^{N} U(|x_i - x_j|)$$

Kadanoff-Baym equations, $1 = (x, t, \sigma)$

$$\left\{ \mathrm{i}\partial_t - \left(-\frac{1}{2}\nabla_x^2 + V(x,t) \right) \right\} G(1,1') = \delta_{\mathcal{C}}(1-1') + \int_{\mathcal{C}} \mathrm{d}2\, \Sigma[G,U](1,2)\, G(2,1')$$

$+$ adjoint equation $t \leftrightarrow t'$

Spin-polarized/restricted ansatz
(spin degeneracy $\xi \in \{1, 2\}$)

$\xi = 1$: $|\uparrow\rangle\ |\uparrow\rangle\ |\uparrow\rangle \ldots$
$\xi = 2$: $|\uparrow\downarrow\rangle\ |\uparrow\downarrow\rangle \ldots$

$$G(1,1') \to G(xt, x't') \,, \qquad \Sigma[G,U](1,1') \to \Sigma_\xi[G,U](xt, x't')$$

Numerical representation of $G(xt, x't')$

treatment of times t, t'

- times t, t' vary on full Keldysh contour $\mathcal{C} \rightarrow$ 2D (complex) grid

treatment of coordinates x, x'

- 2D grid: intuitive but inefficient (huge grid required)
- basis expansion: works but problematic for spatially extended hamiltonians (extremely large basis set required)

+ alternative

combine grid and basis methods

$+$

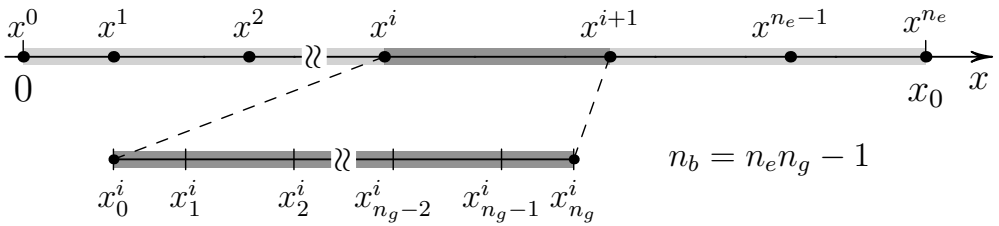
use quadrature rule based integrations

$\Downarrow$

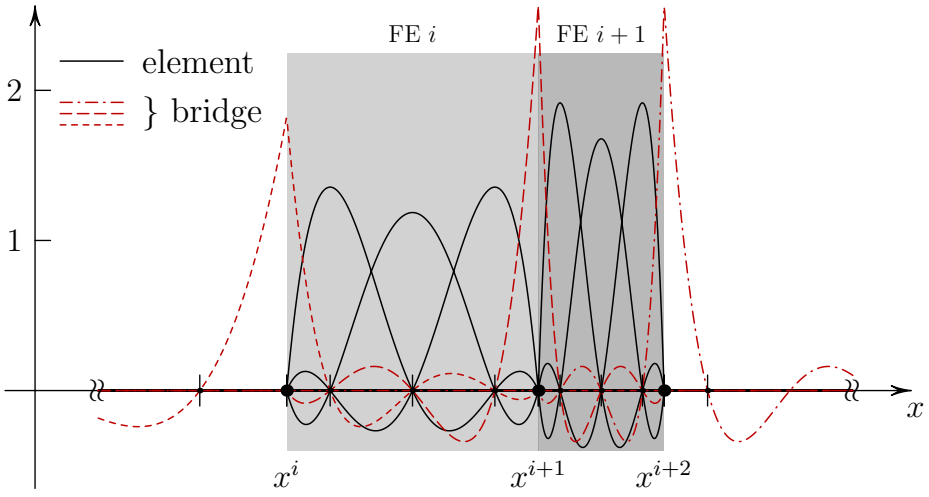
finite-element discrete variable representation[1] (FE-DVR)

[1] with respect to the TDSE e.g. T.N. Rescigno, and C.W. McCurdy PRA **62**, 032706 (2000), B.I. Schneider, L.A. Collins, and S.X. Hu, PRE **73**, 036708 (2006)

Finite-element DVR



i. partition $[0, x_0]$ into n_e FEs i



ii. $\forall$ FEs there exist points x_m^i and weigths w_m^i of the generalized Gauss-Lobatto quadrature

$\Rightarrow$ construct a local DVR basis $\chi_m^i(x)$

$$\chi_m^i(x) = \frac{1}{\sqrt{w_m^i}} \prod_{n \neq m} \frac{x - x_n^i}{x_m^i - x_n^i}$$

FE-DVR ansatz[1] ($n_b = n_e n_g - 1$)

$$G(xt, x't') = \sum_{im} \sum_{\bar{i}\bar{m}} \chi_m^i(x)\, \chi_{\bar{m}}^{\bar{i}}(x')\, G_{m\bar{m}}^{i\bar{i}}(t, t') \,, \qquad x, x' \in [0, x_0]$$

[1] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A **81**, 022510 (2010)

KBE in FE-DVR representation[1]

KBEs transform into EoM for matrix $G^{i\bar{i}}_{m\bar{m}}(t,t')$ — Einstein notation!

$$\left\{\mathrm{i}\partial_t - \left(T^{i\bar{i}}_{m\bar{m}} + V^{i\bar{i}}_{m\bar{m}}(t)\right)\right\} G^{\bar{i}i'}_{\bar{m}m'}(t,t') = \delta_{\mathcal{C}}(t-t') + \int_{\mathcal{C}} \mathrm{d}\bar{t}\, \Sigma^{i\bar{i}}_{\xi,m\bar{m}}[G,U](t,\bar{t})\, G^{\bar{i}i'}_{\bar{m}m'}(\bar{t},t')$$

$+$ adjoint equation $t \leftrightarrow t'$

FE-DVR matrix elements:

$V^{i\bar{i}}_{m\bar{m}}(t) \propto \delta_{ii'}\delta_{mm'}$ is diagonal

$T^{i\bar{i}}_{m\bar{m}}$ is block-diagonal

computed by the generalized Gauss-Lobatto quadrature rule

Self-energy $\Sigma^{i\bar{i}}_{\xi,m\bar{m}}[G,U](t,\bar{t})$ involves matrix elements of $U(|x-x'|)$

$$U^{i_1 i_2, i_3 i_4}_{m_1 m_2, m_3 m_4} = \int_0^{x_0} \mathrm{d}x \int_0^{x_0} \mathrm{d}x'\, \chi^{i_1}_{m_1}(x)\, \chi^{i_3}_{m_3}(x')\, U(|x-x'|)\, \chi^{i_2}_{m_2}(x)\, \chi^{i_4}_{m_4}(x')$$
$$= \delta_{i_1 i_2}\delta_{i_3 i_4}\delta_{m_1 m_2}\delta_{m_3 m_4}\, \tilde{U}^{i_1 i_3}_{m_1 m_3} \quad \text{(high degree of diagonality)}$$

[1] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A **81**, 022510 (2010)

Self-energy functionals

Self-energy in FE-DVR representation ($\xi \in \{1, 2\}$)

$$\Sigma^{ii'}_{\xi,mm'}(t,t') = \delta_{\mathcal{C}}(t-t')\Sigma^{\mathrm{HF},ii'}_{\xi,mm'}(t) + \Sigma^{\mathrm{Corr},ii'}_{\xi,mm'}(t,t')$$

Hartree-Fock (HF) contribution[1]:

$\mathcal{O}(n_b) \quad \neg\,\mathcal{O}(n_b^2)$

$$\Sigma^{\mathrm{HF},ii'}_{\xi,mm'}(t) = -\mathrm{i}\left\{\delta_{ii'}\delta_{mm'}\xi\sum_{i_1 m_1} G^{i_1 i_1}_{m_1 m_1}(t,t^+)\,\tilde{U}^{ii_1}_{mm_1} - G^{i'i}_{m'm}(t,t^+)\,\tilde{U}^{i'i}_{m'm}\right\}$$

Correlations in second Born (2ndB) approximation[1]:

$$\Sigma^{\mathrm{Corr},ii'}_{\xi,mm'}(t,t') = \sum_{i_1 m_1}\sum_{i_2 m_2}\left\{\xi\, G^{ii'}_{mm'}(t,t')\, G^{i_1 i_2}_{m_1 m_2}(t,t') - G^{ii_2}_{mm_2}(t,t')\, G^{i_1 i'}_{m_1 m'}(t,t')\right\}\times$$

$\mathcal{O}(n_b^2)$
$\neg\,\mathcal{O}(n_b^6)$

$$\times\; G^{i_2 i_1}_{m_2 m_1}(t',t)\,\tilde{U}^{ii_2}_{mm_2}\,\tilde{U}^{i'i_1}_{m'm_1}$$

[1] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A **81**, 022510 (2010)

Code parallelization

Why develop a parallel code?

Extensive runtime: r.h.s of KBE: collision integrals $I^{\gtrless}$, self-energies $\Sigma^{\gtrless}$
together with many/small time steps, huge memory requirements

Typical resources needed for 2-time solution

$$G(xt, x't') \to G^{i\bar{i}}_{m\bar{m}}(t,t') \in \mathbb{C}$$

RAM (double precision): $\mathcal{O}(16\, {n_t}^2 {n_b}^2)$ bytes

Example:

Two-time plane $\mathcal{P}(t_1, t_2)$: 50 a.u. with resolution $\delta t = 0.01$ a.u. $\Rightarrow n_t = 5000$

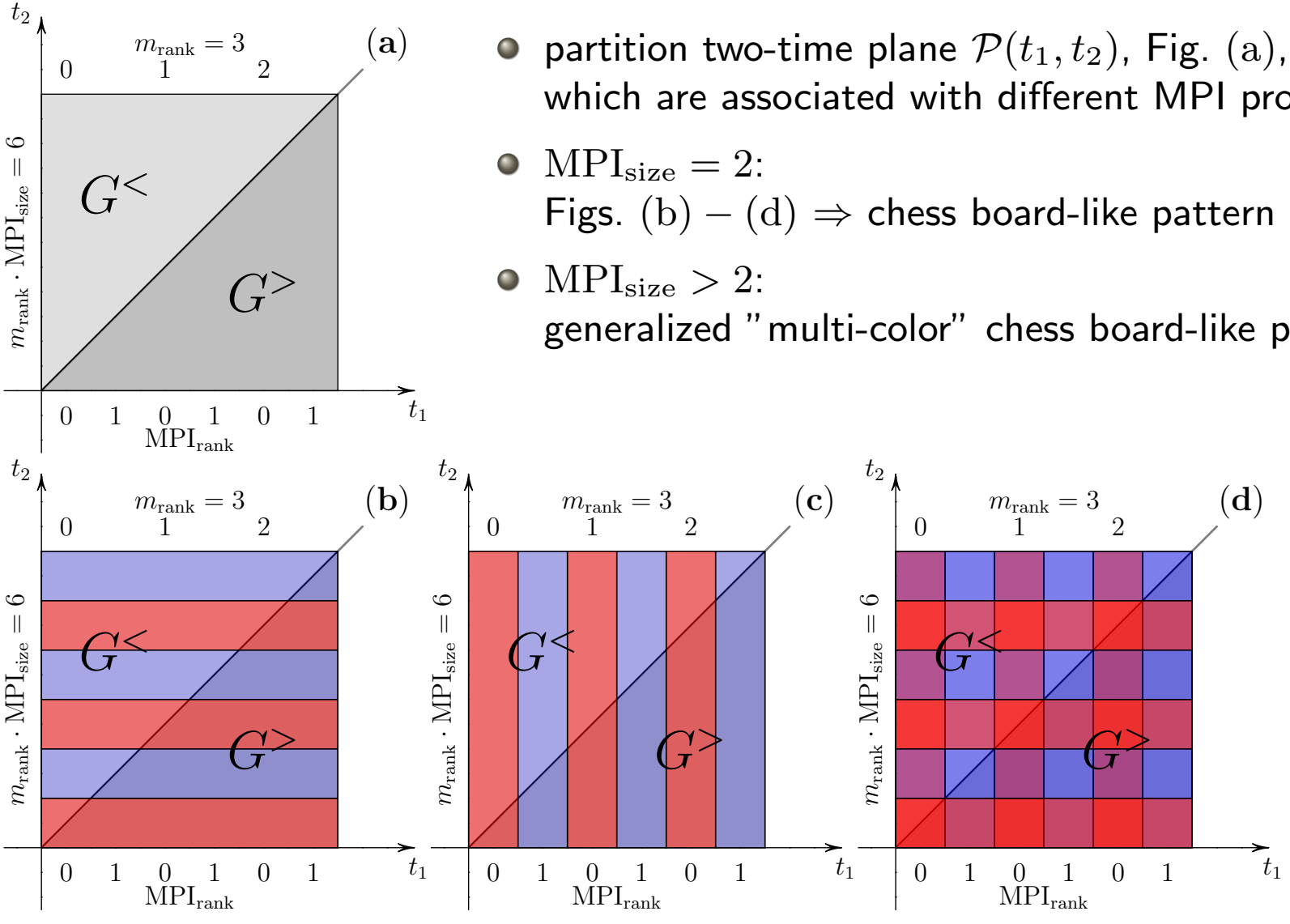
Minimum FE-DVR basis: $n_b = 50$

$$16\, 50^2 5000^2 \text{ Bytes} = 1 \times 10^{12} \text{ bytes} = 1 \text{ tera byte}$$

Why MPI?

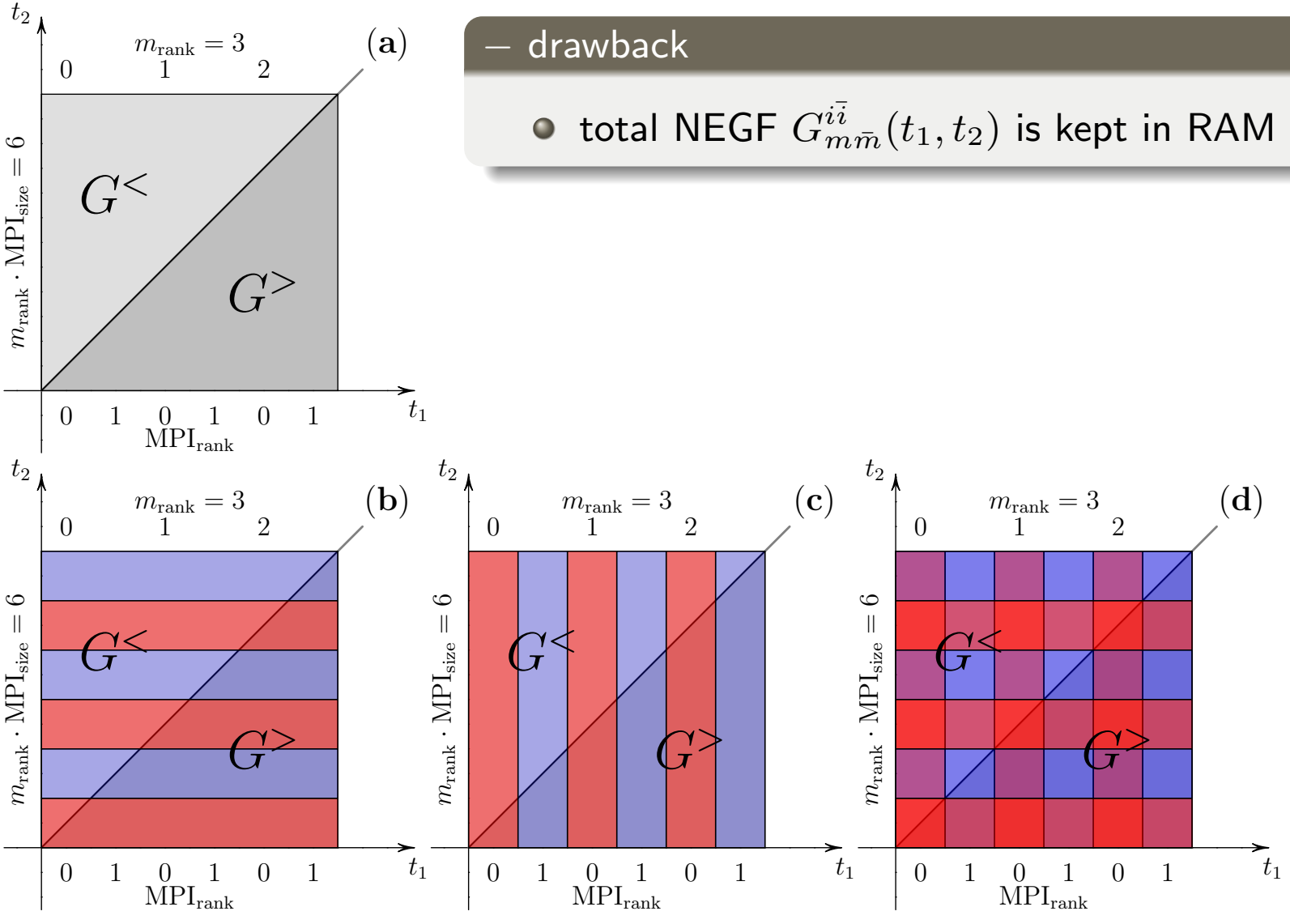
Memory requirements (>1 TB) are beyond typical shared memory setups!

Distributed memory concept



- partition two-time plane $\mathcal{P}(t_1, t_2)$, Fig. (a), in blocks which are associated with different MPI processes
- $\text{MPI}_{\text{size}} = 2$:
  Figs. (b) – (d) $\Rightarrow$ chess board-like pattern
- $\text{MPI}_{\text{size}} > 2$:
  generalized "multi-color" chess board-like pattern

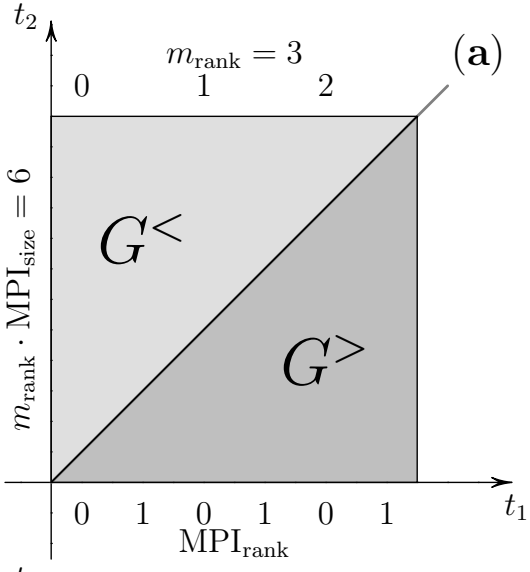
Distributed memory concept



– drawback

- total NEGF $G^{i\bar{i}}_{m\bar{m}}(t_1, t_2)$ is kept in RAM twice

Distributed memory concept

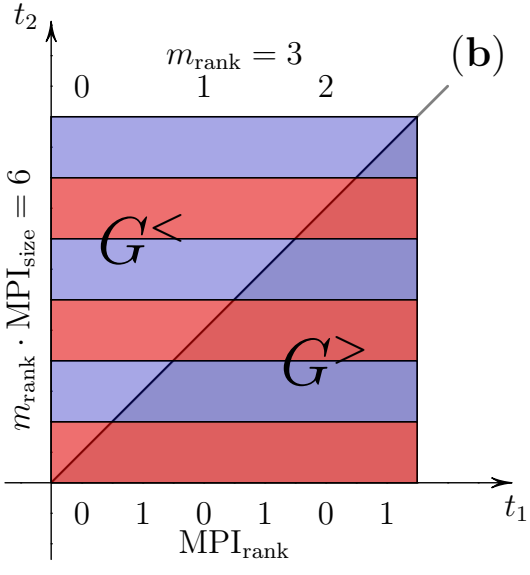


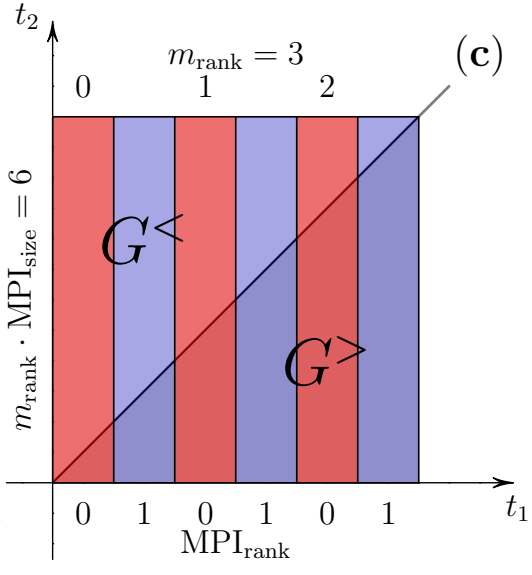
– drawback

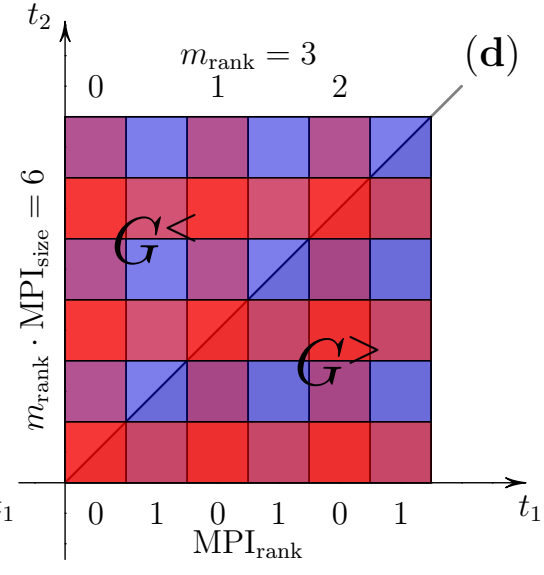
- total NEGF $G^{i\bar{i}}_{m\bar{m}}(t_1, t_2)$ is kept in RAM twice

+ benefit

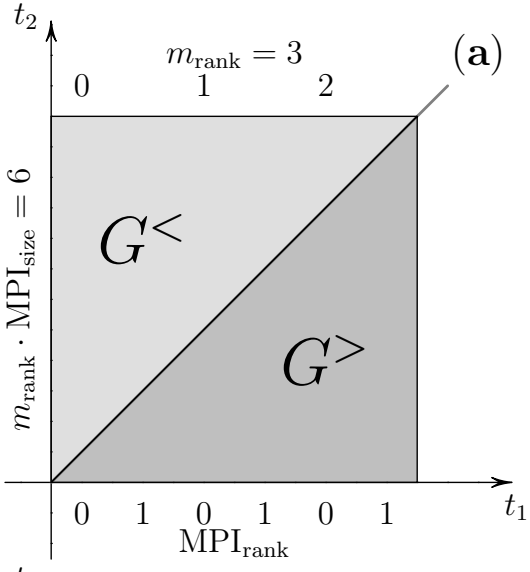
- minimum MPI (inter-process) communication







Distributed memory concept

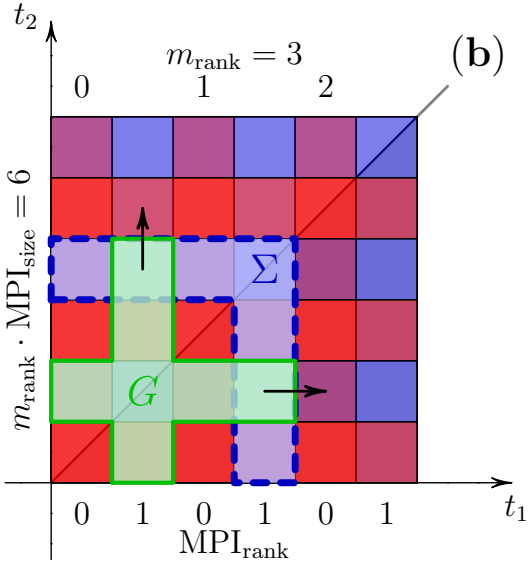


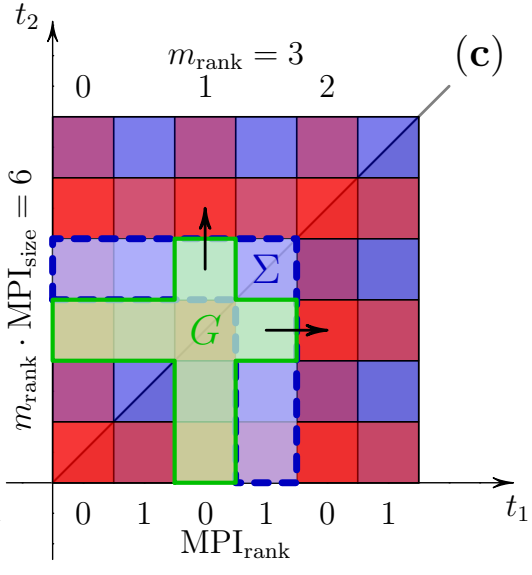
collision integrals $I^{\gtrless}$ involve

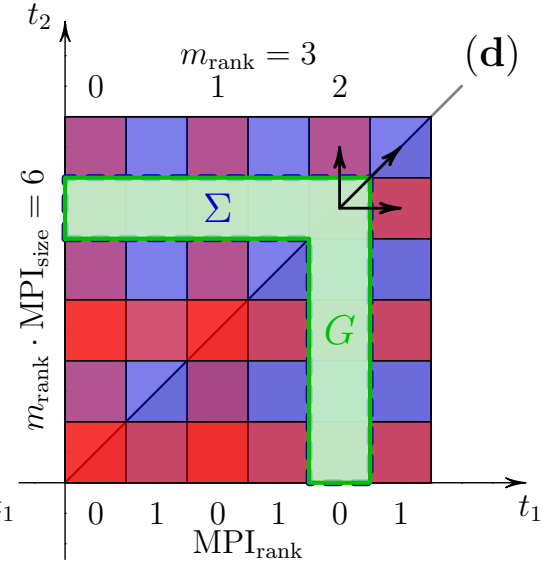
- self-energy $\Sigma^{\gtrless}$
- nonequilibrium Green's function $G^{\gtrless}$

Figs. (b) – (d): relevant contributions for different steps

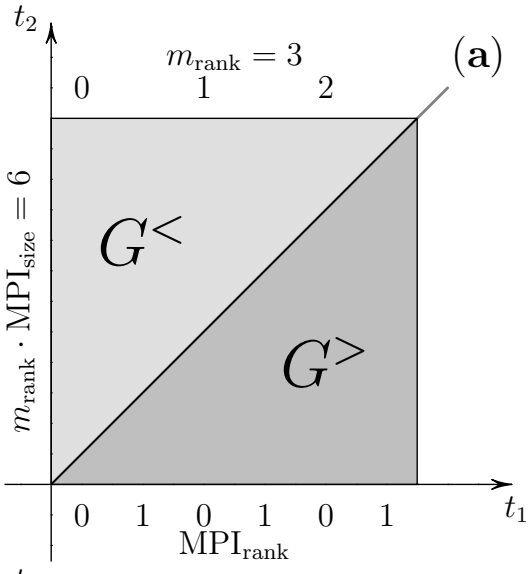
$$G^{\gtrless}(t) \rightarrow G^{\gtrless}(t + \delta t)$$





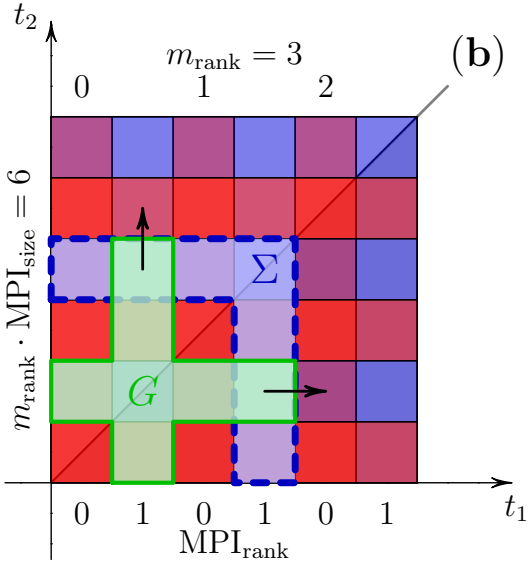


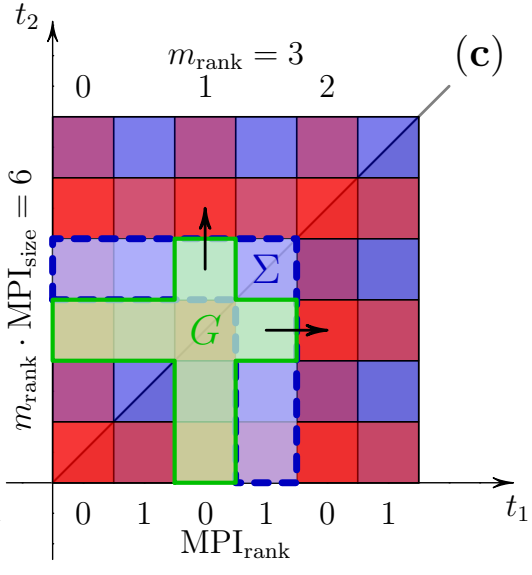
Distributed memory concept

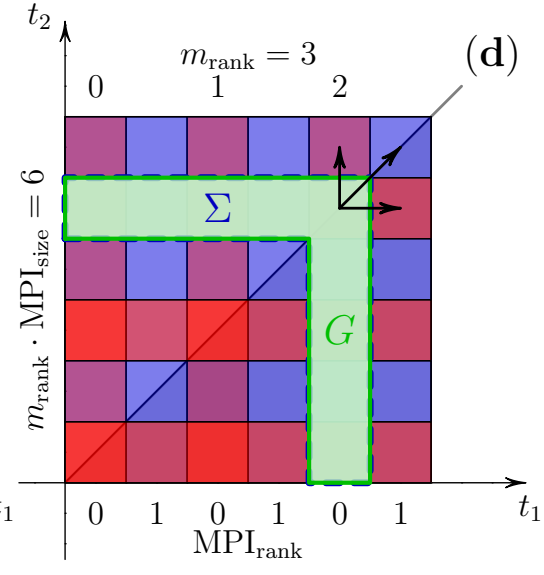


+ features

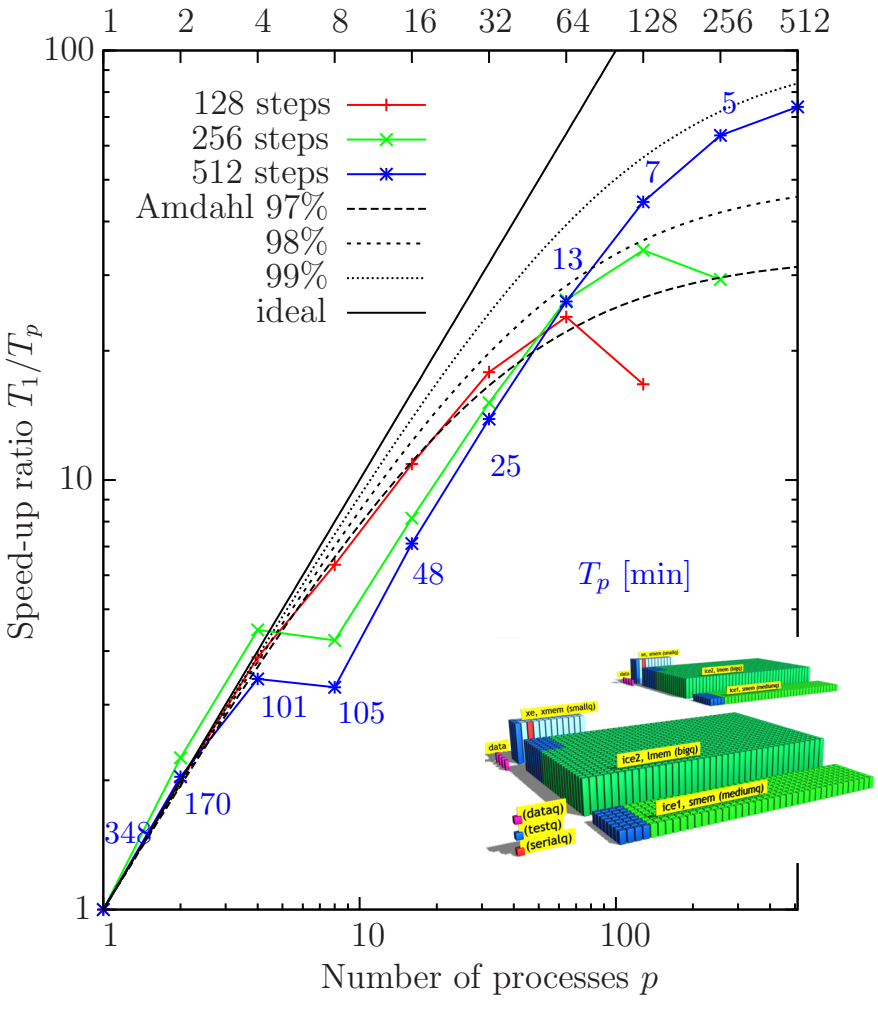
- minimum MPI communication:
  i. broadcast self-energies $\Sigma^{\gtrless}$
  ii. sort newly-calculated NEGFs $G^{\gtrless}$ into the "multi-color" chess board
- MPI_{size} steps parallel:
  steps for $G^<$ and $G^>$ are bunched in a single MPI process







MPI performance



NEGF $G^{i\bar{i}}_{m\bar{m}}(t_1, t_2)$ with $n_b = 23$ FE-DVR basis functions (1D helium model)

+ properties

- 1-512 MPI processes: optimal speed-up behavior
- more than 95% is parallelizable

Amdahl's law: $$\frac{T_1}{T_p} = \frac{1}{(1-\alpha) + \alpha/p} ,$$

$$\alpha > 0.95$$

ZIB RRZN

Outline

He, H_2 and LiH—One-dimensional models

Ne^--Hamiltonian [in a.u.]

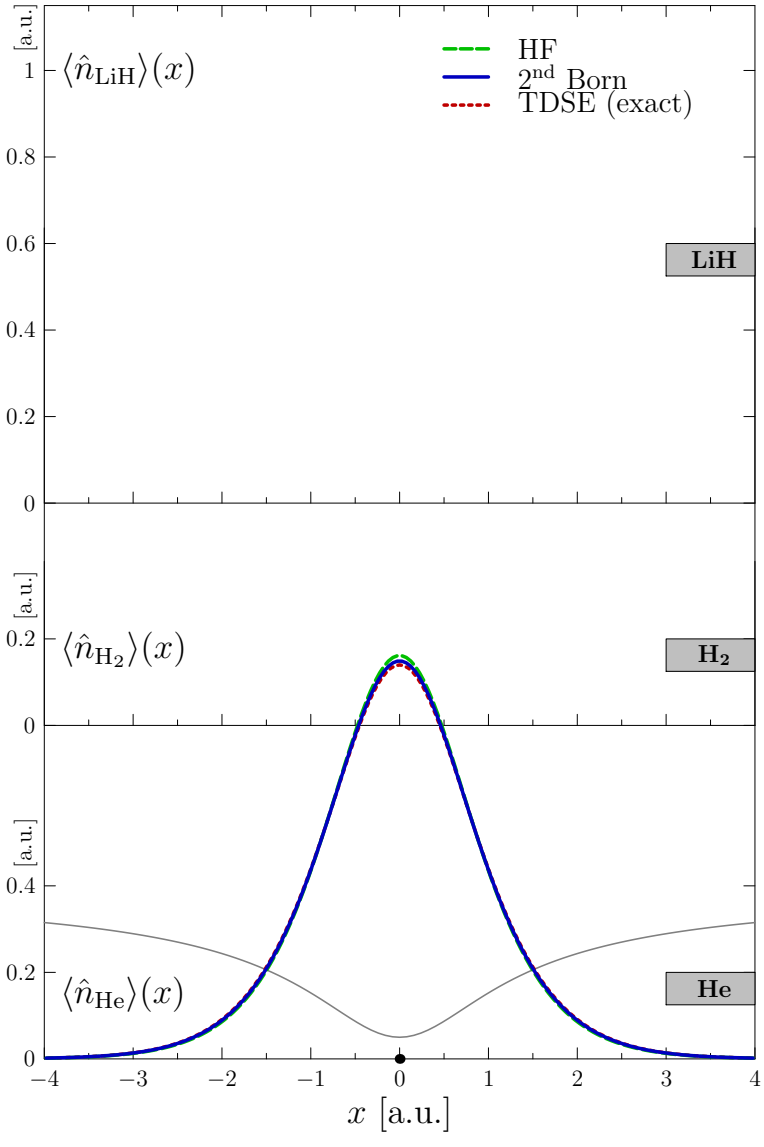
$$\hat{H} = \hat{T} + \hat{V} + \hat{U}$$
$$= \sum_{i=1}^{N} \left\{ -\frac{1}{2}\nabla_i^2 + \sum_{n=1}^{N_c} \frac{-Z_n}{\sqrt{(x_i - \bar{x}_n)^2 + c_n}} \right\} + \sum_{i<j} \frac{1}{\sqrt{(x_i - x_j)^2 + c}}$$

N_c: number of nuclei
Z_n: atomic number of nucleus n
$\bar{x}_n$: nuclei positions, determine molecular geometry
$c_n = c = 1 \; \forall \; n$: soft-core Coulomb potentials/interaction

Helium (He, $2e^-$)	$N_c = 1$	$Z_1 = 2$	$\bar{x}_1 = \frac{1}{2}x_0$
Hydrogen (H_2, $2e^-$)	$N_c = 2$	$Z_{1,2} = 1$	$\bar{x}_{1,2} = \frac{1}{2}(x_0 \pm d)$
Lithium hydride (LiH, $4e^-$)	$N_c = 2$	$Z_1 = 3$, $Z_2 = 1$	$\bar{x}_{1,2} = \frac{1}{2}(x_0 \pm d)$

d: interatomic distance

$1e^-$-densities, energies and bond lengths[1]



He $(2e^-)$

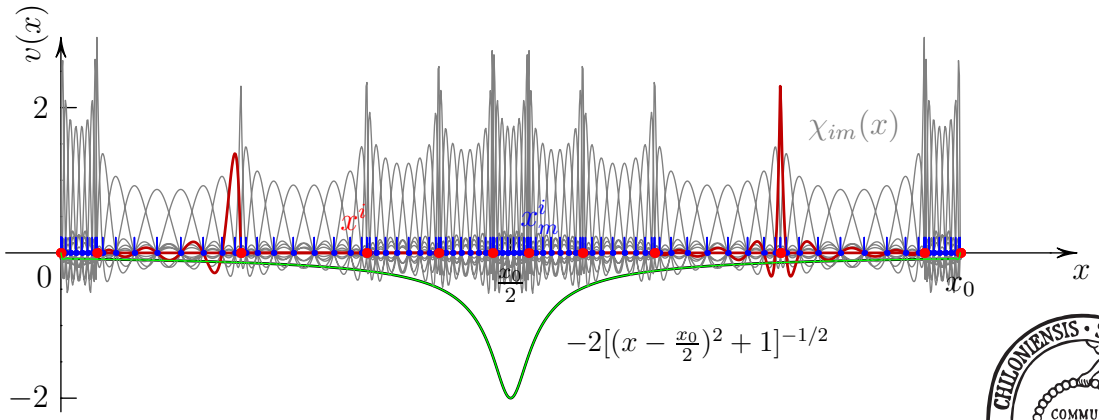
Parameters:

$x_0 = 50$ a.u.

$n_b = 153$ FE-DVR basis functions

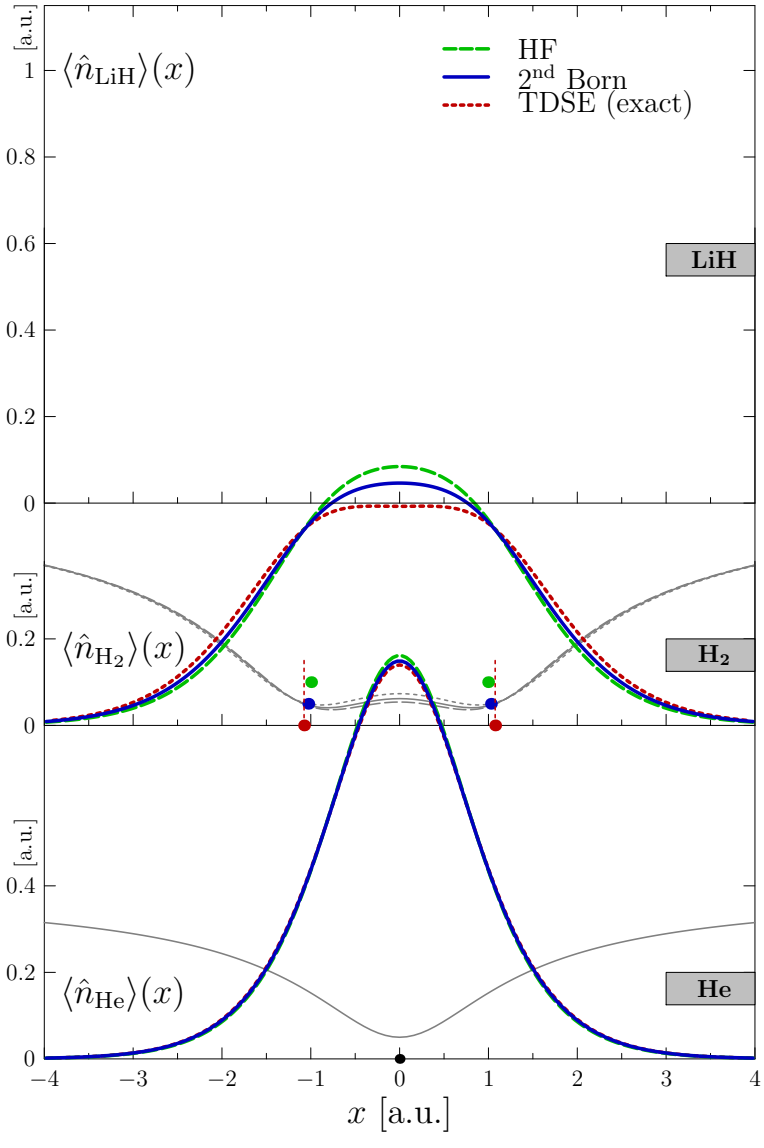
Ground state energy E_{gs} [Ha]:

HF	-2.224210
2ndB	$-2.233419 \approx 65\%$ of corr. energy
exact	-2.238258



[1] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A **81**, 022510 (2010)

$1e^-$-densities, energies and bond lengths[1]



H_2 $(2e^-)$ and LiH $(4e^-)$

- self-consistent results obtained by scanning the potential energy surface (PES)

Bond-length d_b [a.u.]:

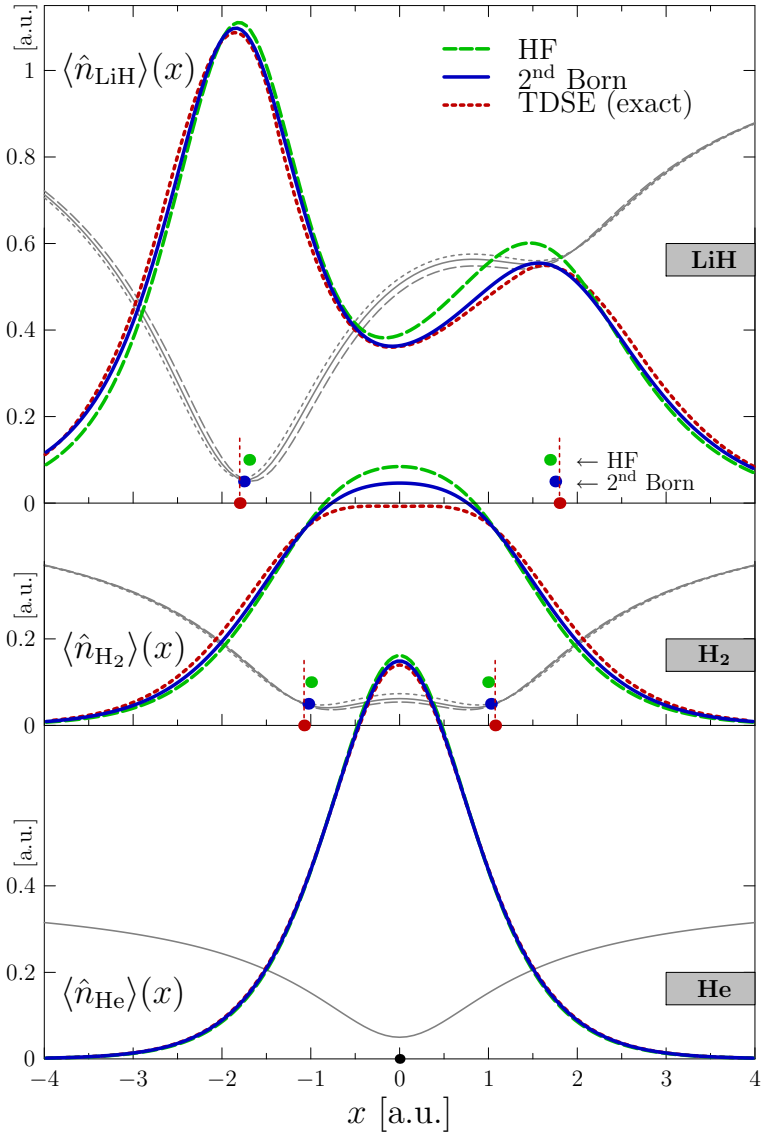
	HF	2ndB	exact
H_2	1.9925	2.0561	2.151
LiH	3.3860	3.5053	$3.6\cdot\cdot$

Binding energy E_b [Ha]:

	HF	2ndB	exact
H_2	-1.3531	-1.3740	-1.391
LiH	-4.8534	-4.8886	$-4.91\cdot$

[1] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A **81**, 022510 (2010)

$1e^-$-densities, energies and bond lengths[1]



H_2 $(2e^-)$ and LiH $(4e^-)$

- self-consistent results obtained by scanning the potential energy surface (PES)

Bond-length d_b [a.u.]:

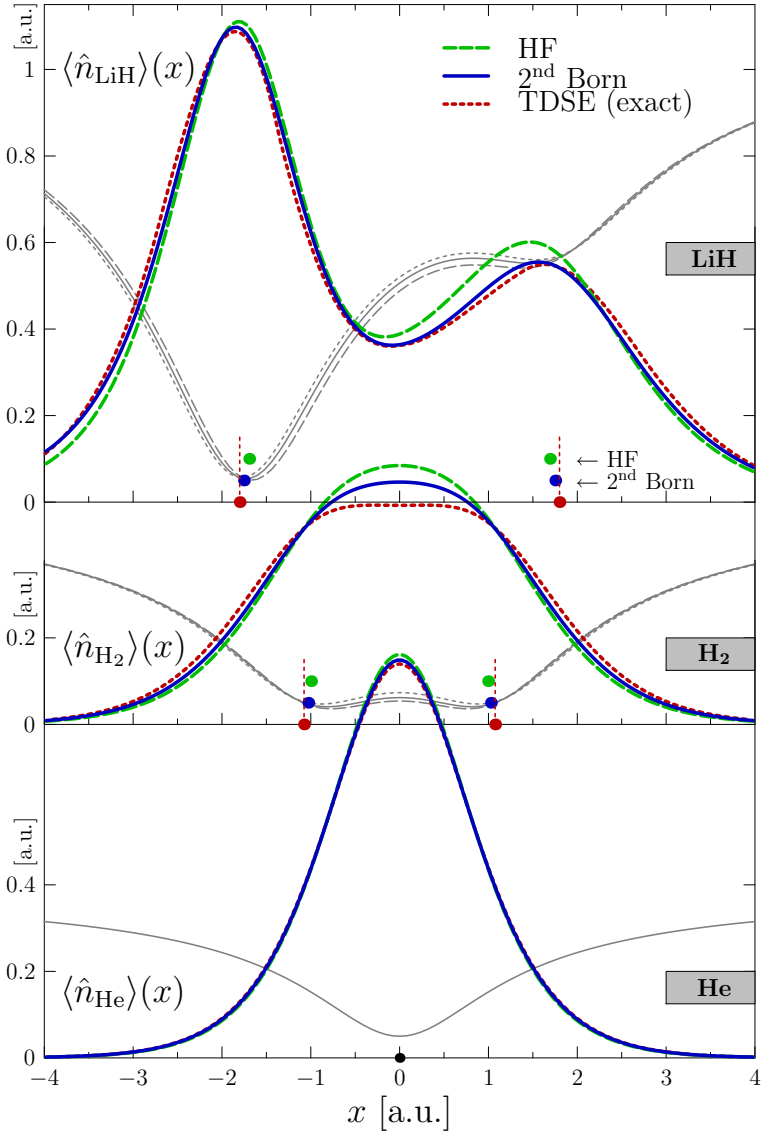
	HF	2ndB	exact
H_2	1.9925	2.0561	2.151
LiH	3.3860	3.5053	$3.6\cdot\cdot$

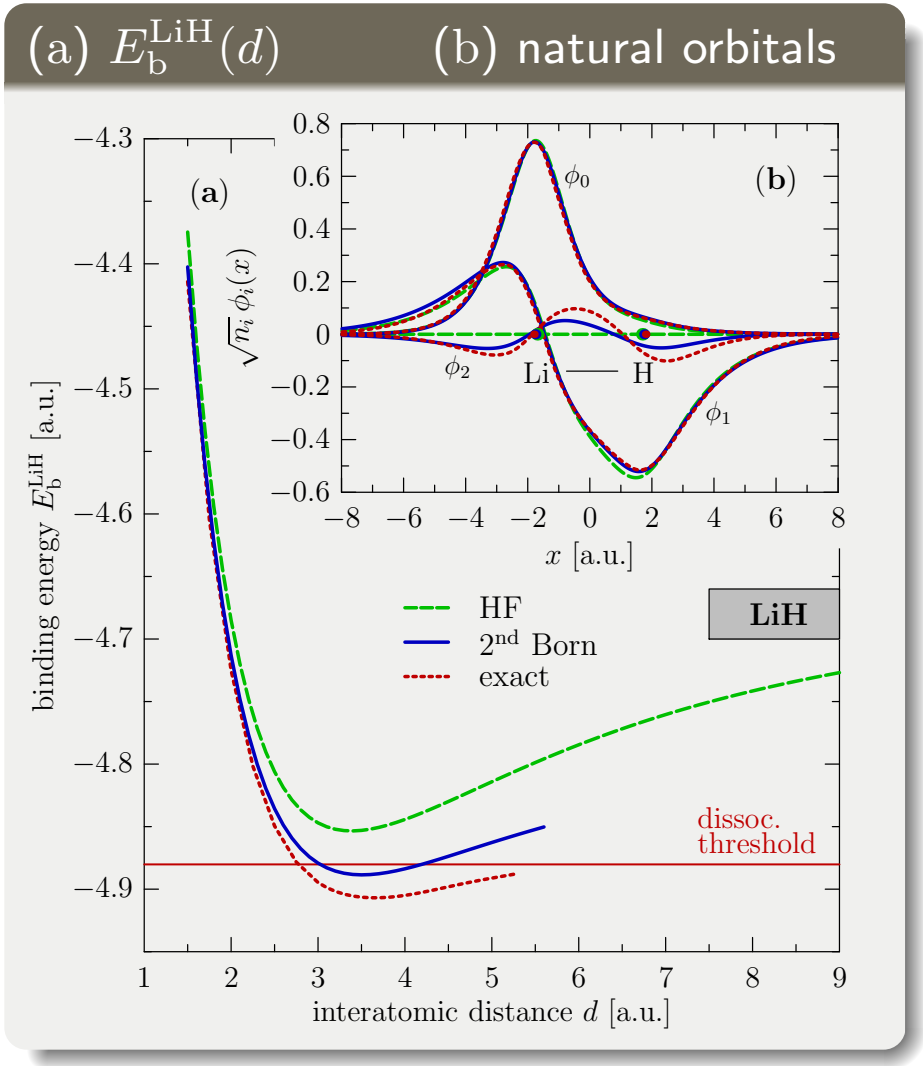
Binding energy E_b [Ha]:

	HF	2ndB	exact
H_2	-1.3531	-1.3740	-1.391
LiH	-4.8534	-4.8886	$-4.91\cdot$

[1] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A **81**, 022510 (2010)

$1e^-$-densities, energies and bond lengths[1]





[1] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A **81**, 022510 (2010)

Nonequilibrium behavior

Time-dependent Ne^--Hamiltonian [in a.u.]

$$\begin{aligned}\hat{H}(t) &= \hat{T} + \hat{V} + \hat{V}_{\text{ext}}(t) + \hat{U} \\ &= \sum_{i=1}^{N} \left\{ -\frac{1}{2}\nabla_i^2 + \sum_{n=1}^{N_c} \frac{-Z_n}{\sqrt{(x_i - \bar{x}_n)^2 + c_n}} + E_0 \cos(\omega\, t) x_i \right\} \\ &\quad + \sum_{i<j} \frac{1}{\sqrt{(x_i - x_j)^2 + c}}\end{aligned}$$

E_0: electric field strength
ω: laser frequency

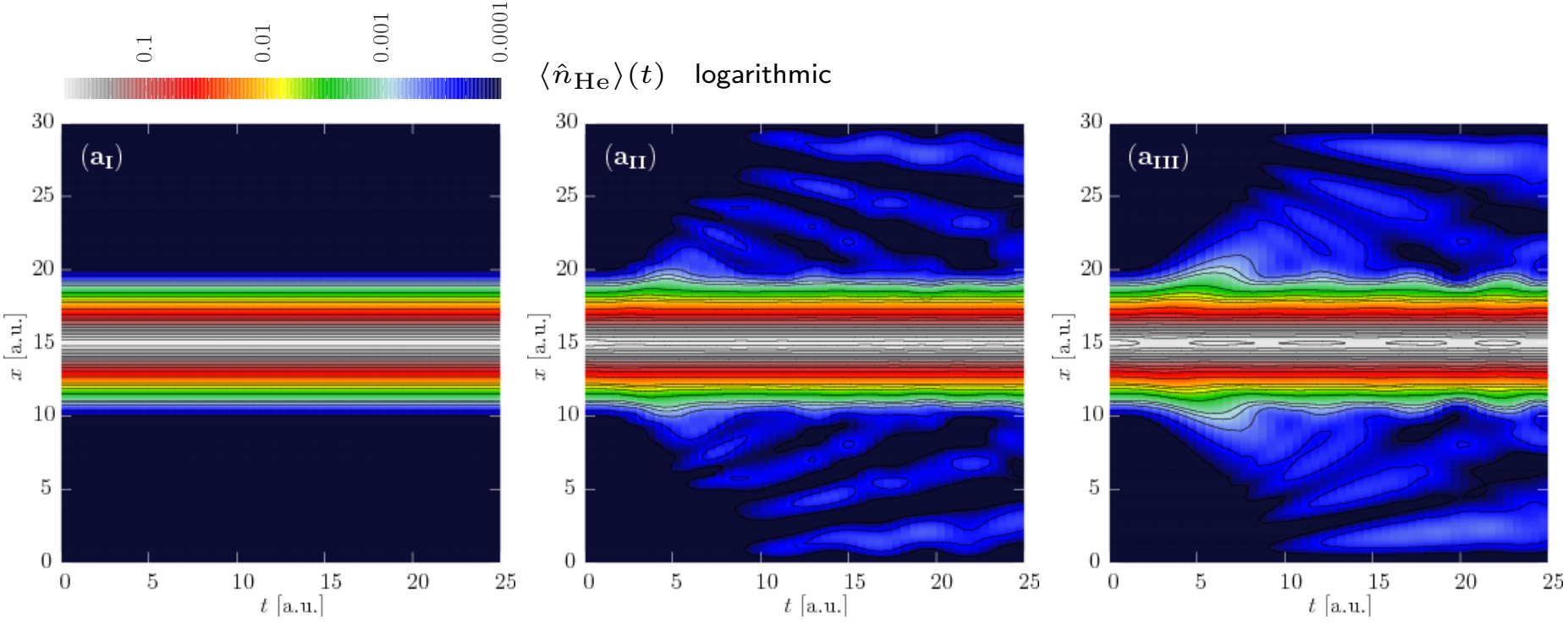
intensity regimes—E_0

$E_0 = 0.01 \rightarrow 3.51 \times 10^{12}$ W/cm^2
$E_0 = 0.1 \rightarrow 3.51 \times 10^{14}$ W/cm^2
$E_0 = 1.0 \rightarrow 3.51 \times 10^{16}$ W/cm^2

frequency regimes—ω

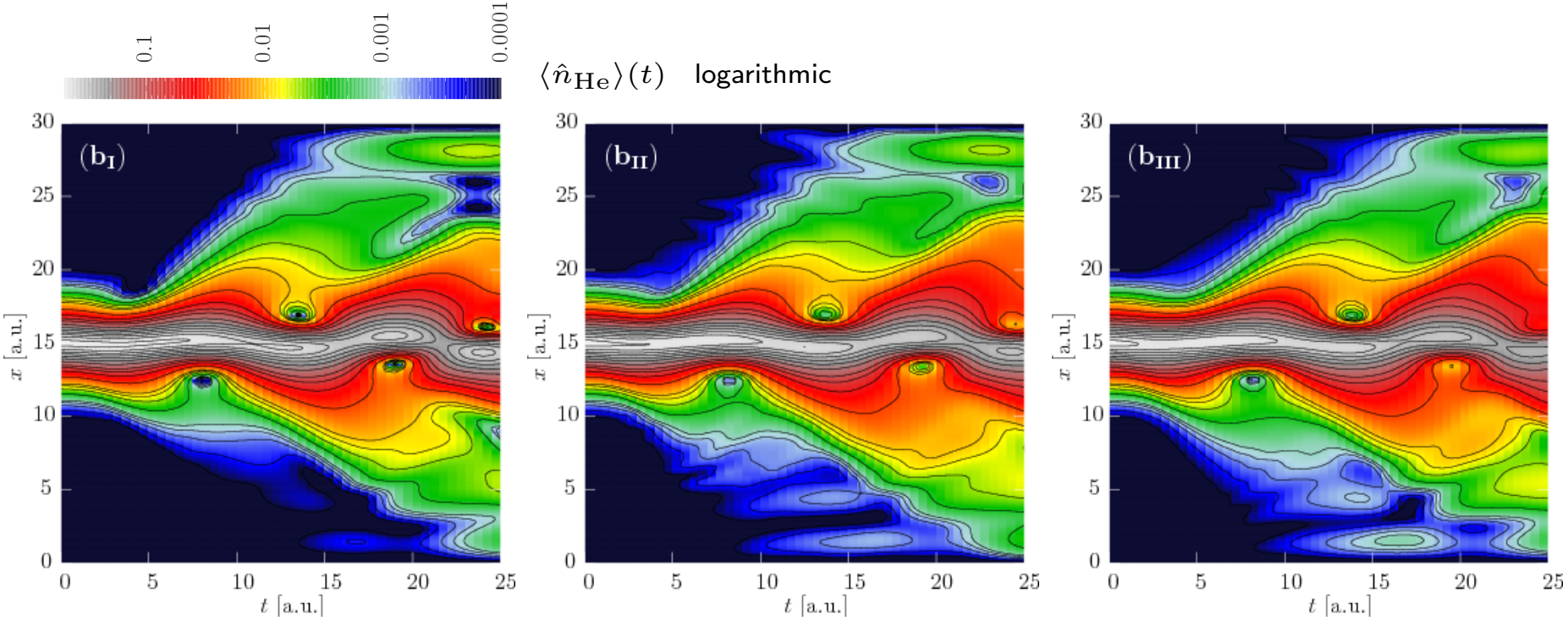
IR: $\omega < 0.06 \rightarrow$ >780 nm
UV: $\omega = 0.1 \ldots 1 \rightarrow$ <400 nm
XUV: $\omega = 1 \ldots 45 \rightarrow$ >30 eV

He: time-dependent $1e^-$-density



- $(\mathrm{a_{I-III}})$: no laser field, atom prepared in HF singlet state
- TDSE: initial wave fuction $\psi(x, x'; 0)$ from HF Slater determinant

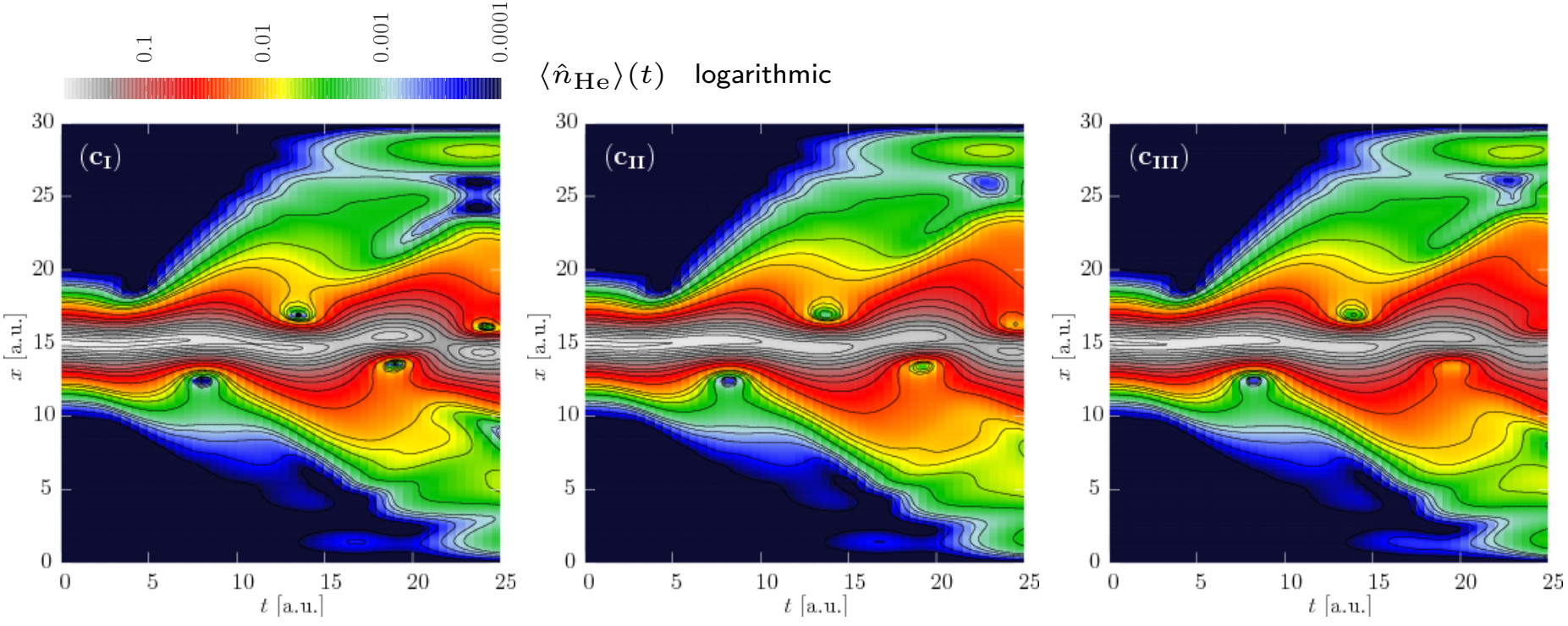
He: time-dependent $1e^-$-density



TDHF TD2ndB TDSE

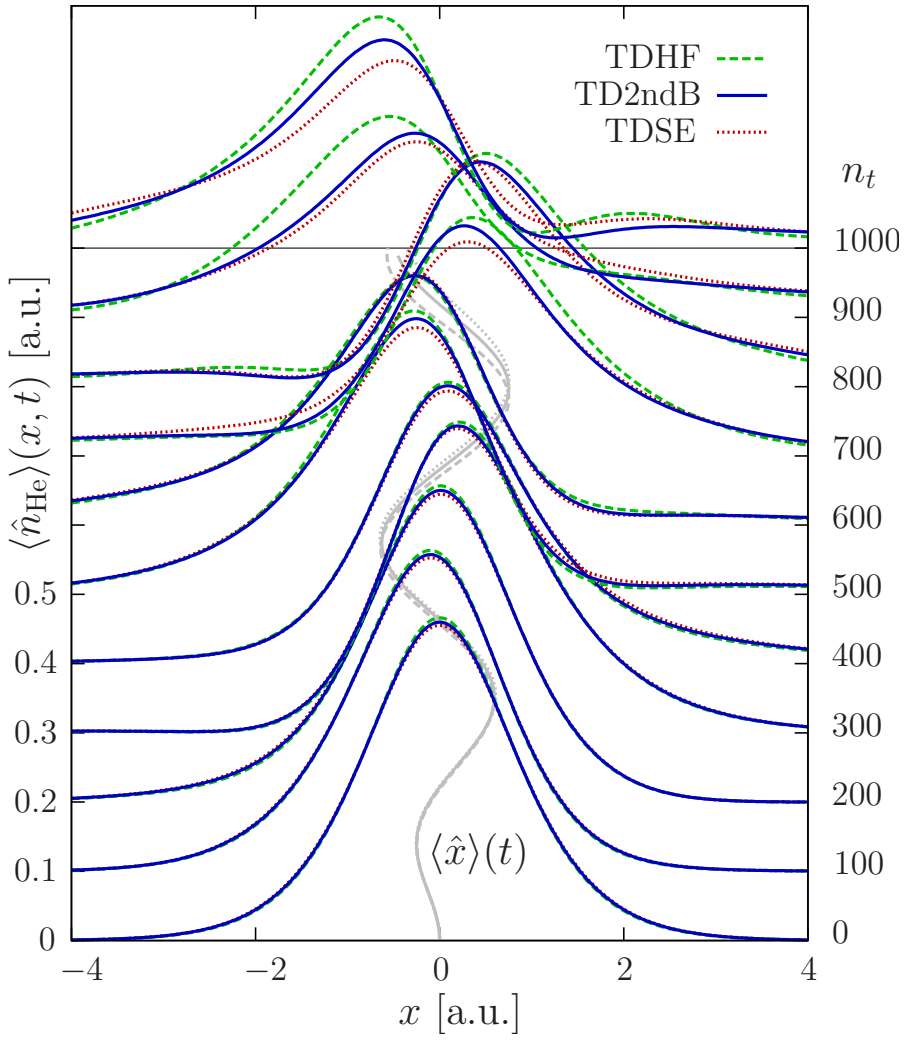
- $(\mathrm{b_{I-III}})$: response to a permanent UV laser field with $E_0 = 0.1$ and $\omega = 0.54$, atom prepared in HF singlet state
- TDSE: $\psi(x, x'; 0)$ from HF Slater determinant

He: time-dependent $1e^-$-density



- $(\mathrm{c_{I-III}})$: response to a permanent UV laser field with $E_0 = 0.1$ and $\omega = 0.54$, atom prepared in self-consistent eigenstate
- $(\mathrm{c_I})$: uncorrelated (HF) initial state $(\mathrm{c_{II}})$: 2ndB initial state, $(\mathrm{c_{III}})$: fully correlated initial state

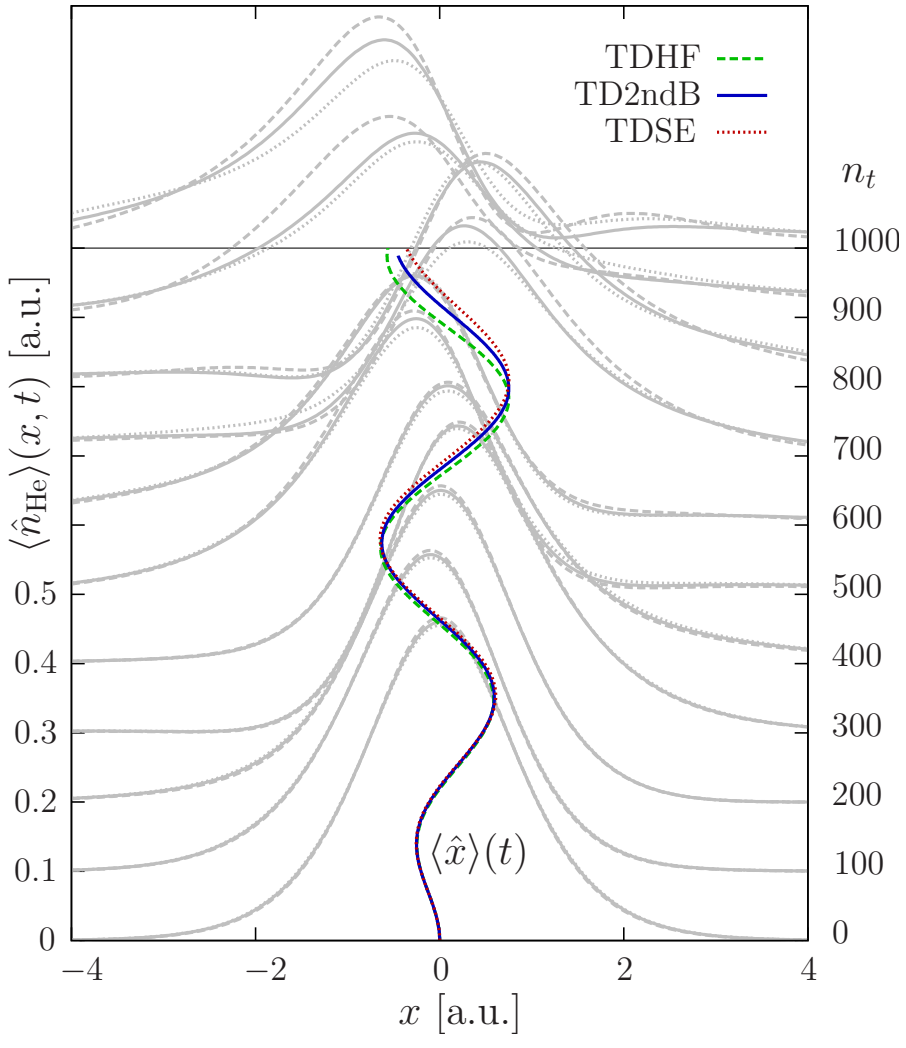
He: time-dependent $1e^-$-density



$\langle\hat{n}_{\mathrm{He}}\rangle(x,t)$—non-logarithmic, $\langle\hat{x}\rangle(t)$

- Qualitatively, TD2ndB gives good results!

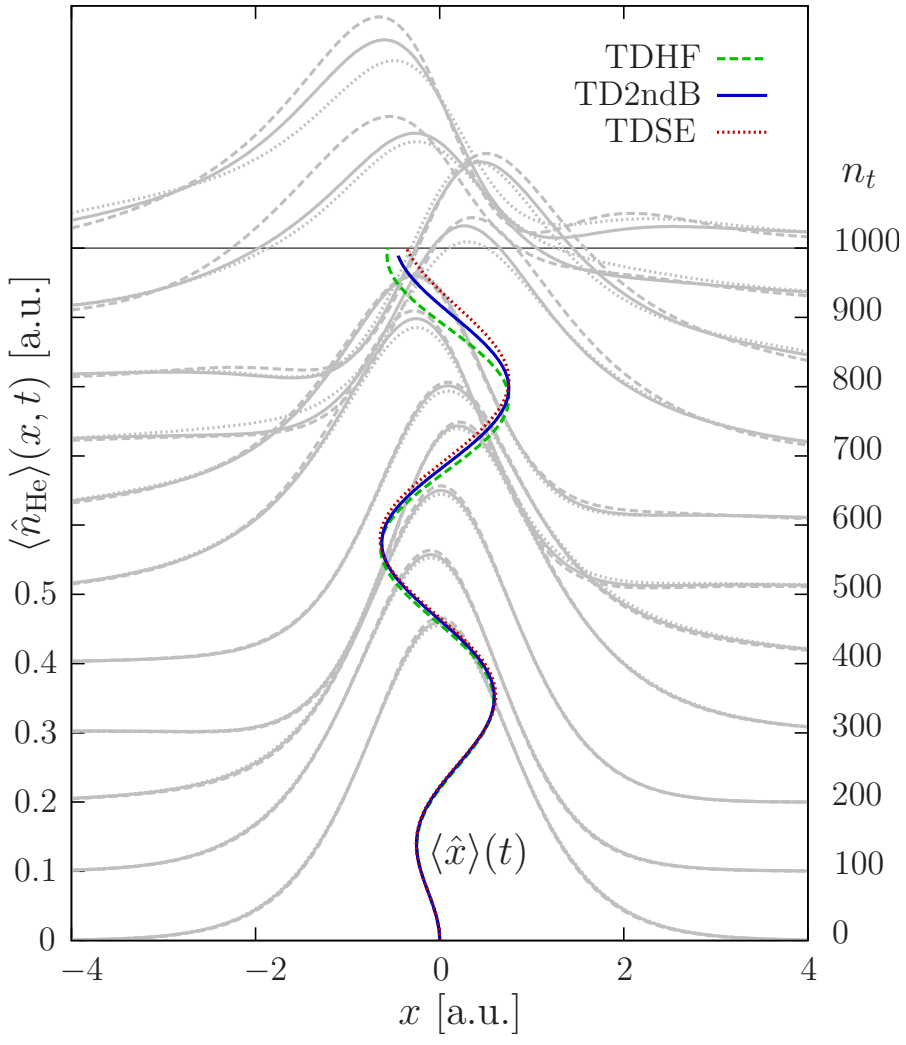
He: time-dependent $1e^-$-density



$\langle\hat{n}_{\mathrm{He}}\rangle(x,t)$—non-logarithmic, $\langle\hat{x}\rangle(t)$

- Qualitatively, TD2ndB gives good results!

He: time-dependent $1e^-$-density



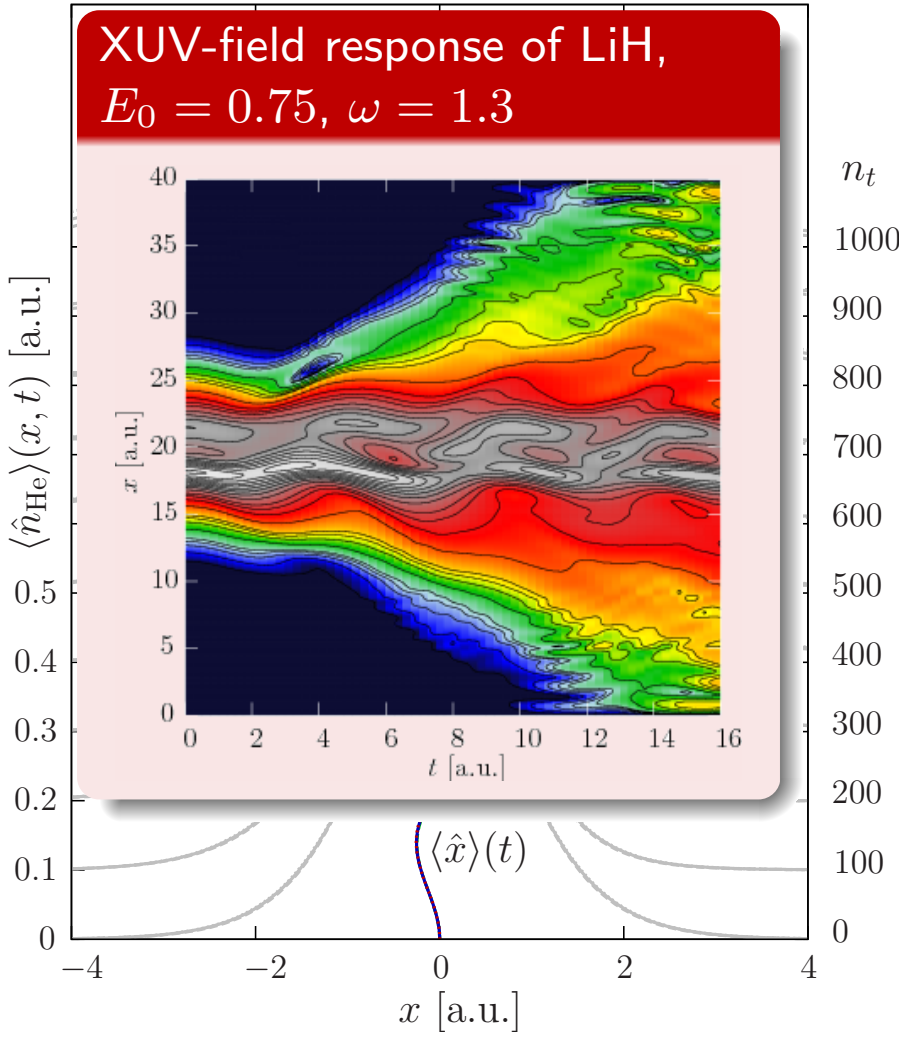
$\langle\hat{n}_{\mathrm{He}}\rangle(x,t)$—non-logarithmic, $\langle\hat{x}\rangle(t)$

- Qualitatively, TD2ndB gives good results!

direct applications

- perform extended calculations with $t \gtrsim 100$ a.u. $\Rightarrow$ compute dipole spectra from DFT of $\langle\hat{x}\rangle(t)$
- study nonequilibrium behavior of other systems, atoms or molecules with $> 2e^-$

He: time-dependent $1e^-$-density



$\langle\hat{n}_{\mathrm{He}}\rangle(x,t)$—non-logarithmic, $\langle\hat{x}\rangle(t)$

- Qualitatively, TD2ndB gives good results!

direct applications

- perform extended calculations with $t \gtrsim 100$ a.u. $\Rightarrow$ compute dipole spectra from DFT of $\langle\hat{x}\rangle(t)$
- study nonequilibrium behavior of other systems, atoms or molecules with $> 2e^-$

Outline

Conclusions

2-time KBE for inhomogeneous systems

FE-DVR applied on $G(1,1')$:

i. allows for an optimal and flexible combination of grid and basis methods
ii. (semi-)analytic matrix for elements $\hat{T}$, $\hat{V}$ and $\hat{U}$ become available
iii. very simple structure of self-energies $\Sigma(1,1')$ obtained

MPI parallelization

Large cluster computation enabled:

i. 2-time propagation can performed parallel with many processes
ii. minimum MPI communication possible due to clever-distributed memory
iii. adequate RAM becomes available for full 2-time propagation

FE-DVR method + MPI code

Opens up new NEGF perspectives!

Conclusions

2-time KBE for inhomogeneous systems

FE-DVR applied on $G(1, 1')$:

i. allows for an optimal and flexible c
methods
ii. (semi-)analytic matrix for elements
iii. very simple structure of self-energi

MPI parallelization

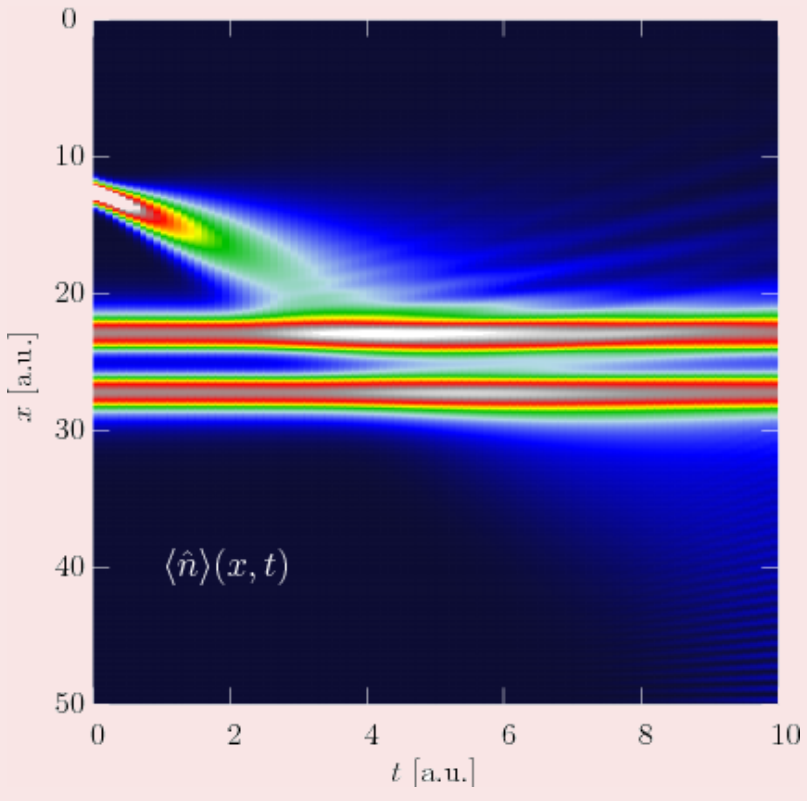
Large cluster computation enabled:

i. 2-time propagation can performed
ii. minimum MPI communication pos
memory
iii. adequate RAM becomes available

FE-DVR method + MPI code

Opens up new NEGF perspectives!

e.g. wave-packet scattering



Conclusions

2-time KBE for inhomogeneous systems

FE-DVR applied on $G(1, 1')$:

i. allows for an optimal and flexible c
methods
ii. (semi-)analytic matrix for elements
iii. very simple structure of self-energi

MPI parallelization

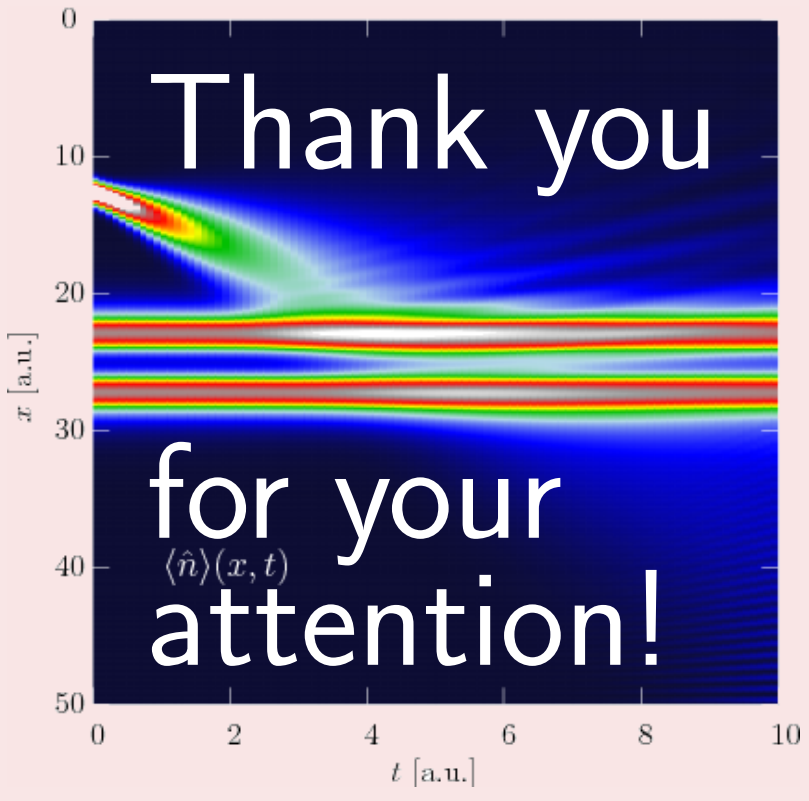
Large cluster computation enabled:

i. 2-time propagation can performed
ii. minimum MPI communication pos
memory
iii. adequate RAM becomes available

FE-DVR method + MPI code

Opens up new NEGF perspectives!

e.g. wave-packet scattering



Outline