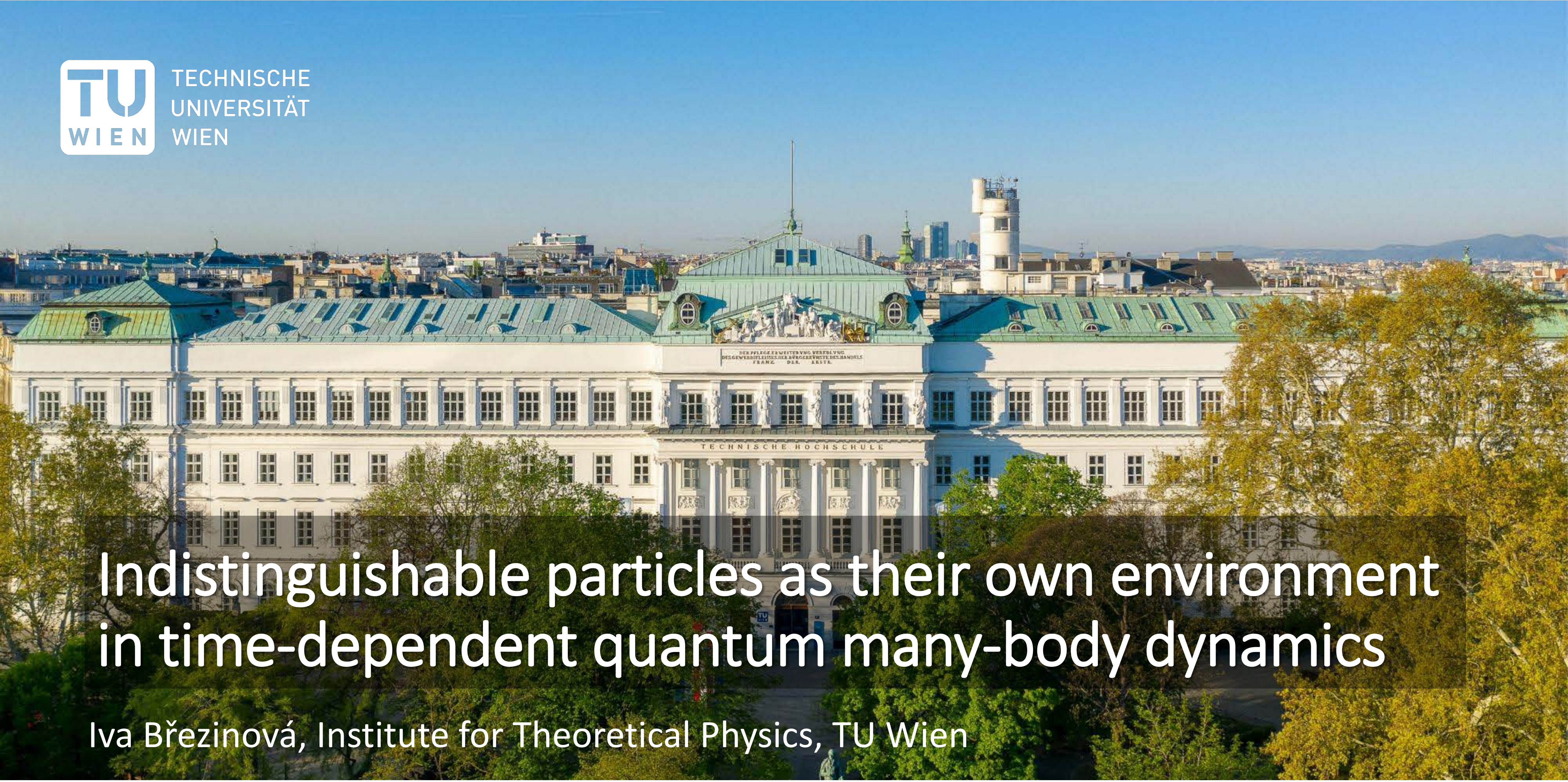

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Indistinguishable particles as their own environment in time-dependent quantum many-body dynamics

Iva Březinová, Institute for Theoretical Physics, TU Wien

New trends in Quantum Thermodynamics, University of Surrey, July 8, 2024

Thanks to collaborators

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quantA

FWF Der Wissenschaftsfonds.

WWTF

VCQ Vienna Center for Quantum Science and Technology

VIENNA SCIENTIFIC CLUSTER

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Indistinguishable particles as their own environment in time-dependent quantum many-body dynamics

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Institute for Theoretical Physics
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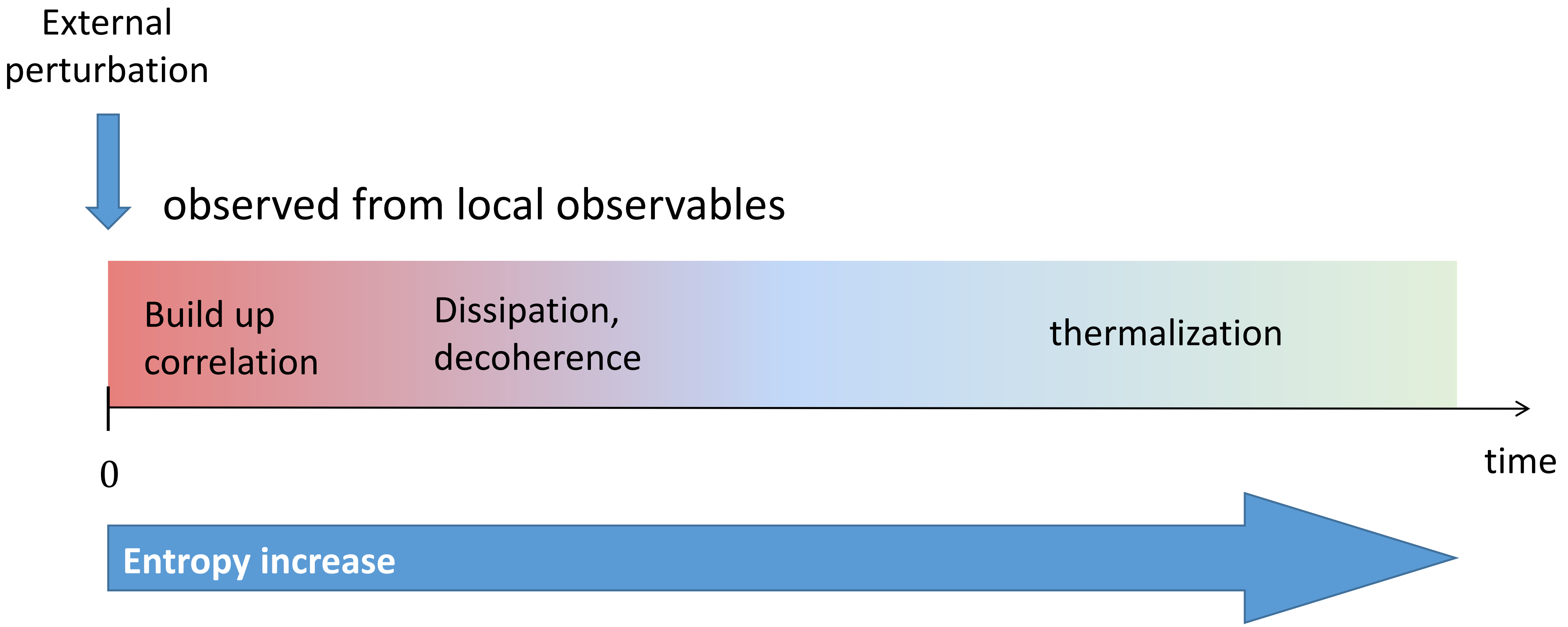
New trends in Quantum Thermodynamics, University of Surrey, July 8, 2024

Time-evolution of quantum systems



The time-dependent Schrödinger equation

$$i\hbar\partial_t |\psi\rangle = \widehat{H}|\psi\rangle$$

Solution impossible!

$$\hat{H} = \sum_{j=1}^{N_e} \frac{(\vec{p}_j + e\vec{A}/c)^2}{2m_e} + V_e(\vec{r}_j) + \sum_{i<j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

electrons

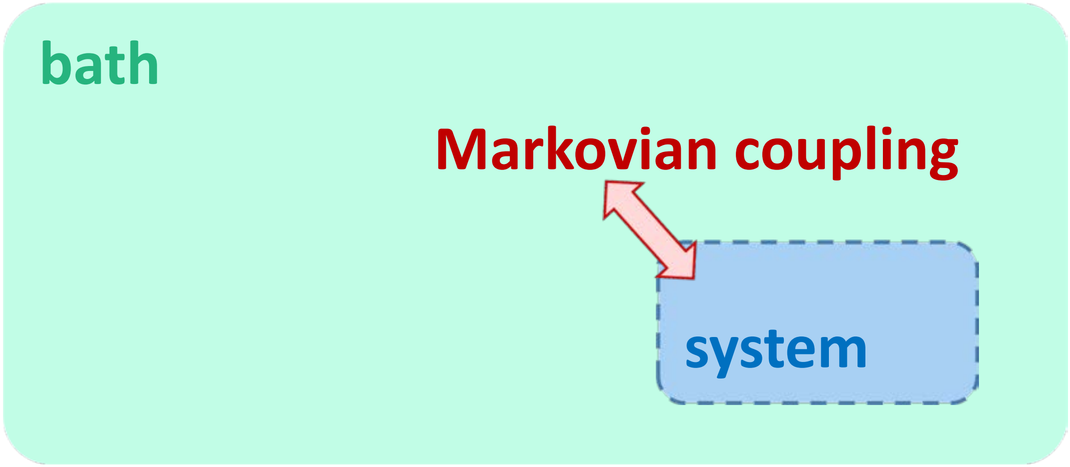
$$+ \sum_{n=1}^{N_n} \frac{(\vec{P}_n^2 + Z_n e\vec{A}/c)^2}{2M_n} + V_n(\vec{r}_n) + \sum_{n<m} \frac{e^2}{|\vec{R}_n - \vec{R}_m|}$$

nuclei

$$- \sum_{j,n} \frac{Z_n e^2}{|\vec{r}_j - \vec{R}_n|}$$

interaction

Open quantum systems



Wavefunction replaced by density matrix

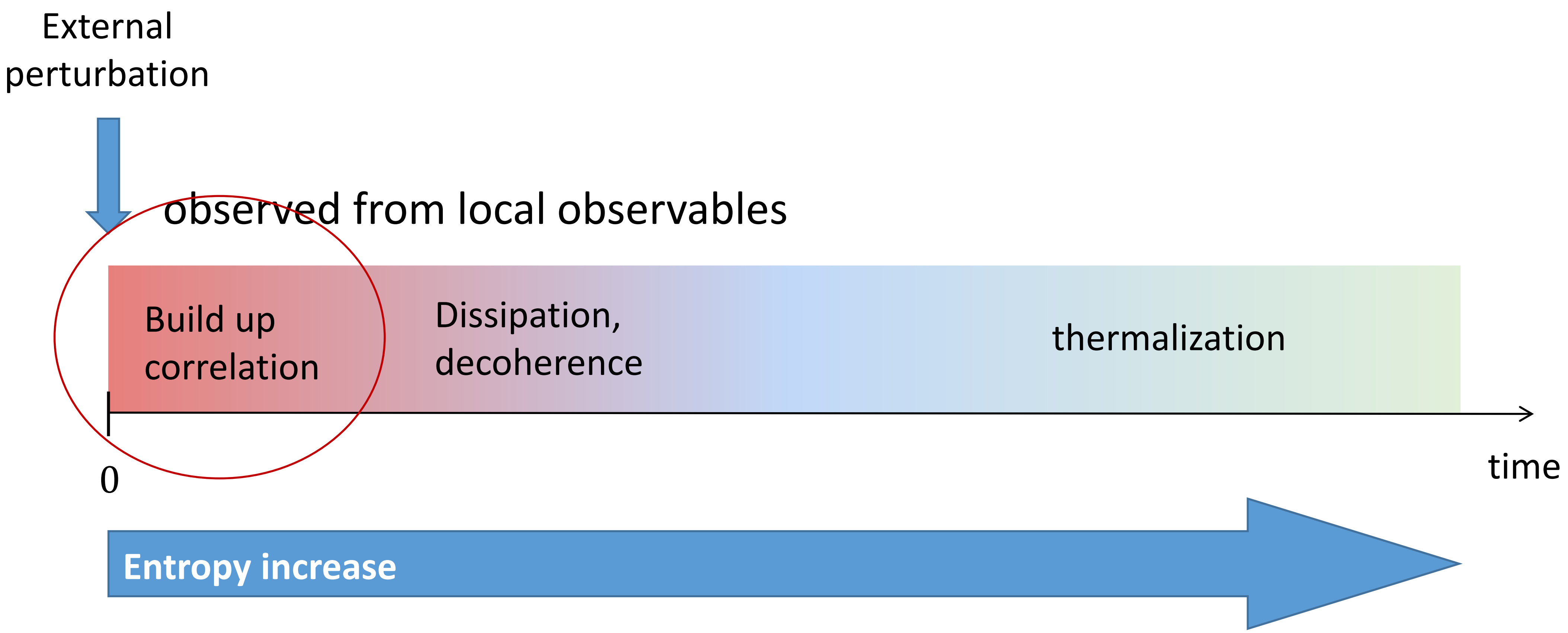
$$|\psi\rangle \rightarrow \widehat{\rho_S}$$

Schrödinger equation replaced by Lindblad equation

$$i\hbar\partial_t\hat{\rho}_S = [\hat{H}_S, \hat{\rho}_S] + \sum_j \gamma_j \left(L_j \hat{\rho}_S L_j^\dagger - \frac{1}{2}\left\{ L_j^\dagger L_j, \hat{\rho}_S \right\} \right)$$

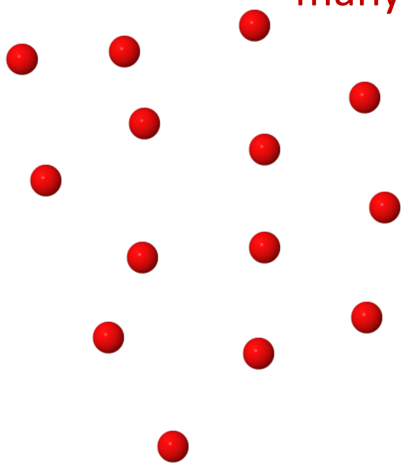
Decoherence and dissipation

Time-evolution of quantum systems



Many indistinguishable fermions

many electrons



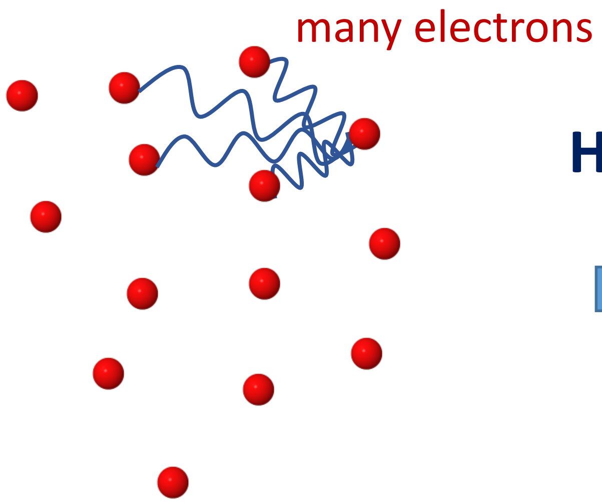
How to describe their correlated dynamics efficiently?

→ **Reduced density matrices**

Outlook:

- Time-dependent two-particle reduced density matrix method (TD2RDM)
- Application to fermionic condensation

Many indistinguishable fermions



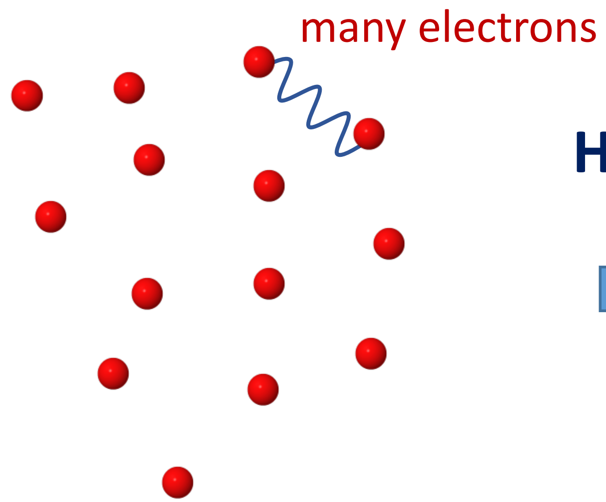
How to describe their correlated dynamics efficiently?

Reduced density matrices

1RDM: $D_1 = N \mathrm{Tr}_{2\ldots N} |\Psi\rangle\langle\Psi|$

$$D_1(\vec{r}, \vec{r}', t) = N \int d^3r_2 \ldots d^3r_N \, \psi(\vec{r}, \vec{r}_2, \ldots, \vec{r}_N)\psi^*(\vec{r}', \vec{r}_2, \ldots, \vec{r}_N)$$

Many indistinguishable fermions



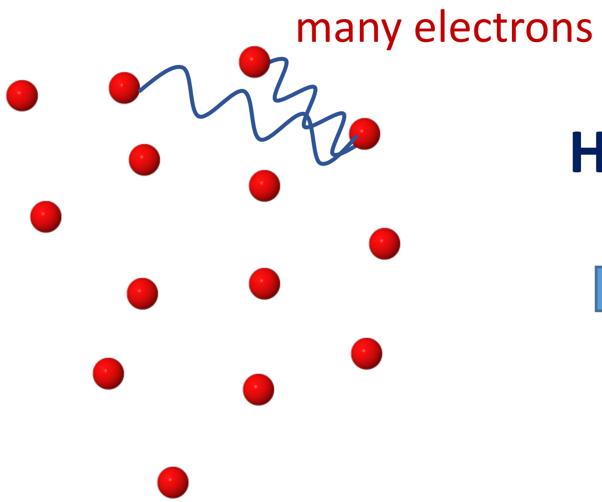
How to describe their correlated dynamics efficiently?

Reduced density matrices

1RDM: $D_1 = N\mathrm{Tr}_{2\dots N}|\Psi\rangle\langle\Psi|$

$$i\partial_t D_1 = [H_1, D_1] \quad +\mathrm{Tr}_2[W_{12}, D_{12}]$$

Many indistinguishable fermions



How to describe their correlated dynamics efficiently?

Reduced density matrices

1RDM: $D_1 = N\mathrm{Tr}_{2\ldots N}|\Psi\rangle\langle\Psi|$ $\quad i\partial_t D_1 = [H_1, D_1] + \mathrm{Tr}_2[W_{12}, D_{12}]$

2RDM: $D_{12} = N(N-1)\mathrm{Tr}_{3\ldots N}|\Psi\rangle\langle\Psi|$ $\quad i\partial_t D_{12} = [H_{12}, D_{12}] + \mathrm{Tr}_3[W_{13} + W_{23}, D_{123}]$

$\vdots$ $\quad\quad$ $\vdots$

BBGKY-hierarchy

The physics of the 2RDM

Cumulant decomposition

Two-particle cumulant

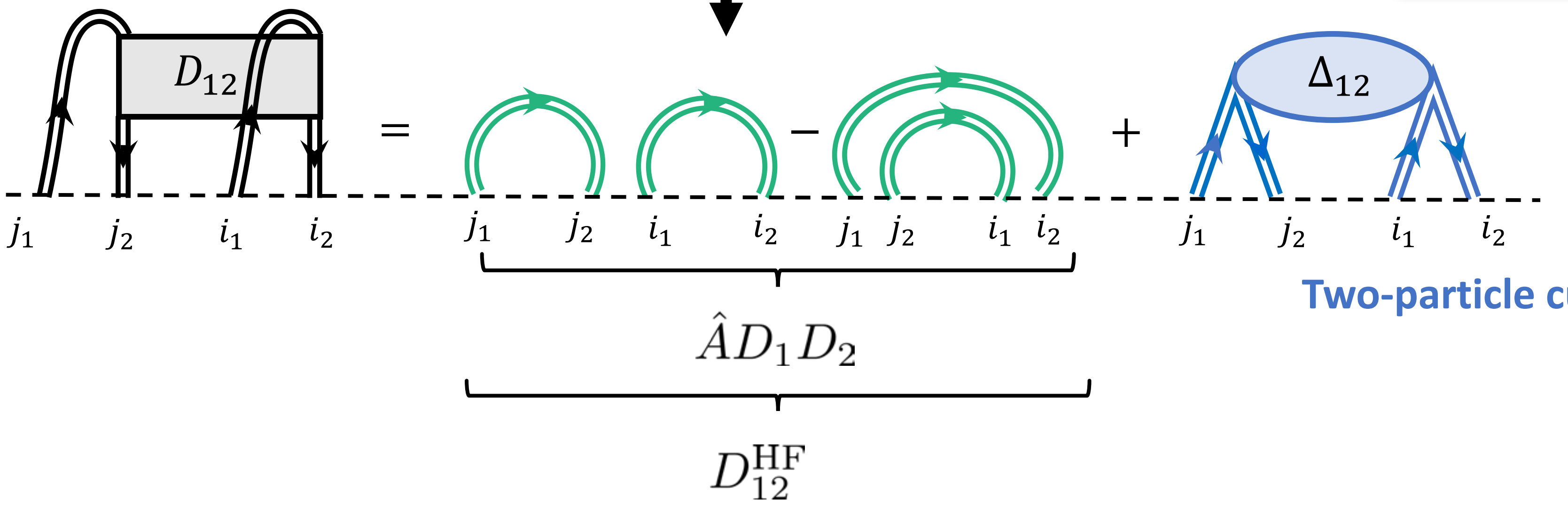
$$D_{12} = \hat{A}D_1D_2 + \Delta_{12}$$

Two statistically independent single-particle processes

Statistically depende particle processes

Within TD2RDM full two-particle correlations included!

Diagrammatic expression



All connected diagrams included.

Two-particle cumulant

Closure of equations of motion

Equation of motion for the 2RDM

Reconstruction functional

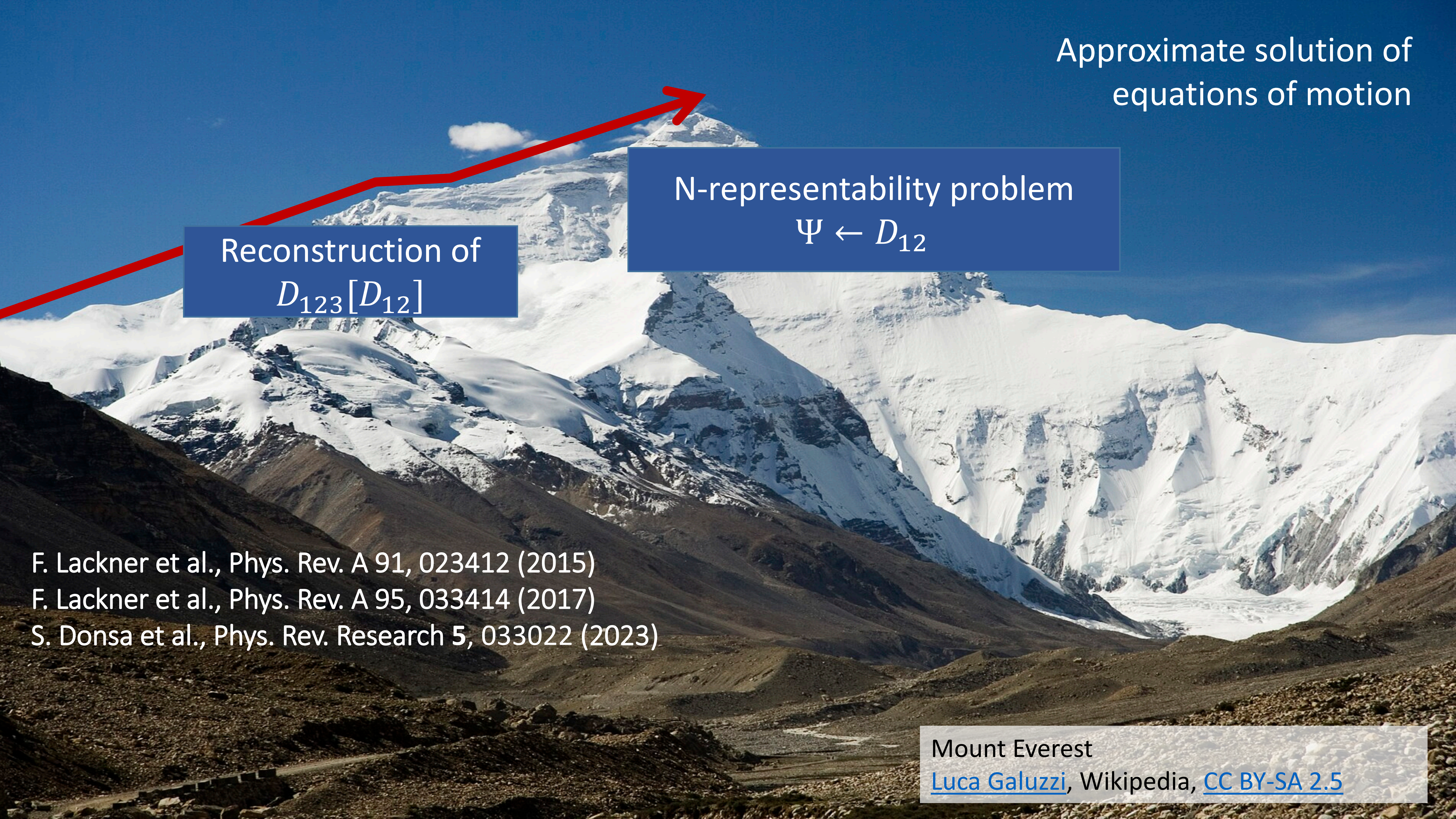
$$i\partial_t D_{12} = [H_{12}, D_{12}] + \mathrm{Tr}_3[W_{13} + W_{23}, D_{123}]$$

$$D^{\mathrm{R}}_{123}\{D_{12}\}$$

closure

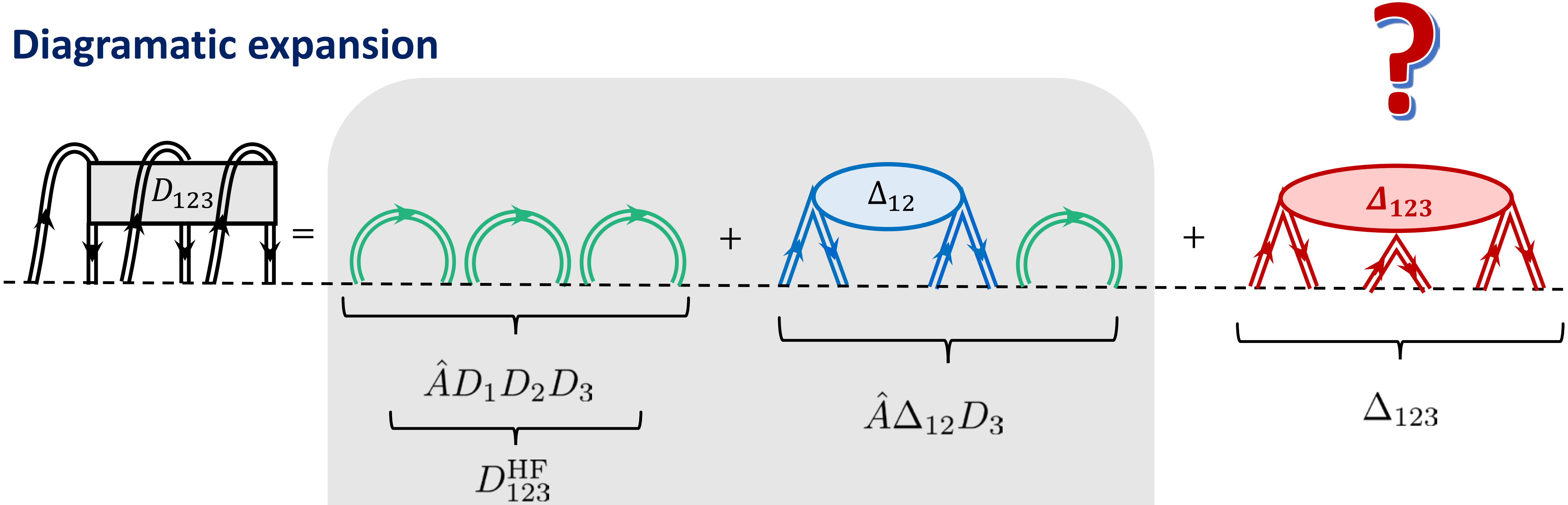
⇒ Time-dependent two-particle reduced density matrix (TD2RDM) method

N. N. Bogoliubov and K. P. Gurov. Kinetic Equations in Quantum Mechanics. JETP 17, 614 (1947)
P. C. Martin and J. Schwinger. Theory of Many-Particle Systems. I. Phys. Rev. 115,1342 (1959)
K.-J. Schmitt, P.-G. Reinhard, and C. Toepffer. Truncation of time-dependent manybody theories. Z. Phys. A 336, 123 (1990)
W. Cassing and A. Pfitzner. Self-consistent truncation of the BBGKY hierarchy on the two-body level. Z. Phys. A 342, 161 (1992)
M. Tohyama and P. Schuck. Truncation scheme of time-dependent density-matrix approach. Eur. Phys. J. A 50, 1 (2014)
B. Schäfer-Bung and M. Nest. Correlated dynamics of electrons with reduced twoelectron density matrices. Phys. Rev. A 78, 012512 (2008)
A. Akbari et al. PRB 85, 235121 (2012)
...


Approximate solution of equations of motion
N-representability problem
$\Psi \leftarrow D_{12}$
Reconstruction of
$D_{123}[D_{12}]$
F. Lackner et al., Phys. Rev. A 91, 023412 (2015)
F. Lackner et al., Phys. Rev. A 95, 033414 (2017)
S. Donsa et al., Phys. Rev. Research **5**, 033022 (2023)
Mount Everest
Luca Galuzzi, Wikipedia, CC BY-SA 2.5

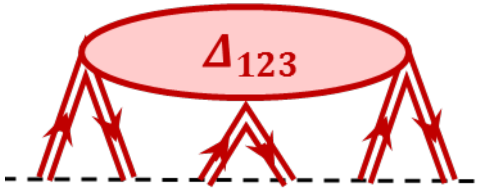
Cumulant decomposition of D_{123}

Diagramatic expansion



corresponds to **time local reconstruction functional**

The three-particle cumulant



Unitary decomposition for 6th order tensor

$$M_{123} = M_{123;\perp}\{M_{12}\} + M_{123;K}$$

known functional

trace free

$$\Delta_{123} = \Delta_{123;\perp}\{D_{12}\} + \Delta_{123;K}$$?

This guarantees contraction consistency

$$D_{12} = \frac{1}{N-2}\mathrm{Tr}_3 D^R_{123}$$

F. Lackner et al., Phys. Rev. A 91, 023412 (2015)
F. Lackner et al., Phys. Rev. A 95, 033414 (2017)
S. Donsa et al., Phys. Rev. Research 5, 033022 (2023)

The N-representability problem

Properties of the 2RDM:

- Hermitian
- Positive-semidefinite
- Antisymmetric
- Normalized

Not enough to guarantee

$$D_{12} \leftarrow |\Psi\rangle$$

N-representability problem: What are the **necessary and sufficient properties** to guarantee the existence of at least one many-body wavefunction that contracts to the given reduced density matrix?

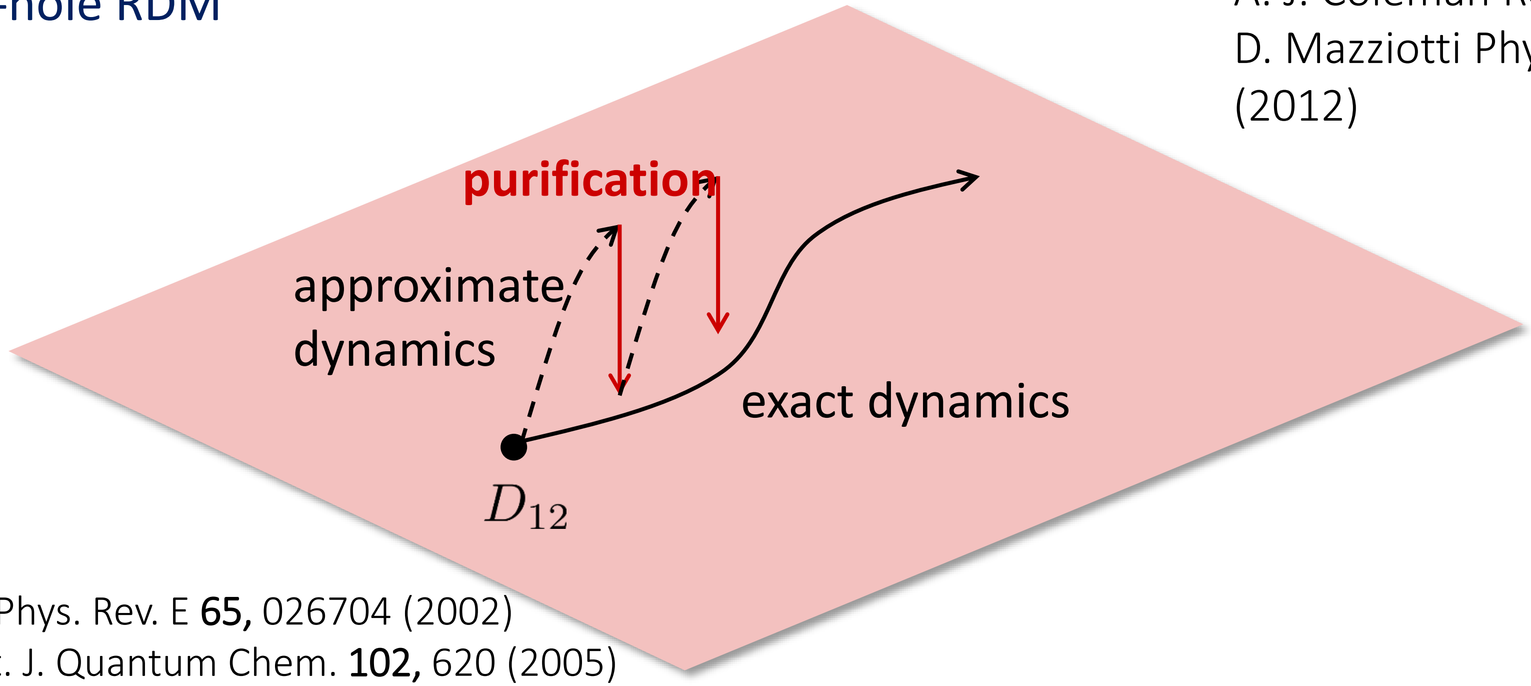
A. J. Coleman Rev. Mod. Phys. 35, 668 (1963)
D. Mazziotti Phys. Rev. Lett 108, 263002 (2012)

Purification

Space of 2RDMs belonging to a wavefunction (N-representability)

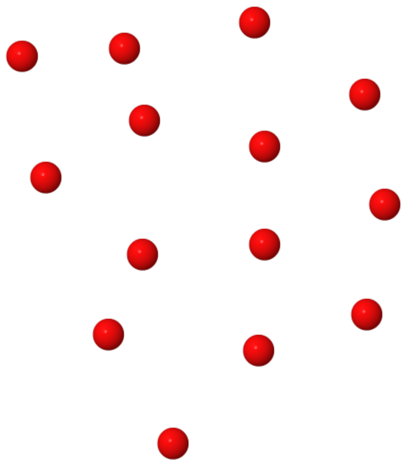
A. J. Coleman Rev. Mod. Phys. 35, 668 (1963)
D. Mazziotti Phys. Rev. Lett 108, 263002 (2012)

Enforcing **positive semi-definiteness** of 2RDM and two-hole RDM



D. A. Mazziotti, Phys. Rev. E **65,** 026704 (2002)
Alcoba et al., Int. J. Quantum Chem. **102,** 620 (2005)
F. Lackner et al., Phys. Rev. A 95, 033414 (2017)
Joost et al., Phys. Rev. B
I. Brezinova et al, Phys. Rev. B,

Many indistinguishable fermions



How to describe their correlated dynamics efficiently ?

→ **Reduced density matrices**

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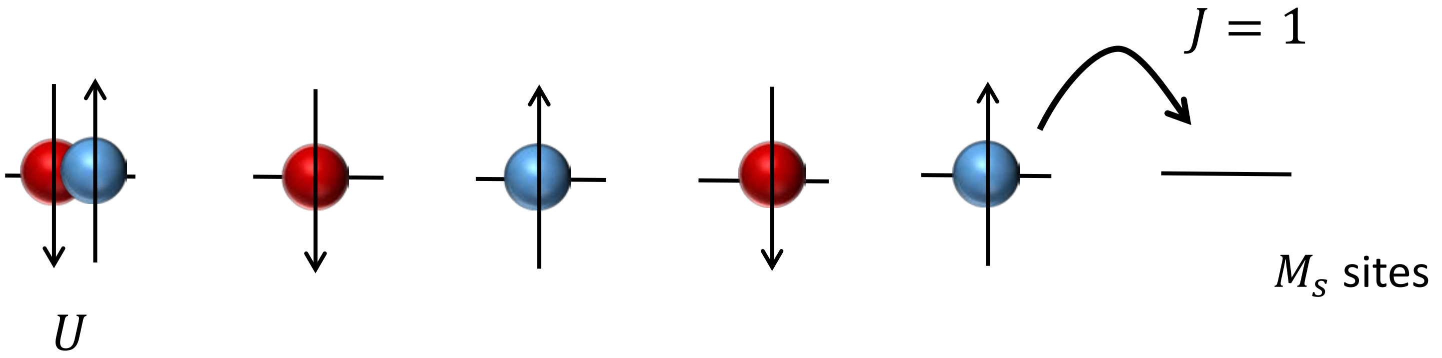
System under investigation – large lattice systems

Fermi-Hubbard model in 1D

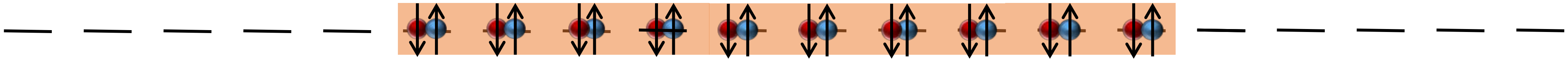


hopping **on-site pair interaction**

$$H = -J \sum_{\langle i,j \rangle;\sigma} a^{\dagger}_{i,\sigma} a_{j,\sigma} + a^{\dagger}_{j,\sigma} a_{i,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

Correlation dynamics

$M_s = 20$
$U = 0.1\,J$

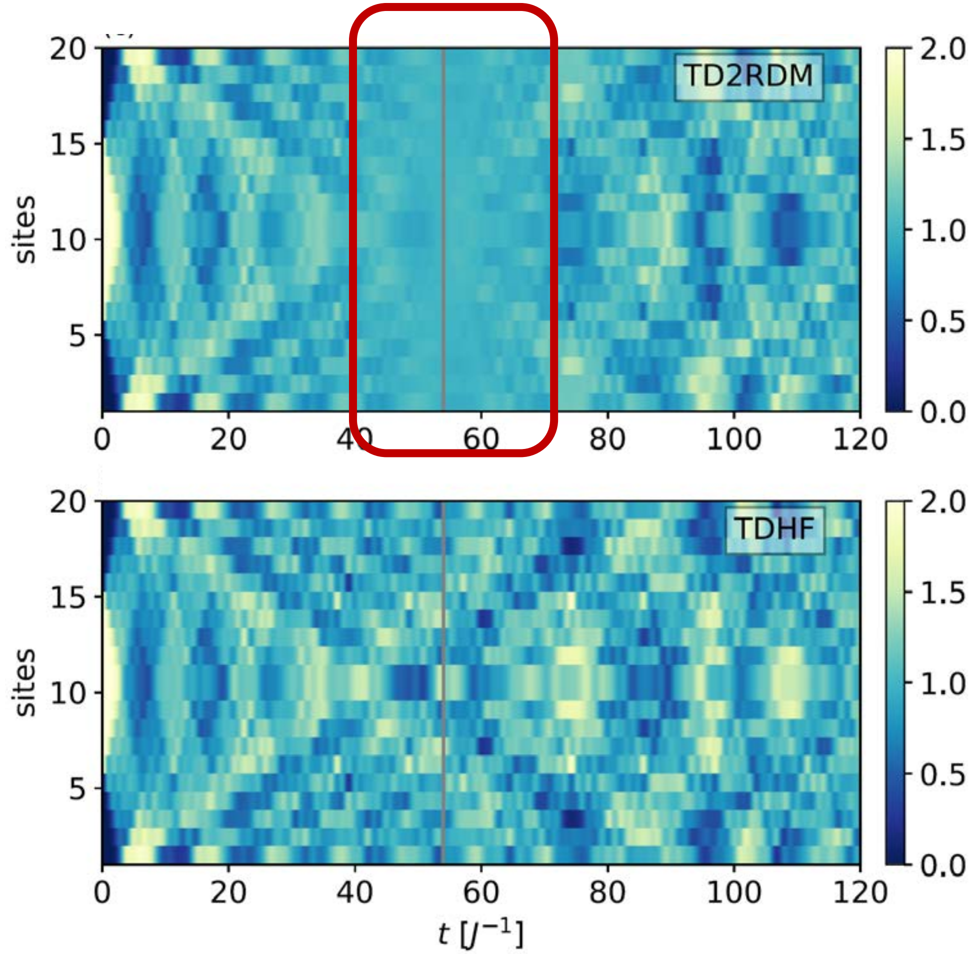


Density fluctuations disappear.

Entropies

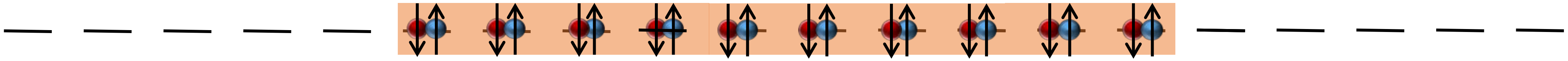
$$D_1 = \sum n_i \, |n_i\rangle\langle n_i| \;\Longrightarrow\; S_1 = -\sum n_i \ln(n_i)$$

$$D_{12} = \sum g_i \, |g_i\rangle\langle g_i| \;\Longrightarrow\; S_2 = -\sum g_i \ln(g_i)$$



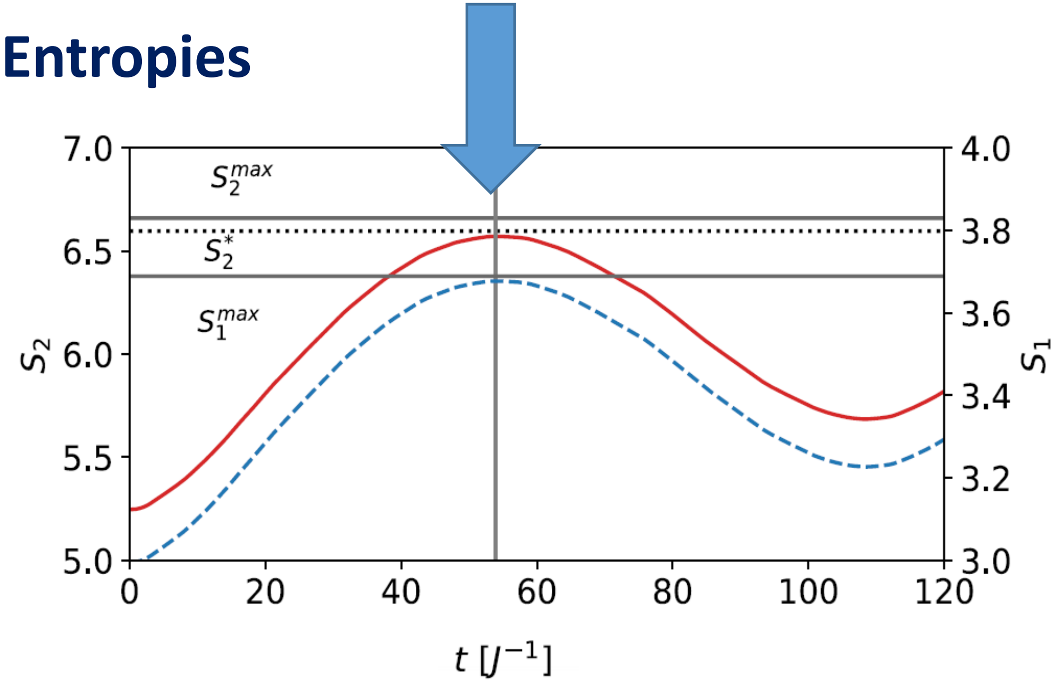
Increase of entropy

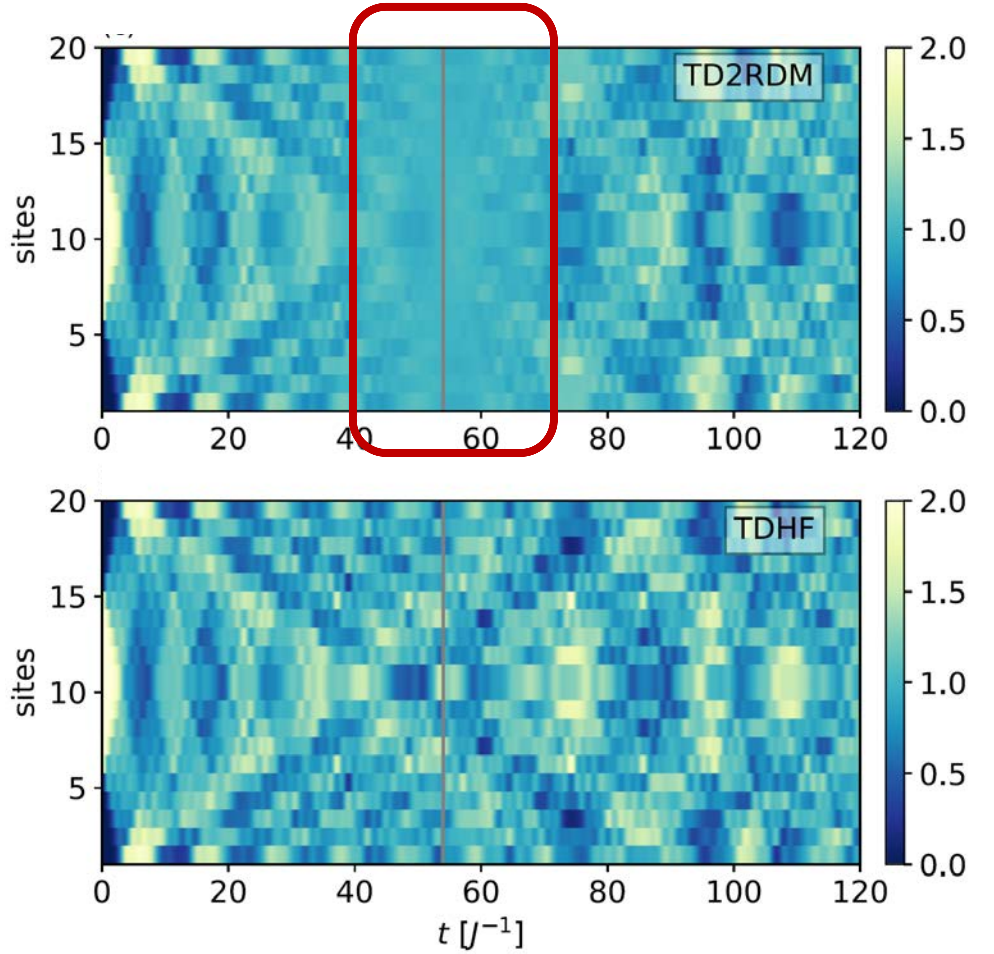
$M_s = 20$
$U = 0.1\,J$



Entropy increases strongly.

Entropies

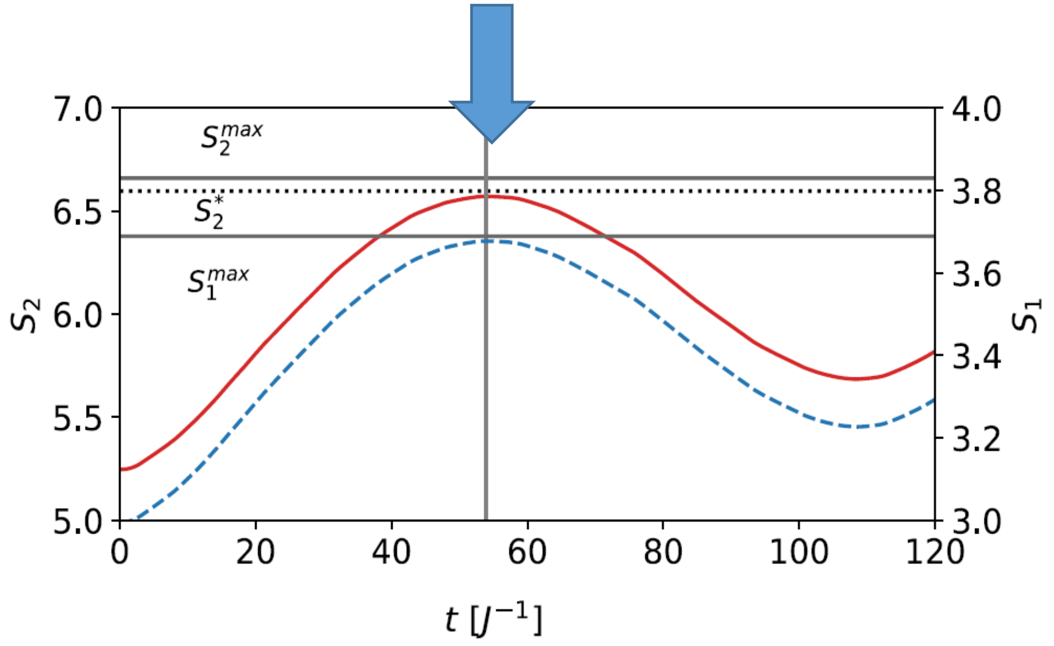


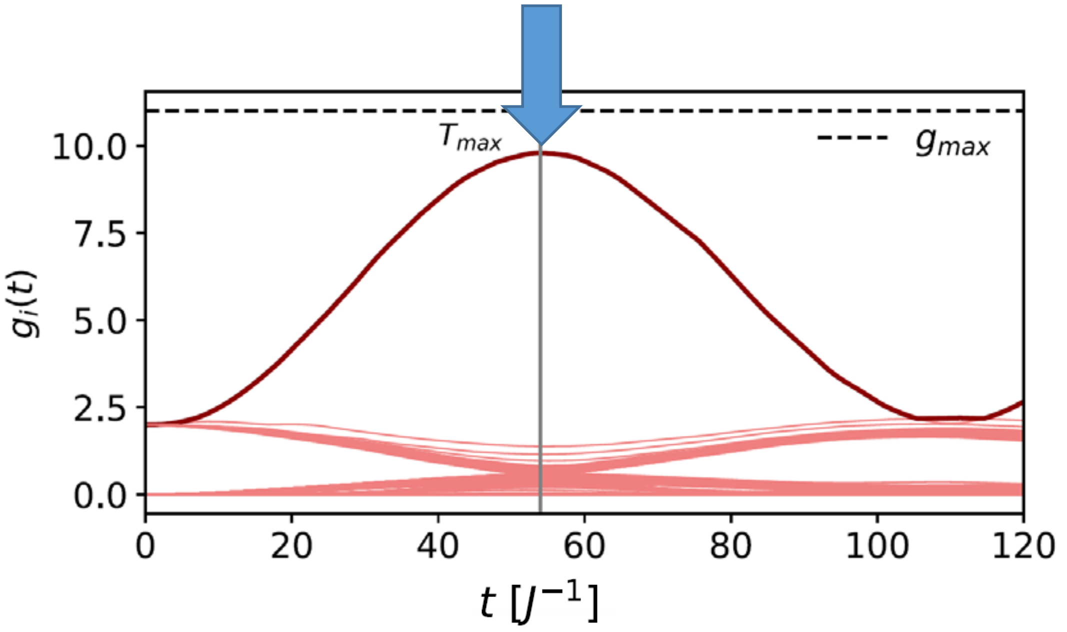


Fermionic quasi-condensation

Large S_2 goes hand in hand with **macroscopic occupation** of one **eigenstate of the 2RDM**

$$D_{12} = \sum g_i \, |g_i\rangle\langle g_i|$$ fermionic condensation if $g_1 \sim O(N)$





I. Březinová et al. Phys. Rev. B **109**, 174308 (2024)

Fermionic quasi-condensation

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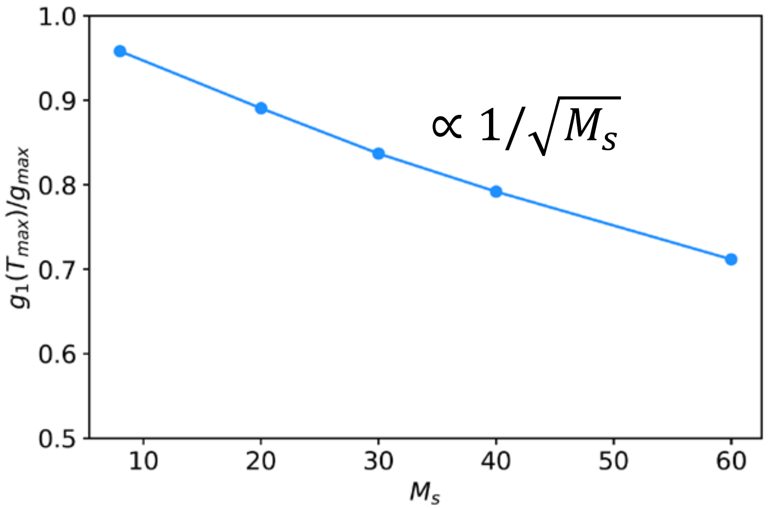
$$D_{12} = \sum g_i \, |g_i\rangle\langle g_i|$$ fermionic condensation if $g_1 \sim O(N)$

Increase number of sites up to $M_s = 60$
At half filling this corresponds to a Hilbert space dimension of $\sim 1.4 \times 10^{34}$

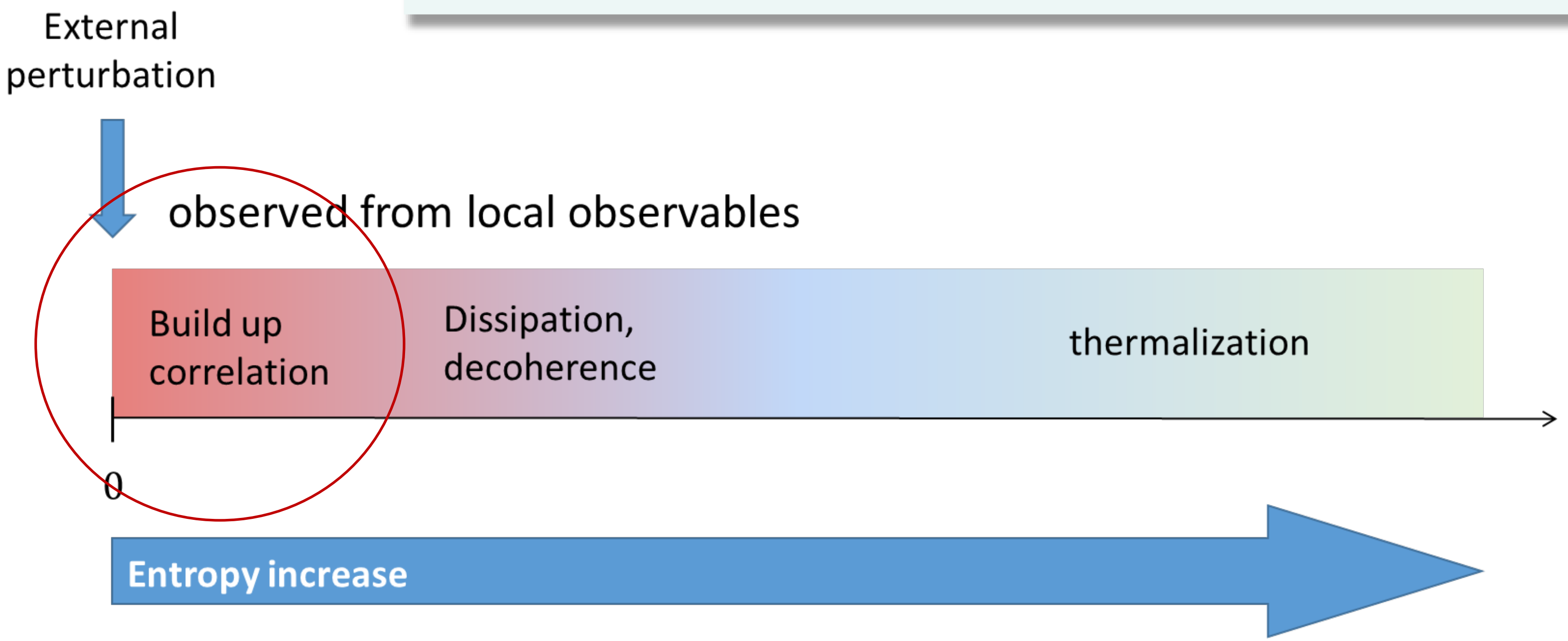


The effect probably disappears in the thermodynamic limit

I. Březinová et al. Phys. Rev. B **109**, 174308 (2024)

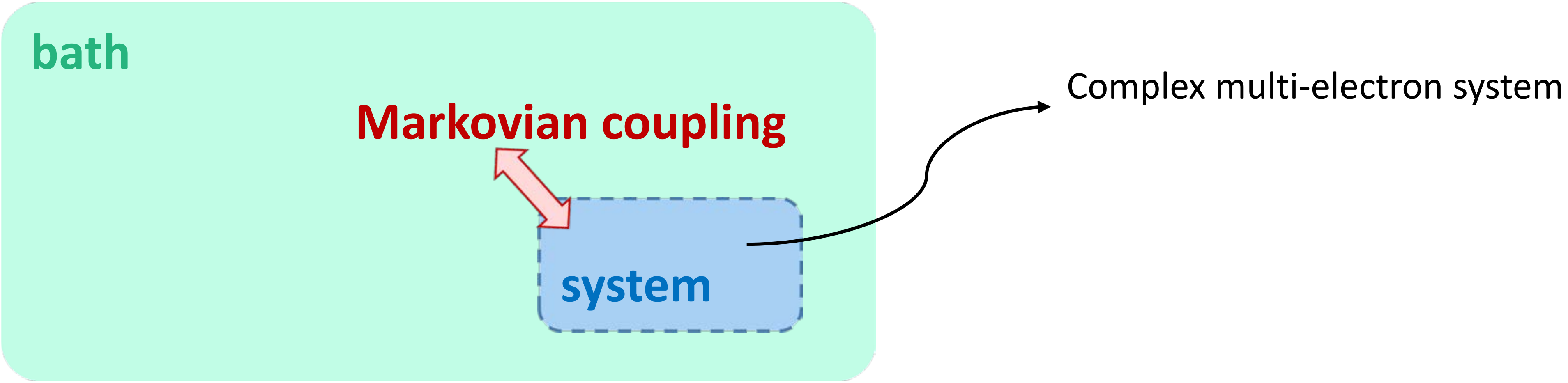
Summary and Conclusions

- New method based on time-dependent two-particle reduced density matrix (TD2RDM)
- Suitable to describe correlated dynamics of multi-electron systems
- Even strong correlation effects well captured



Outlook

- Connecting TD2RDM with formalism of open quantum systems



$$i\hbar\partial_t \hat{D}_{12} = [\hat{H}_{12}, \hat{D}_{12}] + \mathrm{Tr}_3[W_{13} + W_{23}, D_{123}] + \sum_j \gamma_j \left(L_j \hat{D}_{12} L_j^\dagger - \frac{1}{2}\left\{ L_j^\dagger L_j, D_{12} \right\} \right)$$