Numerical Challenges in the Propagation of the KBEs

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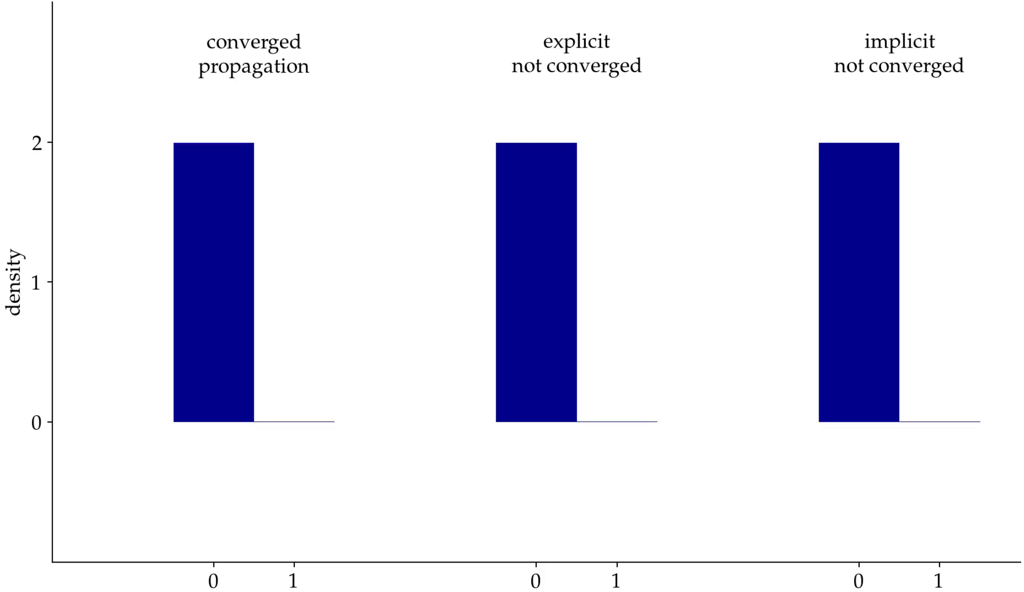
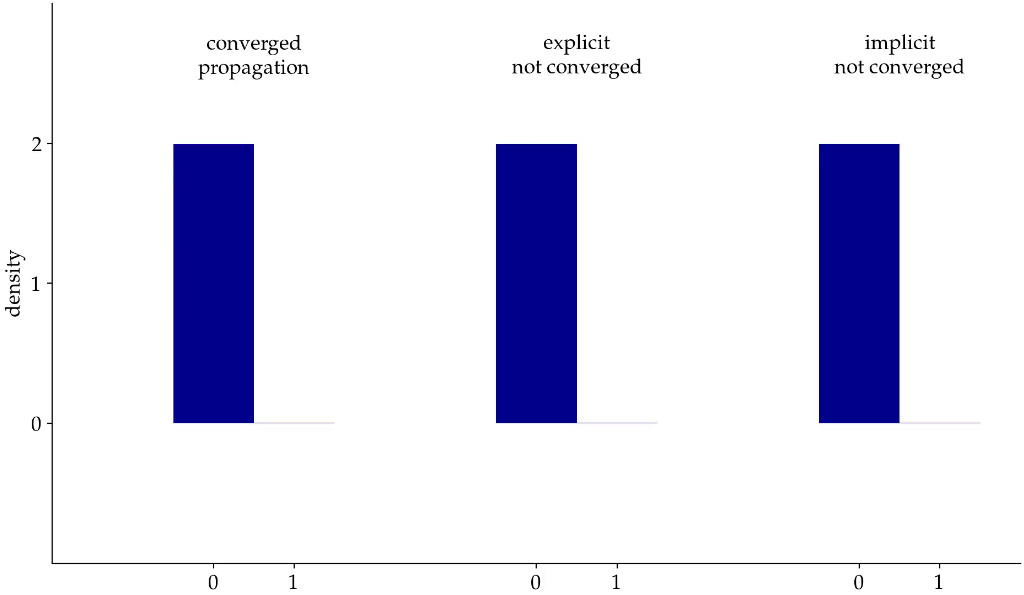
Numerical Challenges



Numerical Challenges



PHYSICAL REVIEW B **96**, 117101 (2017)

Comment on "On the unphysical solutions of the Kadanoff-Baym equations in linear response: Correlation-induced homogeneous density-distribution and attractors"

N. Schlünzen, J.-P. Joost, and M. Bonitz
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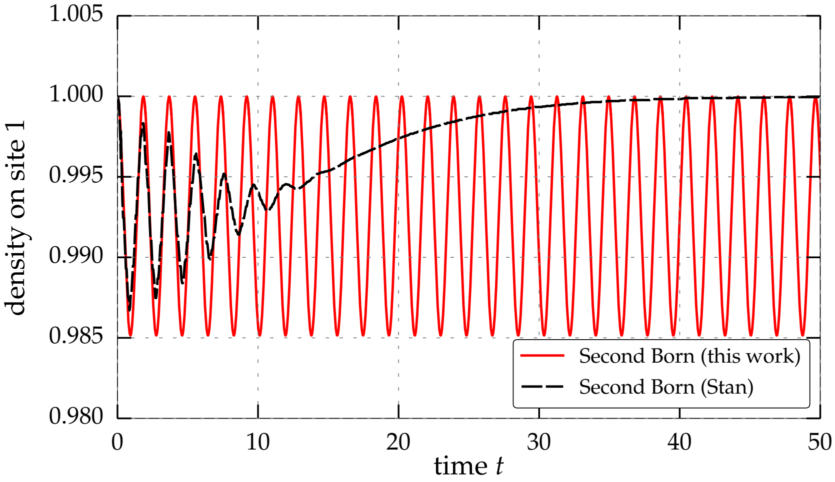
(Received 16 May 2016; published 18 September 2017)

In a recent Rapid Communication [A. Stan, Phys. Rev. B **93**, 041103(R) (2016)], the reliability of the Keldysh-Kadanoff-Baym equations (KBE) using correlated self-energy approximations applied to linear and nonlinear response has been questioned. In particular, the existence of a universal attractor has been predicted that would drive the dynamics of any correlated system towards an unphysical homogeneous density distribution regardless of the system type, the interaction, and the many-body approximation. Moreover, it was conjectured that even the mean-field dynamics would be damped. Here, by performing accurate solutions of the KBE for situations studied in that paper, we prove these claims wrong, being caused by numerical inaccuracies.

DOI: 10.1103/PhysRevB.96.117101

N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. B **96**, 117101 (2017).

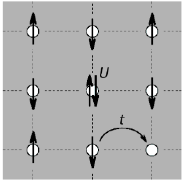
Numerical Challenges



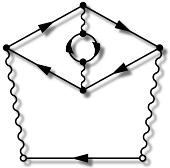
- numerical damping mistaken for artificial damping of the KBEs

N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. B **96**, 117101 (2017).

Theory



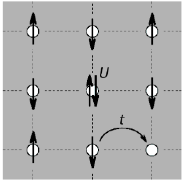
Hubbard model



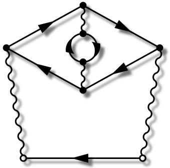
NEGF

Outline

Theory



Hubbard model



NEGF

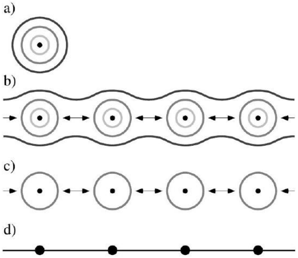
Numerics

$$\frac{\mathrm{d}G}{\mathrm{d}t}$$

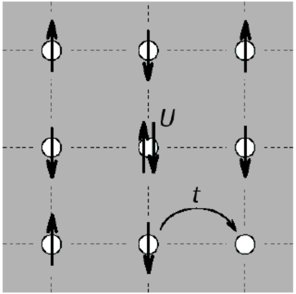
KBEs

$$I_{\mathrm{coll}} = \int_C \Sigma G$$

Collision integral



$\Rightarrow$



$$\boxed{\hat{H}(t) = J \sum_{ij,\,\alpha} h_{ij}\, \hat{c}^\dagger_{i\alpha}\hat{c}_{j\alpha} + U \sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow} + \sum_{ij,\alpha\beta} f_{ij,\alpha\beta}(t)\, \hat{c}^\dagger_{i\alpha}\hat{c}_{j\beta}}$$

$h_{ij} = -\delta_{\langle i,\,j\rangle}$ and $\delta_{\langle i,\,j\rangle} = 1$, if (i,j) nearest neighbors, $\delta_{\langle i,\,j\rangle} = 0$ otherwise;
on-site repulsion ($U > 0$) or attraction ($U < 0$), U favors *doublons* (correlations)

- f: excitation (1-particle hamiltonian): EM field, quench, particle impact etc.
- finite inhomogeneous system, size and geometry dependence

Keldysh Green Functions (NEGF)

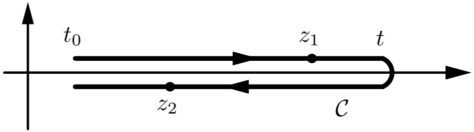
two times $z, z' \in \mathcal{C}$ ("Keldysh contour"), arbitrary one-particle basis $|\phi_i\rangle$

$$\boxed{G_{ij}(z,z') = \frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}} \hat{c}_i(z) \hat{c}_j^\dagger(z') \right\rangle}$$

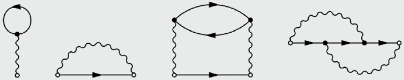
average with ρ^N

Keldysh–Kadanoff–Baym equations (KBE) on $\mathcal{C}$ (2×2 matrix):

$$\sum_k \left\{ \mathrm{i}\hbar \frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z) \right\} G_{kj}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} - \mathrm{i}\hbar \sum_{klm} \int_{\mathcal{C}} \mathrm{d}\bar{z}\, w_{iklm}(z^+,\bar{z}) G^{(2)}_{lmjk}(z,\bar{z};z',\bar{z}^+)$$



- $\int_{\mathcal{C}} wG^{(2)} \to \int_{\mathcal{C}} \Sigma G$, Selfenergy
- Nonequilibrium Diagram technique
  Example: Hartree–Fock + Second Born selfenergy



KBE: first equation of Martin–Schwinger hierarchy for $G, G^{(2)} \dots G^{(n)}$

Real-Time Keldysh-Kadanoff-Baym Equations

- Contour Green function mapped to real-time matrix Green function

$$\boxed{\mathbf{G}_{ij} = \begin{pmatrix} G^{\mathsf{R}}_{ij} & G^{<}_{ij} \\ 0 & G^{\mathsf{A}}_{ij} \end{pmatrix}}$$

$$G^{<}_{ij}(t_1,t_2) = \mp\mathrm{i}\left\langle \hat{c}^{\dagger}_j(t_2)\hat{c}_i(t_1)\right\rangle$$
$$G^{>}_{ij}(t_1,t_2) = -\mathrm{i}\left\langle \hat{c}_i(t_1)\hat{c}^{\dagger}_j(t_2)\right\rangle$$

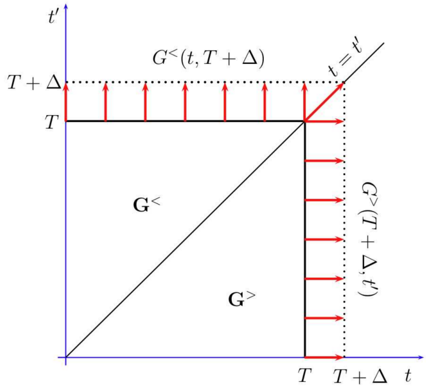
- Propagators (spectral properties)

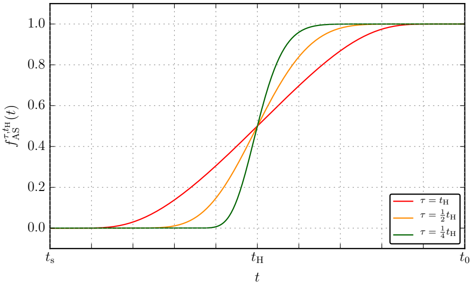
$$G^{\mathsf{R/A}}(t_1,t_2) = \pm\theta\left[\pm(t_1-t_2)\right]\left\{G^{>}(t_1,t_2) - G^{<}(t_1,t_2)\right\}$$

- Correlation functions $G^{\gtrless}$ (statistical properties) obey real-time KBE

$$\left[\mathrm{i}\partial_{t_1} - h_0(t_1)\right]G^{<}(t_1,t_2) = \int \mathrm{d}t_3\,\Sigma^{\mathsf{R}}(t_1,t_3)G^{<}(t_3,t_2) + \int \mathrm{d}t_3\,\Sigma^{<}(t_1,t_3)G^{\mathsf{A}}(t_3,t_2)\,,$$
$$G^{<}(t_1,t_2)\left[-\mathrm{i}\partial_{t_2} - h_0(t_2)\right] = \int \mathrm{d}t_3\,G^{\mathsf{R}}(t_1,t_3)\Sigma^{<}(t_3,t_2) + \int \mathrm{d}t_3\,\Sigma^{\mathsf{A}}(t_1,t_3)G^{<}(t_3,t_2)$$

K. Balzer and M. Bonitz. *Nonequilibrium Green's Function Approach to Inhomogeneous Systems.* Lecture Notes in Phys. Springer London, 2012.





- propagate $G^{\gtrless}(t, t')$ in $t - t'$ plane
- cubic scaling in time and basis size

1. Uncorrelated initial state ($t \to -\infty$)
2. adiabatically slow switch-on of interaction for $t, t' \leq t_0$

$$f_{\mathrm{AS}}^{\tau,t_{\mathrm{H}}}(t) = \exp\left(-\frac{A_{t_{\mathrm{H}}}^{\tau}}{t/(2t_{\mathrm{H}})}\exp\left(\frac{B_{t_{\mathrm{H}}}^{\tau}}{t/(2t_{\mathrm{H}})-1}\right)\right)$$

$$B_{t_{\mathrm{H}}}^{\tau} := \frac{t_{\mathrm{H}}}{\tau\ln(2)} - \frac{1}{2}, \quad A_{t_{\mathrm{H}}}^{\tau} := \frac{\ln(2)}{2}e^{2B_{t_{\mathrm{H}}}^{\tau}}$$

3. solve KBE in $t - t'$ plane for $G^{\gtrless}(t, t')$

A. Rios et al., Ann. Phys. **326**, 1274 (2011)

S. Hermanns et al., Phys. Scr. **T151**, 014036 (2012)

M. Watanabe and W. P. Reinhardt, Phys. Rev. Lett. **65**, 3301 (1990)

Equations of Motion

- equations of motion in the two time directions and along the diagonal

$$\begin{aligned}
-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t'}G^{<}_{ij}(t,t') &= \sum_l G^{<}_{il}(t,t')h^{\mathsf{eff}}_{lj}(t) + I^{(1),<}_{ij}(t,t')\,, \\
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}G^{>}_{ij}(t,t') &= \sum_l h^{\mathsf{eff}}_{il}(t)G^{>}_{lj}(t,t') + I^{(2),>}_{ij}(t,t')\,, \\
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}G^{<}_{ij}(t,t) &= \left[h^{\mathsf{eff}}(t), G^{<}(t,t)\right]_{ij} + I^{(2),>}_{ij}(t,t) - I^{(1),<}_{ij}(t,t)
\end{aligned}$$

- for the missing components

$$G^{\gtrless}_{ij}(t,t') = -\left[G^{\gtrless}_{ji}(t',t)\right]^*$$

- effective hamiltonian h^{eff}

$$h^{\mathsf{eff}}(t) = -J\delta_{\langle i,j\rangle} + \delta_{i,j}U(t)n_i(t)$$

J : hopping amplitude, $\qquad U$: interaction strength

N. Schlünzen and M. Bonitz, Contrib. Plasma Phys. **56**, 5 (2016)

- components of the collision integral

$$I^{(1),<}_{il}(t<T) = \int_{t_s}^{t} \mathrm{d}\bar{t} \sum_k \left\{ G^{>}_{ik}(t>\bar{t})\Sigma^{<}_{kl}(\bar{t}<T) - \left(G^{<}_{ki}(\bar{t}<t)\Sigma^{>}_{lk}(T>\bar{t})\right)^* \right\}$$
$$+ \int_{t}^{T} \mathrm{d}\bar{t} \sum_k \left\{ G^{<}_{ik}(t<\bar{t})\Sigma^{<}_{kl}(\bar{t}<T) + G^{<}_{ik}(t<\bar{t}) \left(\Sigma^{>}_{lk}(T>\bar{t})\right)^* \right\},$$

$$I^{(2),>}_{lj}(T>t') = \int_{t_s}^{t'} \mathrm{d}\bar{t} \sum_k \left\{ \Sigma^{>}_{lk}(T>\bar{t})G^{<}_{kj}(\bar{t}<t') - \left(\Sigma^{<}_{kl}(\bar{t}<T)G^{>}_{jk}(t'>\bar{t})\right)^* \right\}$$
$$+ \int_{t'}^{T} \mathrm{d}\bar{t} \sum_k \left\{ \Sigma^{>}_{lk}(T>\bar{t})G^{>}_{kj}(\bar{t}>t') + G^{>}_{kj}(\bar{t}>t') \left(\Sigma^{>}_{kl}(\bar{t}<T)\right)^* \right\}$$

- self-energy in 2B (second Born) approximation

$$\Sigma^{>}_{ij}(t>t') = U(t)U(t')G^{>}_{ij}(t>t')G^{>}_{ij}(t>t')G^{<}_{ji}(t'<t)\,,$$
$$\Sigma^{<}_{ij}(t<t') = U(t)U(t')G^{<}_{ij}(t<t')G^{<}_{ij}(t<t')G^{>}_{ji}(t'>t)$$

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- propagation of the KBE requires two integration procedures
  - (A) the time propagation of the equations of motion, e.g.

$$-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t'}G^{<}_{ij}(t,t') = \sum_l G^{<}_{il}(t,t')h^{\mathsf{eff}}_{lj}(t) + I^{(1),<}_{ij}(t,t')$$

  - (B) the evaluation of the collision integral in every time step, e.g.

$$\begin{aligned} I^{(1),<}_{il}(t<T) = &\int_{t_{\mathsf{s}}}^{t}\mathrm{d}\bar{t}\sum_k\left\{G^{>}_{ik}(t>\bar{t})\Sigma^{<}_{kl}(\bar{t}<T) - \left(G^{<}_{ki}(\bar{t}<t)\Sigma^{>}_{lk}(T>\bar{t})\right)^*\right\} \\ &+\int_{t}^{T}\mathrm{d}\bar{t}\sum_k\left\{G^{<}_{ik}(t<\bar{t})\Sigma^{<}_{kl}(\bar{t}<T) + G^{<}_{ik}(t<\bar{t})\left(\Sigma^{>}_{lk}(T>\bar{t})\right)^*\right\}\end{aligned}$$

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$$+\int_{t}^{T}\mathrm{d}\bar{t}\sum_{k}\left\{G^{<}_{ik}(t<\bar{t})\Sigma^{<}_{kl}(\bar{t}<T) + G^{<}_{ik}(t<\bar{t})\left(\Sigma^{>}_{lk}(T>\bar{t})\right)^{*}\right\}$$

Equations of Motion - HF

- equations of motion in the two time directions and along the diagonal

$$
\begin{aligned}
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$$

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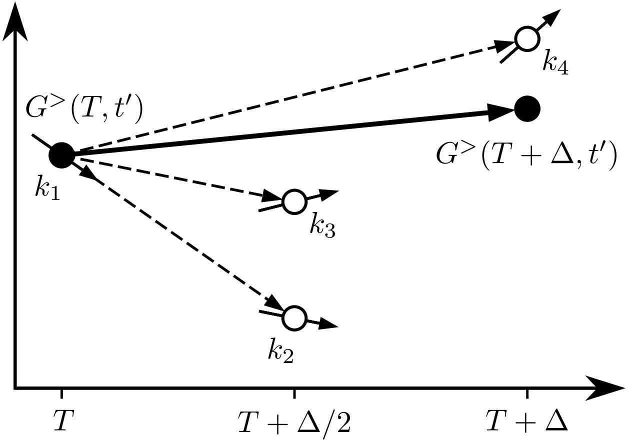
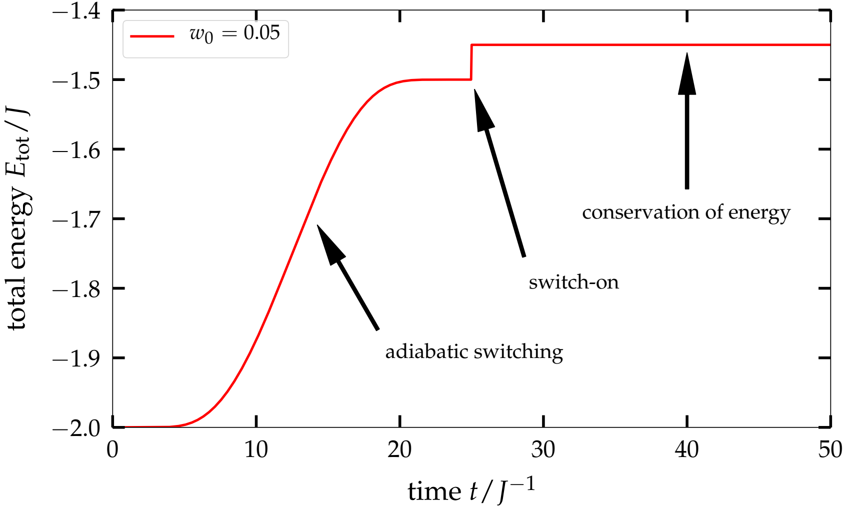
- propagation equation for the Runge Kutta 4 (RK4) method

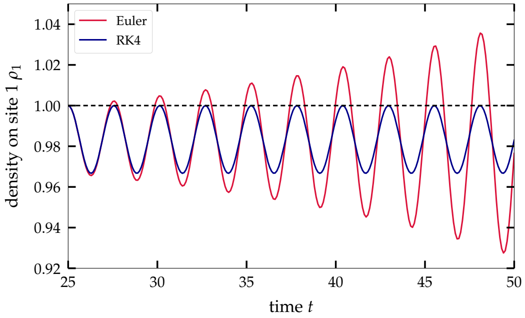
$$G^{>}_{ij}(T+\Delta,t') \quad = \quad G^{>}_{ij}(T,t') + \frac{\Delta}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

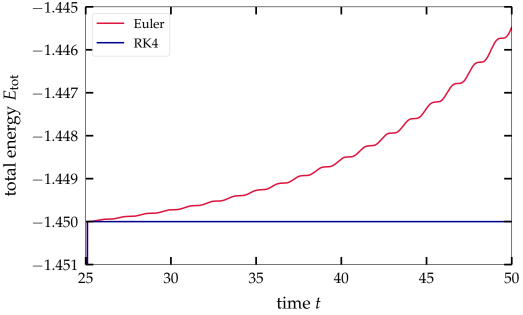


Setup for Testing

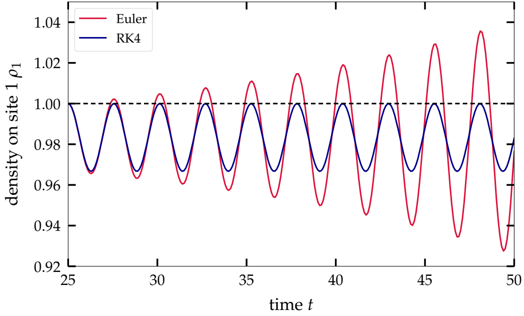


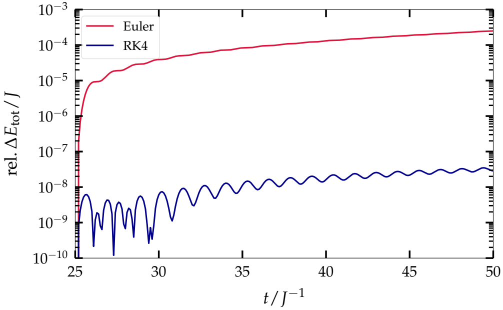
- use conservation of energy to test the quality of the numerical calculations
- two-site setup at half filling





- time step $\Delta = 0.1J^{-1}$
- RK4 shows huge improvement over Euler
- density and energy are conserved better by several orders of magnitude





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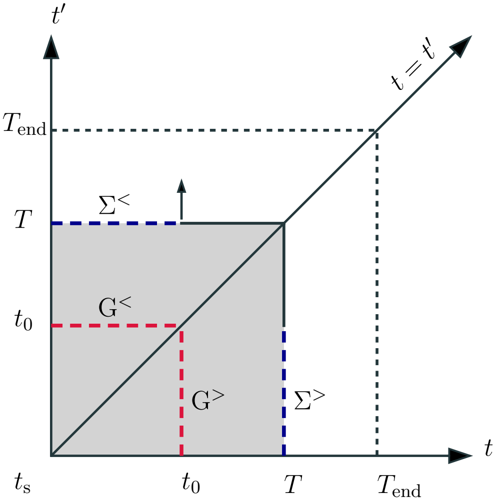
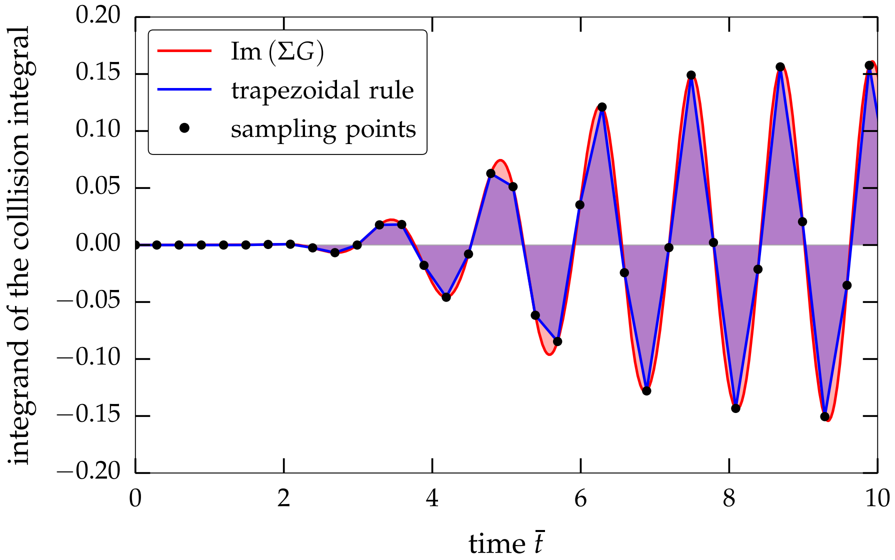
The Collision Integral



$$I_{il}^{(1),<}(t_0 < T) = \int_{t_{\mathrm{s}}}^{t_0} \mathrm{d}\bar{t} \sum_k \left\{ G_{ik}^{>}(t_0 > \bar{t}) \Sigma_{kl}^{<}(\bar{t} < T) - \left(G_{ki}^{<}(\bar{t} < t_0) \Sigma_{lk}^{>}(T > \bar{t}) \right)^* \right\} + \ldots$$

The Collision Integral



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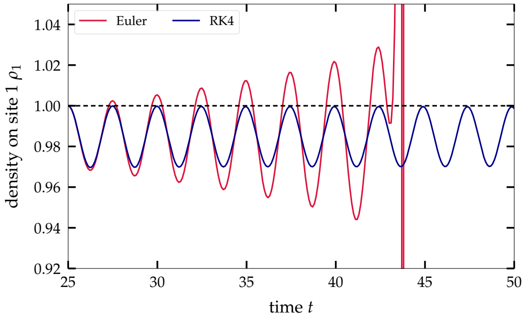

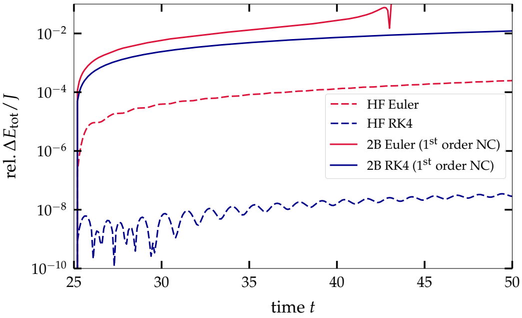

- time step $\Delta = 0.1J^{-1}$
- Euler calculation becomes instable at $t \approx 43J^{-1}$
- RK4 barely improves the accuracy of the calculation
- numerical error due to the integral is huge
  $\rightarrow$ trapezoidal rule is not sufficient

- integral to be calculated

$$I(f) = \int_a^b \mathrm{d}x\, f(x)$$

- with Newton–Cotes integration $I(f)$ can be approximated by an expression that only depends on values for discrete sampling points $f_i := f(x_i)$

$$I(f) \approx dh \sum_{i=0}^{d} f_i w_i^d \qquad \text{with}$$

$$w_i^d := \int_0^1 \mathrm{d}\hat{x} \prod_{\substack{j=0 \\ j\neq i}}^{d} \frac{\hat{x}d - j}{i - j}$$

  where $h := \frac{x_n - x_0}{d}$ and order d.

- the error is of the order $\mathcal{O}\left(h^{d+2}\left|f^{(d+1)}\right|\right)$, if d is odd and of the order $\mathcal{O}\left(h^{d+3}\left|f^{(d+2)}\right|\right)$, if d is even

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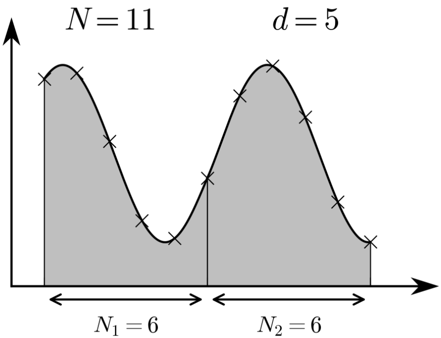
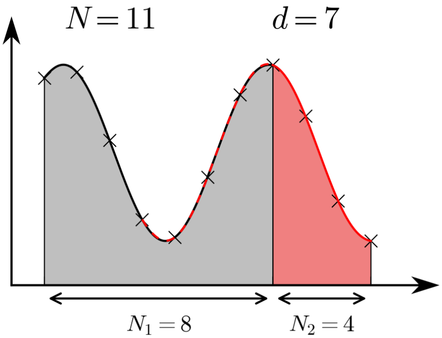
Composite Rule

Two different way of integrating long integrands with Newton–Cotes:

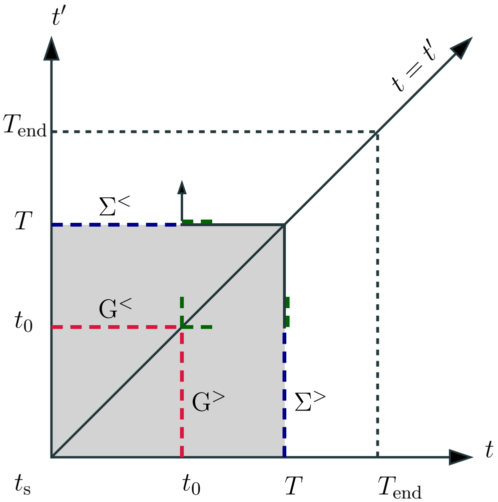




- divide the integrand into smaller parts
- choose the length of the integrals in a way so that the smallest order is optimal

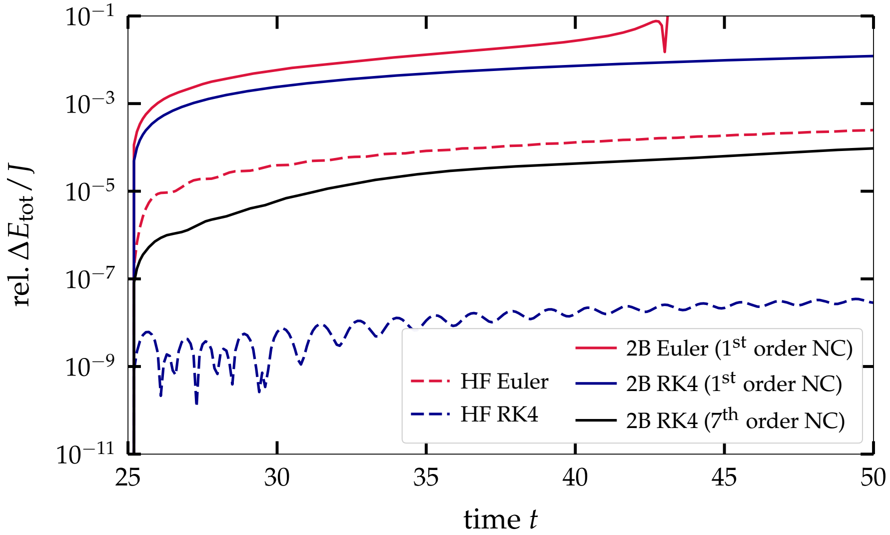
- divide the integrand into parts of the highest order
- integrate the remaining integral by reusing points of the adjacent interval

Extended Integrals

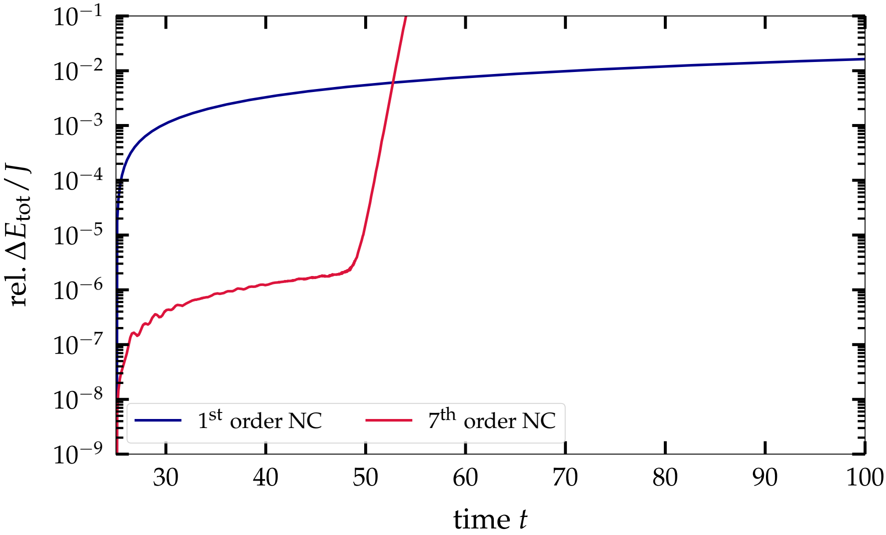


- problem: high order integrals require many sampling points
- short integrals can be expanded by adding additional points
- this way all integrals are calculated in the highest possible order

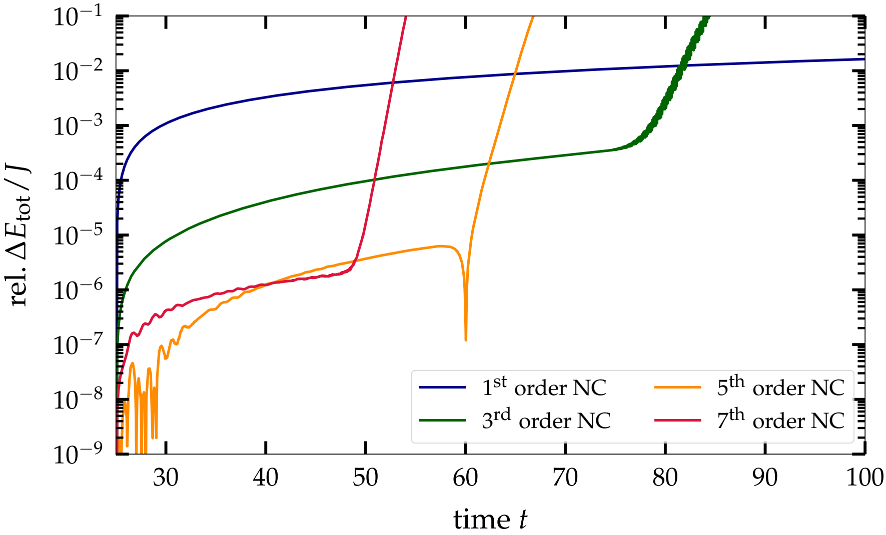
$$I_{il}^{(1),<}(t_0 < T) = \int_{t_{\mathrm{s}}}^{t_0} \mathrm{d}\bar{t} \sum_k \left\{ G_{ik}^>(t_0 > \bar{t})\Sigma_{kl}^<(\bar{t} < T) - \left(G_{ki}^<(\bar{t} < t_0)\Sigma_{lk}^>(T > \bar{t})\right)^* \right\} + \ldots$$



- high-order integration increases accuracy by two orders of magnitude

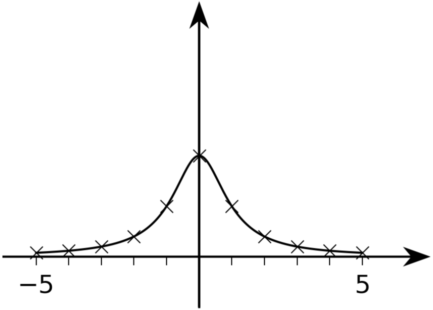


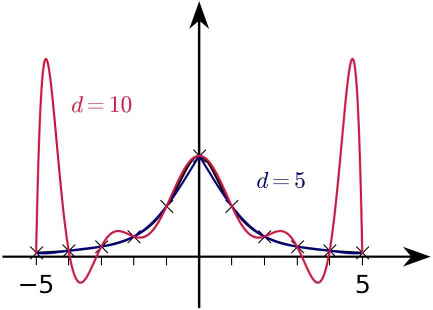
- high-order integration diverges despite time step of $\Delta = 0.04 J^{-1}$



- all high-order integrals show instability: can we do something about this?

Runge's Phenomenon



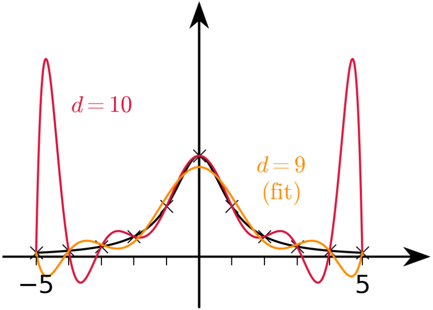


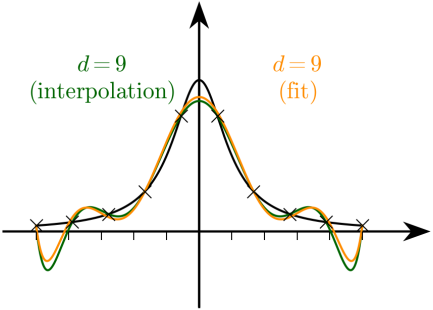
- Runge function

$$f(x) = \frac{1}{1 + x^2}$$

- high order interpolation polynomials show strong oszillations at the edges of the interval
- most common way to mitigate the effect is using non-equidistant points
  $\rightarrow$ not possible here

Runge's Phenomenon





- another solution is using regression instead of interpolation
- advantage: weights can be calculated in advance as in the Newton–Cotes method
- a fit of order 9 shows better behavior than the interpolation polynomial of order 9
- another way: use Fourier basis functions (Fourier extension)

J. P. Boyd, Journal of Computational Physics **178 (2002).**

- new weights for regression

$$w_i^d \;:=\; \sum_{j=0}^{d-1} q_j(x_i) \int_0^1 \mathrm{d}\hat{x}\, q_j(\hat{x})$$

with orthogonal polynomials

$$q_n(x) = \frac{1}{||p_n||_u} p_n(x), \qquad ||f||_u := \sqrt{u(f,f)}, \qquad u(f,g) = \sum_{j=1}^{N} f(x_j) g(x_j)$$

- obtainable by solving the recurrence relation

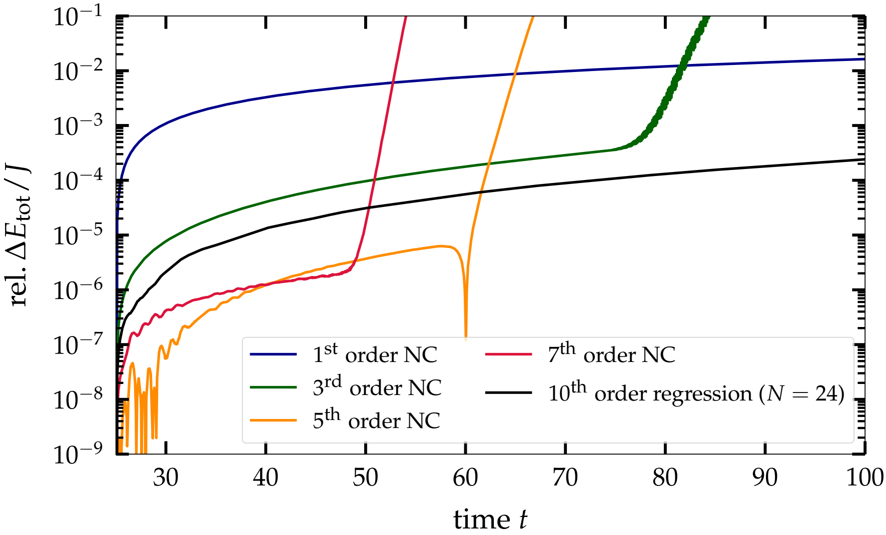
$$p_n(x) = (x - \alpha_n) p_{n-1}(x) - \beta_n p_{n-2}(x), \qquad n = 2, 3, \ldots, N-1$$

with the coefficients

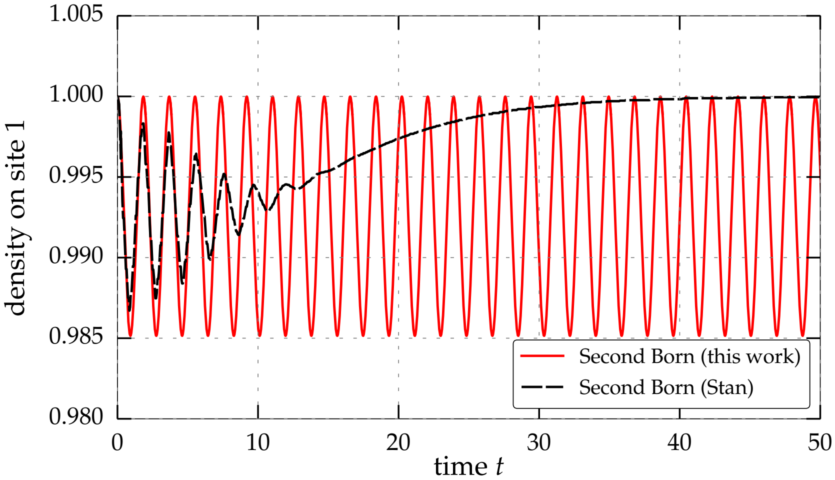
$$\alpha_n(x) = \frac{v(x p_{n-1}, p_{n-1})}{v(p_{n-1}, p_{n-1})}, \qquad \beta_n(x) = \frac{v(x p_{n-1}, p_{n-2})}{v(p_{n-2}, p_{n-2})}$$

$$p_{-1}(x) \equiv 0 \qquad \text{and} \qquad p_0(x) = 1$$

D. Huybrechs, *Stable high-order quadrature rules with equidistant points.* Journal of Computational and Applied Mathematics **231**, 933 (2009).

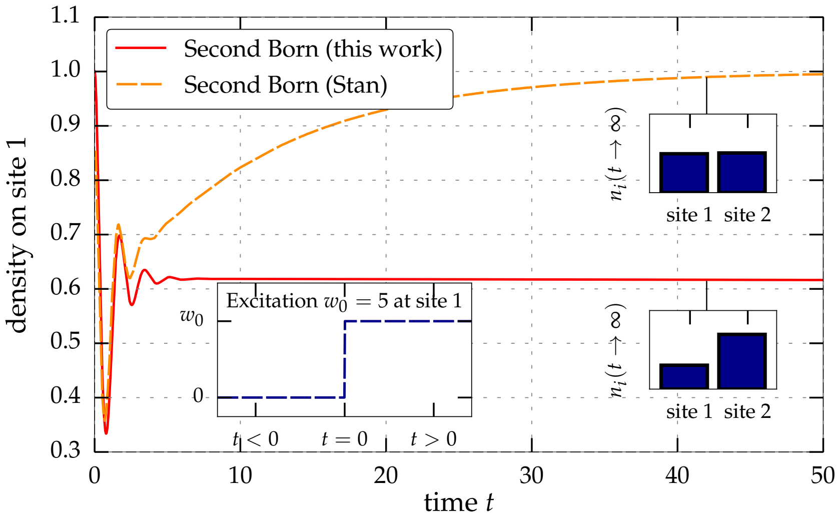


- regression method shows slightly worse energy conservation but no instability



- numerical damping mistaken for artificial damping of the KBEs

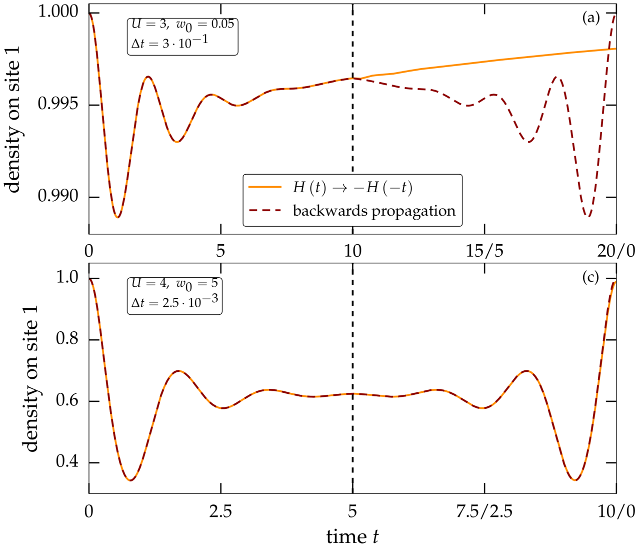
N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. B **96**, 117101 (2017).



- inaccurate calculation leads to wrong steady state

N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. B **96**, 117101 (2017).

Time Reversibility



- if done correctly, time reversibility is an ideal check for your numerics
- sign of Hamiltonian has to be changed
- top: weak excitation, numerical damping, correct time reversion fails
- bottom: strong excitation, intrinsic damping, correct time reversion succeeds

N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. B **96**, 117101 (2017).

M. Scharnke, N. Schlünzen and M. Bonitz, Journal of Mathematical Physics **58**, 061903 (2017).

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Mathematisch-Naturwissenschaftliche Fakultät

optimizations:

- RK4 method (or U-equivalent) is sufficient for the propagation of the KBEs
- integration in the collision integral is far more error-prone
  $\rightarrow$ high-order Newton–Cotes integration rules
- short integrals can be improved with additional data points
- mitigating the effect of the Runge phenomenon for high-order integrals by using regression polynomials or Fourier extension

advantages:

- conservation of energy is $2-3$ orders of magnitude better than for trivial approaches
  $\rightarrow$ perform more precise calculations in a shorter time

not shown:

- also applicable for the integration in the self-energy (GW, T-matrix)

J.-P. Joost, Master's Thesis, CAU Kiel (2017).