Acceleration of Non-Equilibrium Quantum Dynamics Calculations Using Data Compression

Thomas Blommel

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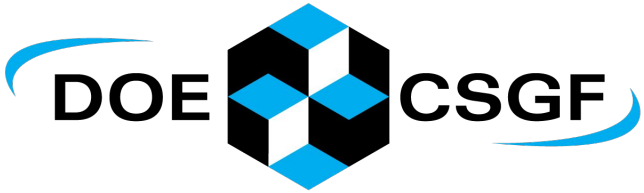
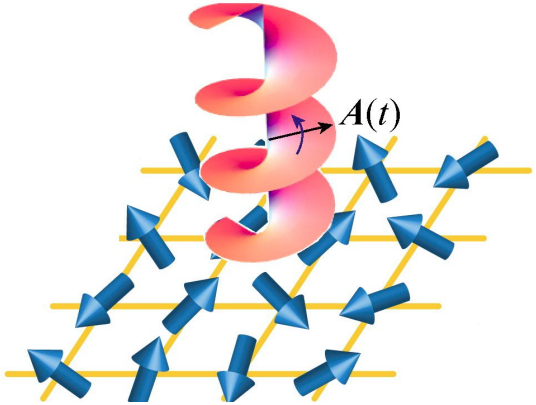


Motivations

- Condensed matter physics seeks to describe the physical and electronic properties of materials
- These materials consist of many interacting, quantum particles
- We can use Quantum Field Theory to describe many condensed matter systems both in and out of equilibrium
  - Ultrafast pump-probe spectroscopy
  - Molecular nano-junctions
  - Dynamical Mean-Field Theory and Impurity models
  - Floquet physics
  - Photoexcitation of superconductors
  - Etc



1. Phys. Rev. A 92, 033419
2. Guy Cohen Group
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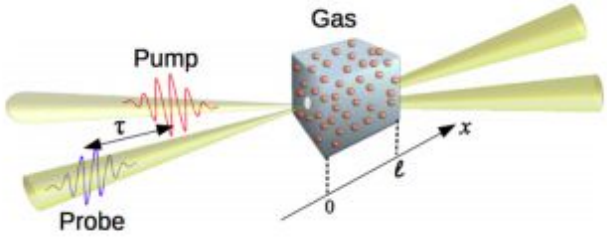
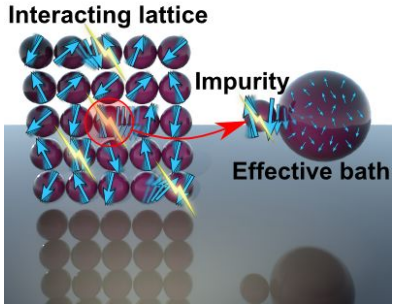
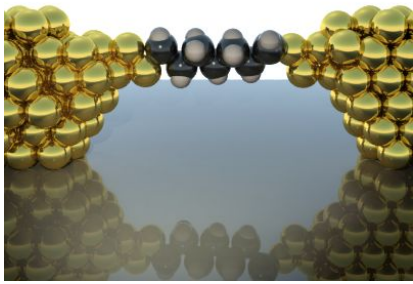
4. Annual Review of Condensed Matter Physics 2019 10:1, 387-408
5. Nature Physics volume 11, pages 421–426 (2015)







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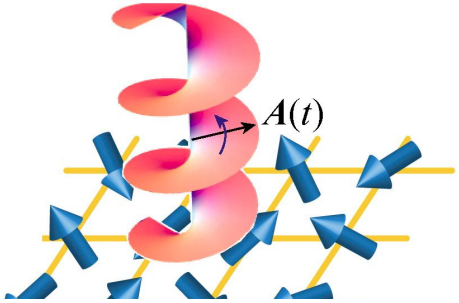

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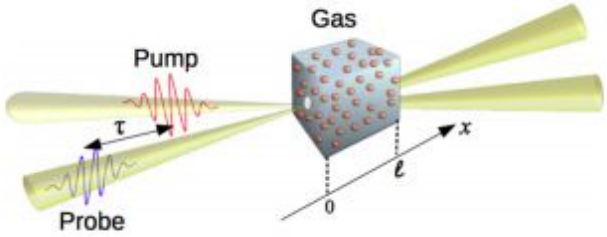
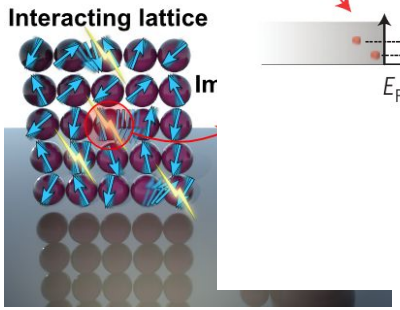
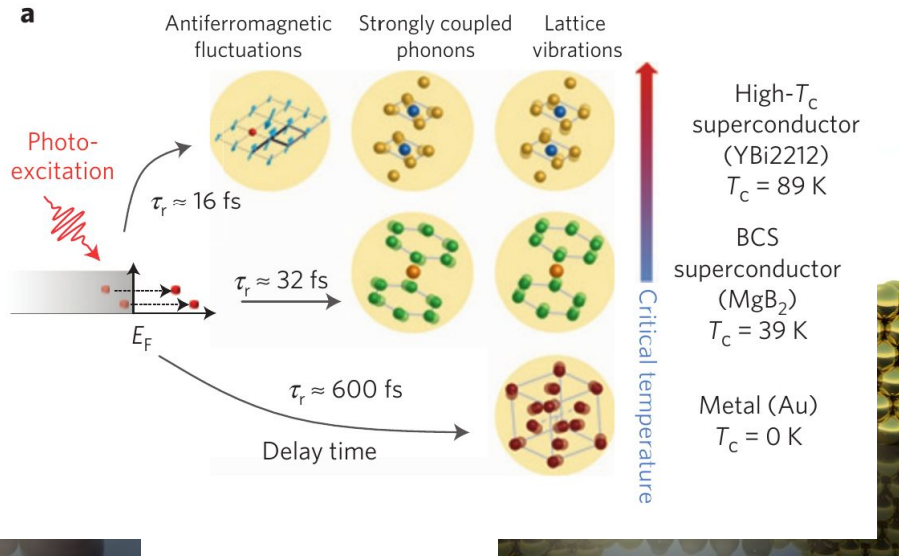
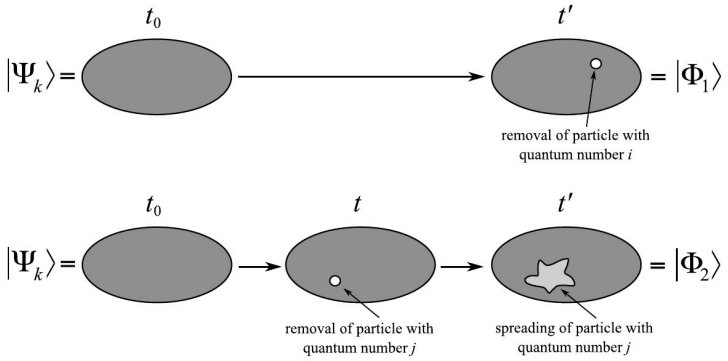






Non-Equilibrium Green's Functions

- The Non-Equilibrium Green's Function, $G_{ij}(t,t')$, is a matrix-valued correlation function in QFT
- Measures correlation between two quantum states, where a particle is removed from two different positions at two different times
- Contains information about many physically observable quantities
  - Current
  - Density
  - Probability of finding particles with certain energies and momenta
  - Phonon (lattice vibration) displacements
  - Photoabsorption and emission spectra
  - Order parameters (magnetic, superconducting, etc.)



1. Stefanucci, van Leeuwen, Nonequilibrium Many-Body Theory of Quantum Systems (2013)

Equation of Motion

- The dynamics of the Green's Function is governed by the integro-differential equation, the Kadanoff Baym Equation

$$i\partial_t G_{ij}(t,t') = h_{ik}(t) G_{kj}(t,t') + \int_0^t d\bar{t}\, \Sigma_{ik}(t,\bar{t}) G_{kj}(\bar{t},t')$$

- Dynamics of particles without interactions
- History integral which introduces memory
- System dependent functional of G, accounts for Many-Body interactions

Equation of Motion

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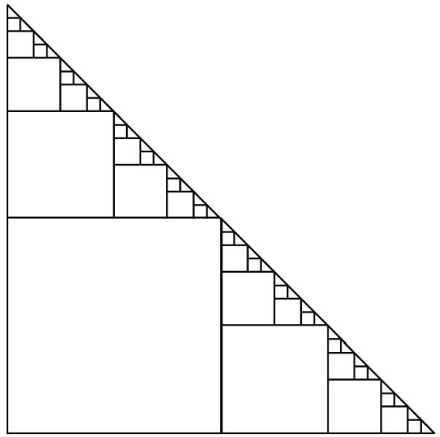
- When integrating this equation for N timesteps, the computational cost scales as N^3 and the memory required scales as N^2
- This scaling (in both cost and memory) prevents investigation of long-time limit phenomena
- In practice, researchers typically make approximations that reduce the scaling of these equations, however these approximations are unconstrained, i.e., they have no small parameter to converge with

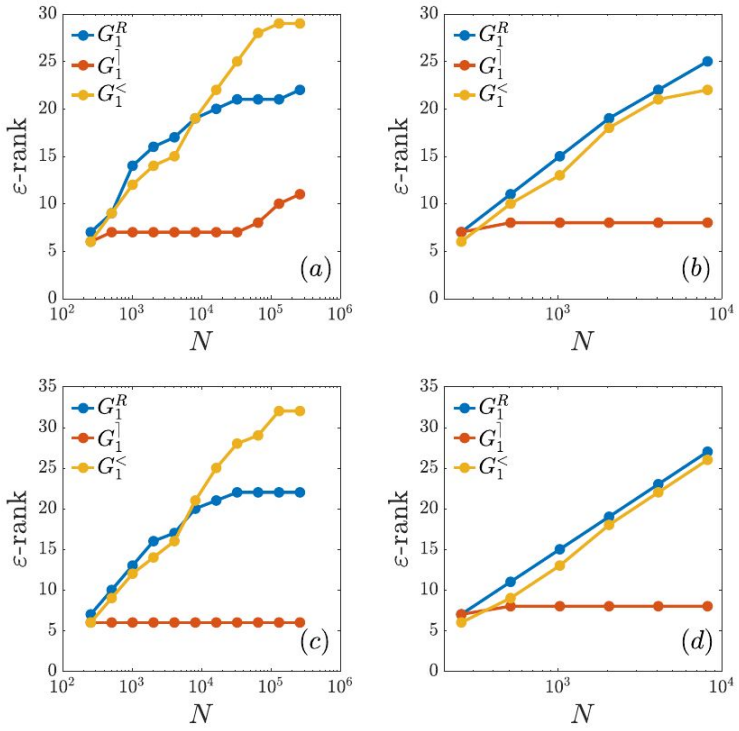
Hierarchical decomposition

- Key idea: G(t,t') is a correlation function, and as $|t-t'| \gg 0$, we expect the correlations to decay to zero.
- This leads to the ansatz that, since less information is contained in this region, there should be a low-rank representation
- Matrices with this property are known as hierarchically off-diagonal low-rank (hodlr)
- Recursively partition matrix and perform SVD on each block
- Performing one timestep amounts to adding a single row to the lower triangular matrix
- Fast SVD updates mean full block is never stored



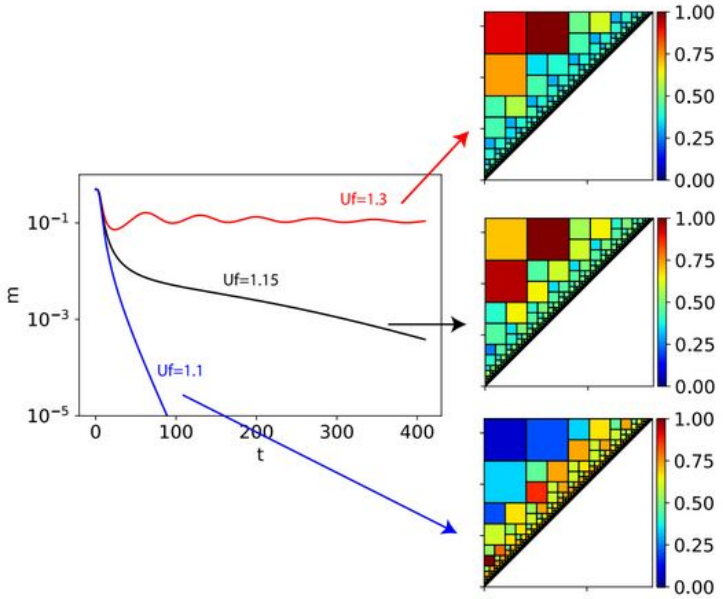
Decomposition results

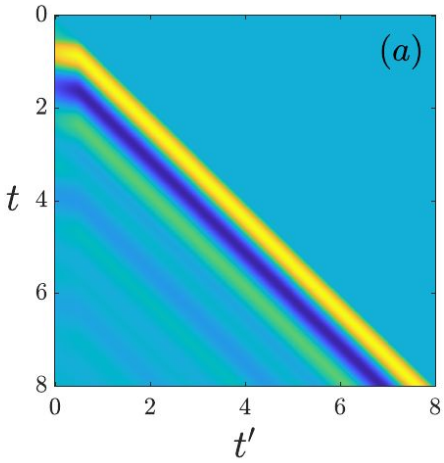
- Ranks of blocks for most interesting physical systems grow logarithmically with size of block
- We evaluate history integrals using SVDs, which reduces scaling
- Reduction of computational cost $N^3 \rightarrow N^2 \log(N)$
- Memory requirements $N^2 \rightarrow N \log(N)$

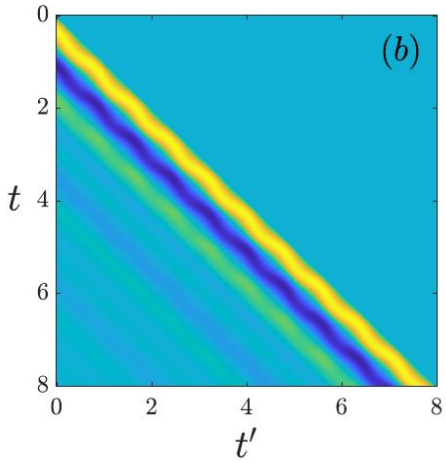


Decomposition results

- Scalar Hubbard model with two external potential fields applied: one ramp and one floquet
- Calculation that now takes 26.5 hrs with 3.8 GB on a laptop
- Would have taken: 5 months with 2.2 TB







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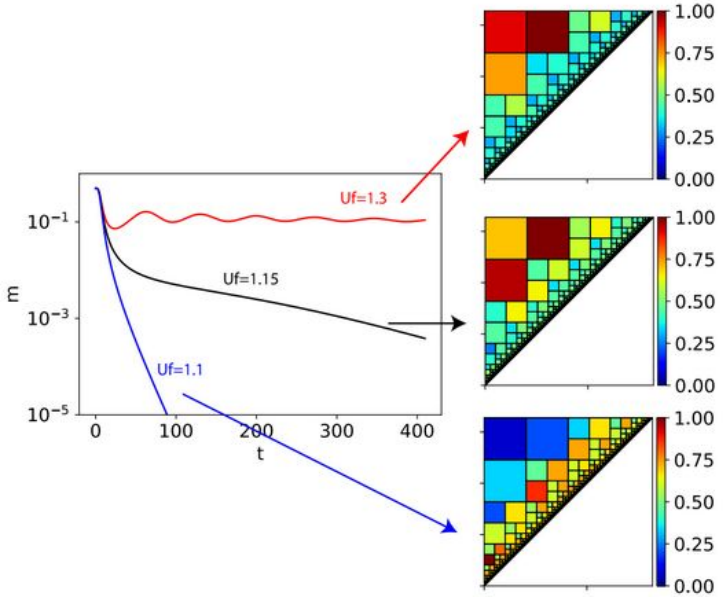
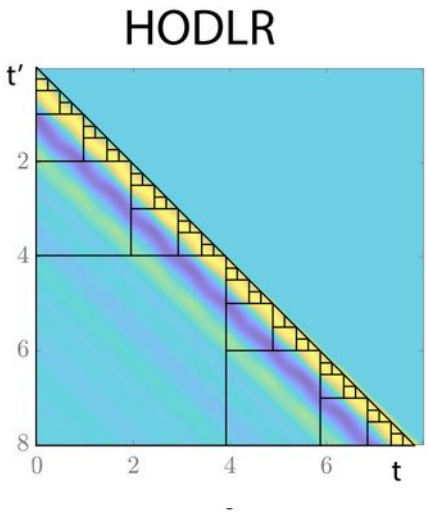
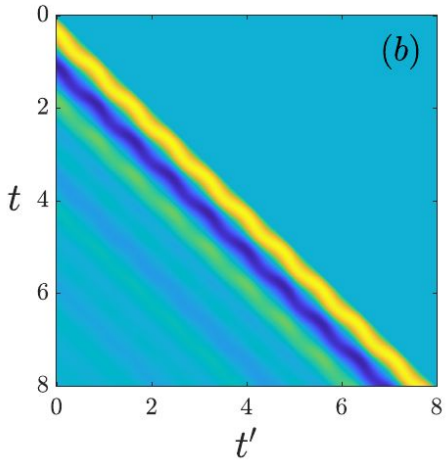
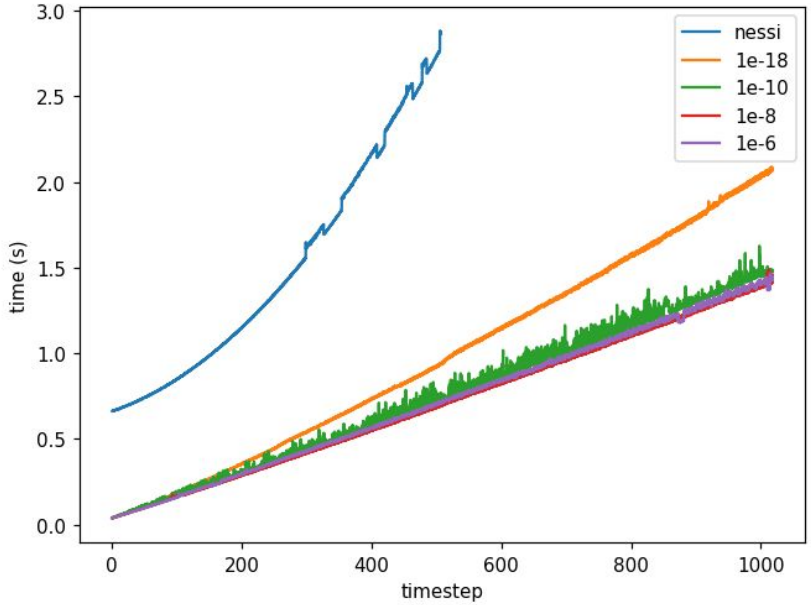


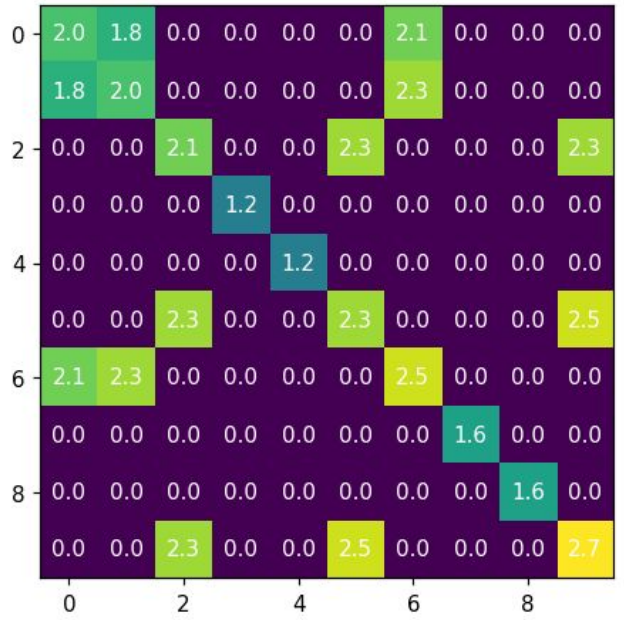




Helium gas results

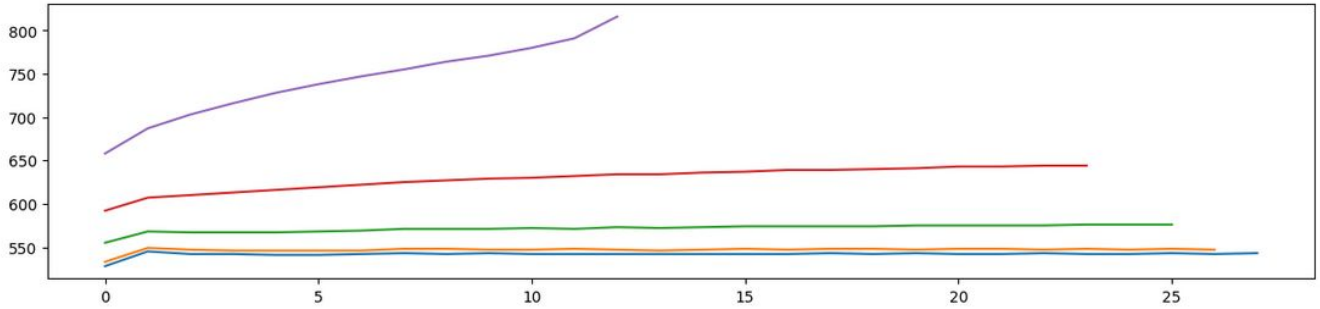
- We couple Helium gas to external electric field representing a laser
- Electrons in certain orbitals are excited and transitions occur
- GF of orbitals not involved in process is zero, making information redundant

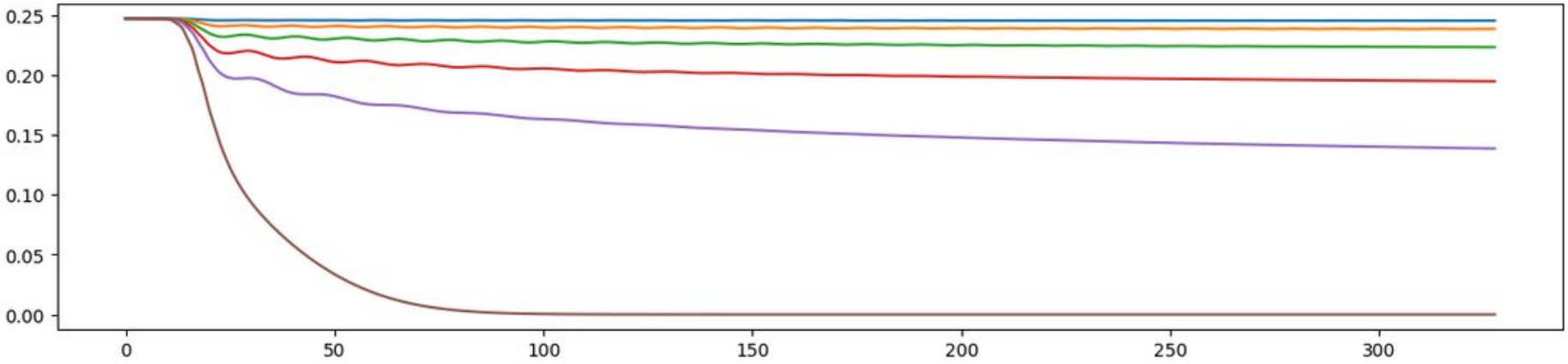




Superconductor results

- Shine a laser on a superconducting system and follow evolution of order parameter
- For large laser intensity, enough energy is deposited to “melt” system and cause a phase transition
- For intermediate pulse strengths, we see deformation of potential responsible for formation of Cooper pairs
- Calculations take 10 hrs with less than a GB of memory
- Previously 1 month with 34 GB of memory



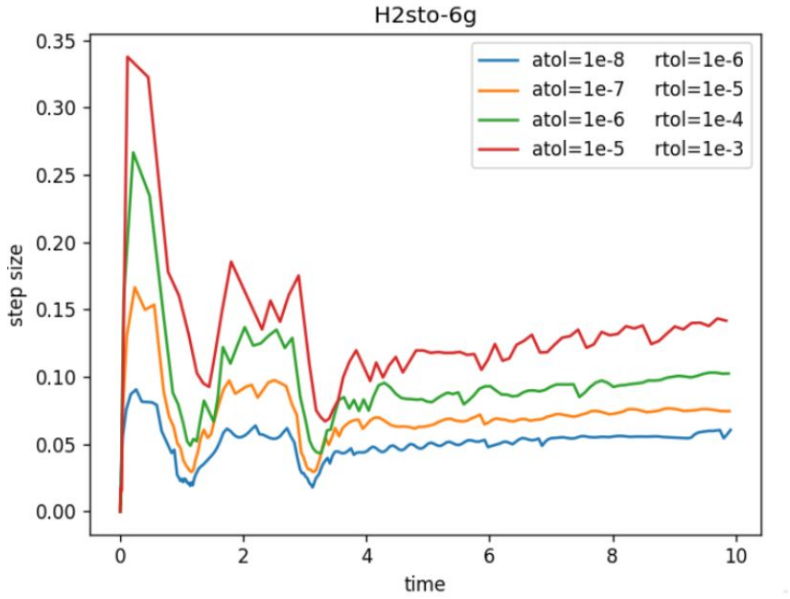


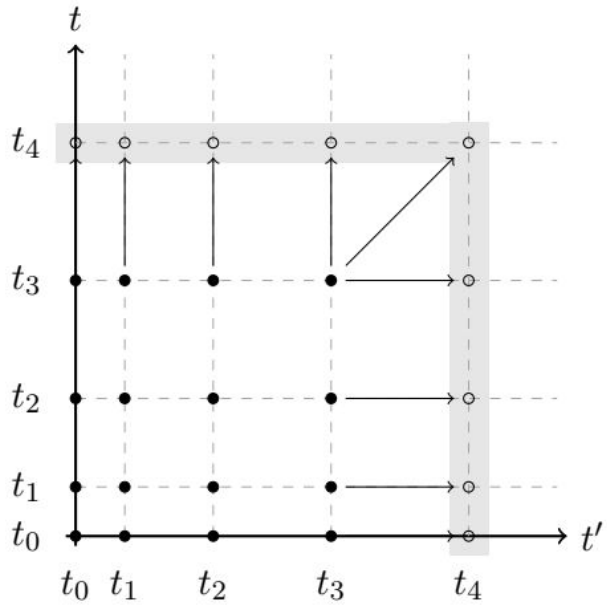
Adaptive stepping

- Often there are multiple time scales in a problem we are looking to integrate
- Laser pulses or potential quenches can be very short and fast compared to system's response
- Being able to adapt timestep sizes would be very helpful in integrating to much longer times
- CVODE, part of the sundials package at LLNL adaptively solves y'=f(t,y)

Adaptive stepping

- At each step, our solution vector grows in size
- CVODE assumes solution vector size is constant for entire calculation
- We are working on implementing the ability to change solution vector size at each timestep
- This functionality will be useful for many applications outside of our own (time dependent system boundaries, mesh refinement)





Conclusion and Future Work

- We have developed timestepping schemes for the Kadanoff-Baym equations which scales as $N^2\log(N)$ instead of N^3
- This had lead to several orders of magnitude decrease in computational cost
- CVODE functionality which allows for dynamic solution vector sizes

- High order integration schemes still need to be implemented (currently capped at order 2)
- Compression scheme will be implemented into current state-of-the-art quantum system timestepping package (Nessi)