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Implementation of Configuration Interaction in the Auxiliary Master Equation Approach

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Motivation

- The Auxiliary Master Equation Approach[1] (AMEA) allows to simulate an impurity in contact with arbitrary environments. Using the Configuration Interaction[2,3] (CI) approximation reduces the computation time and allows to increase the accuracy of the calculation.

Physical and auxiliary system

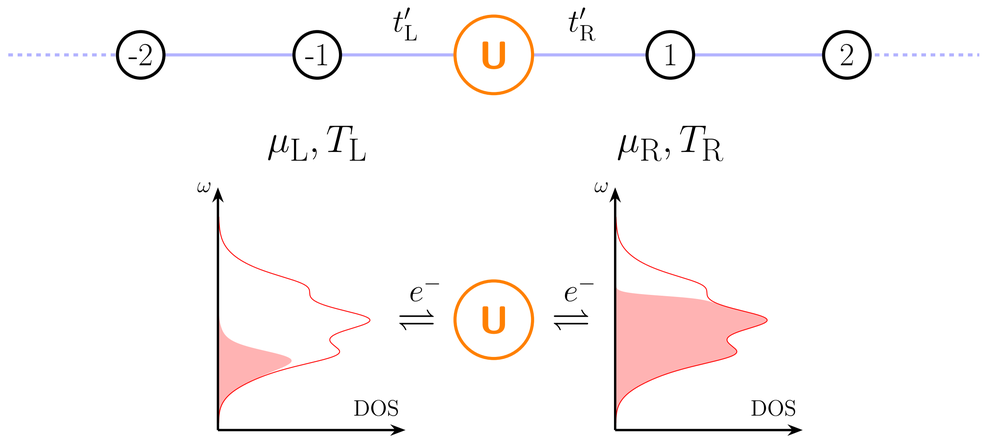

Fig. 1. The upper part depicts the physical system as two semi-infinite chains connected to the impurity. The one below represents those chains in terms of their density of states.

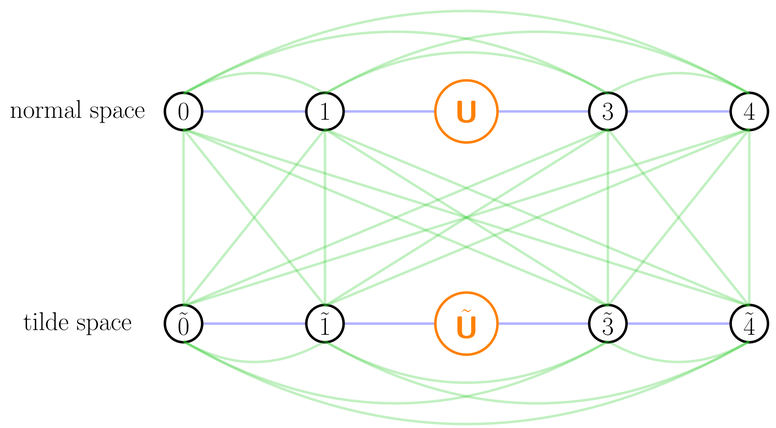

Fig. 2. Visualisation of the auxiliary system. The green and blue lines show how the sites are connected, and correspond to fitting parameters.

- Figure 2 illustrates the Lindblad equation in superfermion representation[4]. The blue lines represent the unitary part, and the green ones the disspative part.
- The real system is modelled by the auxiliary one, by recreating the hybridization function as good as possible[5].

Configuration Interaction

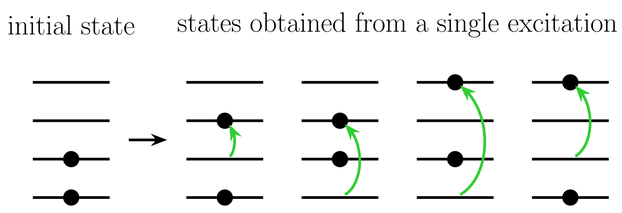

Fig. 3. We choose an initial state and add excitations in terms of annihilations and creations.

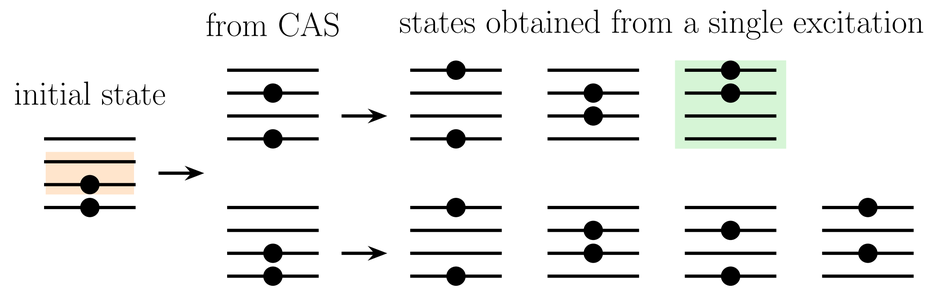

Fig. 4. Here we obtain two initial states from our Complete Active Space (orange).

- CASCI/CI keeps the Hilbert space small.

Results

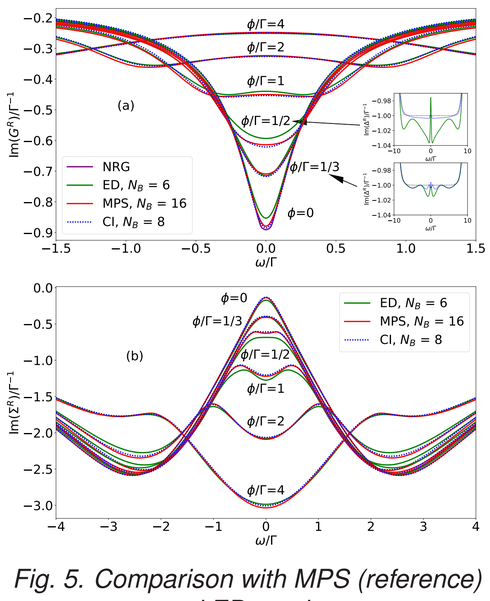

Fig. 5. Comparison with MPS (reference) and ED results.

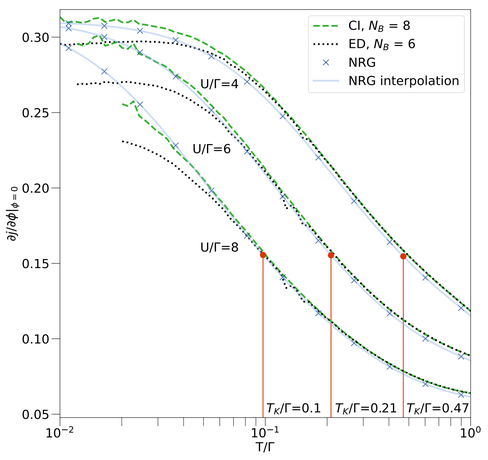

Fig. 6. Comparison with NRG (reference) and ED for equilibrium.

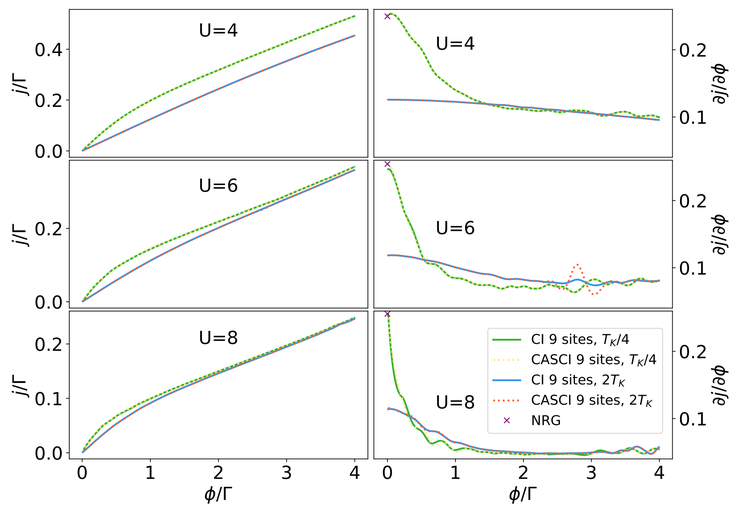

Fig. 7. Current (lhs) and the respective conductance (rhs) over voltage.

- Good agreement with MPS[6] and NRG[7] results.
- Reproduces physical behaviour for the current.

Outlook

- Use as impurity solver for DMFT.
- Implement natural orbital basis to improve accuracy.

References

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This project is funded by

FWF Der Wissenschaftsfonds.
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