Löwdin's Symmetry Dilemma in Correlated Systems - Green Functions Theory Results

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Abstract

The Hubbard model is a key system in the theory of strongly correlated electrons in solids, and it is realized with atoms in optical lattices. In the well-studied one-dimensional case, exact solutions are provided by analytic methods and density-matrix-renormalization-group (DMRG) simulations. In 2D and 3D, Green functions combined with many body approximations (GFMBA) present a reliable approach[1]. Here we present results demonstrating the capability of GFMBA to produce reliable data for the Hubbard gap energy despite its approximate character. We observed an improvement to the gap energy when lifting restrictions on spin symmetry and spatial homogeneity coupled with a spontaneous breaking of symmetry. This "symmetry dilemma" was described by Löwdin[2] for Hartree Fock wave function calculations, and is extended here to GFMBA beyond Hartree-Fock[3].

Hubbard Model

- Simplified model of correlated lattice systems
- Hubbard Hamiltonian:

$$\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}}$$

- **Nearest-neighbor** hopping
- Constant **on-site** interaction

$$\hat{H}_{\text{hop}} = -J \sum_{\langle \boldsymbol{s},\boldsymbol{s}' \rangle} \sum_{\sigma=\uparrow,\downarrow} \hat{c}^{\dagger}_{\boldsymbol{i},\sigma} \hat{c}_{\boldsymbol{j},\sigma} \qquad \hat{H}_{\text{int}} = U \sum_{\boldsymbol{i}} \hat{n}^{\uparrow}_{\boldsymbol{i}} \hat{n}^{\downarrow}_{\boldsymbol{i}}$$

with $\langle \boldsymbol{i}, \boldsymbol{j} \rangle$ nearest-neighbor sites, $\hat{c}^{\dagger}_{\boldsymbol{i},\sigma}$, $\hat{c}_{\boldsymbol{i},\sigma}$ creation and annihilation operator on site $\boldsymbol{i}$ with spin σ and $\hat{n}^{\sigma}_{\boldsymbol{i}} = \hat{c}^{\dagger}_{\boldsymbol{i},\sigma} \hat{c}_{\boldsymbol{i},\sigma}$.

- Hubbard interaction U and hopping amplitude J specify the system state

Green Function Theory

- The one-particle nonequilibrium Green function is defined by

$$G^{\sigma}_{\boldsymbol{ij}}(z, z') = -\frac{\mathrm{i}}{\hbar} \left\langle T_{\mathcal{C}} \hat{c}_{\boldsymbol{i},\sigma}(z) \hat{c}^{\dagger}_{\boldsymbol{j},\sigma}(z') \right\rangle$$

with the time-ordering operator $\hat{T}_{\mathcal{C}}$ on the Keldysh contour $\mathcal{C}$.

- The equations of motion are given by the **Keldysh-Kadanoff-Baym equations**[4] (KBE), where all correlations are included in the **self-energy** Σ:

$$\left(\mathrm{i}\hbar \frac{\partial}{\partial z} \delta_{\boldsymbol{i},\boldsymbol{l}} - h^{\sigma}_{\boldsymbol{il}} \right) G^{\sigma}_{\boldsymbol{lj}}(z, z') = \delta_{\mathcal{C}}(z - z') \delta_{\boldsymbol{i},\boldsymbol{j}} + \int_{\mathcal{C}} \mathrm{d}\bar{z}\, \Sigma^{\sigma}_{\boldsymbol{il}}(z, \bar{z}) G^{\sigma}_{\boldsymbol{lj}}(\bar{z}, z')\,,$$

and the adjoint equation, respectively.

- $\Sigma^{\sigma}_{i,j}(z, z_0)$ includes the time-diagonal Hartree–Fock (HF) self-energy as well as the time non-local correlation part. Here the second-order (Born) approximation (SOA) is used.

$$\begin{aligned}
\Sigma^{\sigma}_{\boldsymbol{ij}}(z, z') &= \Sigma^{\mathrm{HF},\sigma}_{\boldsymbol{ij}}(z, z') + \Sigma^{\mathrm{SOA},\sigma}_{\boldsymbol{ij}}(z, z') \\
\Sigma^{\mathrm{HF},\uparrow(\downarrow)}_{\boldsymbol{ij}}(z, z') &= -\mathrm{i}\hbar\, \delta_{\boldsymbol{i},\boldsymbol{j}} \delta_{\mathcal{C}}(z - z')\, U(z) G^{\downarrow(\uparrow)}_{\boldsymbol{ii}}(z, z) \\
\Sigma^{\mathrm{SOA},\uparrow(\downarrow)}_{\boldsymbol{ij}}(z, z') &= -(\mathrm{i}\hbar)^2\, U(z) G^{\uparrow}_{\boldsymbol{ij}}(z, z')\, G^{\downarrow}_{\boldsymbol{ij}}(z, z') \\
&\qquad G^{\downarrow(\uparrow)}_{\boldsymbol{ji}}(z', z) U(z')
\end{aligned}$$

Groundstate Generation

- **Iterative approach**:
  - In equilibrium the KBE depend only on the time difference and can be rewritten in frequency space in form of the Dyson-equation:

$$G(\omega) = G_0(\omega) + G_0(\omega) \Sigma(\omega) G(\omega)$$

  - Starting with $G(\omega) = G_0(\omega)$ the solution can be improved by iterating until $G(\omega)$ no longer changes between iterations.

- **Adiabatic switching**:
  - Time propagation starts from non-interacting state.
  - Interaction strength U(t) is switched on adiabatically.

Results

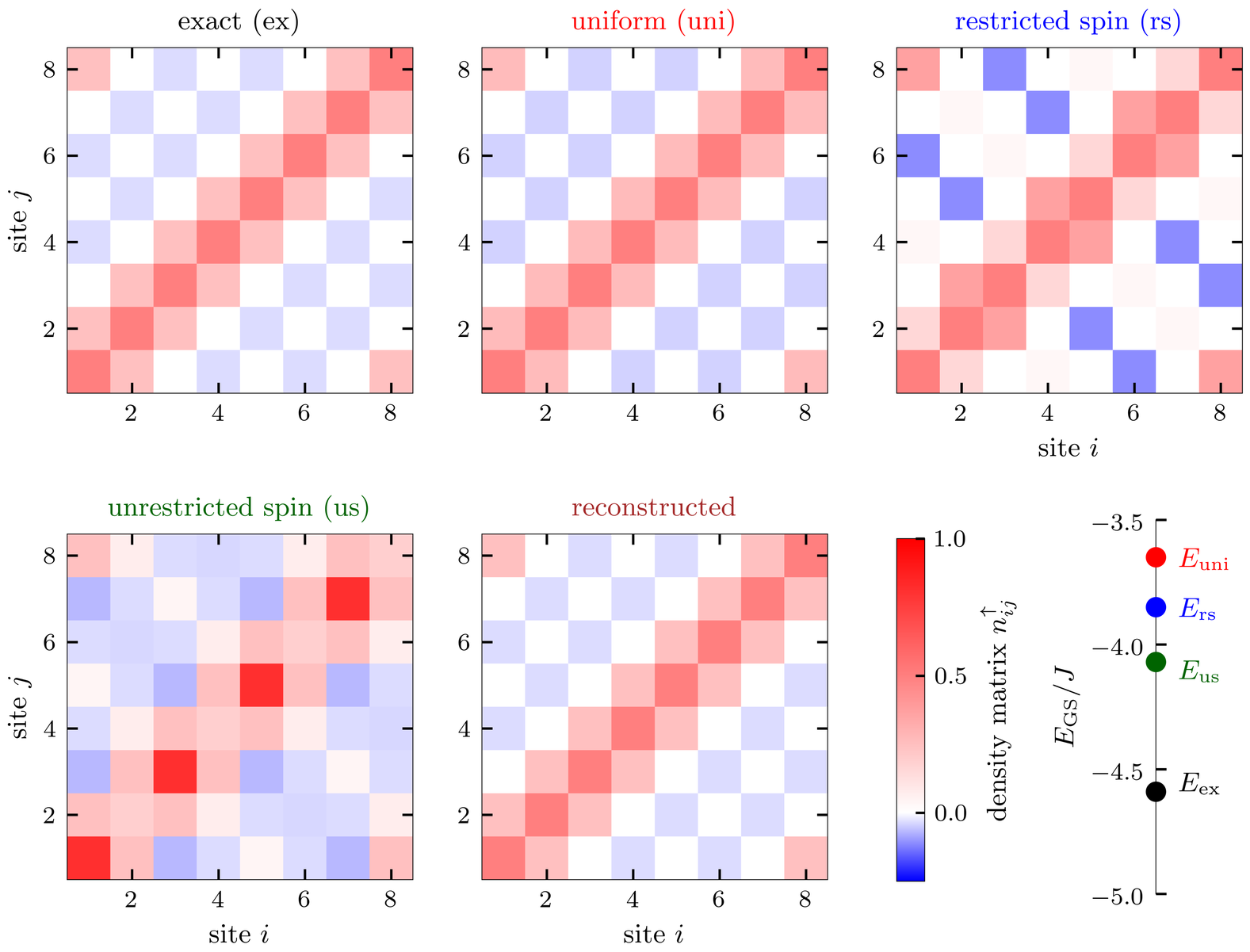

FIG. 1: Comparison of density matrix structures
All calculations used a half-filled, one-dimensional Hubbard chain with 8-sites, periodic boundary conditions and employed the SOA approximation with $U = 4J$.
The uniform approach (top center) reproduces the structure of the exact density matrix (top left), but exhibits no Hubbard gap (see FIG. 2.) and has a significantly higher energy (bottom right). The restricted spin method (top right) keeps the uniform structure only on the diagonal, but improves on both the energy and the Hubbard gap. Lifting the restrictions on spin (bottom left) produces a broken-symmetry state improving even further on the groundstate energy and the density of states while exhibiting a spin-density wave. From these broken symmetry states a spatially homogeneous density matrix (bottom center) can be recovered by resymmentrization[5].

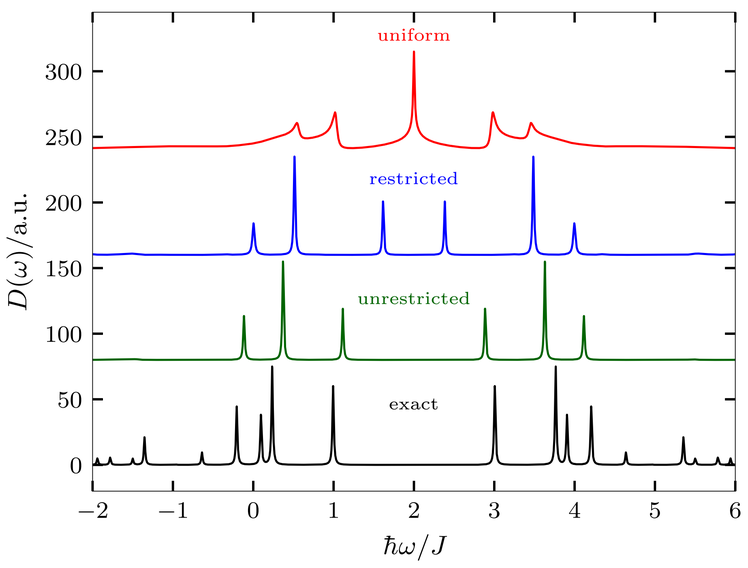

FIG. 2: Density of states for the different approaches
Same setup as in FIG. 1. The gap is non-existent for the uniform results, appears for the spin restricted calculation and closely matches the exact one when allowing unrestricted spins.

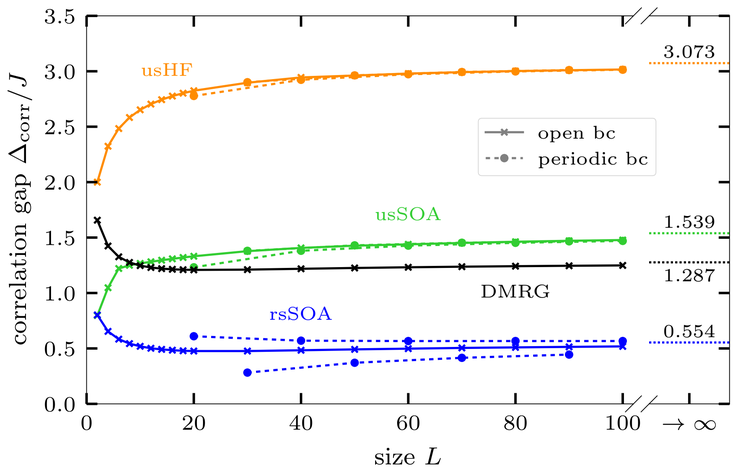

FIG. 3: Correlation gap size
Correlation gap energies for one-dimensional, half-filled Hubbard chains of different lengths L and $U = 4J$. Solid lines indicate open and dashed lines periodic boundary conditions. One the right the extrapolations for the limit $L \to \infty$ are given by the dotted lines.

Conclusion

- Forcing the uniformity of the density matrix does not reproduce the exact solution and shows worse results in spectral information and groundstate energy.
- Giving up the spatial uniformity constraint while still restricting the spin improves the energy and opens the Hubbard gap.
- The **unrestricted** approach produces broken-symmetry states even beyond Hartree-Fock and shows good agreement with the exact density of states and a better groundstate energy than restricted calculations.
- The reconstructed state from both possible unrestricted states reproduces the spacial uniformity of the exact density matrix.

Outlook

- First calculations for **higher order approximations** (GW, T-matrix, etc.) have shown similar results but need to be studied further.
- Extend the calculations to **two-dimensional** lattices.
- Investigations whether symmetry broken states persist in **non-equilibrium** circumstances.
- Calculating both spin directions allows for systems with unbalanced spin populations.

References

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