A Two-Subsystem Ground State Approximation

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1. Introduction

In modern solid-state physics the problem of addressing strong correlations of particles leads to exponentially large numerical problems.

This work was inspired by the Automated Multilevel Sub-structuring Method (AMLS, [1]). It relies on partitioning the physical space into smaller pieces wherein the eigenproblem is solved as a starting point for the calculation of the full system eigenvalues.

2. Partitioning the Occupation Number State Space

- Partition the Occupation Number space by the number of particles contained in each of two equally sized sub-systems
- Primary partition: equal amount of particles ($N/2$) in both sub-systems
- Further partitions: one, two or more particles *hopped* away from equilibrium configuration

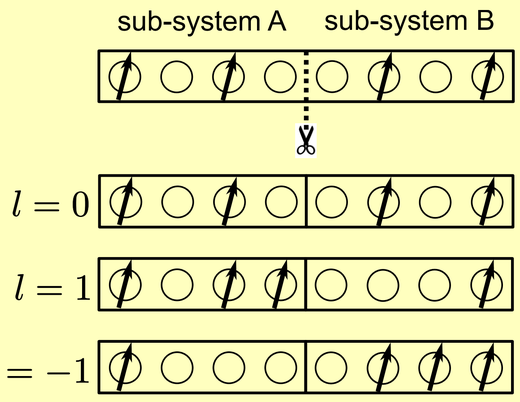

FIGURE 1: *Partitioning the Occupation Number state space by the number of particles in each sub-system. Here, representatives of each partition are depicted.*

- Particle numbers in partition i: $N/2+l_i$ and $N/2-l_i$ for sub-systems A and B, respectively
- The number of particles away from equilibrium is varied up to a maximum ($l=0,\pm1,..\pm l_{\max}$).

3. Hamiltonian Structure

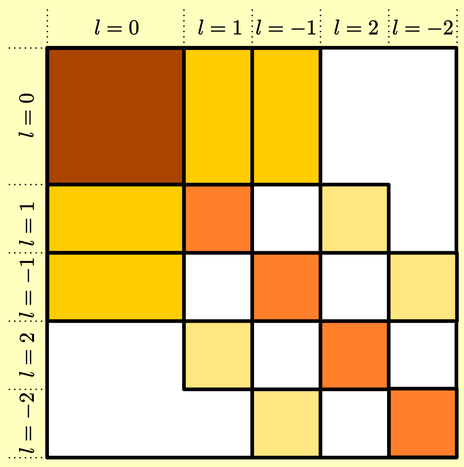

FIGURE 2: *Block-structured Hamiltonian: partitioning according to previous section ($l_{\max}=2$)*

4. Hamiltonian Transformation

- Consider the following exemplary Hamiltonian:

$$H=\begin{pmatrix} H_1 & H_{1,2} & H_{1,3} \\ H_{1,2}^\dagger & H_2 & 0 \\ H_{1,3}^\dagger & 0 & H_3 \end{pmatrix}$$

- Rotate the Hamiltonian orthogonally by a rotation matrix $V=\mathrm{diag}(V_1,V_2,V_3)$
- V_i are the partition eigenvalues ($H_iV_i=V_iD_i$):

$$H_r=V^\dagger HV=\begin{pmatrix} D_1 & V_1^\dagger H_{1,2}V_2 & V_1^\dagger H_{1,3}V_3 \\ V_2^\dagger H_{1,2}^\dagger V_1 & D_2 & 0 \\ V_3^\dagger H_{1,3}^\dagger V_1 & 0 & D_3 \end{pmatrix}$$

- The effective Hamiltonian can be limited in size by modal reduction of the partition eigensystems (e.g. use only an amount of vectors at the lower end of the spectrum)

5. Application to the Hubbard Model

Diagonal Blocks

Each partition Hamiltonian can be written as a tensor product of the sub-systems A and B with fixed number of particles:

$$H_i=H_{i,A}\otimes E_{i,B}+E_{i,A}\otimes H_{i,B} \qquad (1)$$

with $E_{i,X}$ the identity matrix. The partition eigenvalues D_i and eigenvectors V_i can be obtained from the sub-systems:

$$D_i=D_{i,A}\oplus D_{i,B}$$
$$V_i=V_{i,A}\otimes V_{i,B}$$

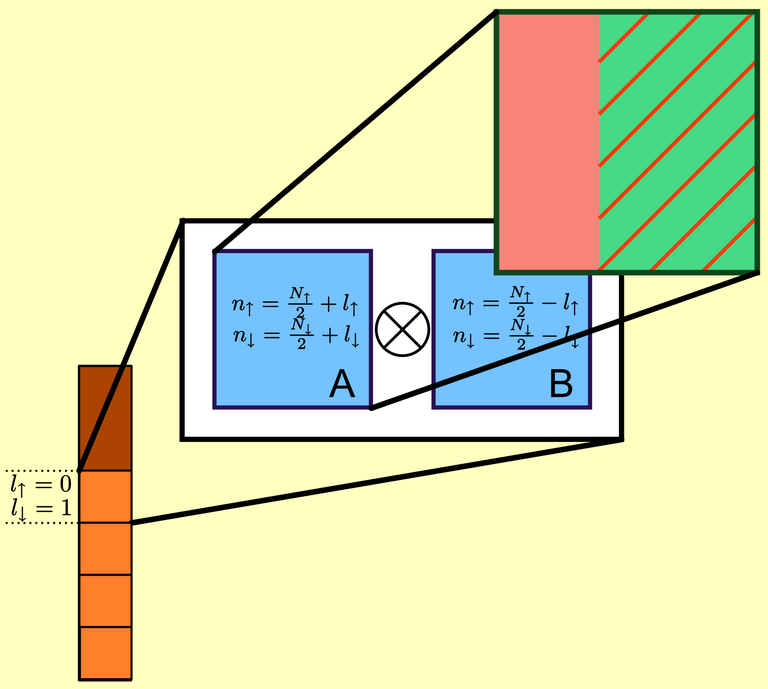

FIGURE 3: *The new basis V is constructed by individual partitions V_i (brown, orange), which are tensor products of the corresponding eigenvectors $V_{i,X}$ (blue). A modal reduction decreases the complexity (red, green).*

Off-Diagonal Blocks

The off-diagonal blocks can be represented by a sum over all possible particle exchange paths between the sub-systems:

$$H_{i,j}=\sum_\alpha \quad o_{\alpha,A}\otimes o_{\alpha,B}$$

The matrices $o_{\alpha,X}$ (indices i,j dropped) correspond to the annihilation and creation operators of quantum mechanics. The transformed blocks become:

$$V_i^\dagger H_{i,j}V_j=\sum_\alpha (V_{i,A}^\dagger o_{\alpha,A}V_{j,A})\otimes(V_{i,B}^\dagger o_{\alpha,B}V_{j,B})$$

6. Numerical Results

Croppings	E	$\lvert E-E_0\rvert$	$\left\lvert\frac{E-E_0}{E_0}\right\rvert$
80/60	-3.114643	0.1177	0.0361
80/60/30	-3.221613	0.0108	0.0033
80/60/40	-3.222737	0.0096	0.0030
80/60/50	-3.224861	0.0075	0.0023
80/60/50/20	-3.226303	0.0060	0.0019

TABLE 1: *Ground state energies of a Hubbard system ($L=12, N_\uparrow=N_\downarrow=6, U=10$) as estimated by TSGSA compared to Exact Diagonalization (Lanczos, basis size: 853776, $E_0=-3.232383$). The first column shows the croppings for the individual partitions used (e.g. for the first line 80 eigenmodes were used for the partition $l=0$, 60 for the partitions $l=\pm1$, etc.).*

System	Crop.	E	E_{DMRG}	$\left\lvert\frac{E-E_{\mathrm{DMRG}}}{E_{\mathrm{DMRG}}}\right\rvert$
$L=4,\ N_\uparrow=N_\downarrow=2$	4/2	-0.882	-0.911	0.032
$L=8,\ N_\uparrow=N_\downarrow=4$	36/24	-1.937	-1.975	0.019
$L=12,\ N_\uparrow=N_\downarrow=6$	50/25	-2.949	-3.041	0.030
$L=16,\ N_\uparrow=N_\downarrow=8$	50/25	-3.961	-4.109	0.036
$L=20,\ N_\uparrow=N_\downarrow=10$	50/25	-5.021	-5.178	0.030
$L=24,\ N_\uparrow=N_\downarrow=12$	50/25	-6.090	-6.245	0.025

TABLE 2: *Hubbard-TSGSA for multiple Hubbard system sizes compared with DMRG.*

7. Conclusions and Outlook

Advantages of the presented approach

- Selection of partitions by importance
- Each partition described by tensor product
- TSGSA basis completely obtained using subsystem complexity
- Modal reduction of sub-system solutions
- Explicit matrix representation available
- Easily adopted to multi-dimensional systems

Further possibilities

- Sophisticated selection of sub-system eigenmodes
- Calculation of dynamic properties

References

[1] Jeffrey K. Bennighof and R. B. Lehoucq. An automated multilevel substructuring method for eigenspace computation in linear elastodynamics. *SIAM Journal on Scientific Computing*, 25(6):2084–2106, 2004.