Exercise 6 (optional): DMRG for the particle on-a-chain problem

In this exercise, we will use the Density Matrix Renormalization Group (DMRG) method to optain the ground state energy for the particle on-a-chain problem. The Hamiltonian we will consider is

$$H = -t\sum_{i=1}^{L-1}\left(|i\rangle\langle i+1| + |i+1\rangle\langle i|\right) + 2\sum_{i=1}^{L}|i\rangle\langle i|$$

where the state $|i\rangle$ corresponds to a localized tight-binding orbital on site i. The value 2 on the diagonal is chosen so that this operator is just the discretization of the second derivative operator $-\partial^2/\partial x$.

Let's divide the system up into four pieces, called blocks. Block-1 (the "left block") consists of sites 1...s; block-2 and -3 are single sites being $s+1$ and $s+2$; and block-4 (the "right block") consists of sites $s+3$...L. So the total length of our chain is L. During the course of the algorithm, the dividing point s will be moved back and forth through the system, so that every site except the first and last is represented by one of the two middle sites during a "sweep".

We represent each block by a single basis state, which lead us to diagonalize only 4x4 matrices. For the middle blocks it is exact, but for the left and right this is a severe limitation. In this basis the wavefunction ϕ_j, with $j = 1, \ldots, L$, is writen as

$$\phi_j = \begin{cases} a_1 L_j & j \leq s \\ a_2 & j = s+1 \\ a_3 & j = s+2 \\ a_4 R_j & j \geq s+3 \end{cases}$$

The Hamiltonian matrix in our restricted basis is written as

$$\langle\phi|H|\phi'\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}^T \begin{pmatrix} H_{11} & T_{12} & 0 & 0 \\ T_{21} & 2 & -1 & 0 \\ 0 & -1 & 2 & T_{34} \\ 0 & 0 & T_{43} & H_{44} \end{pmatrix} \begin{pmatrix} a'_1 \\ a'_2 \\ a'_3 \\ a'_4 \end{pmatrix},$$

where $H_{11} = \langle L|H|L\rangle$, $H_{44} = \langle R|H|R\rangle$, $T_{12} = T_{21} = \langle L|H|s+1\rangle = -L_s$ and $T_{34} = T_{43} = \langle s+2|H|R\rangle = -R_{s+3}$. The basis states L and R are defined only in the corresponding blocks and normalized by $\langle L|L\rangle = \langle R|R\rangle = 1$.

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In order to find the ground state of the system we should improve the set of basis states, $\{L(s)\}$ and $\{R(s)\}$. To do so, we improved the basis state $L(s+1)$ using the known $L(s)$ and $R(s+3)$, and proceed though the lattice to the right. Once the right end is reached, we reverse the procedure improving $R(s+2)$, given $L(s)$ and $R(s+3)$ sweeping in reverse direction and eventually improving the whole set $\{R(s)\}$.

1. *Warm up sweep: Left-to-right.*

   - Diagonalize the initial 4x4 matrix and obtain the ground state wavefunction written as (a_1, a_2, a_3, a_4).
   - Normalize a_1 and a_2 as $a_1' = a_1/N$ and $a_2' = a_2/N$, where $N = \sqrt{a_1^2 + a_2^2}$. Such that, the new basis state properly normalized is

   $$L(s+1)' = \begin{pmatrix} a_1' L(s)_1 \\ \vdots \\ a_1' L(s)_s \\ a_2' \end{pmatrix}$$

   - Calculate the new Hamiltonian matrix element, needed to construct H for the next step:

   $$\langle L(s+1)'|H|L(s+1)'\rangle = a_1'^2 \langle L(s)|H|L(s)\rangle + 2a_2' - 2a_1' a_2' L(s)_s$$

   Note: Starting with a $L = 4$ system, the left and right blocks are just single sites with trivial $L = L(1)$ and $R = R(1)$. Use this system to get an approximate $L(2)$ for the $L = 6$ system and for the right block let's use the reflection of $L(2)$. At each additional step, use a reflection of the left block for the right one. In this way, the system gradually grows up to the desired size L, generating an initial set of $\{L(s)\}$ and $\{R(s)\}$.

2. *Finite system sweeps.*

   - To perform the right-to-left sweep using the $L(s)$ basis states, you need to calculate the Hamiltonian matrix element in a similar way as before:

   $$\langle R(s+2)'|H|R(s+2)'\rangle = a_2'^2 \langle R(s+3)|H|R(s+3)\rangle + 2a_1' - 2a_1' a_2' R(s+3)_{s+3},$$

   where $a_1' = a_3/N$ and $a_2' = a_4/N$ with $N = \sqrt{a_3^2 + a_4^2}$.

3. *Calculate the observables.*

   - Keep track of the energy through out the sweeps, you will realized how fast is the convergency to the ground state value, which you can calculate analytically for this particular example.