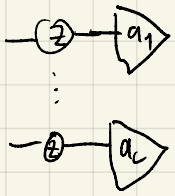
$$P = \prod_{j=1}^{L} Z_j = Z \otimes \cdots \otimes Z.$$

(a) Show that the eigenstates of P are precisely the computational basis states $|a_1\rangle \otimes \cdots \otimes |a_L\rangle \equiv |a_1 \dots a_L\rangle$ with $a_j \in \{0, 1\}$ for all j, with corresponding eigenvalues ± 1. How is the eigenvalue related to the bit string $a_1 \dots a_L$?

$Z \cdot |0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle$ $\quad Z \cdot |1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -1\,|1\rangle$

$P\,|a_1 \dots a_L\rangle =$ 

$= s_1 |a_1\rangle \otimes \dots \otimes s_L |a_L\rangle = (s_1 \cdot \dots \cdot s_L) \cdot |a_1 \dots a_L\rangle = \pm |a_1 \dots a_L\rangle$

$s_j = \begin{cases} 1 & \text{if } a_j = 0 \\ -1 & \text{if } a_j = 1 \end{cases}$

$\Rightarrow \pm 1$ eigenvalue

$\Rightarrow |a_1 \dots a_L\rangle$ eigenvector

For bit-string $a_1 \dots a_L$ eigenvalue is 1 if number of 1s is even (even number of $s_j = -1 \Rightarrow (-1)\cdot(-1) = 1$)

In the following, we associate the overall quantum number 0 with eigenvalue 1 of P, and the overall quantum number 1 with eigenvalue -1, such that $\lambda = (-1)^q$, where λ is the eigenvalue and q the quantum number. Addition of quantum numbers is understood modulo 2.

(b) At each lattice site, we likewise attach the (local) quantum number 0 to $|0\rangle$ and 1 to $|1\rangle$. Based on the sparsity pattern of I_2, X and Z, decide which of these matrices leave the quantum number invariant, and which change it (equivalent to incrementing it by 1 modulo 2).

$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\Rightarrow I_2$ and Z leave the quantum number invariant (diagonal matrix)

$\Rightarrow X$ changes the number

Recall that the Ising Hamiltonian admits a MPO representation, with tensors (for the current convention)

$$A^1 = \begin{pmatrix} -gZ & -JX & I_2 \end{pmatrix}, \quad A^j = \begin{pmatrix} I_2 & 0 & 0 \\ X & 0 & 0 \\ -gZ & -JX & I_2 \end{pmatrix} \; \forall j = 2, \dots, L-1, \quad A^L = \begin{pmatrix} I_2 \\ X \\ -gZ \end{pmatrix}.$$

(c) Assign quantum numbers 0 and 1 to the virtual bonds (the finite automaton "states" a, b, c from the lecture, or equivalently the input and output channels of A^j) such that they are compatible with the behavior of the entries I_2, X and Z of A^j found in (b).

a is $|0\rangle$ because $-gZ\,|0\rangle = -g\,|0\rangle \Rightarrow$ leaves quantum number unchanged

$\Rightarrow$ c is $|0\rangle \Rightarrow$ number needs to stay the same

b is $|1\rangle \longrightarrow X \cdot a = X \cdot |0\rangle = |1\rangle \Rightarrow -JX \cdot b = |0\rangle \Rightarrow$ fits to c

exercise11.2_template

July 12, 2022

1 DMRG and TEBD algorithms

[1]:
```
import numpy as np
from scipy.linalg import expm
from scipy import sparse
import scipy.sparse.linalg as scila
from copy import deepcopy
import matplotlib.pyplot as plt
```

1.1 Utility functions

[2]:
```
def crandn(size):
    """
    Draw random samples from the standard complex normal (Gaussian)␣
 ↪distribution.
    """
    # 1/sqrt(2) is a normalization factor
    return (np.random.normal(size=size) + 1j*np.random.normal(size=size)) / np.
 ↪sqrt(2)
```

[3]:
```
def retained_bond_indices(s, tol):
    """
    Indices of retained singular values based on given tolerance.
    """
    w = np.linalg.norm(s)
    if w == 0:
        return np.array([], dtype=int)
    # normalized squares
    s = (s / w)**2
    # accumulate values from smallest to largest
    sort_idx = np.argsort(s)
    s[sort_idx] = np.cumsum(s[sort_idx])
    return np.where(s > tol)[0]
```

[4]:
```
def split_matrix_svd(A, tol):
    """
    Split a matrix by singular value decomposition,
```

```
    and truncate small singular values based on tolerance.
    """
    assert A.ndim == 2
    u, s, v = np.linalg.svd(A, full_matrices=False)
    # truncate small singular values
    idx = retained_bond_indices(s, tol)
    u = u[:, idx]
    v = v[idx, :]
    s = s[idx]
    return u, s, v
```

1.2 MPS class and related utility functions

[5]:
```
def local_orthonormalize_left_qr(A, Anext):
    """
    Left-orthonormalize a MPS tensor `A` by a QR decomposition,
    and update tensor at next site.
    """
    # perform QR decomposition and replace A by reshaped Q matrix
    s = A.shape
    assert len(s) == 3
    Q, R = np.linalg.qr(np.reshape(A, (s[0]*s[1], s[2])), mode='reduced')
    A = np.reshape(Q, (s[0], s[1], Q.shape[1]))
    # update Anext tensor: multiply with R from left
    Anext = np.transpose(np.tensordot(R, Anext, (1, 1)), (1, 0, 2))
    return A, Anext
```

[6]:
```
def local_orthonormalize_right_qr(A, Aprev):
    """
    Right-orthonormalize a MPS tensor `A` by a QR decomposition,
    and update tensor at previous site.
    """
    # flip left and right virtual bond dimensions
    A = np.transpose(A, (0, 2, 1))
    # perform QR decomposition and replace A by reshaped Q matrix
    s = A.shape
    assert len(s) == 3
    Q, R = np.linalg.qr(np.reshape(A, (s[0]*s[1], s[2])), mode='reduced')
    A = np.transpose(np.reshape(Q, (s[0], s[1], Q.shape[1])), (0, 2, 1))
    # update Aprev tensor: multiply with R from right
    Aprev = np.tensordot(Aprev, R, (2, 1))
    return A, Aprev
```

[7]:
```
def merge_mps_tensor_pair(A0, A1):
    """
    Merge two neighboring MPS tensors.
```

```
    """
    A = np.tensordot(A0, A1, (2, 1))
    # pair original physical dimensions of A0 and A1
    A = A.transpose((0, 2, 1, 3))
    # combine original physical dimensions
    A = A.reshape((A.shape[0]*A.shape[1], A.shape[2], A.shape[3]))
    return A
```

[8]:
```
class MPS(object):
    """
    Matrix product state (MPS) class.

    The i-th MPS tensor has dimension `[d, D[i], D[i+1]]` with `d` the physical
    dimension at each site and `D` the list of virtual bond dimensions.
    """

    def __init__(self, d, D, fill='zero'):
        """
        Create a matrix product state.
        """
        self.d = d
        # leading and trailing bond dimensions must agree (typically 1)
        assert D[0] == D[-1]
        if fill == 'zero':
            self.A = [np.zeros((d, D[i], D[i+1])) for i in range(len(D)-1)]
        elif fill == 'random real':
            # random real entries
            self.A = [np.random.normal(size=(d, D[i], D[i+1])) / np.
 ↪sqrt(d*D[i]*D[i+1]) for i in range(len(D)-1)]
        elif fill == 'random complex':
            # random complex entries
            self.A = [crandn(size=(d, D[i], D[i+1])) / np.sqrt(d*D[i]*D[i+1])␣
 ↪for i in range(len(D)-1)]
        else:
            raise ValueError('fill = {} invalid.'.format(fill))

    @property
    def local_dim(self):
        """Local (physical) dimension at each lattice site."""
        return self.d

    @property
    def nsites(self):
        """Number of lattice sites."""
        return len(self.A)

    @property
```

```
    def bond_dims(self):
        """Virtual bond dimensions."""
        if len(self.A) == 0:
            return []
        else:
            D = [self.A[i].shape[1] for i in range(len(self.A))]
            D.append(self.A[-1].shape[2])
            return D

    @property
    def dtype(self):
        """Data type of tensor entries."""
        return self.A[0].dtype

    def orthonormalize(self, mode='left'):
        """Left- or right-orthonormalize the MPS using QR decompositions."""
        if len(self.A) == 0:
            return

        if mode == 'left':
            for i in range(len(self.A) - 1):
                self.A[i], self.A[i+1] = local_orthonormalize_left_qr(self.
↪A[i], self.A[i+1])
            # last tensor
            self.A[-1], T = local_orthonormalize_left_qr(self.A[-1], np.
↪array([[[1.0]]]))
            # normalization factor (real-valued since diagonal of R matrix is␣
↪real)
            assert T.shape == (1, 1, 1)
            nrm = T[0, 0, 0].real
            if nrm < 0:
                # flip sign such that normalization factor is always␣
↪non-negative
                self.A[-1] = -self.A[-1]
                nrm = -nrm
            return nrm
        elif mode == 'right':
            for i in reversed(range(1, len(self.A))):
                self.A[i], self.A[i-1] = local_orthonormalize_right_qr(self.
↪A[i], self.A[i-1])
            # first tensor
            self.A[0], T = local_orthonormalize_right_qr(self.A[0], np.
↪array([[[1.0]]]))
            # normalization factor (real-valued since diagonal of R matrix is␣
↪real)
            assert T.shape == (1, 1, 1)
```

```
            nrm = T[0, 0, 0].real
            if nrm < 0:
                # flip sign such that normalization factor is always␣
↪non-negative
                self.A[0] = -self.A[0]
                nrm = -nrm
            return nrm
        else:
            raise ValueError('mode = {} invalid; must be "left" or "right".'.
↪format(mode))

    def as_vector(self):
        """Merge all tensors to obtain the vector representation on the full␣
↪Hilbert space."""
        psi = self.A[0]
        for i in range(1, len(self.A)):
            psi = merge_mps_tensor_pair(psi, self.A[i])
        assert psi.ndim == 3
        # contract leftmost and rightmost virtual bond (has no influence if␣
↪these virtual bond dimensions are 1)
        psi = np.trace(psi, axis1=1, axis2=2)
        return psi
```

[9]:
```
def split_mps_tensor(A, d0, d1, svd_distr, tol=0):
    """
    Split a MPS tensor with dimension `d0*d1 x D0 x D2` into two MPS tensors
    with dimensions `d0 x D0 x D1` and `d1 x D1 x D2`, respectively.
    """
    assert A.ndim == 3
    assert d0 * d1 == A.shape[0], 'physical dimension of MPS tensor must be␣
↪equal to d0 * d1'
    # reshape as matrix and split by SVD
    A = np.transpose(np.reshape(A, (d0, d1, A.shape[1], A.shape[2])), (0, 2, 1,␣
↪3))
    s = A.shape
    A0, sigma, A1 = split_matrix_svd(A.reshape((s[0]*s[1], s[2]*s[3])), tol)
    A0.shape = (s[0], s[1], len(sigma))
    A1.shape = (len(sigma), s[2], s[3])
    # use broadcasting to distribute singular values
    if svd_distr == 'left':
        A0 = A0 * sigma
    elif svd_distr == 'right':
        A1 = A1 * sigma[:, None, None]
    elif svd_distr == 'sqrt':
        s = np.sqrt(sigma)
        A0 = A0 * s
```

```
        A1 = A1 * s[:, None, None]
    else:
        raise ValueError('svd_distr parameter must be "left", "right" or "sqrt".
↪')
    # move physical dimension to the front
    A1 = A1.transpose((1, 0, 2))
    return A0, A1
```

[10]:
```
def is_left_orthonormal(A):
    """
    Test whether a MPS tensor `A` is left-orthonormal.
    """
    s = A.shape
    assert len(s) == 3
    A = np.reshape(A, (s[0]*s[1], s[2]))
    return np.allclose(A.conj().T @ A, np.identity(s[2]))
```

[11]:
```
def is_right_orthonormal(A):
    """
    Test whether a MPS tensor `A` is right-orthonormal.
    """
    # call `is_left_orthonormal` with flipped left and right virtual bond␣
↪dimensions
    return is_left_orthonormal(np.transpose(A, (0, 2, 1)))
```

1.3 MPO class and related utility functions

[12]:
```
def merge_mpo_tensor_pair(A0, A1):
    """
    Merge two neighboring MPO tensors.
    """
    A = np.tensordot(A0, A1, (3, 2))
    # pair original physical dimensions of A0 and A1
    A = np.transpose(A, (0, 3, 1, 4, 2, 5))
    # combine original physical dimensions
    A = A.reshape((A.shape[0]*A.shape[1], A.shape[2]*A.shape[3], A.shape[4], A.
↪shape[5]))
    return A
```

[13]:
```
class MPO(object):
    """
    Matrix product operator (MPO) class.

    The i-th MPO tensor has dimension `[d, d, D[i], D[i+1]]` with `d` the␣
↪physical
    dimension at each site and `D` the list of virtual bond dimensions.
```

```
    """

    def __init__(self, Alist):
        """
        Create a matrix product operator.
        """
        self.A = [np.array(Aj) for Aj in Alist]
        # consistency checks
        for i in range(len(self.A)-1):
            assert self.A[i].ndim == 4
            assert self.A[i].shape[3] == self.A[i+1].shape[2]
        assert self.A[0].shape[2] == self.A[-1].shape[3]

    @property
    def nsites(self):
        """Number of lattice sites."""
        return len(self.A)

    @property
    def bond_dims(self):
        """Virtual bond dimensions."""
        if len(self.A) == 0:
            return []
        else:
            D = [self.A[i].shape[2] for i in range(len(self.A))]
            D.append(self.A[-1].shape[3])
            return D

    def as_matrix(self):
        """Merge all tensors to obtain the matrix representation on the full␣
↪Hilbert space."""
        op = self.A[0]
        for i in range(1, len(self.A)):
            op = merge_mpo_tensor_pair(op, self.A[i])
        assert op.ndim == 4
        # contract leftmost and rightmost virtual bond (has no influence if␣
↪these virtual bond dimensions are 1)
        op = np.trace(op, axis1=2, axis2=3)
        return op
```

1.4 Transverse-field Ising model

1.4.1 Construct Ising Hamiltonian as MPO

[14]:
```
def construct_ising_hamiltonian_mpo(J, g, L, pbc=False):
    """
    Construct Ising Hamiltonian on a 1D lattice with `L` sites as MPO,
    for interaction parameter `J` and external field parameter `g`.
    """
    # Pauli-X and Z matrices
    X = np.array([[0., 1.], [1.,  0.]])
    Z = np.array([[1., 0.], [0., -1.]])
    I = np.identity(2)
    O = np.zeros((2, 2))
    A = np.array([[I, O, O], [Z, O, O], [-g*X, -J*Z, I]])
    # flip the ordering of the virtual bond dimensions and physical dimensions
    A = np.transpose(A, (2, 3, 0, 1))
    if pbc:
        # periodic boundary conditions:
        # add a direct transition b -> a which applies -J Z at the rightmost␣
↪lattice site
        AL = np.array([[-g*X, -J*Z, I], [Z, O, O]])
        AR = np.array([[I, -J*Z], [Z, O], [-g*X, O]])
        # flip the ordering of the virtual bond dimensions and physical␣
↪dimensions
        AL = np.transpose(AL, (2, 3, 0, 1))
        AR = np.transpose(AR, (2, 3, 0, 1))
        return MPO([AL if i == 0 else A if i < L-1 else AR for i in range(L)])
    else:
        return MPO([A[:, :, 2:3, :] if i == 0 else A if i < L-1 else A[:, :, :,␣
↪0:1] for i in range(L)])
```

1.4.2 Construct Ising Hamiltonian as sparse matrix (for comparison and testing)

[15]:
```
def adjacency_1D_lattice(L, pbc=True):
    """
    Construct the adjacency matrix for a 1D lattice with `L` sites.
    The optional parameter `pbc` specifies whether periodic boundary conditions
    should be used.
    """
    assert L > 1
    # special case
    if L == 2:
        return np.array([[0, 1], [1, 0]])
    if pbc:
        # periodic boundary conditions
```

```
        return np.roll(np.identity(L, dtype=int), -1, axis=0) + np.roll(np.
↪identity(L, dtype=int), 1, axis=0)
    else:
        # open boundary conditions
        return np.diag(np.ones(L - 1, dtype=int), k=-1) + np.diag(np.ones(L -␣
↪1, dtype=int), k=1)
```

[16]:
```
# should be symmetric
np.linalg.norm(adjacency_1D_lattice(6) - adjacency_1D_lattice(6).T)
```

[16]:
```
0.0
```

[17]:
```
# each site should have 2 neighbors (for periodic boundary conditions)
np.sum(adjacency_1D_lattice(6), axis=0)
```

[17]:
```
array([2, 2, 2, 2, 2, 2])
```

[18]:
```
# example
adjacency_1D_lattice(6, pbc=False)
```

[18]:
```
array([[0, 1, 0, 0, 0, 0],
       [1, 0, 1, 0, 0, 0],
       [0, 1, 0, 1, 0, 0],
       [0, 0, 1, 0, 1, 0],
       [0, 0, 0, 1, 0, 1],
       [0, 0, 0, 0, 1, 0]])
```

[19]:
```
def construct_ising_hamiltonian_sparse(J, g, adj):
    """
    Construct Ising Hamiltonian as sparse matrix,
    for interaction parameter `J` and external field parameter `g`.
    `adj` is the adjacency matrix of the underlying lattice.
    """
    # Pauli-X and Z matrices
    X = sparse.csr_matrix([[0., 1.], [1.,  0.]])
    Z = sparse.csr_matrix([[1., 0.], [0., -1.]])
    # overall number of lattice sites
    L = adj.shape[0]
    H = sparse.csr_matrix((2**L, 2**L), dtype=float)
    for j in range(L):
        for k in range(j+1, L):
            if adj[j, k] > 0:
                H -= J * sparse.kron(sparse.eye(2**j),
                         sparse.kron(Z,
                         sparse.kron(sparse.eye(2**(k-j-1)),
                         sparse.kron(Z,
                                     sparse.eye(2**(L-k-1))))))
```

```
    # external field
    for j in range(L):
        H -= g * sparse.kron(sparse.eye(2**j), sparse.kron(X, sparse.
 ↪eye(2**(L-j-1))))
    return H
```

[20]:
```
# example
Hising_sparse = construct_ising_hamiltonian_sparse(1.1, 0.7,␣
 ↪adjacency_1D_lattice(6, pbc=False))
Hising_sparse
```

[20]:
```
<64x64 sparse matrix of type '<class 'numpy.float64'>'
        with 448 stored elements in Compressed Sparse Row format>
```

[21]:
```
# convert to NumPy array to show entries
Hising_sparse.toarray()
```

[21]:
```
array([[-5.5, -0.7, -0.7, …,  0. ,  0. ,  0. ],
       [-0.7, -3.3,  0. , …,  0. ,  0. ,  0. ],
       [-0.7,  0. , -1.1, …,  0. ,  0. ,  0. ],
       …,
       [ 0. ,  0. ,  0. , …, -1.1,  0. , -0.7],
       [ 0. ,  0. ,  0. , …,  0. , -3.3, -0.7],
       [ 0. ,  0. ,  0. , …, -0.7, -0.7, -5.5]])
```

[22]:
```
# compare (difference should be zero)
np.linalg.norm(Hising_sparse - construct_ising_hamiltonian_mpo(1.1, 0.7, 6).
 ↪as_matrix())
```

[22]:
```
0.0
```

[23]:
```
# compare for periodic boundary conditions (difference should be zero)
np.linalg.norm(construct_ising_hamiltonian_sparse(1.1, 0.7,␣
 ↪adjacency_1D_lattice(6, pbc=True)) - construct_ising_hamiltonian_mpo(1.1, 0.
 ↪7, 6, pbc=True).as_matrix())
```

[23]:
```
0.0
```

1.4.3 Construct Ising Hamiltonian as sum of local interaction terms (for TEBD)

[24]:
```
def construct_ising_hamiltonian_local_terms(J, g, L):
    """
    Construct Ising Hamiltonian on a one-dimensional lattice
    with open boundary conditions as sum of local interaction terms,
    for interaction parameter `J` and external field parameter `g`.
    """
    # Pauli-X and Z matrices
```

```
    X = np.array([[0., 1.], [1.,  0.]])
    Z = np.array([[1., 0.], [0., -1.]])
    I = np.identity(2)
    return [-J*np.kron(Z, Z) - g*(np.kron(X, I) + 0.5*np.kron(I, X)) if i == 0␣
↪else
            -J*np.kron(Z, Z) - g*0.5*(np.kron(X, I) + np.kron(I, X)) if i < L-2␣
↪else
            -J*np.kron(Z, Z) - g*(0.5*np.kron(X, I) + np.kron(I, X))
                for i in range(L-1)]
```

[25]:
```
# example
hloc = construct_ising_hamiltonian_local_terms(1.1, 0.7, 6)
hloc
```

[25]:
```
[array([[-1.1 , -0.35, -0.7 , -0.  ],
        [-0.35,  1.1 , -0.  , -0.7 ],
        [-0.7 , -0.  ,  1.1 , -0.35],
        [-0.  , -0.7 , -0.35, -1.1 ]]),
 array([[-1.1 , -0.35, -0.35, -0.  ],
        [-0.35,  1.1 , -0.  , -0.35],
        [-0.35, -0.  ,  1.1 , -0.35],
        [-0.  , -0.35, -0.35, -1.1 ]]),
 array([[-1.1 , -0.35, -0.35, -0.  ],
        [-0.35,  1.1 , -0.  , -0.35],
        [-0.35, -0.  ,  1.1 , -0.35],
        [-0.  , -0.35, -0.35, -1.1 ]]),
 array([[-1.1 , -0.35, -0.35, -0.  ],
        [-0.35,  1.1 , -0.  , -0.35],
        [-0.35, -0.  ,  1.1 , -0.35],
        [-0.  , -0.35, -0.35, -1.1 ]]),
 array([[-1.1 , -0.7 , -0.35, -0.  ],
        [-0.7 ,  1.1 , -0.  , -0.35],
        [-0.35, -0.  ,  1.1 , -0.7 ],
        [-0.  , -0.35, -0.7 , -1.1 ]])]
```

[26]:
```
# for testing: construct overall sparse matrix representation of H from local␣
↪terms
Hloc = sparse.csr_matrix((2**6, 2**6), dtype=float)
for j in range(6-1):
    Hloc += sparse.kron(sparse.eye(2**j),
            sparse.kron(hloc[j],
                        sparse.eye(2**(6-j-2))))
```

[27]:
```
# compare (difference should be zero)
np.linalg.norm(Hising_sparse.toarray() - Hloc)
```

[27]: 0.0

1.5 Core DMRG algorithm

[28]:
```
def contract_left_block(A, W, L):
    """
    Contraction step from left to right, with a matrix product operator
    sandwiched in between.

    To-be contracted tensor network::


      ---------           -----
     /         \         /     \
     |        0|---   ---|1 A 2|---
     |         |         \__0__/
     |         |            |
     |         |
     |         |          __|__
     |         |         /  1  \
     |    L   1|---   ---|2 W 3|---
     |         |         \__0__/
     |         |            |
     |         |
     |         |          __|__
     |         |         /  0  \
     |        2|---   ---|1 A*2|---
     \_________/         \_____/
    """

    assert A.ndim == 3
    assert W.ndim == 4
    assert L.ndim == 3

    # multiply with conjugated A tensor
    T = np.tensordot(L, A.conj(), axes=(2, 1))

    # multiply with W tensor
    T = np.tensordot(W, T, axes=((0, 2), (2, 1)))

    # multiply with A tensor
    Lnext = np.tensordot(A, T, axes=((0, 1), (0, 2)))

    return Lnext
```

[29]:
```
def contract_right_block(A, W, R):
    """
    Contraction step from right to left, with a matrix product operator
    sandwiched in between.
```

```
    To-be contracted tensor network::

         _____           _________
        /     \         /         \
      ---|1 A 2|---   ---|0        |
        \__0__/         |         |
           |            |         |
                        |         |
         __|__          |         |
        /  1  \         |         |
      ---|2 W 3|---   ---|1   R    |
        \__0__/         |         |
           |            |         |
                        |         |
         __|__          |         |
        /  0  \         |         |
      ---|1 A*2|---   ---|2        |
        \_____/         \_________/
    """

    T = np.tensordot(R, A.conj(), axes=(2, 2))

    T = np.tensordot(W, T, axes=((3, 0), (1, 2)))

    T = np.tensordot(A, T, ((2, 0), (2, 0)))

    return T
```

[30]:
```
def compute_right_operator_blocks(psi, op):
    """
    Compute all partial contractions from the right.
    """
    L = psi.nsites
    assert L == op.nsites
    BR = [None for _ in range(L)]
    # initialize rightmost dummy block
    BR[-1] = np.array([[[1]]], dtype=psi.dtype)
    for i in reversed(range(L-1)):
        BR[i] = contract_right_block(psi.A[i+1], op.A[i+1], BR[i+1])
    return BR
```

[31]:
```
def construct_local_two_site_hamiltonian(V, W, L, R):
    """
    Construct the two-site local Hamiltonian operator.

    To-be contracted tensor network (the indices at the open legs
    show the ordering for the output tensor of degree 8)::
```

```
                6       4               5       7
 _________      |       |               |       |     _________
/         \     |       |               |       |    /         \
|        0|---/        |               |       \---|0        |
|         |            |               |           |         |
|         |            |               |           |         |
|         |            |               |           |         |
|         |            |               |           |         |
|         |          __|__           __|__         |         |
|         |         /  1  \         /  1  \         |         |
|    L   1|---   ---|2 V 3|---   ---|2 W 3|---   ---|1   R    |
|         |         \__0__/         \__0__/         |         |
|         |            |               |           |         |
|         |            |               |           |         |
|         |            |               |           |         |
|         |            |               |           |         |
|         |            |               |           |         |
|        2|---\        |               |        /--|2        |
\_________/    |       |               |       |   \_________/
               |       |               |       |
               2       0               1       3
    """
    # repeated indices are summed over
    return np.einsum(V, (0, 1, 2, 3), W, (4, 5, 3, 6), L, (7, 2, 8), R, (9, 6,␣
↪10), (0, 4, 8, 10, 1, 5, 7, 9))
```

[32]:
```
def dmrg_two_site(H:MPO, psi:MPS, numsweeps, tol=1e-5):
    """
    Approximate the ground state MPS by left and right sweeps and local␣
↪two-site optimizations.

    Args:
        H: Hamiltonian as MPO
        psi: initial MPS used for optimization; will be overwritten
        numsweeps: maximum number of left and right sweeps
        tol: "tolerance" for SVD truncation

    Returns:
        numpy.ndarray: array of approximate ground state energies after each␣
↪iteration
    """

    # number of lattice sites
    L = H.nsites
    assert L == psi.nsites

    # right-normalize input matrix product state
    psi.orthonormalize(mode='right')
```

```
    # left and right operator blocks
    # initialize leftmost block by 1x1x1 identity
    BR = compute_right_operator_blocks(psi, H)
    BL = [None for _ in range(L)]
    BL[0] = np.array([[[1.0]]], dtype=BR[0].dtype)

    en_min = np.zeros(numsweeps)

    # Number of iterations should be determined by tolerance and some␣
↪convergence measure
    for n in range(numsweeps):
        en = 0

        # sweep from left to right (rightmost two lattice sites are handled by␣
↪right-to-left sweep)
        for i in range(L - 2):
            Hloc = construct_local_two_site_hamiltonian(H.A[i], H.A[i+1],␣
↪BL[i], BR[i+1])
            s = Hloc.shape
            assert s[0] == s[1] == psi.local_dim
            assert s[4] == s[5] == psi.local_dim
            # reshape into a matrix
            Hloc = np.reshape(Hloc, (s[0]*s[1]*s[2]*s[3], s[4]*s[5]*s[6]*s[7]))
            # The following can be accelerated by Krylov methods and a "matrix␣
↪free" application of the local Hamiltonian.
            wloc, vloc = np.linalg.eigh(Hloc)
            # select first eigenvector corresponding to lowest energy
            en = wloc[0]
            # optimized local tensor for two sites
            Aloc = np.reshape(vloc[:, 0], (s[0]*s[1], s[2], s[3]))
            #TODO: call "split_mps_tensor" here with the appropriate␣
↪distribution direction of singluar values, and also pass the 'tol' parameter
            psi.A[i], psi.A[i+1] = split_mps_tensor(Aloc, s[0], s[1], 'right',␣
↪tol=tol)
            assert is_left_orthonormal(psi.A[i])
            # update the left blocks
            BL[i+1] = contract_left_block(psi.A[i], H.A[i], BL[i])

        # sweep from right to left
        for i in reversed(range(L - 1)):
            Hloc = construct_local_two_site_hamiltonian(H.A[i], H.A[i+1],␣
↪BL[i], BR[i+1])
            s = Hloc.shape
            assert s[0] == s[1] == psi.local_dim
            assert s[4] == s[5] == psi.local_dim
```

```
            # reshape into a matrix
            Hloc = np.reshape(Hloc, (s[0]*s[1]*s[2]*s[3], s[4]*s[5]*s[6]*s[7]))
            # The following can be accelerated by Krylov methods and a "matrix␣
↪free" application of the local Hamiltonian.
            wloc, vloc = np.linalg.eigh(Hloc)
            # select first eigenvector corresponding to lowest energy
            en = wloc[0]
            # optimized local tensor for two sites
            Aloc = np.reshape(vloc[:, 0], (s[0]*s[1], s[2], s[3]))
            # TODO: call "split_mps_tensor" here with the appropriate␣
↪distribution direction of singluar values, and also pass the 'tol' parameter
            psi.A[i], psi.A[i+1] = split_mps_tensor(Aloc, s[0], s[1], 'left',␣
↪tol=tol)

            assert is_right_orthonormal(psi.A[i+1])
            # update the right blocks
            BR[i] = contract_right_block(psi.A[i+1], H.A[i+1], BR[i+1])

        # right-normalize leftmost tensor to ensure that 'psi' is normalized
        psi.A[0], _ = local_orthonormalize_right_qr(psi.A[0], np.array([[[1.
↪0]]]))

        # record energy after each sweep
        en_min[n] = en

        print("sweep {} completed, current energy: {}".format(n+1, en))

    return en_min
```

[33]:
```
def operator_average(op:MPO, psi:MPS):
    """
    Compute the expectation value `<psi | op | psi>`.

    Args:
        psi: wavefunction represented as MPS
        op:  operator represented as MPO

    Returns:
        complex: `<psi | op | psi>`
    """

    assert psi.nsites == op.nsites

    if psi.nsites == 0:
        return 0

    # initialize T by identity matrix
```

```
    T = np.identity(psi.A[-1].shape[2], dtype=psi.dtype)
    T = np.reshape(T, (psi.A[-1].shape[2], 1, psi.A[-1].shape[2]))

    for i in reversed(range(psi.nsites)):
        T = contract_right_block(psi.A[i], op.A[i], T)

    # T should now be a 1x1x1 tensor
    assert T.shape == (1, 1, 1)

    return T[0, 0, 0]
```

1.6 Example run of DMRG

[34]:
```
L = 14
J = 1.0
g = 1.05
```

[35]:
```
Hising = construct_ising_hamiltonian_mpo(J, g, L)
```

[36]:
```
# H as sparse matrix, for comparison
Hising_sparse = construct_ising_hamiltonian_sparse(J, g,␣
 ↪adjacency_1D_lattice(L, pbc=False))
Hising_sparse
```

[36]:
```
<16384x16384 sparse matrix of type '<class 'numpy.float64'>'
        with 245760 stored elements in Compressed Sparse Row format>
```

[37]:
```
# compute algebraically smallest few eigenvalues and corresponding␣
 ↪eigenvectors, as reference
en_ref, ref = sparse.linalg.eigsh(Hising_sparse, k=5, which='SA')
en_ref = en_ref[0]
ref = ref[:, 0]
```

[38]:
```
# reference ground state energy
en_ref
```

[38]:
```
-17.981355609315436
```

[39]:
```
# to-be optimized quantum state as MPS
dmrg = MPS(2, [1] + (L-1)*[5] + [1], fill="random real")
```

[40]:
```
dmrg.local_dim
```

[40]:
```
2
```

[41]:
```
dmrg.bond_dims
```

[41]:
```
[1, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 1]
```

[42]:
```
dmrg.nsites
```

[42]:
```
14
```

[43]:
```
numsweeps = 5
en_sweeps = dmrg_two_site(Hising,  dmrg, numsweeps, tol=1e-8)
```

```
sweep 1 completed, current energy: -17.98135545454854
sweep 2 completed, current energy: -17.981355507888622
sweep 3 completed, current energy: -17.981355507887876
sweep 4 completed, current energy: -17.98135550788785
sweep 5 completed, current energy: -17.98135550788783
```

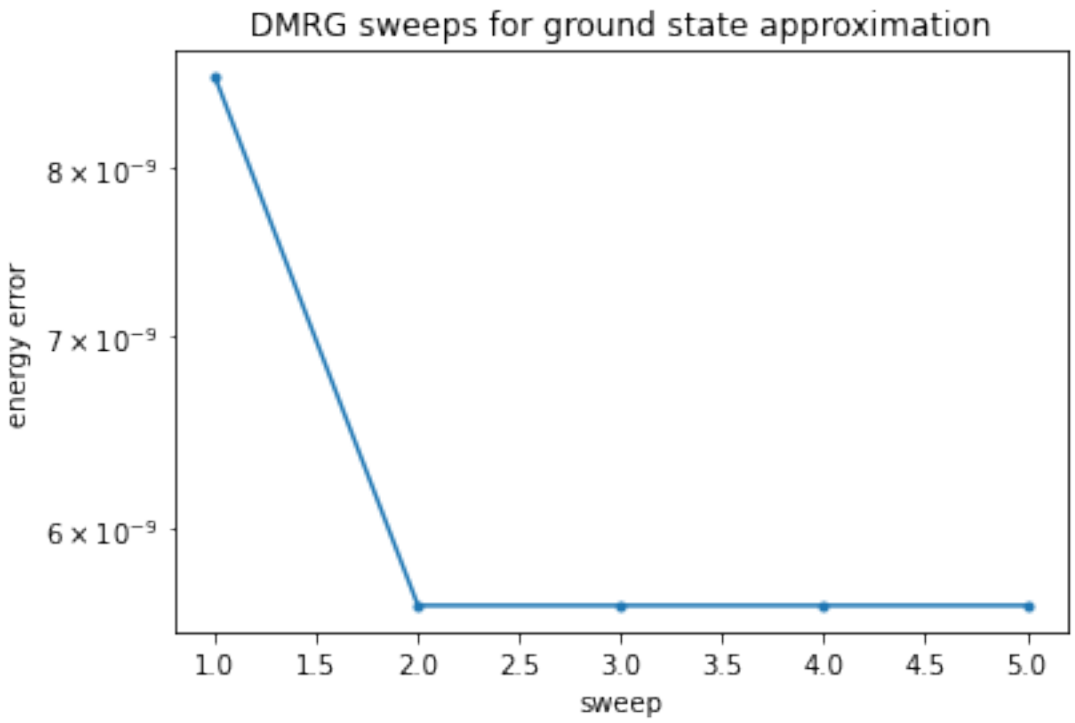
[44]:
```
# bond dimensions after optimization
dmrg.bond_dims
```

[44]:
```
[1, 2, 4, 6, 6, 6, 6, 6, 6, 6, 6, 6, 4, 2, 1]
```

[45]:
```
# check: should all be true
[is_right_orthonormal(Aj) for Aj in  dmrg.A]
```

[45]:
```
[True,
 True,
 True,
 True,
 True,
 True,
 True,
 True,
 True,
 True,
 True,
 True,
 True,
 True,
 True]
```

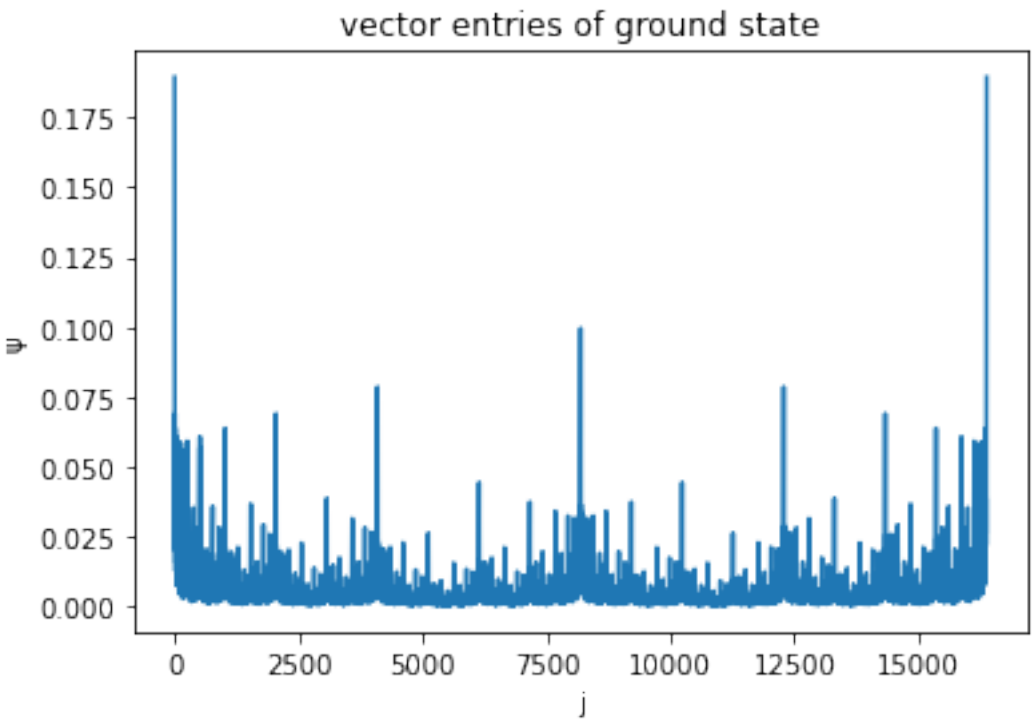
[46]:
```
# convergence plot
plt.semilogy(range(1, numsweeps+1), abs((en_sweeps - en_ref)/en_ref), '.-')
plt.xlabel("sweep")
plt.ylabel("energy error")
plt.title("DMRG sweeps for ground state approximation")
plt.show()
```



[47]:
```
# alternative way to compute energy expectation value
operator_average(Hising, dmrg)
```

[47]: -17.981355507887812

[48]:
```
# show vector entries of ground state (although not very insightful)
plt.plot( dmrg.as_vector())
plt.xlabel("j")
plt.ylabel(" ")
plt.title("vector entries of ground state")
plt.show()
```



1.7 TEBD algorithm

[49]:
```
def tebd_step(psi:MPS, U, tol=1e-5):
    """
    Single step of the TEBD algorithm, for time-evolving a quantum state `psi`
    via Trotter splitting.
    Each unitary matrix `U[i]` performs a time step at lattices sites (i, i+1).
    """
    for s in [0, 1]: # even or odd
        # time step for pairs (i, i+1) with i even or odd
        for i in range(s, psi.nsites-1, 2):
            # TODO: complete the implementation (apply U[i] to merged tensor␣
↪pair psi.A[i] and psi.A[i+1]).
            A = merge_mps_tensor_pair(psi.A[i], psi.A[i+1])
            A = np.tensordot(U[i], A, (0, 0))
            psi.A[i], psi.A[i+1] = split_mps_tensor(A, psi.A[i].shape[0], psi.
↪A[i+1].shape[0], 'sqrt', tol=tol)
            # The functions `merge_mps_tensor_pair` and `split_mps_tensor`␣
↪might be useful.
    # psi has been updated in-place
```

[50]:
```
def calculate_tebd_unitaries_imagtime(hloc, dt):
    """
```

```
    Calculate the local unitary blocks for TEBD imaginary-time evolution.
    """
    return [expm(-dt*h) for h in hloc]
```

[51]:
```
def calculate_tebd_unitaries_realtime(hloc, dt):
    """
    Calculate the local unitary blocks for TEBD real-time evolution.
    """
    return [expm(-1j*dt*h) for h in hloc]
```

1.8 Example run of TEBD for ground state approximation

[52]:
```
hloc = construct_ising_hamiltonian_local_terms(J, g, L)
```

[53]:
```
Uloc_imag = calculate_tebd_unitaries_imagtime(hloc, 0.1)
```

[54]:
```
# show dimensions
[U.shape for U in Uloc_imag]
```

[54]:
```
[(4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4),
 (4, 4)]
```

[55]:
```
# to-be optimized quantum state as MPS
tebd = MPS(2, [1] + (L-1)*[5] + [1], fill="random real")
tebd.orthonormalize("left");
```

[56]:
```
tebd.local_dim
```

[56]:
```
2
```

[57]:
```
tebd.bond_dims
```

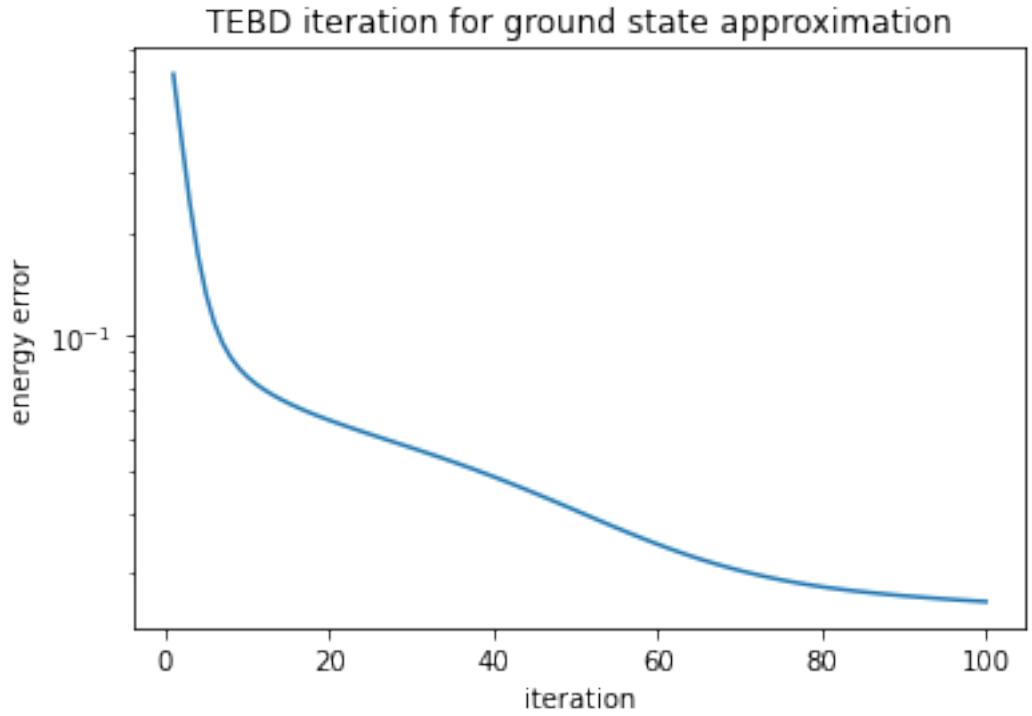
[57]:
```
[1, 2, 4, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 1]
```

[58]:
```
# run TEBD
numsteps = 100
en_iter_tebd = np.zeros(numsteps)
for n in range(numsteps):
    tebd_step( tebd, Uloc_imag)
    # re-normalize
     tebd.orthonormalize("left")
    en_iter_tebd[n] = operator_average(Hising,  tebd)
```

[59]:
```
# bond dimensions after optimization
 tebd.bond_dims
```

[59]: [1, 2, 4, 8, 11, 10, 8, 8, 9, 8, 6, 6, 4, 2, 1]

[60]:
```
# convergence plot
plt.semilogy(range(1, numsteps+1), abs((en_iter_tebd - en_ref)/en_ref))
plt.xlabel("iteration")
plt.ylabel("energy error")
plt.title("TEBD iteration for ground state approximation")
plt.show()
```



1.9 Example run of TEBD for real time evolution

[61]:
```
# initial quantum state as MPS
0 = MPS(2, [1] + (L-1)*[5] + [1], fill="random real")
0.orthonormalize("left");
```

[62]:
```
tmax = 2
```

[63]:
```
# reference time-evolved state
t_ref = scila.expm_multiply(-1j*tmax*Hising_sparse, 0.as_vector())
```

[64]:
```
# real-time evolution via TEBD for different time steps
# virtual bond dimensions are expected to increase quite rapidly
dt_list = [0.5**k for k in range(6)]
err_t_tebd = np.zeros(len(dt_list))
for n, dt in enumerate(dt_list):
    t_tebd = deepcopy( 0)
    Uloc = calculate_tebd_unitaries_realtime(hloc, dt)
    nsteps = round(tmax / dt)
    print("nsteps:", nsteps)
    for _ in range(nsteps):
        tebd_step( t_tebd, Uloc, tol=1e-7)
    # record error
    err_t_tebd[n] = np.linalg.norm( t_tebd.as_vector() - t_ref)
    print(" t_tebd.bond_dims:", t_tebd.bond_dims)
```

```
nsteps: 2
 t_tebd.bond_dims: [1, 2, 4, 8, 16, 32, 64, 40, 76, 40, 16, 8, 4, 2, 1]
nsteps: 4
 t_tebd.bond_dims: [1, 2, 4, 8, 16, 32, 64, 95, 64, 32, 16, 8, 4, 2, 1]
nsteps: 8
 t_tebd.bond_dims: [1, 2, 4, 8, 16, 32, 64, 98, 64, 32, 16, 8, 4, 2, 1]
nsteps: 16
 t_tebd.bond_dims: [1, 2, 4, 8, 16, 32, 64, 92, 64, 32, 16, 8, 4, 2, 1]
nsteps: 32
 t_tebd.bond_dims: [1, 2, 4, 8, 16, 32, 64, 84, 64, 32, 16, 8, 4, 2, 1]
nsteps: 64
 t_tebd.bond_dims: [1, 2, 4, 8, 16, 32, 61, 73, 61, 32, 16, 8, 4, 2, 1]
```

[65]:
```
# convergence plot
plt.loglog(dt_list, err_t_tebd, '.-', label="data")
# dashed line shows first order scaling from Trotter splitting;
# order can be improved, e.g., via Strang splitting, almost without increase of␣
 ↪computational cost
plt.loglog(dt_list, 1.5*np.array(dt_list), '--', label="Δt")
plt.xlabel("Δt")
plt.ylabel("error")
```

```
plt.legend()
plt.title("TEBD real time evolution up to t = {}".format(tmax))
plt.show()
```