Exercise Sheet No. 5

Exercise 1: Spin correlations of the one-dimensional Heisenberg modeL

Xiongxiao Wang, Pulkit Kukreja

Here we focus on the isotropic Heisenberg model in dimension d = 1 with open boundary conditions

$$H = -J \sum_{i=1}^{N-1} \vec{S}_i \vec{S}_{i+1}$$

with J = −1 (the antiferromagnetic case). We are interested in the spin correlations between sites 1 and n, $\chi_{1n} =< \vec{S}_1 \cdot \vec{S}_n >$, for both zero and finite temperature.

a)Calculate $\chi_{1n} =< \psi_g | \vec{S}_1 \cdot \vec{S}_n | \psi_g >$ for the ground state $|\psi_g >$ of a Heisenberg chain with N = 10 sites and n = 1, . . . , 10. Note that for an even number of sites N, the ground state of the antiferromagnetic Heisenberg chain is non-degenerate

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
from numpy import linalg as LA
import pandas as pd
```

In [2]:

```
def Hmatrix(N,J_x,J_y,J_z):
    n_states = 2**N
    matrix = np.zeros((n_states,n_states))
    for n in range(n_states):
        z = np.zeros(N,dtype = int)
        nz = n
        for z_i in range(N):
            if nz//2 >= 0:
                z[z_i] = nz%2
                nz = nz//2

        for p in range(1,N+1):
            for q in range(p+1,N+1):
                s = (2*z[p-1]-1)*(2*z[q-1]-1)
                l =n + (1-2*z[p-1])*2**(p-1) + (1-2*z[q-1])*2**(q-1)
                x_link =  0.25*  J_x[p-1,q-1]
                y_link = -0.25*s*J_y[p-1,q-1]
                z_link =  0.25*s*J_z[p-1,q-1]

                matrix[l,n]-= x_link
                matrix[l,n]-= y_link
                matrix[n,n]-= z_link
    return(matrix)
```

To calculate the ground state we use the code from last assigment and pay attention that the H only consider the neighboring sites

$$H = -J \sum_{i=1}^{N-1} \vec{S}_i \vec{S}_{i+1}$$

In [3]:

```
# Isotropic Heisenberg model with neighboing sites, set N = 10, J=-1

N=10

J_x_model = np.zeros((2**N,2**N))
J_y_model = np.zeros((2**N,2**N))
J_z_model = np.zeros((2**N,2**N))
for i in range(N-1):
    J_x_model[i,i+1] = -1
    J_y_model[i,i+1] = -1
    J_z_model[i,i+1] = -1

H_model = Hmatrix(N,J_x_model,J_y_model,J_z_model)
w_model,v_model = LA.eig(H_model)
print(H_model)

ground_indice = np.argmin(w_model)
fig,ax = plt.subplots(1,2,figsize=(10,5))

ax[0].plot(w_model,'.')
ax[0].set_title('Eigenvalues of Heisenberg model sites '+str(N))
ax[0].set_xlabel('states')
ax[0].set_ylabel('Eigenenergy')
ground_state = v_model[ground_indice]
print('The ground state is ',ground_state)
ax[1].plot(ground_state,'.')
ax[1].set_title('Ground state vectors')
ax[1].set_xlabel('states')
ax[1].set_ylabel('probability amplitude ')
```

```
[[2.25 0.   0.   ... 0.   0.   0.  ]
 [0.   1.75 0.5  ... 0.   0.   0.  ]
 [0.   0.5  1.25 ... 0.   0.   0.  ]
 ...
 [0.   0.   0.   ... 1.25 0.5  0.  ]
 [0.   0.   0.   ... 0.5  1.75 0.  ]
 [0.   0.   0.   ... 0.   0.   2.25]]
The ground state is  [0.        +0.j 0.        +0.j 0.        +0.j ... 0.018
93372+0.j
 0.        +0.j 0.        +0.j]

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_.py:1333: ComplexWarning: Casting complex values to real discards the imagi
nary part
  return np.asarray(x, float)
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_.py:1333: ComplexWarning: Casting complex values to real discards the imagi
nary part
  return np.asarray(x, float)
```
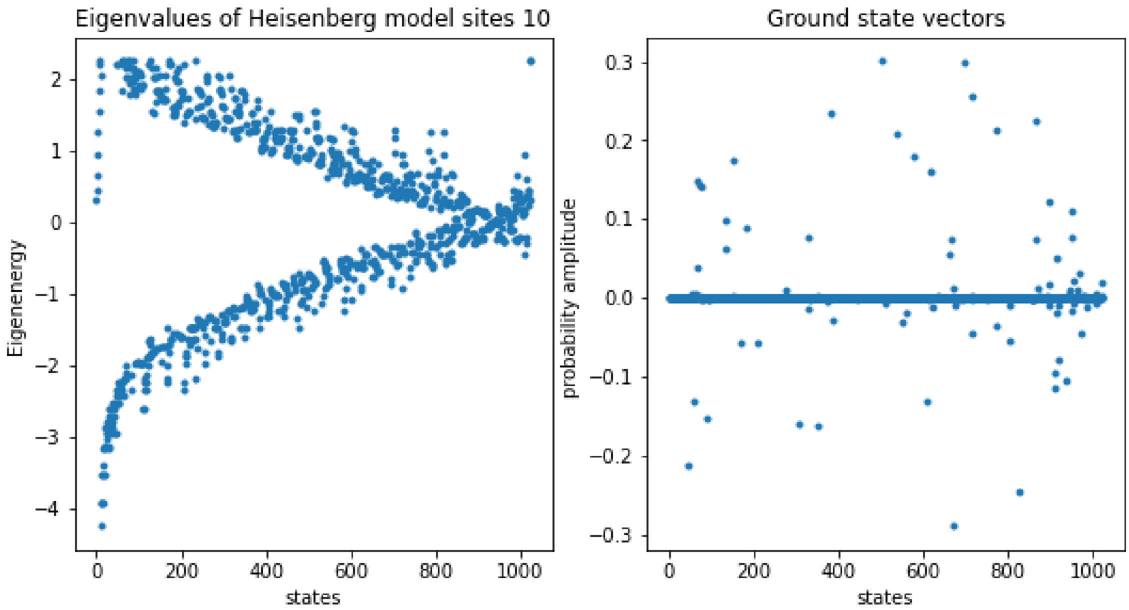

Out[3]:

```
Text(0, 0.5, 'probability amplitude ')
```



To calculate $\chi_{1n} =< \psi_g|\vec{S}_1 \cdot \vec{S}_n|\psi_g >$, firstly we define matrix $\vec{\chi}$ as $\vec{S}_1 \cdot \vec{S}_n$. Using the similar algorithm of calcualting Hmatrix, it's easy to find the matrix of $\vec{\chi}$ by setting J_{1n} = -1 and the other J = 0.

But there is one special case we should pay attention to, when the n = 1 which means $\vec{S}_1 \cdot \vec{S}_n = \vec{S}_1 \cdot \vec{S}_1$, the algorithm of calculating Hmatrix() doesn't include this case any more because Hmatrix() only concerns about two different spins. So we should modify the algorithm to include this case

In [4]:

```
def Cmatrix(N,J_x,J_y,J_z):
    n_states = 2**N
    matrix = np.zeros((n_states,n_states))
    for n in range(n_states):
        z = np.zeros(N,dtype = int)
        nz = n
        for z_i in range(N):
            if nz//2 >= 0:
                z[z_i] = nz%2
                nz = nz//2

        for p in range(1,N+1):
            for q in range(p,N+1):
                s = (2*z[p-1]-1)*(2*z[q-1]-1)
                l =n + (1-2*z[p-1])*2**(p-1) + (1-2*z[q-1])*2**(q-1)
                #print(n,l)
                x_link =  0.25*  J_x[p-1,q-1]
                y_link = -0.25*s*J_y[p-1,q-1]
                z_link =  0.25*s*J_z[p-1,q-1]


                matrix[(l+n_states)%n_states,n]-= x_link
                matrix[(l+n_states)%n_states,n]-= y_link
                matrix[n,n]-= z_link
    return(matrix)
```

In [5]:

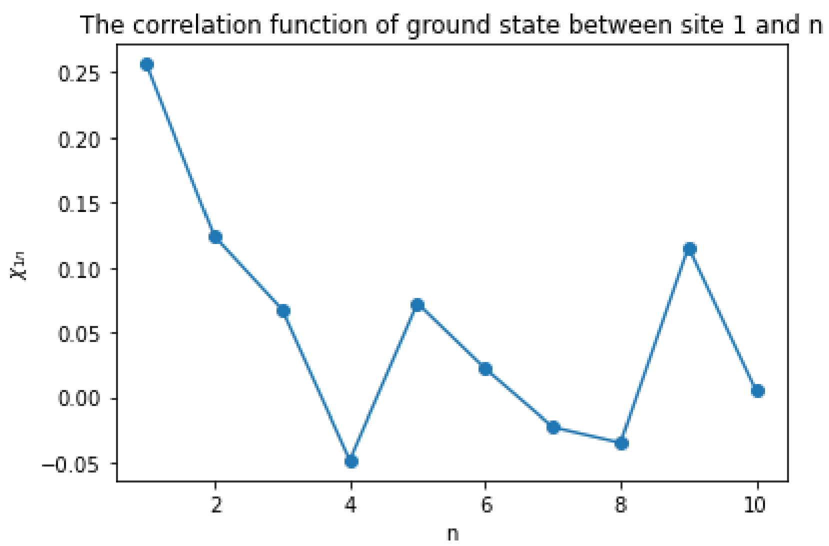
```
# The chi matrix
chi_1n = []
for n in range(N):
    J_x = np.zeros((N,N))
    J_y = np.zeros((N,N))
    J_z = np.zeros((N,N))
    J_x[0,n] = -1
    J_y[0,n] = -1
    J_z[0,n] = -1
    chi_matrix = Cmatrix(N,J_x,J_y,J_z)
    #print(chi_matrix)
    chi_1n.append(np.matmul(np.matmul(ground_state,chi_matrix),ground_state.T))
```

In [6]:

```
n_list = [i for i in range(1,N+1)]
plt.plot(n_list,chi_1n,'-o')
plt.title(r'The correlation function of ground state between site 1 and n')
plt.xlabel('n')
plt.ylabel(r'$\chi_{1n}$')
```

Out[6]:

```
Text(0, 0.5, '$\\chi_{1n}$')
```



b) Calculate the temperature dependence of the spin correlation

$$\chi_{1n}(T) = \frac{1}{Z}\sum_l < l|\vec{S}_1 \cdot \vec{S}_n|l > e^{-\beta E_l}$$

with $Z = \sum_i e^{-\beta E_l}$ the partition function, β = 1/(kBT) (k_B can be set to 1), and |l> the eigenstates of H with eigenenergies El , for temperatures T = 0.5, 2,and 10

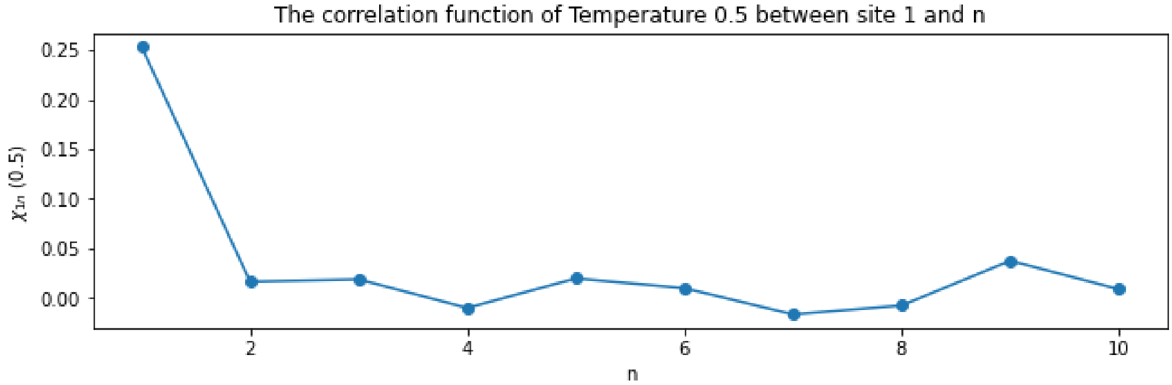
In [7]:

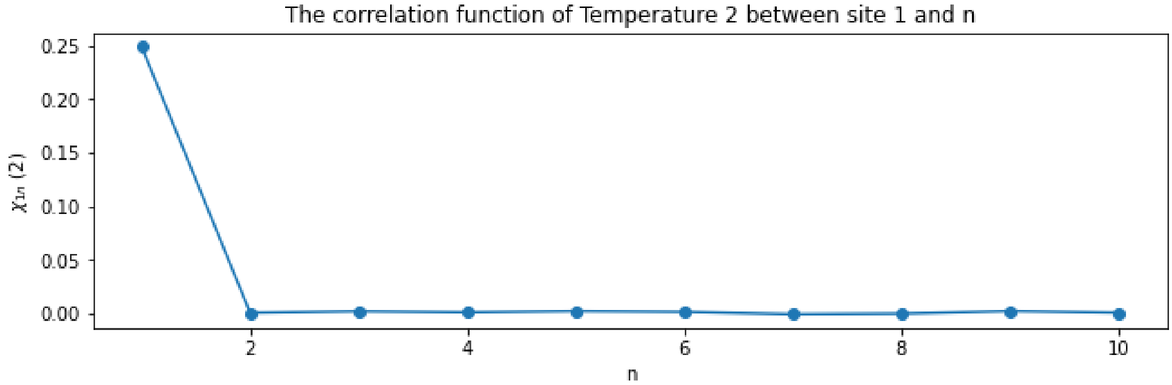
```
eigenvalue, eigenvector = w_model,v_model

T = [0.5,2,10]
index = 0
fig,ax = plt.subplots(len(T),1,figsize = (9,9),constrained_layout=True)
chi_1n_T_dataframe = pd.DataFrame({'site':n_list})
for Ti in T: #Loop temperature
    beta = 1/Ti
    Z = np.sum(np.exp(-beta*eigenvalue))
    chi_1n_T = []
    for n in range(N): #Loop site n from 1 to N
        J_x = np.zeros((N,N))
        J_y = np.zeros((N,N))
        J_z = np.zeros((N,N))
        J_x[0,n] = -1
        J_y[0,n] = -1
        J_z[0,n] = -1
        chi_matrix = Cmatrix(N,J_x,J_y,J_z)
        sum = 0
        for l in range(2**N):#Loop eigenstates
            sum+=np.matmul(np.matmul(eigenvector[l],chi_matrix),eigenvector[l].T)*np.exp(-b

        chi_1n_T.append(sum/Z)
    ax[index].plot(n_list,chi_1n_T,'-o')
    ax[index].set_title(r'The correlation function of Temperature '+str(Ti)+' between site
    ax[index].set_xlabel('n')
    ax[index].set_ylabel(r'$\chi_{1n}$ ('+str(Ti)+')')
    index+=1
    chi_1n_T_dataframe['Temperature'+str(Ti)] = chi_1n_T
print('The spin correlation chi(1n) in three different Temperature')
chi_1n_T_dataframe.set_index('site')
```

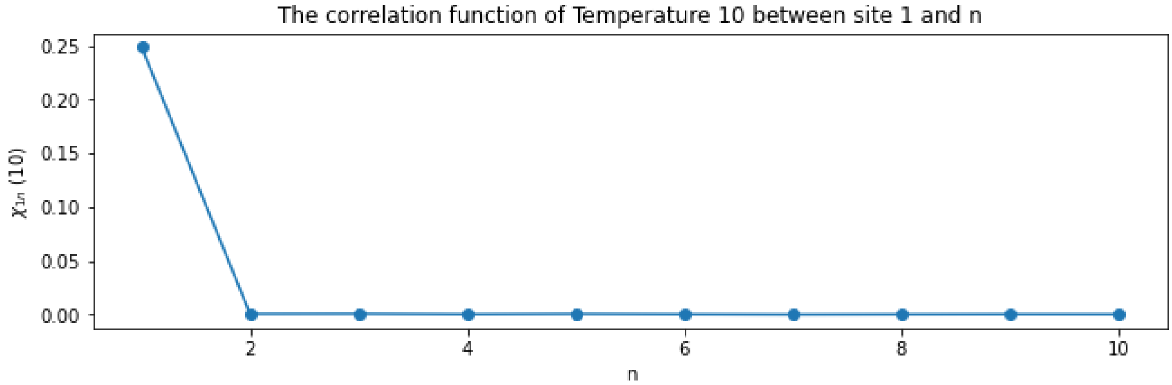
```
The spin correlation chi(1n) in three different Temperature
```

Out[7]:

site	Temperature0.5	Temperature2	Temperature10
1	0.253419-0.000000j	0.249331-0.000000j	0.248840-0.000000j
2	0.016281+0.000050j	0.000542+0.000145j	0.000414+0.000149j
3	0.018577+0.000048j	0.001902+0.000006j	0.000500-0.000020j
4	-0.010254+0.000138j	0.000987+0.000188j	0.000063+0.000181j
5	0.019535-0.000124j	0.002064-0.000165j	0.000388-0.000178j
6	0.009689-0.000129j	0.001406-0.000126j	0.000055-0.000117j
7	-0.016775+0.000087j	-0.000839+0.000141j	-0.000166+0.000122j
8	-0.007781+0.000143j	-0.000265+0.000196j	-0.000006+0.000188j
9	0.037356+0.000127j	0.002105+0.000200j	0.000098+0.000189j
10	0.008641+0.000134j	0.000625+0.000174j	0.000026+0.000183j







c) Show numerically that, in the limit $T \rightarrow 0$, the finite-temperature spin-correlation $\chi_{1n}(T)$ of part b) corresponds to the zero-temperature spin-correlation of part a). (2 points)

In [8]:

```
T0 = 0.01
beta = 1/T0
Z = np.sum(np.exp(-beta*eigenvalue))
chi_1n_T0 = []
for n in range(N): #loop site n from 1 to N
    J_x = np.zeros((N,N))
    J_y = np.zeros((N,N))
    J_z = np.zeros((N,N))
    J_x[0,n] = -1
    J_y[0,n] = -1
    J_z[0,n] = -1
    chi_matrix = Cmatrix(N,J_x,J_y,J_z)
    sum = 0
    for l in range(2**N):#loop eigenstates
        sum+=np.matmul(np.matmul(eigenvector[l],chi_matrix),eigenvector[l].T)*np.exp(-beta*

    chi_1n_T0.append(sum/Z)
```

In [11]:

```
print('The spin correlation chi(1n) of T = 0.01 and ground state')
chi_1n_g0_df = pd.DataFrame({'site':n_list,'$\chi_{1n}$ of T = 0.01':chi_1n_T0,'$\chi_{1n}$
chi_1n_g0_df.set_index('site')
```

```
The spin correlation chi(1n) of T = 0.01 and ground state
```

Out[11]:

site	χ_{1n} of T = 0.01	χ_{1n} of ground state
1	0.256334+0.000000j	0.256334+0.000000j
2	0.124048+0.000028j	0.124048+0.000028j
3	0.067674+0.000037j	0.067674+0.000037j
4	-0.048182+0.000037j	-0.048182+0.000037j
5	0.072508-0.000038j	0.072508-0.000038j
6	0.022278+0.002280j	0.022278+0.002280j
7	-0.022621-0.000049j	-0.022621-0.000049j
8	-0.034672+0.000041j	-0.034672+0.000041j
9	0.115693+0.000041j	0.115693+0.000041j
10	0.005170+0.000041j	0.005170+0.000041j

In [10]:

```
fig,ax1 = plt.subplots(2,figsize = (6,6),sharex = True)
ax1[0].plot(n_list,chi_1n_T0,'-o',label = r'T = 0.01')
ax1[1].plot(n_list,chi_1n,'-o',label = 'Ground state')
ax1[0].set_title(r'The correlation function of T $\rightarrow$ 0  ')
ax1[1].set_title(r'The correlation function of  ground state ')
ax1[0].set_xlabel('n')
ax1[0].set_ylabel(r'$\chi_{1n}$')
ax1[1].set_xlabel('n')
ax1[1].set_ylabel(r'$\chi_{1n}$')
ax1[0].legend()
ax1[1].legend()
```

```
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_.py:1333: ComplexWarning: Casting complex values to real discards the imagi
nary part
  return np.asarray(x, float)
```
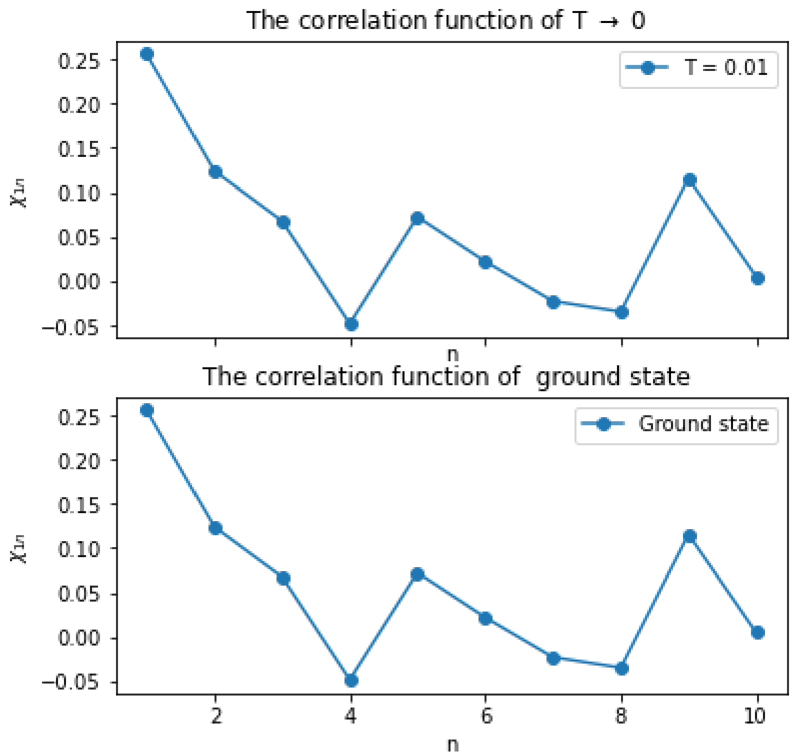

Out[10]:

```
<matplotlib.legend.Legend at 0x23eaae43550>
```



These show in the limit $T \to 0$, the finite-temperature spin-correlation $\chi 1n(T)$ of part b) corresponds to the zero-temperature spin-correlation of part a).

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Exercise 2: Reduced density matrix and entanglement entropy

a) $|\psi\rangle = \sum_{i=1}^{2}\sum_{j=1}^{2} \psi_{ij} |i\rangle |j\rangle$

$|\psi\rangle_1 = |\uparrow\rangle_A |\downarrow\rangle_B$

$|\psi\rangle_2 = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_A |\downarrow\rangle_B - |\downarrow\rangle_A |\uparrow\rangle_B\right)$

$|\psi\rangle_3 = \frac{1}{2}\left(|\uparrow\rangle_A + |\downarrow\rangle_A\right)\left(|\uparrow\rangle_B + |\downarrow\rangle_B\right)$

$$|\psi\rangle = \sum_{\sigma_1=\uparrow,\downarrow}\sum_{\sigma_2=\uparrow,\downarrow} \psi_{\sigma_1,\sigma_2} |\sigma_1\rangle |\sigma_2\rangle$$

$$= \left(|\uparrow\rangle_A \ |\downarrow\rangle_A\right)\begin{pmatrix} \psi_{\uparrow\uparrow} & \psi_{\uparrow\downarrow} \\ \psi_{\downarrow\uparrow} & \psi_{\downarrow\downarrow} \end{pmatrix}\begin{pmatrix} |\uparrow\rangle_B \\ |\downarrow\rangle_B \end{pmatrix}$$

$$|\psi\rangle_1 = \left(|\uparrow\rangle_A \ \ |\downarrow\rangle_A\right)\cdot\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} |\uparrow\rangle_B \\ |\downarrow\rangle_B \end{pmatrix}$$

$$|\psi\rangle_2 = \left(|\uparrow\rangle_A \ \ |\downarrow\rangle_A\right)\cdot\begin{pmatrix} 0 & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & 0 \end{pmatrix}\begin{pmatrix} |\uparrow\rangle_B \\ |\downarrow\rangle_B \end{pmatrix}$$

$$|\psi\rangle_3 = \left(|\uparrow\rangle_A \ \ |\downarrow\rangle_A\right)\cdot\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}\begin{pmatrix} |\uparrow\rangle_B \\ |\downarrow\rangle_B \end{pmatrix}$$

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b) $\hat{\rho} \equiv \mathrm{Tr}_B(|\psi\rangle\langle\psi|) = \sum_{j=1}^{2} \langle j|\psi\rangle\langle\psi|j\rangle$

with the matrix elements $\rho_{ii'} = \langle i|\hat{\rho}|i'\rangle = \sum_j \psi_{ij}\psi^*_{i'j}$

$$\hat{\rho}_A = (|\uparrow\rangle_A \quad |\downarrow\rangle_A) \underbrace{\begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix}}_{\rho_{\sigma_1\sigma_2}} \begin{pmatrix} \langle\uparrow|_A \\ \langle\downarrow|_A \end{pmatrix}$$

$$\hat{\rho}_{A1} = \mathrm{Tr}_B(|\psi\rangle_1\langle\psi|_1) = \underbrace{\langle\uparrow_B|\psi_1\rangle}_{=\underbrace{\langle\uparrow_B|\downarrow_B\rangle}_{=0}|\uparrow_A\rangle}\langle\psi_1|\uparrow_B\rangle + \underbrace{\langle\downarrow_B|\psi_1\rangle}_{=\underbrace{\langle\downarrow_B|\downarrow_B\rangle}_{1}|\uparrow_A\rangle}\underbrace{\langle\psi_1|\downarrow_B\rangle}_{=\langle\uparrow_A|\underbrace{\langle\downarrow_B|\downarrow_B\rangle}_{1}}$$

$$\hat{\rho}_{A1} = |\uparrow_A\rangle\langle\uparrow_A| \qquad \rho_{\sigma_1\sigma_2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\hat{\rho}_{A2} = \mathrm{Tr}_B(|\psi\rangle_2\langle\psi_2|) = \langle\uparrow_B|\psi_2\rangle\langle\psi_2|\uparrow_B\rangle + \langle\downarrow_B|\psi_2\rangle\langle\psi_2|\downarrow_B\rangle$$

$\langle\uparrow_B|\psi_2\rangle = \frac{-1}{\sqrt{2}}\langle\uparrow_B|\uparrow_B\rangle|\downarrow_A\rangle = -\frac{1}{\sqrt{2}}\cdot|\downarrow_A\rangle \qquad \langle\psi_2|\uparrow_B\rangle = -\frac{1}{\sqrt{2}}\cdot\langle\downarrow_A|$

$\langle\downarrow_B|\psi_2\rangle = \frac{1}{\sqrt{2}}|\uparrow_A\rangle \qquad \langle\psi_2|\downarrow_B\rangle = \frac{1}{\sqrt{2}}\cdot\langle\uparrow_A|$

$$\hat{\rho}_{A2} = \frac{1}{2}|\downarrow_A\rangle\langle\downarrow_A| + \frac{1}{2}|\uparrow_A\rangle\langle\uparrow_A| \qquad \rho_{\sigma_1\sigma_2} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

$$\hat{\rho}_{A3} = \mathrm{Tr}_B(|\psi_3\rangle\langle\psi_3|) = \langle\uparrow_B|\psi_3\rangle\langle\psi_3|\uparrow_B\rangle + \langle\downarrow_B|\psi_3\rangle\langle\psi_3|\downarrow_B\rangle$$

$\langle\uparrow_B|\psi_3\rangle = \frac{1}{2}(|\uparrow\rangle_A + |\downarrow\rangle_A) \qquad \langle\psi_3|\uparrow_B\rangle = \frac{1}{2}(\langle\uparrow|_A + \langle\downarrow|_A)$

$\langle\downarrow_B|\psi_3\rangle = \frac{1}{2}(|\uparrow\rangle_A + |\downarrow\rangle_A) \qquad \langle\psi_3|\downarrow_B\rangle = \frac{1}{2}(\langle\uparrow|_A + \langle\downarrow|_A)$

$$\hat{\rho}_{A3} = \frac{1}{2}(|\uparrow\rangle_A + |\downarrow\rangle_A)(\langle\uparrow|_A + \langle\downarrow|_A) \qquad \rho_{\sigma_1\sigma_2} = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

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Entanglement entropy S_e:

$$S_e = -\mathrm{Tr}_A\left[\hat{\rho}_A \ln \hat{\rho}_A\right] = -\sum_\alpha w_\alpha \ln w_\alpha$$

For state $|\psi_1\rangle$ $\quad \overline{\Psi}_{\sigma_1\sigma_2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ eigenvalue: $w_1 = 1$, $w_2 = 0$

$$S_e = -w_1 \ln w_1 - w_2 \ln w_2 = \underbrace{-0\ln 0}_{\lim\limits_{x\to 0} x\cdot\ln x = 0} - 1\cdot\ln 1 = 0$$

For state $|\psi_2\rangle$ $\quad \overline{\Psi}_{\sigma_1\sigma_2} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$ $\quad w_1 = \frac{1}{2} \quad w_2 = \frac{1}{2}$

$$S_e = -\frac{1}{2}\ln\left(\frac{1}{2}\right) - \frac{1}{2}\ln\left(\frac{1}{2}\right) = \ln 2$$

For state $|\psi_3\rangle$ $\quad \overline{\Psi}_{\sigma_1\sigma_2} = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix}$

$$\det\left(\overline{\Psi}_{\sigma_1\sigma_2} - \lambda E\right) = \begin{vmatrix} \frac{1}{4}-\lambda & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4}-\lambda \end{vmatrix} = \left(\frac{1}{4}-\lambda\right)^2 - \frac{1}{16} = 0 \Rightarrow \lambda_1 = \frac{1}{2} \quad \lambda_2 = 0$$

$$\Rightarrow w_1 = \frac{1}{2} \quad w_2 = 0$$

$$S_e = -\frac{1}{2}\ln\left(\frac{1}{2}\right) - 0\ln 0 = \frac{1}{2}\ln 2$$

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