Computational Many-Body Physics - Sheet 5

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The full implementation of all exercises can be found under `https://github.com/Fhoeddinghaus/cmbp22-exercises/tree/main/sheet_5`.

1. Spin correlations of the one-dimensional Heisenberg model

Consider the isotropic Heisenberg model in $d = 1$ dimension with open boundary conditions

$$\begin{aligned} H &= -J \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1} \\ &= -J \sum_{i=1}^{N-1} \left(\frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + S_i^z S_{i+1}^z \right) \end{aligned}$$

with $J = -1$ (antiferromagnetic case).
The spin correlation between site 1 and n is

$$\chi_{1n} = \langle \vec{S}_1 \cdot \vec{S}_n \rangle$$

a).

The spin correlation for zero-temperature is

$$\chi_{nm} = \langle \vec{S}_n \vec{S}_m \rangle = \langle \psi_g | \vec{S}_n \cdot \vec{S}_m | \psi_g \rangle = \langle \psi_g | H_{nm} | \psi_g \rangle$$

with

$$H_{nm} = \vec{S}_n \cdot \vec{S}_m$$

which can be interpeted as a Hamiltonian coupling only m and n with $J = -1$.
In the case of $n = m$, it is

$$\vec{S}_n^2 = (S_n^x)^2 + (S_n^y)^2 + (S_n^z)^2 = \frac{3}{4} \cdot \hat{\mathbf{1}}.$$

We can use this to implement a function to calculate the spin correlation using the function `calculate_hamilton_matrix()`[1] from the last exercise:

```
function spin_correlation(N,ψ, n,m; H_sc = false)
    if n == m
        # the algorithm for hamilton matrix works only for n≠m,
        # manually:
        return 3/4 * ψ' * ψ # 1/4 for each α=x,y,z
    end
    if H_sc == false
        # construct the Hamilton matrix for the coupling between (n,m)
        Js_sc = reset_Js(N)
        # only coupling between (n,m) for all α
        Js_sc[1][n,m] = -1
        Js_sc[2][n,m] = -1
        Js_sc[3][n,m] = -1
        H_sc = calculate_hamilton_matrix(Js_sc, N)
    end # else: H_sc is given, e.g.for multiple calculations for the same (n,m)
        for different states, no re-calculation is needed

    return (ψ' * H_sc * ψ)[1] # 1x1 matrix to scalar
end
```

Listing 1: Function to calculate the spin-correlation for a given state and sites n and m using a given H_{nm} Hamilton matrix `H_sc` or by calculating H_{nm} first using `calculate_hamilton_matrix()`.

To now calculate χ_{1n} for the ground state of a Heisenberg chain with $N = 10$ sites and $n = 1, \ldots, N$, we first have to calculate the corresponding Hamilton matrix for the Heisenberg chain, again using `calculate_hamilton_matrix()` with the $(i, i+1)$-couplings like this:

```
J = -1
N = 10

Js = reset_Js(N)

# coupling between (i,i+1) for α=x (1)
for i in 1:(N-1)
    Js[1][i,i+1] = J
end

# coupling between (i,i+1) for α=y,z (2,3)
Js[2] = Js[1]
Js[3] = Js[1]

H = rationalize.(calculate_hamilton_matrix(Js, N))
```

Listing 2: Calculation of the Hamilton matrix for the Heisenberg chain in one dimension.

Using `eigvecs(Matrix(H))[:,1];` from `LinearAlgebra.jl`, we can calculate the ground state $|\psi_g\rangle$ and then calculate the spin correlations between the sites 1 and $n = 1, \ldots, N$:

$$\chi_{1,1} \approx 0.750 \qquad \chi_{1,2} \approx -0.658 \qquad \chi_{1,3} \approx 0.198$$
$$\chi_{1,4} \approx -0.222 \qquad \chi_{1,5} \approx 0.108 \qquad \chi_{1,6} \approx -0.131$$
$$\chi_{1,7} \approx 0.070 \qquad \chi_{1,8} \approx -0.092 \qquad \chi_{1,9} \approx 0.045$$
$$\chi_{1,10} \approx -0.068$$

[1] This function is again implemented in `hamilton_spins.jl` in the repository

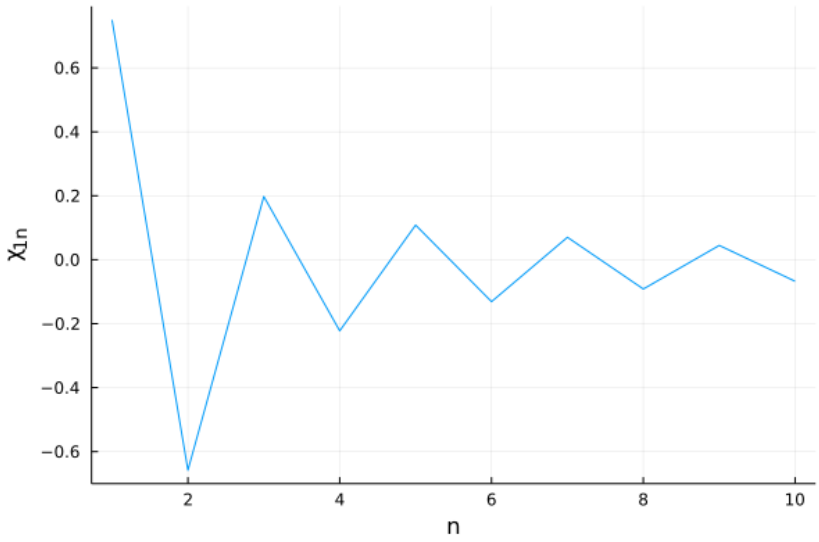

Figure 1.1

b).

The temperature dependence of the spin correlation is

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

with $Z = \sum_l e^{-\beta E_l}$ (partition function), $|l\rangle$ eigenstates and eigenenergies E_l.
With

- `β(T) = 1/T` (for $k_B = 1$) and
- `Z(T, Es) = sum([exp(-β(T) * E) for E in Es])` (partition function)

we can implement the following function, that calculates $\chi_{1n}(T)$:

```
function spin_correlation_temperature(T, n, H, N; ls = false, Es = false)
    # eigenstates
    if ls == false
        ls = round.(eigvecs(Matrix(H)); digits=9)
    end
    # eigenenergies
    if Es == false
        Es = eigvals(Matrix(H))
    end

    # (from spin_correlation(...))
    if n == 1
        # manually:
        return 1/Z(T, Es) * sum([spin_correlation(N, ls[:,i], 1, 1) * exp(-β(T)
            * Es[i]) for i in 1:length(Es)])
    end
    # calculate the Hamilton matrix only one time
    Js_sc = reset_Js(N)
    # only coupling between (1,n) for all α
    Js_sc[1][1,n] = -1
    Js_sc[2][1,n] = -1
    Js_sc[3][1,n] = -1
    H_sc = calculate_hamilton_matrix(Js_sc, N)

    return 1/Z(T, Es) * sum([spin_correlation(N, ls[:,i], 1, n; H_sc = H_sc) *
        exp(-β(T) * Es[i]) for i in 1:length(Es)])
end
```

Listing 3: Function to calculate $\chi_{1n}(T)$ for a given n, T using the Eigenstates `ls` and Eigenenergies `Es` (or calculating them first from `H`). For $n > 1$, the function first calculates H_{1n} (s.t. only one calculation is necessary) and then returns $\chi_{1n}(T)$ using `spin_correlation()` for the different $|l\rangle$.

We can then calculate $\chi_{1n}(T)$ for $n = 1, \ldots, 10$ and $T = 0.5, 2, 10$ as

```
Ts = [0.5, 2, 10]
χs = zeros(length(Ts),10)

# (from spin_correlation_temperature(...))
# eigenstates
ls = round.(eigvecs(Matrix(H)); digits=9)
# eigenenergies
Es = eigvals(Matrix(H))

@time for i in 1:length(Ts)
    T = Ts[i]
    for n in 1:10
        χs[i,n] = spin_correlation_temperature(T, n, H, N; ls = ls, Es = Es)
    end
end
```

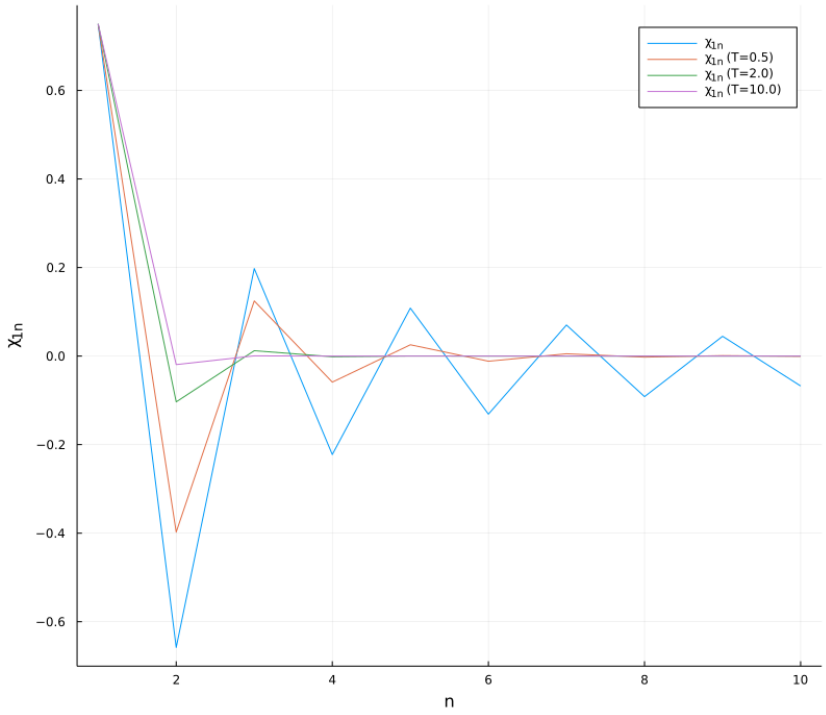

Figure 1.2

c).

To show, that $\lim_{T \to 0} \chi_{1n}(T) \overset{!}{=} \chi_{1n}$, we can look at the absolute difference $\Delta\chi = |\chi_{1n} - \chi_{1n}(T)|$ for different values of T and the sum of errors squared $\Delta_{total} = \sum_{n=1}^{N} (\chi_{1n} - \chi_{1n}(T))^2$.

Using the code from above for e.g. $T = 0.5, 0.25, 0.1, 0.01$ and calculating $\Delta\chi_{1n}(T)$, we get:

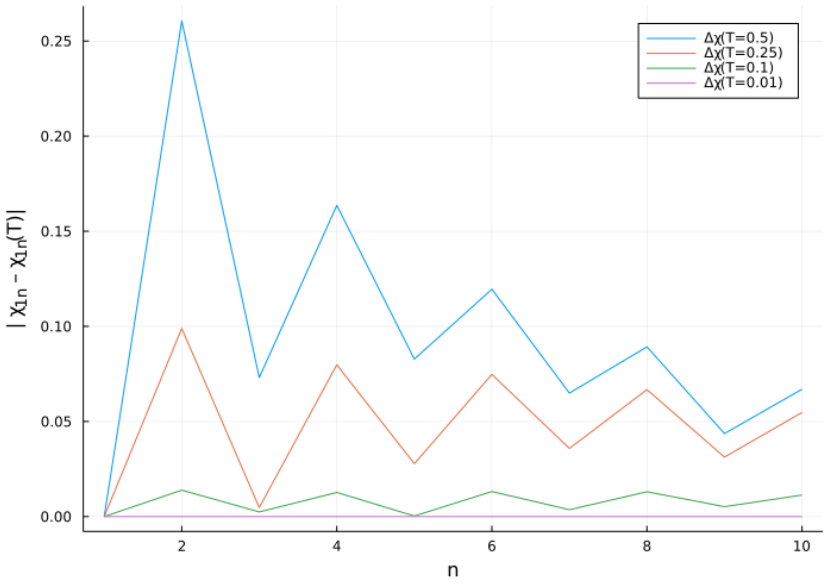

Figure 1.3

Looking at Δ_{total}, we see for the different values of T:

$$\Delta_{total}(T = 0.5) \approx 0.140 \qquad \Delta_{total}(T = 0.25) \approx 0.0322$$
$$\Delta_{total}(T = 0.1) \approx 0.000873 \qquad \Delta_{total}(T = 0.01) = 2.589 \cdot 10^{-29} \approx 0$$

For a few more values of T, we find:

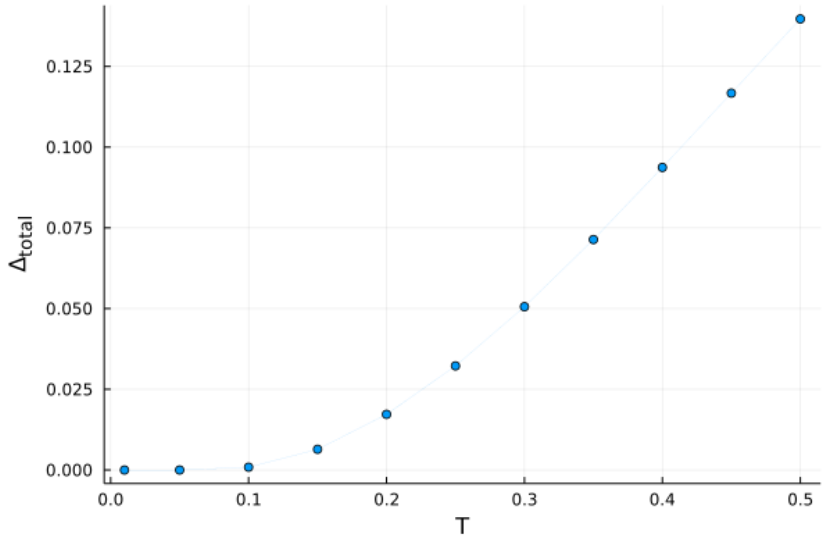

Figure 1.4

Therefore, for $T \to 0 : \Delta_{total} \to 0 \Rightarrow \chi_{1n}(T) \xrightarrow{T \to 0} \chi_{1n}$.

2. Reduced density matrix and entanglement entropy

Consider a two-site system with sites A and B with a two-dimensional basis $\{|i\rangle\} = \{|\uparrow\rangle_A, |\downarrow\rangle_A\}$, $\{|j\rangle\} = \{|\uparrow\rangle_B, |\downarrow\rangle_B\}$.

A given state $|\psi\rangle$ can be expressed in this basis as

$$|\psi\rangle = \sum_{i=\uparrow,\downarrow} \sum_{j=\uparrow,\downarrow} \psi_{ij} |i\rangle |j\rangle \tag{2.1}$$

Consider the following three states:

$$\begin{aligned}
|\psi\rangle_1 &= |\uparrow\rangle_A |\downarrow\rangle_B , \\
|\psi\rangle_2 &= \frac{1}{\sqrt{2}}(|\uparrow\rangle_A |\downarrow\rangle_B - |\downarrow\rangle_A |\uparrow\rangle_B), \\
|\psi\rangle_3 &= \frac{1}{2}(|\uparrow\rangle_A + |\downarrow\rangle_A)(|\uparrow\rangle_B + |\downarrow\rangle_B).
\end{aligned}$$

a).

a).1. $|\psi\rangle_1$

$$\begin{aligned}
|\psi\rangle_1 &= |\uparrow\rangle_A |\downarrow\rangle_B \\
&= 0 |\uparrow\rangle |\uparrow\rangle + 1 |\uparrow\rangle |\downarrow\rangle + 0 |\downarrow\rangle |\uparrow\rangle + 0 |\downarrow\rangle |\downarrow\rangle \\
\Rightarrow \underline{\underline{\bar{\psi}_1}} &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}
\end{aligned}$$

a).2. $|\psi\rangle_2$

$$\begin{aligned}
|\psi\rangle_2 &= \frac{1}{\sqrt{2}}(|\uparrow\rangle_A |\downarrow\rangle_B - |\downarrow\rangle_A |\uparrow\rangle_B) \\
&= 0 |\uparrow\rangle |\uparrow\rangle + \frac{1}{\sqrt{2}} |\uparrow\rangle |\downarrow\rangle - \frac{1}{\sqrt{2}} |\downarrow\rangle |\uparrow\rangle + 0 |\downarrow\rangle |\downarrow\rangle \\
\Rightarrow \underline{\underline{\bar{\psi}_2}} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}
\end{aligned}$$

a).3. $|\psi\rangle_3$

$$\begin{aligned}
|\psi\rangle_3 &= \frac{1}{2}(|\uparrow\rangle_A + |\downarrow\rangle_A)(|\uparrow\rangle_B + |\downarrow\rangle_B) \\
&= \frac{1}{2} |\uparrow\rangle |\uparrow\rangle + \frac{1}{2} |\uparrow\rangle |\downarrow\rangle + \frac{1}{2} |\downarrow\rangle |\uparrow\rangle + \frac{1}{2} |\downarrow\rangle |\downarrow\rangle \\
\Rightarrow \underline{\underline{\bar{\psi}_3}} &= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}
\end{aligned}$$

b).

The reduced density operator $\hat{\rho}$ is defined as

$$\hat{\rho}_A = \mathrm{Tr}_B(|\psi\rangle \langle\psi|) = \sum_{j=\uparrow,\downarrow} \langle j|\psi\rangle\langle\psi|j\rangle$$

with matrix elements $\rho_{ii'} = \langle i|\hat{\rho}|i'\rangle = \sum_{j=\uparrow,\downarrow} \psi_{ij}\psi_{i'j}$.

b).1. $|\psi\rangle_1$

$$\begin{aligned}
\langle\uparrow|\hat{\rho}_1|\uparrow\rangle &= (\bar{\psi}_1)_{\uparrow\uparrow}(\bar{\psi}_1)_{\uparrow\uparrow} + (\bar{\psi}_1)_{\uparrow\downarrow}(\bar{\psi}_1)_{\uparrow\downarrow} = 0 + 1 = 1\\
\langle\uparrow|\hat{\rho}_1|\downarrow\rangle &= (\bar{\psi}_1)_{\uparrow\uparrow}(\bar{\psi}_1)_{\downarrow\uparrow} + (\bar{\psi}_1)_{\uparrow\downarrow}(\bar{\psi}_1)_{\downarrow\downarrow} = 0 + 0 = 0\\
\langle\downarrow|\hat{\rho}_1|\uparrow\rangle &= (\bar{\psi}_1)_{\downarrow\uparrow}(\bar{\psi}_1)_{\uparrow\uparrow} + (\bar{\psi}_1)_{\downarrow\downarrow}(\bar{\psi}_1)_{\uparrow\downarrow} = 0 + 0 = 0\\
\langle\downarrow|\hat{\rho}_1|\downarrow\rangle &= (\bar{\psi}_1)_{\downarrow\uparrow}(\bar{\psi}_1)_{\downarrow\uparrow} + (\bar{\psi}_1)_{\downarrow\downarrow}(\bar{\psi}_1)_{\downarrow\downarrow} = 0 + 0 = 0\\
\Rightarrow \underline{\underline{\hat{\rho}_1}} &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}
\end{aligned}$$

b).2. $|\psi\rangle_2$

$$\begin{aligned}
\langle\uparrow|\hat{\rho}_2|\uparrow\rangle &= (\bar{\psi}_2)_{\uparrow\uparrow}(\bar{\psi}_2)_{\uparrow\uparrow} + (\bar{\psi}_2)_{\uparrow\downarrow}(\bar{\psi}_2)_{\uparrow\downarrow} = 0 + \frac{1}{2} = \frac{1}{2}\\
\langle\uparrow|\hat{\rho}_2|\downarrow\rangle &= (\bar{\psi}_2)_{\uparrow\uparrow}(\bar{\psi}_2)_{\downarrow\uparrow} + (\bar{\psi}_2)_{\uparrow\downarrow}(\bar{\psi}_2)_{\downarrow\downarrow} = 0 + 0 = 0\\
\langle\downarrow|\hat{\rho}_2|\uparrow\rangle &= (\bar{\psi}_2)_{\downarrow\uparrow}(\bar{\psi}_2)_{\uparrow\uparrow} + (\bar{\psi}_2)_{\downarrow\downarrow}(\bar{\psi}_2)_{\uparrow\downarrow} = 0 + 0 = 0\\
\langle\downarrow|\hat{\rho}_2|\downarrow\rangle &= (\bar{\psi}_2)_{\downarrow\uparrow}(\bar{\psi}_2)_{\downarrow\uparrow} + (\bar{\psi}_2)_{\downarrow\downarrow}(\bar{\psi}_2)_{\downarrow\downarrow} = \frac{1}{2} + 0 = \frac{1}{2}\\
\Rightarrow \underline{\underline{\hat{\rho}_2}} &= \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\end{aligned}$$

b).3. $|\psi\rangle_3$

$$\begin{aligned}
\langle\uparrow|\hat{\rho}_3|\uparrow\rangle &= (\bar{\psi}_3)_{\uparrow\uparrow}(\bar{\psi}_3)_{\uparrow\uparrow} + (\bar{\psi}_3)_{\uparrow\downarrow}(\bar{\psi}_3)_{\uparrow\downarrow} = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}\\
\langle\uparrow|\hat{\rho}_3|\downarrow\rangle &= (\bar{\psi}_3)_{\uparrow\uparrow}(\bar{\psi}_3)_{\downarrow\uparrow} + (\bar{\psi}_3)_{\uparrow\downarrow}(\bar{\psi}_3)_{\downarrow\downarrow} = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}\\
\langle\downarrow|\hat{\rho}_3|\uparrow\rangle &= (\bar{\psi}_3)_{\downarrow\uparrow}(\bar{\psi}_3)_{\uparrow\uparrow} + (\bar{\psi}_3)_{\downarrow\downarrow}(\bar{\psi}_3)_{\uparrow\downarrow} = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}\\
\langle\downarrow|\hat{\rho}_3|\downarrow\rangle &= (\bar{\psi}_3)_{\downarrow\uparrow}(\bar{\psi}_3)_{\downarrow\uparrow} + (\bar{\psi}_3)_{\downarrow\downarrow}(\bar{\psi}_3)_{\downarrow\downarrow} = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}\\
\Rightarrow \underline{\underline{\hat{\rho}_3}} &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}
\end{aligned}$$

c).

The entanglement entropy is defined as

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

with w_α the eigenvalues of the reduced density matrix.

c).1. $|\psi\rangle_1$

The eigenvalues of $\hat{\rho}_1$ are

$$w_1 = 0, \qquad\qquad w_2 = 1,$$

therefore, the entanglement entropy is

$$\begin{aligned}
\rightsquigarrow \underline{\underline{S_e^{(1)}}} &= -w_1 \ln w_1 - w_2 \ln w_2\\
&= -\underbrace{0 \cdot \ln 0}_{\lim_{x\to 0} x \ln x = 0} - 1 \ln 1 = \underline{0}
\end{aligned}$$

$\rightsquigarrow |\psi\rangle_1$ is **not entangled**.

c).2. $|\psi\rangle_2$

The eigenvalues of $\hat{\rho}_2$ are

$$w_1 = w_2 = \frac{1}{2},$$

therefore, the entanglement entropy is

$$\begin{aligned} \rightsquigarrow \underline{\underline{S_e^{(2)}}} &= -w_1 \ln w_1 - w_2 \ln w_2 \\ &= -2 \cdot \frac{1}{2} \ln \frac{1}{2} = \underline{\underline{\ln 2}} \approx 0.693 \end{aligned}$$

$\rightsquigarrow |\psi\rangle_2$ is **entangled**.

c).3. $|\psi\rangle_3$

The eigenvalues of $\hat{\rho}_3$ are

$$w_1 = 0, \qquad\qquad w_2 = 1,$$

therefore, the entanglement entropy is

$$\begin{aligned} \rightsquigarrow \underline{\underline{S_e^{(3)}}} &= -w_1 \ln w_1 - w_2 \ln w_2 \\ &= - \underbrace{0 \cdot \ln 0}_{\lim\limits_{x \to 0} x \ln x = 0} - 1 \ln 1 = \underline{\underline{0}} \end{aligned}$$

$\rightsquigarrow |\psi\rangle_3$ is **not entangled**.