Exercise sheet 2, ANM

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Problem 7.1

a) there are two states $|\frac{1}{2},\frac{1}{2}\rangle$ and $|\frac{1}{2},-\frac{1}{2}\rangle$ representing spin up & down

$\Rightarrow \hat{S}^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2}\sigma^z$

$\hat{S}^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$

$\hat{S}^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

$\hat{S}^z|\frac{1}{2},\frac{1}{2}\rangle = \frac{1}{2}|\frac{1}{2},\frac{1}{2}\rangle$

$\hat{S}^z|\frac{1}{2},-\frac{1}{2}\rangle = -\frac{1}{2}|\frac{1}{2},-\frac{1}{2}\rangle$

$S^+|\frac{1}{2},\frac{1}{2}\rangle = \sqrt{\frac{1}{2}(\frac{1}{2}+1)-\frac{1}{2}(\frac{1}{2}+1)}\,|\frac{1}{2},\frac{3}{2}\rangle = 0$

$S^+|\frac{1}{2},-\frac{1}{2}\rangle = \sqrt{\frac{1}{2}(\frac{1}{2}+1)+\frac{1}{2}(-\frac{1}{2})}\,|\frac{1}{2},\frac{1}{2}\rangle$

$= \sqrt{\frac{3}{4}+\frac{1}{4}}\,|\frac{1}{2},\frac{1}{2}\rangle = 1|\frac{1}{2},\frac{1}{2}\rangle$

$S^-|\frac{1}{2},-\frac{1}{2}\rangle = 0$

$S^-|\frac{1}{2},\frac{1}{2}\rangle = \sqrt{\frac{3}{4}-\frac{1}{2}(-\frac{1}{2})}\,|\frac{1}{2},-\frac{1}{2}\rangle = |\frac{1}{2},-\frac{1}{2}\rangle$

b) states are $|1,1\rangle = |\uparrow\rangle$, $|1,0\rangle = |0\rangle$, $|1,-1\rangle = |\downarrow\rangle$

general form form of matrix: $\hat{Q} = \begin{pmatrix} \langle\uparrow|\hat{Q}|\uparrow\rangle & \langle\uparrow|\hat{Q}|0\rangle & \langle\uparrow|\hat{Q}|\downarrow\rangle \\ \langle 0|\hat{Q}|\uparrow\rangle & \langle 0|\hat{Q}|0\rangle & \langle 0|\hat{Q}|\downarrow\rangle \\ \langle\downarrow|\hat{Q}|\uparrow\rangle & \langle\downarrow|\hat{Q}|0\rangle & \langle\downarrow|\hat{Q}|\downarrow\rangle \end{pmatrix}$

where $\hat{Q} \in \{\hat{S}^z, \hat{S}^+, \hat{S}^-\}$

$\Rightarrow$ for $\hat{S}^z$

$\left.\begin{aligned} \hat{S}^z|\uparrow\rangle &= |\uparrow\rangle \\ \hat{S}^z|0\rangle &= 0 \\ \hat{S}^z|\downarrow\rangle &= -|\downarrow\rangle \end{aligned}\right\} \hat{S}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

$\Rightarrow$ for $\hat{S}^+$

$\left.\begin{aligned} \hat{S}^+|\uparrow\rangle &= 0 \\ \hat{S}^+|0\rangle &= \sqrt{2}|\uparrow\rangle \\ \hat{S}^+|\downarrow\rangle &= \sqrt{2}|0\rangle \end{aligned}\right\} \hat{S}^+ = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}\sqrt{2}$

$\Rightarrow$ for $\hat{S}^-$

$\left.\begin{aligned} \hat{S}^-|\uparrow\rangle &= \sqrt{2}|0\rangle \\ \hat{S}^-|0\rangle &= \sqrt{2}|\downarrow\rangle \\ \hat{S}^-|\downarrow\rangle &= 0 \end{aligned}\right\} \hat{S}^- = \sqrt{2}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

Exercise 7.1.a and 7.1.b computed results

For code see Hamiltonian.py

S=1/2 Heisenberg model

Hamiltonian is :
```
 [[ 0.25  0.    0.    0.  ]
 [ 0.   -0.25  0.5   0.  ]
 [ 0.    0.5  -0.25  0.  ]
 [ 0.    0.    0.    0.25]]
```
With eigenvalue:

```
[-0.75  0.25  0.25  0.25]
```
and eigenvectors:

```
[[ 0.      1.      0.      0.    ]
 [ 0.7071  0.      0.7071  0.    ]
 [-0.7071  0.      0.7071  0.    ]
 [ 0.      0.      0.      1.    ]]
```

S=1 Heisenberg model

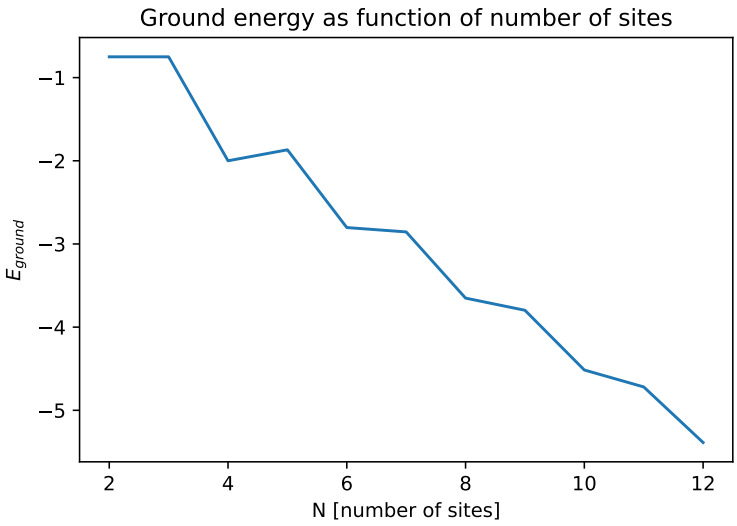
Hamiltonian is :
```
 [[1. 0. 0. 0. 0. 0. 0. 0. 0.]
 [0. 1. 0. 1. 0. 0. 0. 0. 0.]
 [0. 0. 1. 0. 1. 0. 0. 0. 0.]
 [0. 1. 0. 1. 0. 0. 0. 0. 0.]
 [0. 0. 1. 0. 1. 0. 1. 0. 0.]
 [0. 0. 0. 0. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 1. 0. 1. 0. 0.]
 [0. 0. 0. 0. 0. 1. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 0. 0. 1.]]
```

With eigenvalue:

```
[-0.4142 -0.     -0.      1.      1.      1.      2.      2.      2.4142]
```
and eigenvectors:

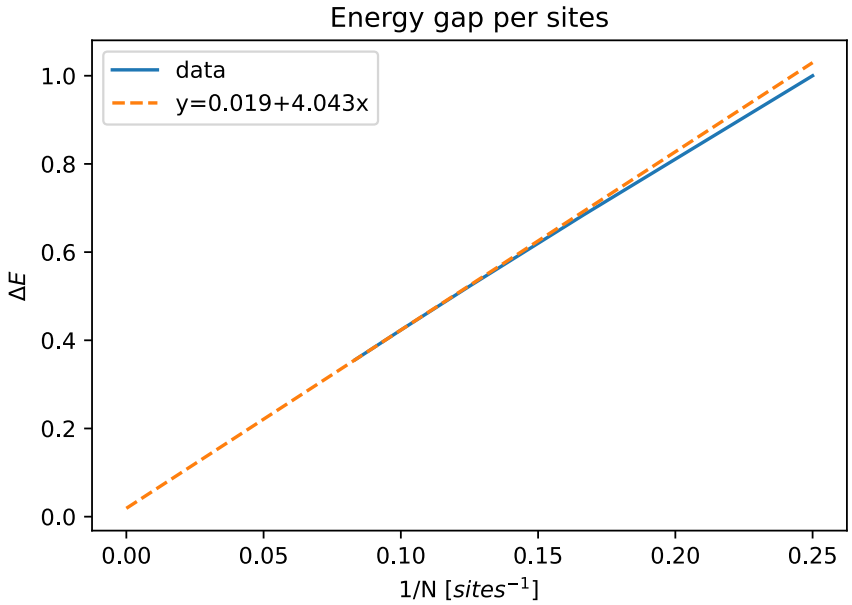
```
[[ 0.     -0.     -0.      1.      0.      0.      0.      0.      0.    ]
 [ 0.     -0.7071 -0.      0.      0.      0.      0.     -0.7071  0.    ]
 [ 0.5    0.     -0.      0.      0.      0.7071  0.      0.     -0.5   ]
 [ 0.      0.7071 -0.      0.      0.      0.      0.     -0.7071  0.    ]
 [-0.7071 -0.     -0.      0.      0.     -0.      0.      0.     -0.7071]
 [ 0.     -0.      0.7071  0.      0.      0.      0.7071  0.      0.    ]
 [ 0.5    -0.      0.      0.      0.     -0.7071  0.      0.     -0.5   ]
 [ 0.     -0.     -0.7071  0.      0.      0.      0.7071  0.      0.    ]
 [ 0.     -0.     -0.      0.      1.      0.      0.      0.      0.    ]]
```

Exercise 7.2.4



Due to the ground state existing of a system with all spins down the first excited state is due to a spin flip. Where the spin changes from down to up for the S=1/2 system.
This is the cause for the oscillation because the increase in the system size (number of sites) results in a lower ground state. For odd numbered system sizes there is always one spin that is flipped to an up state which results in an increase/slower decrease of the ground energy which can be seen in the figure.

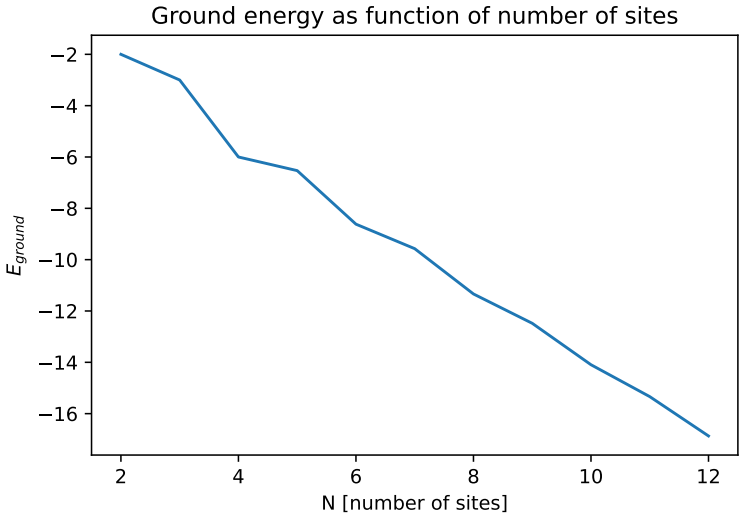
Exercise 7.2.5

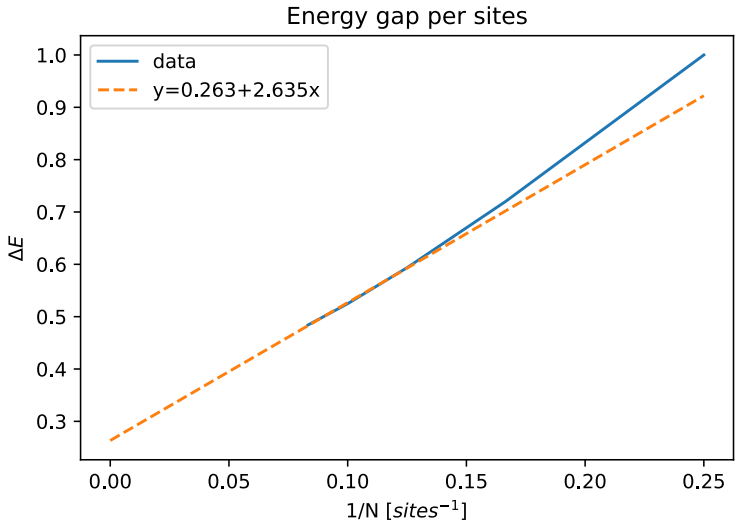


S=1/2 system for system sizes ranging from 2 till 12, the extrapolated energy in the thermodynamic limit is not zero as would be expected but any deviation from zero could result from rounding errors during calculation

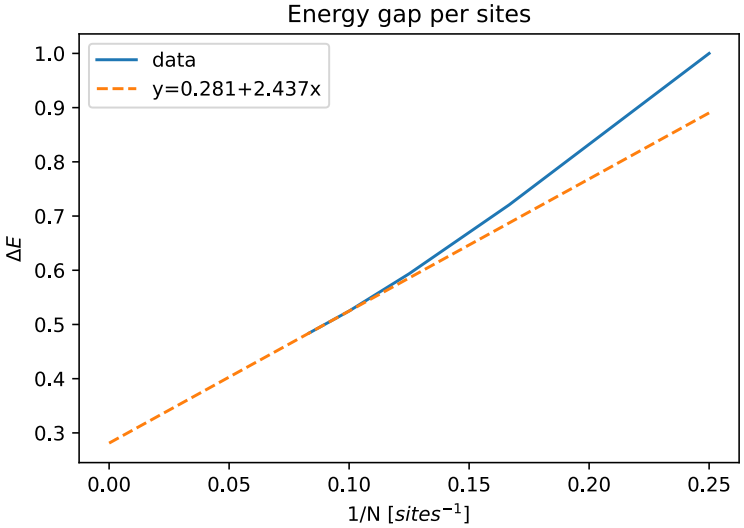
Exercise 7.2.6

For the system sizes the range is taken from 2 till 12 sites





Interpolation for the three largest system sizes, which are 10,11, and 12 sites. The extrapolation results in an energy of 0.263 in the thermodynamic limit.



Interpolation for the two largest system sizes, which are 11, and 12 sites. The extrapolation results in an energy of 0.281 in the thermodynamic limit.