Ground state of the two-qubit Ising model

In[43]:=

```
$Assumptions = {J > 0, h > 0};
```

Define Pauli operators and other

In[44]:=

```
I1 = {{1, 0}, {0, 1}}; MatrixForm[I1]
```

Out[44]//MatrixForm=

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

In[45]:=

```
X = {{0, 1}, {1, 0}}; MatrixForm[X]
```

Out[45]//MatrixForm=

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

In[46]:=

```
Y = {{0, -I}, {I, 0}}; MatrixForm[Y]
```

Out[46]//MatrixForm=

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

In[47]:=

```
Z = {{1, 0}, {0, -1}}; MatrixForm[Z]
```

Out[47]//MatrixForm=

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In[48]:=

$$H = \frac{1}{\mathtt{Sqrt[2]}} \{\{1, 1\}, \{1, -1\}\}; \mathtt{MatrixForm[H]}$$

Out[48]//MatrixForm=

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

In[49]:=

```
I1 = {{1, 0}, {0, 1}}; MatrixForm[I1]
```

Out[49]//MatrixForm=

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

In[50]:=

```
X = {{0, 1}, {1, 0}}; MatrixForm[X]
```

Out[50]//MatrixForm=

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

In[51]:=

```
Y = {{0, -I}, {I, 0}}; MatrixForm[Y]
```

Out[51]//MatrixForm=

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

In[52]:=

```
Z = {{1, 0}, {0, -1}}; MatrixForm[Z]
```

Out[52]//MatrixForm=

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In[53]:=

$$H = \frac{1}{\text{Sqrt[2]}} \{\{1, 1\}, \{1, -1\}\}; \text{MatrixForm[H]}$$

Out[53]//MatrixForm=

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

Define two qubit operators

In[54]:=

```
ZZ = KroneckerProduct[Z, Z];  MatrixForm[ZZ]
```

Out[54]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

In[55]:=

```
IX = KroneckerProduct[I1, X]; MatrixForm[IX]
```

Out[55]//MatrixForm=

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

In[56]:=

```
XI = KroneckerProduct[X, I1]; MatrixForm[XI]
```

Out[56]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Define the Hamiltonian

In[57]:=

```
Hamiltonian[J_, h0_, h1_] = -J ZZ - h0 XI - h1 IX; MatrixForm[Hamiltonian[J, h0, h1]]
```

Out[57]//MatrixForm=

$$\begin{pmatrix} -J & -h1 & -h0 & 0 \\ -h1 & J & 0 & -h0 \\ -h0 & 0 & J & -h1 \\ 0 & -h0 & -h1 & -J \end{pmatrix}$$

Compute eigenvalues and eigenvectors

We consider H0 with no field , and H1 with external field

Hamiltonian with no field

In[58]:=

```
H0 = Hamiltonian[J, 0, 0]; MatrixForm[H0]
```

Out[58]//MatrixForm=

$$\begin{pmatrix} -J & 0 & 0 & 0 \\ 0 & J & 0 & 0 \\ 0 & 0 & J & 0 \\ 0 & 0 & 0 & -J \end{pmatrix}$$

In[59]:=

```
Eigenvalues[H0]
```

Out[59]=

```
{-J, -J, J, J}
```

In[60]:=

```
Eigenvectors[H0]
```

Out[60]=

```
{{0, 0, 0, 1}, {1, 0, 0, 0}, {0, 0, 1, 0}, {0, 1, 0, 0}}
```

The eigenvectors are the basis vectors, if J>0 the ground state is 00 and 11
These are product states with no entanglement

However also combinations of the ground states are eigestates, and the Bell state 00+11 is a ground state

Notably enough this is maximally entangled !!!
So we can have ground state with and without entanglement in the absence of the field

Hamiltonian with field h0=h1=h

In[61]:=

```
H1 = Hamiltonian[J, h, h]; MatrixForm[H1]
```

Out[61]//MatrixForm=

$$\begin{pmatrix} -J & -h & -h & 0 \\ -h & J & 0 & -h \\ -h & 0 & J & -h \\ 0 & -h & -h & -J \end{pmatrix}$$

In[62]:=

```
Eigenvalues[H1]
```

Out[62]=

$$\left\{-J, J, -\sqrt{4 h^2 + J^2}, \sqrt{4 h^2 + J^2}\right\}$$

In[63]:=

```
e1 = Eigenvectors[H1]
```

Out[63]=

$$\left\{\{-1, 0, 0, 1\}, \{0, -1, 1, 0\}, \left\{1, -\frac{J - \sqrt{4 h^2 + J^2}}{2 h}, -\frac{J - \sqrt{4 h^2 + J^2}}{2 h}, 1\right\}, \left\{1, -\frac{J + \sqrt{4 h^2 + J^2}}{2 h}, -\frac{J + \sqrt{4 h^2 + J^2}}{2 h}, 1\right\}\right\}$$

For J>0 degeneracy is broken, and the state with energy -J is -00+11 which is a maximally-entangled Bell state, as the eingevector with energy J i.e. -01+10

The ground state has energy -$\sqrt{}$(4 h^2+J^2) and is also an entangled written as a combination of bell states 00+11 and 01+10

Hamiltonian with h0=h and h1=0

In[64]:=

```
H2 = Hamiltonian[J, h, 0]; MatrixForm[H2]
```

Out[64]//MatrixForm=

$$\begin{pmatrix} -J & 0 & -h & 0 \\ 0 & J & 0 & -h \\ -h & 0 & J & 0 \\ 0 & -h & 0 & -J \end{pmatrix}$$

In[65]:=

```
Eigenvalues[H2]
```

Out[65]=

$$\left\{-\sqrt{h^2 + J^2}, -\sqrt{h^2 + J^2}, \sqrt{h^2 + J^2}, \sqrt{h^2 + J^2}\right\}$$

In[66]:=

```
e2 = Eigenvectors[H2]
```

Out[66]=

$$\left\{\left\{0, -\frac{J-\sqrt{h^2+J^2}}{h}, 0, 1\right\}, \left\{-\frac{-J-\sqrt{h^2+J^2}}{h}, 0, 1, 0\right\}, \left\{0, -\frac{J+\sqrt{h^2+J^2}}{h}, 0, 1\right\}, \left\{-\frac{-J+\sqrt{h^2+J^2}}{h}, 0, 1, 0\right\}\right\}$$

Hamiltonian with field h0 ≠ h1

In[67]:=

```
H1 = Hamiltonian[J, h0, h1]; MatrixForm[H1]
```

Out[67]//MatrixForm=

$$\begin{pmatrix} -J & -h1 & -h0 & 0 \\ -h1 & J & 0 & -h0 \\ -h0 & 0 & J & -h1 \\ 0 & -h0 & -h1 & -J \end{pmatrix}$$

Computing the entanglement of the ground state by schmidt decomposition

Entanglement for H1

Normalize the ground state

In[88]:=

```
Norm[e1[[3]]] // Simplify
```

Out[88]=

$$\sqrt{4+\frac{J\left(J-\sqrt{4 h^2+J^2}\right)}{h^2}}$$

In[68]:=

```
nGS = FullSimplify[Refine[e1[[3]] / Norm[e1[[3]]], Assumptions → J > 0 && h > 0]]; MatrixForm[nGS]
```

Out[68]//MatrixForm=

$$\begin{pmatrix} \frac{h}{\sqrt{4 h^2+J\left(J-\sqrt{4 h^2+J^2}\right)}} \\ \frac{1}{2}\sqrt{1-\frac{J}{\sqrt{4 h^2+J^2}}} \\ \frac{1}{2}\sqrt{1-\frac{J}{\sqrt{4 h^2+J^2}}} \\ \frac{h}{\sqrt{4 h^2+J^2\left(J-\sqrt{4 h^2+J^2}\right)}} \end{pmatrix}$$

In[69]:=

```
Refine[Limit[nGS, h → 0], Assumptions → J > 0]
```

Limit: Warning: Assumptions that involve the limit variable are ignored.

Out[69]=

```
{Indeterminate, 0, 0, Indeterminate}
```

Check normalization

In[70]:=

```
Refine[Norm[nGS], Assumptions → J > 0 && h > 0] // FullSimplify
```

Out[70]=

```
1
```

Extract the coefficient for the ground state of H1 as a 2x2 Matrix

In[71]:=

```
Cij = {{nGS[[1]], nGS[[2]]}, {nGS[[3]], nGS[[4]]}}; MatrixForm[Cij]
```

Out[71]//MatrixForm=

$$\begin{pmatrix} \frac{h}{\sqrt{4h^2+J\left(J-\sqrt{4h^2+J^2}\right)}} & \frac{1}{2}\sqrt{1-\frac{J}{\sqrt{4h^2+J^2}}} \\ \frac{1}{2}\sqrt{1-\frac{J}{\sqrt{4h^2+J^2}}} & \frac{h}{\sqrt{4h^2+J\left(J-\sqrt{4h^2+J^2}\right)}} \end{pmatrix}$$

```
dk = FullSimplify[Eigenvalues[Cij]]
```

Out[72]=

$$\left\{\frac{4h\sqrt{4h^2+J^2}-\sqrt{64h^4+48h^2J^2+8J^4-32h^2J\sqrt{4h^2+J^2}-8J^3\sqrt{4h^2+J^2}}}{4\sqrt{4h^2+J^2}\sqrt{4h^2+J^2-J\sqrt{4h^2+J^2}}},\right.$$
$$\left.\frac{4h\sqrt{4h^2+J^2}+\sqrt{64h^4+48h^2J^2+8J^4-32h^2J\sqrt{4h^2+J^2}-8J^3\sqrt{4h^2+J^2}}}{4\sqrt{4h^2+J^2}\sqrt{4h^2+J^2-J\sqrt{4h^2+J^2}}}\right\}$$

Check eigenvalues

In[73]:=

```
Sum[dk[[j]]^2, {j, 1, 2}] // FullSimplify
```

Out[73]=

```
1
```

In[74]:=

```
Sum[dk[[j]]^2, {j, 1, 2}] /. {J → 1.0, h → 0.5}
```

Out[74]=

```
1.
```

SVD of Cij

In[91]:=

```
{Usvd, dsvd, Vsvd} = SingularValueDecomposition[Cij]
```

Out[91]=

$$\left\{\left\{\left\{\frac{\frac{1}{2}\sqrt{1-\frac{J}{\sqrt{4h^2+J^2}}}-\frac{h(\cdots 1\cdots)}{\sqrt{4h^2+J\cdots 1\cdots}\,(\cdots 1\cdots)}}{\sqrt{\text{Abs}\left[\frac{h}{\sqrt{\cdots 1\cdots}}-\frac{\cdots 1\cdots}{\cdots 1\cdots}\right]^2+\text{Abs}\left[\frac{1}{2}\cdots 1\cdots-\cdots 1\cdots\right]^2}},\frac{\frac{1}{2}\sqrt{1-\frac{J}{\cdots 1\cdots}}-\cdots 1\cdots}{\sqrt{\text{Abs}[\cdots 1\cdots]^2+\cdots 1\cdots^2}}\right\},\left\{\frac{\frac{h}{\cdots 1\cdots}-\cdots 1\cdots}{\sqrt{\cdots 1\cdots^2+\cdots 1\cdots}},\cdots 1\cdots\right\}\right\},\{\cdots 1\cdots\},\{\cdots 1\cdots\}\right\}$$

Full expression not available (original memory size: 0.5 MB)

In[93]:=

```
FullSimplify[dsvd]
```

Out[93]=

$$\left\{\left\{\sqrt{\left(\left(\sqrt{4h^4+2J^3\left(J-\sqrt{4h^2+J^2}\right)+4h^2J\left(2J-\sqrt{4h^2+J^2}\right)}+2h\left(h-\sqrt{2h^2+J^2-J\sqrt{4h^2+J^2}+\sqrt{4h^4+2J^3\left(J-\sqrt{4h^2+J^2}\right)+4h^2J\left(2J-\sqrt{4h^2+J^2}\right)}}\right)\right)\Big/\left(8h^2+2J\left(J-\sqrt{4h^2+J^2}\right)\right)\right)},0\right\},\left\{0,\sqrt{\left(\left(\sqrt{4h^4+2J^3\left(J-\sqrt{4h^2+J^2}\right)+4h^2J\left(2J-\sqrt{4h^2+J^2}\right)}+2h\left(h+\sqrt{2h^2+J^2-J\sqrt{4h^2+J^2}+\sqrt{4h^4+2J^3\left(J-\sqrt{4h^2+J^2}\right)+4h^2J\left(2J-\sqrt{4h^2+J^2}\right)}}\right)\right)\Big/\left(8h^2+2J\left(J-\sqrt{4h^2+J^2}\right)\right)\right)}\right\}\right\}$$

In[96]:=

```
dsvd1 = FullSimplify[dsvd[[1, 1]]]
```

Out[96]=

$$\sqrt{\left(\left(\sqrt{4h^4+2J^3\left(J-\sqrt{4h^2+J^2}\right)+4h^2J\left(2J-\sqrt{4h^2+J^2}\right)}+2h\left(h-\sqrt{2h^2+J^2-J\sqrt{4h^2+J^2}+\sqrt{4h^4+2J^3\left(J-\sqrt{4h^2+J^2}\right)+4h^2J\left(2J-\sqrt{4h^2+J^2}\right)}}\right)\right)\Big/\left(8h^2+2J\left(J-\sqrt{4h^2+J^2}\right)\right)\right)}$$

In[101]:=

```
dsvd2 = FullSimplify[dsvd[[2, 2]]]
```

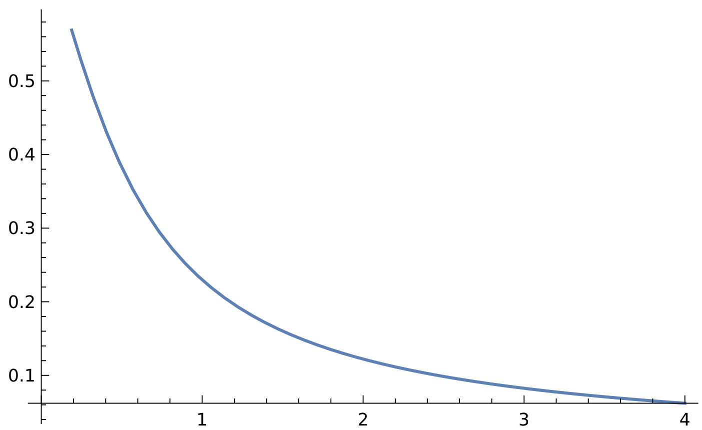
Out[101]=

$$\sqrt{\left(\left(\sqrt{4 h^4 + 2 J^3 \left(J - \sqrt{4 h^2 + J^2}\right) + 4 h^2 J \left(2 J - \sqrt{4 h^2 + J^2}\right)} + 2 h \left(h + \sqrt{2 h^2 + J^2 - J \sqrt{4 h^2 + J^2} + \sqrt{4 h^4 + 2 J^3 \left(J - \sqrt{4 h^2 + J^2}\right) + 4 h^2 J \left(2 J - \sqrt{4 h^2 + J^2}\right)}}\right)\right) \Big/ \left(8 h^2 + 2 J \left(J - \sqrt{4 h^2 + J^2}\right)\right)\right)}$$

In[97]:=

```
Plot[dsvd1 /. J → 1, {h, 0, 4}]
```

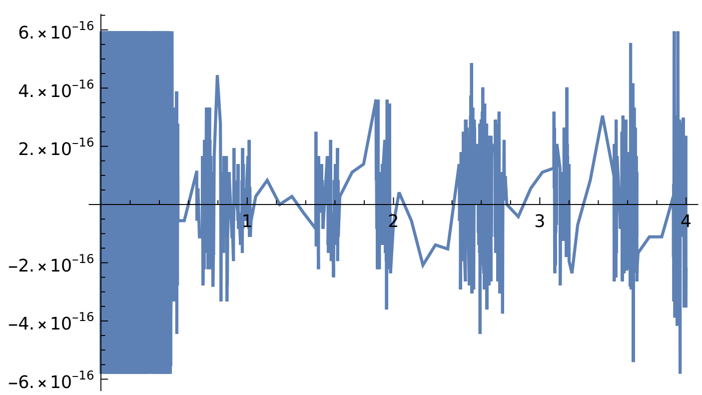
Out[97]=



In[99]:=

```
Plot[dk[[1]] - dsvd1 /. J → 1, {h, 0, 4}]
```

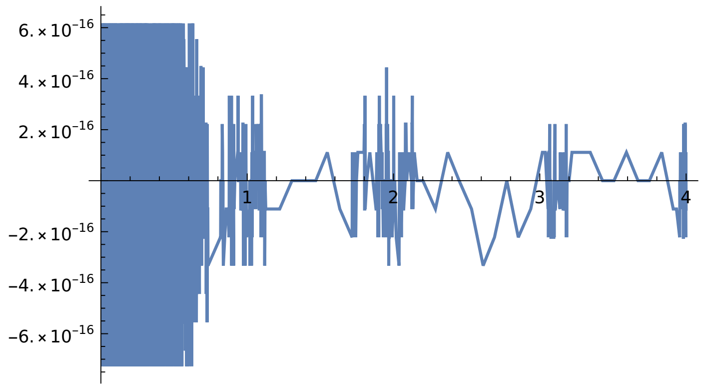
Out[99]=



In[102]:=

```
Plot[dk⟦2⟧ - dsvd2 /. J → 1, {h, 0, 4}]
```

Out[102]=



Entropy of entanglement

In[75]:=

```
entropy = -Sum[dk⟦j⟧^2 × Log2[dk⟦j⟧^2], {j, 1, 2}];
```

In[104]:=

```
FullSimplify[entropy]
```

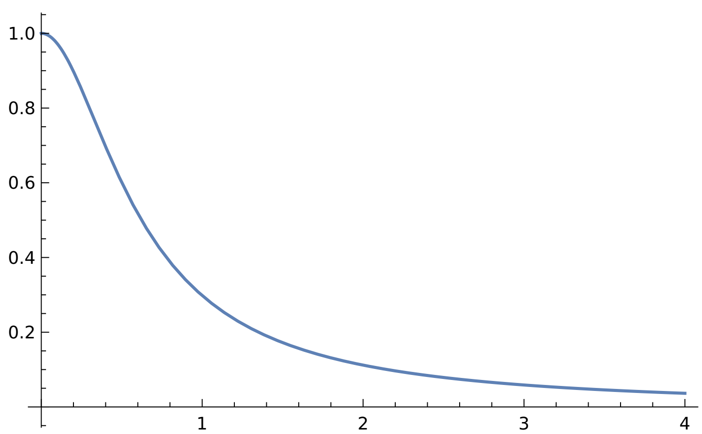
Out[104]=

$$-\frac{\dfrac{4\,h\,\sqrt{4\,h^2+2\,J\left(J-\sqrt{4\,h^2+J^2}\right)}\ \mathrm{ArcCoth}\left[\dfrac{\sqrt{2}\,h}{\sqrt{2\,h^2+J^2-J\,\sqrt{4\,h^2+J^2}}}\right]}{4\,h^2+J\left(J-\sqrt{4\,h^2+J^2}\right)}+\mathrm{Log}\left[\dfrac{J}{2\,\sqrt{4\,h^2+J^2}}\right]}{\mathrm{Log}[2]}$$

In[76]:=

```
Plot[entropy /. J → 1, {h, 0, 4.0}]
```

Out[76]=



In[77]:=

⋮

Out[77]=

⋮

Apparently even a vanishing field introduce entanglement by breaking the degeneracy and making as the ground state the Bell state

For large h the ground state is the product state of the eigenstates of X and no entanglement is present

Entanglement of H2

Normalize the ground state

Note that the ground state is the first eigenvalue

In[78]:=

```
nGS2 = FullSimplify[Refine[e2[[1]] / Norm[e2[[1]]], Assumptions → J > 0 && h > 0]];
MatrixForm[nGS2]
```

Out[78]//MatrixForm=

$$\begin{pmatrix} 0 \\ \frac{1}{\sqrt{2+\frac{2J\left(J+\sqrt{h^2+J^2}\right)}{h^2}}} \\ 0 \\ \frac{1}{\sqrt{2+\frac{2J\left(J-\sqrt{h^2+J^2}\right)}{h^2}}} \end{pmatrix}$$

In[79]:=

```
Refine[Limit[nGS2, h → 0], Assumptions → J > 0]
```

Limit: Warning: Assumptions that involve the limit variable are ignored.

Out[79]=

```
{0, 0, 0, 1}
```

Check normalization

In[80]:=

```
Refine[Norm[nGS2], Assumptions → J > 0 && h > 0] // FullSimplify
```

Out[80]=

```
1
```

Extract the coefficient for the ground state of H2 as a 2x2 Matrix

In[81]:=

```
Cij2 = {{nGS2[[1]], nGS2[[2]]}, {nGS2[[3]], nGS2[[4]]}}; MatrixForm[Cij2]
```

Out[81]//MatrixForm=

$$\begin{pmatrix} 0 & \frac{1}{\sqrt{2+\frac{2J\left(J+\sqrt{h^2+J^2}\right)}{h^2}}} \\ 0 & \frac{1}{\sqrt{2+\frac{2J\left(J-\sqrt{h^2+J^2}\right)}{h^2}}} \end{pmatrix}$$

In[82]:=

```
dk2 = Eigenvalues[Cij2]
```

Out[82]=

$$\left\{0, \frac{1}{\sqrt{2}\ \sqrt{\frac{h^2+J^2-J\ \sqrt{h^2+J^2}}{h^2}}}\right\}$$

This state is not entangled as it has only one Schmidt coefficient non vanishing

Check decomposition

In[83]:=

```
Sum[dk2[[j]]^2, {j, 1, 2}] // FullSimplify
```

Out[83]=

$$\frac{1}{2}\left(1+\frac{J}{\sqrt{h^2+J^2}}\right)$$

In[84]:=

```
Sum[dk2[[j]]^2, {j, 1, 2}] /. {J → 1.0, h → 0.5}
```

Out[84]=

0.947214