Advanced Quantum Theory Homework 8

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Exercise 1

Show that, conversely, as the temperature is driven to zero, $\beta \to \infty$, the density matrix tends towards the pure ground state of the Hamiltonian.

Solution. First note that we can write the density matrix as

$$\hat{\rho} = \sum_{i=0}^{\infty} \frac{e^{-\beta E_i}}{Z} |E_i\rangle\langle E_i| .$$

where Z is the usual partition function. Now we can pull out the first term marked by the property that is has the lowest energy $E_0 \leq E_i$ for all i.

$$\begin{aligned} \hat{\rho} &= e^{-\beta E_0} \sum_{i=0}^{\infty} \frac{e^{-\beta(E_i - E_0)}}{Z} |E_i\rangle\langle E_i| \\ &= e^{-\beta E_0} \left[\frac{1}{Z} |E_0\rangle\langle E_0| + \sum_{i=1}^{\infty} \frac{e^{-\beta(E_i - E_0)}}{Z} |E_i\rangle\langle E_i| \right] \end{aligned} \tag{1}$$

Now let's take a look at the partition function when $\beta \to \infty$.

$$\lim_{\beta\to\infty} Z = \lim_{\beta\to\infty} e^{-\beta E_0} + e^{-\beta E_1} + e^{-\beta E_2} + \cdots \approx e^{-\beta E_0}$$

Where, I don't think this is very rigorous, but makes intuitive sense because every $E_i \geq E_0$, so they go to 0 faster. This allows us to cancel the terms in front of the $|E_0\rangle\langle E_0|$ term, and using the fact that $\lim_{\beta\to\infty} e^{-\beta E} = 0$ we can drop the second term of **??**. This leaves us with

$$\lim_{\beta\to\infty} \hat{\rho} = |E_0\rangle\langle E_0| .$$

I think somewhat equivalently, one could scale all the energies so that $\tilde{E}_0 = 0$, and $\tilde{E}_i = E_i - E_0$. This maybe makes it more clear that the first term isn't going anywhere, but everything else will. I just wasn't sure if that's always valid to scale the energies like that.

Exercise 2

Differentiate Eq.11.16 with respect to λ and show that this derivative is always ≤ 0. Hint: Recall the definition of the variance (of the energy).

Solution. First, we'll put $\hat{H}$ in it's eigenbasis so it's diagonal. That makes these computations much easier.

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\overline{E} = \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{1}{\sum_n \mathrm{e}^{-\lambda E_n}}\sum_n E_n \mathrm{e}^{-\lambda E_n}\right)$$

This is going to get a touch messy so let's break this into two pieces and then apply the chain rule $f' = g'h + gh'$[1] later. So we'll first calculate the derivative of the first and second terms separately.

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{1}{\sum_n \mathrm{e}^{-\lambda E_n}}\right) = \frac{\sum_n E_n \mathrm{e}^{-\lambda E_n}}{\left(\sum_n \mathrm{e}^{-\lambda E_n}\right)^2} \qquad \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\sum_n E_n \mathrm{e}^{-\lambda E_n}\right) = -\sum_n E_n^2 \mathrm{e}^{-\lambda E_n}$$

Putting these back together we have:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\lambda}\overline{E} &= \left(\frac{\sum_n E_n \mathrm{e}^{-\lambda E_n}}{\sum_n \mathrm{e}^{-\lambda E_n}}\right)^2 - \frac{\sum_n E_n^2 \mathrm{e}^{-\lambda E_n}}{\sum_n \mathrm{e}^{-\lambda E_n}} \\ &= \overline{E}^2 - \overline{E^2} \\ &= -(\Delta E)^2\end{aligned}$$

Because we know $\Delta E \geq 0$, we can conclude $\frac{\mathrm{d}E}{\mathrm{d}\lambda} \leq 0$ as desired.

[1] Just in case you forgot ☺.

Exercise 3

Consider a quantum harmonic oscillator of frequency ω in a thermal environment with temperature T.

(a) Calculate its thermal state $\hat{\rho}$.

(b) Explicitly calculate the energy expectation value $\overline{E}(\beta)$ as a function of the inverse temperature β.

Hint: Consider using the geometric series $\sum_{n=0}^{\infty} \mathrm{e}^{-\alpha n} = \sum_{n=0}^{\infty} (\mathrm{e}^{\alpha})^n = 1/(1-\mathrm{e}^{-\alpha})$ which holds for all $\alpha > 0$. Also the derivative of this equation with respect to α is useful.

Solution. **??** In the eigenbasis of the Hamiltonian we have

$$\hat{H} = \begin{bmatrix} E_0 & & & \\ & E_1 & & \\ & & E_2 & \\ & & & \ddots \end{bmatrix}$$

which makes it easy to see that our thermal state is given by the following

$$\hat{\rho} = \frac{1}{\sum_n \mathrm{e}^{-\beta E_n}} \begin{bmatrix} \mathrm{e}^{-\beta E_0} & & & \\ & \mathrm{e}^{-\beta E_1} & & \\ & & \mathrm{e}^{-\beta E_2} & \\ & & & \ddots \end{bmatrix}$$

where $E_n = \hbar\omega(n + \frac{1}{2})$.

?? We start with the equation

$$\overline{E}(\beta) = \frac{1}{\mathrm{tr}\left(\mathrm{e}^{-\beta \hat{H}}\right)} \mathrm{tr}\left(\hat{H} \mathrm{e}^{-\beta \hat{H}}\right).$$

Let's take this step by step and calculate the trace of the simpler $\mathrm{e}^{-\beta \hat{H}}$ first.

$$\begin{aligned} \mathrm{tr}\left(-\beta \hat{H}\right) &= \sum_n \langle n| \mathrm{e}^{-\beta \hat{H}} |n\rangle \\ &= \sum_n \mathrm{e}^{-\beta\hbar\omega(n+\frac{1}{2})} \\ &= \mathrm{e}^{-\beta\hbar\omega/2} \sum_n \mathrm{e}^{-\beta\hbar\omega n} \\ &= \frac{\mathrm{e}^{-\beta\hbar\omega/2}}{1-\mathrm{e}^{-\beta\hbar\omega}} \\ &= \frac{\mathrm{e}^{\beta\hbar\omega/2}}{\mathrm{e}^{\beta\hbar\omega}-1} \end{aligned}$$

Now we'll need the trace of $\mathrm{e}^{-\beta\hat{H}}\hat{H}$ also.

$$\begin{aligned}
\operatorname{tr}\left(\mathrm{e}^{-\beta\hat{H}}\hat{H}\right) &= \sum_n \langle n| \mathrm{e}^{-\beta\hat{H}}\hat{H} |n\rangle \\
&= \sum_n \mathrm{e}^{-\beta\hbar\omega(n+\frac{1}{2})}\left[\hbar\omega\left(n+\frac{1}{2}\right)\right] \\
&= \frac{\hbar\omega}{2}\sum_n \mathrm{e}^{-\beta\hbar\omega(n+\frac{1}{2})} + \hbar\omega\sum_n n\mathrm{e}^{-\beta\hbar\omega(n+\frac{1}{2})} \\
&= \frac{\hbar\omega}{2}\frac{\mathrm{e}^{\beta\hbar\omega/2}}{\mathrm{e}^{\beta\hbar\omega}-1} + \hbar\omega\mathrm{e}^{-\beta\hbar\omega/2}\frac{\mathrm{e}^{-\beta\hbar\omega}}{(1-\mathrm{e}^{-\beta\hbar\omega})^2} \\
&= \frac{\hbar\omega}{2}\frac{\mathrm{e}^{\beta\hbar\omega/2}}{\mathrm{e}^{\beta\hbar\omega}-1} + \hbar\omega\frac{\mathrm{e}^{\beta\hbar\omega/2}}{(\mathrm{e}^{\beta\hbar\omega}-1)^2} \\
&= \hbar\omega\frac{\mathrm{e}^{\beta\hbar\omega/2}}{\mathrm{e}^{\beta\hbar\omega}-1}\left(\frac{1}{2}+\frac{1}{\mathrm{e}^{\beta\hbar\omega}-1}\right)
\end{aligned}$$

Putting these together we have

$$\overline{E}(\beta) = \frac{1}{\operatorname{tr}\left(\mathrm{e}^{-\beta\hat{H}}\right)}\operatorname{tr}\left(\hat{H}\mathrm{e}^{-\beta\hat{H}}\right) = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{\mathrm{e}^{\beta\hbar\omega}-1}.$$

Exercise 1

Assume that the density operator of system A is $\hat{\rho}^{(A)}$ and that $\hat{f}^{(A)}$ is an observable in system A. Then the prediction for $\overline{f}^{(A)}$ is given as always by $\overline{f} = \operatorname{tr}\left(\hat{\rho}^{(A)}\hat{f}^{(A)}\right)$. Now assume that the density operator of a combined system AB happens to be of the form $\hat{\rho}^{(AB)} = \hat{\rho}^{(A)} \otimes \hat{\rho}^{(B)}$. Show that the operator $\hat{f}^{(A)} \otimes \mathbb{1}$ represents the observable $\hat{f}^{(A)}$ on the larger system AB, which means that the prediction $\overline{f}(A)$ can also be calculated within the large system AB, namely as the expectation value of the observable $\hat{f}^{(A)} \otimes \mathbb{1}$. I.e., the task is to show that $\overline{f}^{(A)} = \operatorname{tr}\left(\hat{\rho}^{(AB)}(\hat{f}^{(A)} \otimes \mathbb{1})\right)$.

Solution.

$$
\begin{aligned}
\overline{f}_A^{(A)} &= \operatorname{tr}\left(\hat{\rho}^{(A)}\hat{f}^{(A)}\right) \\
\overline{f}_{AB}^{(A)} &= \operatorname{tr}\left(\hat{\rho}^{(AB)}\left(\hat{f}^{A} \otimes \mathbb{1}\right)\right) \\
&= \operatorname{tr}\left(\hat{\rho}^{(A)} \otimes \hat{\rho}^{(B)}\left(\hat{f}^{A} \otimes \mathbb{1}\right)\right) \\
&= \operatorname{tr}\left(\hat{\rho}^{(A)}\hat{f}^{A} \otimes \hat{\rho}^{(B)}\right) \\
&= \operatorname{tr}\left(\hat{\rho}^{(A)}\hat{f}^{A}\right)\operatorname{tr}\left(\hat{\rho}^{(B)}\right) \\
&= \operatorname{tr}\left(\hat{\rho}^{(A)}\hat{f}^{A}\right) = \overline{f}_A^{(A)}
\end{aligned}
$$

Thus we conclude the observable measured with respect to the system A $\overline{f}_A^{(A)}$ is equal to the observable measured with respect to the combined system AB $\overline{f}_A^{(AB)}$.

Exercise 2

Prove the proposition above. Hint: Notice that the trace on the left hand side is a trace in the large Hilbert space $\mathcal{H}^{(AB)}$ while the trace on the right hand side is a trace over only the Hilbert space $\mathcal{H}^{(A)}$.

Solution. Let's start with the right hand side of the proposition. We'll do this piece by piece since it's messy.

$$\begin{aligned}
\hat{f}^{(A)} \otimes \mathbb{1} &= \left(\sum_{i,j} f_{ij} |a_i\rangle\langle a_j|\right) \otimes \left(\sum_n |b_n\rangle\langle b_n|\right) \\
&= \sum_{i,j,n} f_{ij} |a_i\rangle\langle a_j| \otimes |b_n\rangle\langle b_n| \\
\left(\hat{f}^{(A)} \otimes \mathbb{1}\right)\hat{S}^{(AB)} &= \left[\sum_{i,j,n} f_{ij} |a_i\rangle\langle a_j| \otimes |b_n\rangle\langle b_n|\right] \sum_{r,s,t,u} S_{rstu} |a_r\rangle \otimes |b_s\rangle \langle a_t| \otimes \langle b_n| \\
&= \sum_{i,j,n,t,u} f_{ij} S_{jntu} |a_i\rangle\langle a_t| \otimes |b_n\rangle\langle b_u| \\
&= \sum_{i,j,n,t,u} f_{ij} S_{jntu} (|a_i\rangle \otimes |b_n\rangle)(\langle a_t| \otimes \langle b_u|) \\
\operatorname{tr}\left(\left(\hat{f}^{(A)} \otimes \mathbb{1}\right)\hat{S}^{(AB)}\right) &= \sum_{k,s} \langle a_k| \otimes \langle b_s| \left(\hat{f}^{(A)} \otimes \mathbb{1}\right)\hat{S}^{(AB)} |a_k\rangle \otimes |b_s\rangle \\
&= \sum_{k,j,s} f_{kj} S_{jsks}
\end{aligned}$$

Now the right hand side.

$$\begin{aligned}
\hat{g}^{(A)} &= \sum_i \langle b_i| \left[\sum_{j,k,s,n} S_{jksn} (|a_j\rangle \otimes |b_k\rangle)(\langle a_s| \otimes \langle b_n|)\right] |b_i\rangle \\
&= \sum_{i,j,s} S_{jisi} |a_j\rangle\langle a_s| \\
\hat{f}^{(A)}\hat{g}^{(A)} &= \left[\sum_{i,j} f_{ij} |a_i\rangle\langle a_j|\right]\left[\sum_{i,j,s} S_{jisi} |a_j\rangle\langle a_s|\right] \\
&= \sum_{i,j,s,n} f_{ij} S_{jsns} |a_i\rangle\langle a_n| \\
\operatorname{tr}\left(\hat{f}^{(A)}\hat{g}^{(A)}\right) &= \sum_k \langle a_k| \left[\sum_{i,j,s,n} f_{ij} S_{jsns} |a_i\rangle\langle a_n|\right] |a_k\rangle \\
&= \sum_{k,j,s} f_{kj} S_{jsks}
\end{aligned}$$

Wow I didn't even plan it so the indices match, but they do!

Exercise 3

Consider two systems, A and B, with Hilbert spaces $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(B)}$ which each are only two-dimensional. Assume that $\{|a_1\rangle, |a_2\rangle\}$ and $\{|b_1\rangle, |b_2\rangle\}$ are orthonormal bases of the Hilbert spaces $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(B)}$ respectively. Assume that the composite system AB is in a pure state $|\Omega\rangle \in \mathcal{H}^{(AB)}$ given by:

$$|\Omega\rangle := \alpha(|a_1\rangle |b_2\rangle + 3 |a_2\rangle |b_1\rangle)$$

Here, $\alpha \in \mathbb{R}$ is a constant so that $|\Omega\rangle$ is normalized:$\langle\Omega|\Omega\rangle = 1$.

(a) Calculate α

(b) Is $|\Omega\rangle$ an entangled or unentangled state?

(c) Calculte the density matrix $\hat{\rho}^{(A)}$ of subsystem A. Is it pure or mixed? Hint: you can use your reply to (b).

Solution. **??** All we have to do is ensure the state $|\Omega\rangle$ is normalized.

$$\begin{aligned}
1 = \langle\Omega|\Omega\rangle &= \alpha^2(\langle a_1| \langle b_2| + 3 \langle a_2| \langle b_1|)(|a_1\rangle |b_2\rangle + 3 |a_2\rangle |b_1\rangle) \\
&= \alpha^2(1+9) \\
\alpha &= \pm\frac{1}{\sqrt{10}}
\end{aligned}$$

?? The state $|\Omega\rangle$ is *entangled* because it can't be as a simple product $|\Omega\rangle \neq |\psi\rangle \otimes |\phi\rangle$. This can be shown by assuming they can and arriving at a contradiction.

$$\begin{aligned}
|\Omega\rangle &= |\psi\rangle \otimes |\phi\rangle \\
&= (c_1 |a_1\rangle + c_2 |a_2\rangle) \otimes (d_1 |b_1\rangle + d_2 |d_2\rangle) \\
&= \underbrace{c_1 d_1}_{0} |a_1 b_1\rangle + \underbrace{c_1 d_2}_{\frac{1}{\sqrt{10}}} |a_1 b_2\rangle + \underbrace{c_2 d_1}_{\frac{3}{\sqrt{10}}} |a_2 b_1\rangle + \underbrace{c_1 d_2}_{0} |a_2 b_2\rangle
\end{aligned}$$

The first equation $c_1 d_1 = 0$ tells us c_1 or d_1 is 0, but then both $c_1 d_2 = \frac{1}{\sqrt{10}}$ *and* $c_2 d_1 = \frac{3}{\sqrt{10}}$ are impossible to satisfy simultaneously. Thus it is impossible to write this state as a product and hence it is entangled.

??

$$\begin{aligned}
\rho^{(A)} = \mathrm{tr}_B\left(\rho^{(AB)}\right) &= \sum_{n=1}^{2} \langle b_n|\Omega\rangle \langle\Omega|b_n\rangle \\
&= \frac{1}{10}[|a_1\rangle\langle a_1| + 9 |a_2\rangle\langle a_2|]
\end{aligned}$$

This is clearly of the form $\sum_n p_n |\psi_n\rangle\langle\psi_n|$ with $\sum_n p_n = 1$ and hence is a mixed state. We can also conclude this by the fact that $|\Omega\rangle$ is entangled.

Exercise 1

(a) Show that $\hat{U}(t)$ is unitary.

(b) Calculate $\hat{\rho}^{(AB)}(t)$.

(c) Use the result of (b) to calculate $\hat{\rho}^{(A)}(t)$.

(d) Calculate, therefore, the purity measure $P[\hat{\rho}^{(A)}(t)]$ and sketch a plot of it as a function of time.

(e) Now in our example here, if the initial state were instead $|\Omega(t_0)\rangle = |a_1\rangle\,|b_2\rangle$, what would then be the purity measure of $\hat{\rho}^{(A)}$ as a function of time? Hint: In this case, there is a quick way to get the answer.

Solution. **??** This is really tedious. Why do you make us do this? We'll do this by showing $\hat{U}\hat{U}^\dagger = \mathbb{1}$.

$$\begin{aligned}
\hat{U}\hat{U}^\dagger &= |a_1b_2\rangle\langle a_1b_2| + |a_2b_1\rangle\langle a_2b_1| \\
&\quad + \sin^2(\omega t)\,|a_2b_2\rangle\langle a_2b_2| + \sin\omega t\cos\omega t\,|a_2b_2\rangle\langle a_1b_1| \\
&\quad + \sin^2(\omega t)\,|a_1b_1\rangle\langle a_1b_1| - \sin\omega t\cos\omega t\,|a_1b_1\rangle\langle a_2b_2| \\
&\quad + \cos^2(\omega t)\,|a_2b_2\rangle\langle a_2b_2| - \sin\omega t\cos\omega t\,|a_2b_2\rangle\langle a_1b_1| \\
&\quad + \cos^2(\omega t)\,|a_1b_1\rangle\langle a_1b_1| + \sin\omega t\cos\omega t\,|a_1b_1\rangle\langle a_2b_2| \\
&= |a_1b_2\rangle\langle a_1b_2| + |a_2b_1\rangle\langle a_2b_1| + |a_2b_2\rangle\langle a_2b_2| + |a_1b_1\rangle\langle a_1b_1| \\
&= \sum_{i,j=1}^{2} |a_ib_j\rangle\langle a_ib_j| = \mathbb{1}
\end{aligned}$$

?? First we need to know $|\Omega(t)\rangle = U\,|\Omega(t_0)\rangle = \sin\omega t\,|a_2b_2\rangle + \cos\omega t\,|a_1b_1\rangle$.

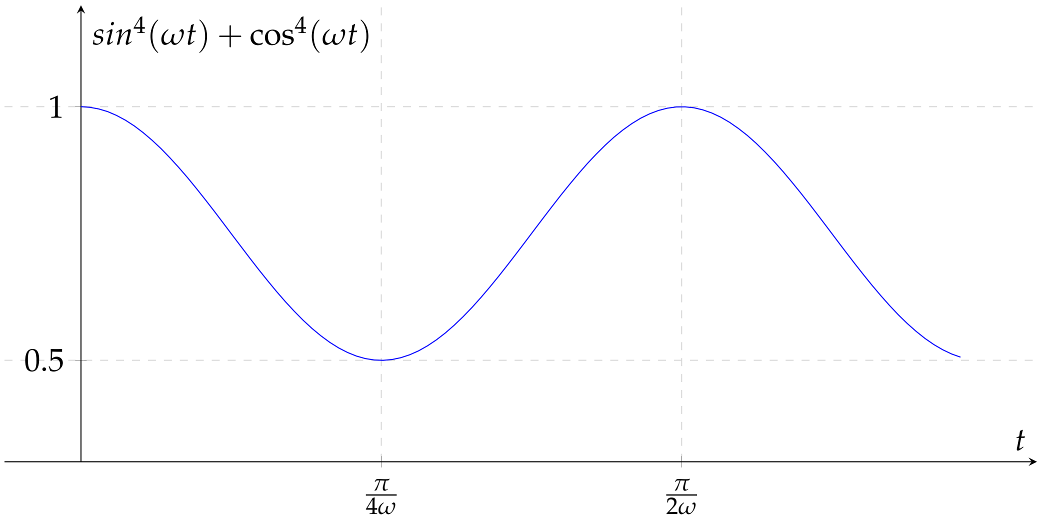
$$\begin{aligned}
\hat{\rho}^{(AB)}(t) &= \hat{U}\,|\Omega(t_0)\rangle\,\langle\Omega(t_0)|\,\hat{U}^\dagger \\
&= \sin^2(\omega t)\,|a_2b_2\rangle\langle a_2b_2| + \sin\omega t\cos\omega t\,|a_2b_2\rangle\langle a_1b_1| \\
&\quad + \sin\omega t\cos\omega t\,|a_1b_1\rangle\langle a_2b_2| + \cos^2(\omega t)\,|a_1b_1\rangle\langle a_1b_1|
\end{aligned}$$

??

$$\begin{aligned}
\hat{\rho}^{(A)}(t) &= \mathrm{tr}_B\left(\hat{\rho}^{(AB)}(t)\right) \\
&= \sum_{n=1}^{2} \langle b_n|\,\hat{\rho}^{(AB)}(t)\,|b_n\rangle \\
&= \sin^2(\omega t)\,|a_2\rangle\langle a_2| + \cos^2(\omega t)\,|a_1\rangle\langle a_1|
\end{aligned}$$

?? We can now calculate the square of the density matrix as $\hat{\rho}^2 = \sin^4(\omega t) + \cos^4(\omega t)$. Below is a plot of this function.

?? Given this new initial state, then the state never picks up any time dependence on evolution $|\Omega(t)\rangle = |a_1b_2\rangle$, and hence this state stays a pure state and hence the purity P remains at 1.


$sin^4(\omega t) + \cos^4(\omega t)$
1
0.5
t
$\frac{\pi}{4\omega}$
$\frac{\pi}{2\omega}$

Exercise 2

Assume a system possesses a Hilbert space that is N-dimensional. Which state ρ is its least pure, i.e., which is its maximally mixed state, and what is the value of the purity $P[\rho]$ of that state?

Solution. The state ρ that is the most mixed is that state that is a uniform distribution across all possible states: $\rho = \frac{1}{N}\mathbb{1}$. The purity of this state is $P[\rho] = \operatorname{tr}(\rho^2) = \frac{1}{N^2}\operatorname{tr}(\mathbb{1}) = \frac{1}{N}$.

Exercise 1

In the example of two identical bosonic subsystems just above, assume now that $\hat{H}^{(A)} |a_j\rangle = E_j |a_j\rangle$ with $E_1 = 0$ and $E_2 = E > 0$.

(a) Calculate the thermal density matrix of the system AA. In particular, what are the probabilities for the three basis states of Eq.16.7 as a function of the temperature?

(b) Determine the temperature dependence of the preference of bosons to be in the same state: Does this preference here increase or decrease as the temperature either goes to zero or to infinity?

Solution. **??** Let's first calculate the action of $\hat{H}^{(AA)}$ on our basis states.

$$\begin{aligned} \hat{H}^{(AA)} |a_1 a_1\rangle &= 0 \\ \hat{H}^{(AA)} |a_2 a_2\rangle &= 2E |a_2 a_2\rangle \\ \hat{H}^{(AA)} \frac{1}{\sqrt{2}}(|a_1 a_2\rangle + |a_2 a_1\rangle) &= E\frac{1}{\sqrt{2}}(|a_1 a_2\rangle + |a_2 a_1\rangle) \end{aligned}$$

So now we know our Hamiltonian takes the form

$$\hat{H}^{(AA)} = \begin{bmatrix} 0 & & \\ & 2E & \\ & & E \end{bmatrix}$$

and hence our density matrix looks like

$$\hat{\rho} = \frac{1}{\mathrm{e}^{-2\beta E} + \mathrm{e}^{-\beta E}} \begin{bmatrix} 0 & & \\ & \mathrm{e}^{-2\beta E} & \\ & & \mathrm{e}^{-\beta E} \end{bmatrix} = \begin{bmatrix} 0 & & \\ & \frac{1}{\mathrm{e}^{\beta E}+1} & \\ & & \frac{\mathrm{e}^{\beta E}}{\mathrm{e}^{\beta E}+1} \end{bmatrix}.$$

Hence the probabilities are exactly those terms on the diagonal.

?? Since the $|a_2 a_2\rangle$ term is the only one representing bosons, we just divide that by the other non-zero term.

$$\text{Bosonic Preference} = \frac{1}{\mathrm{e}^{\beta E}+1} \frac{\mathrm{e}^{\beta E}+1}{\mathrm{e}^{\beta E}} = \mathrm{e}^{-\frac{E}{kT}}$$

As $T \to 0$, this preference goes to 0 and hence the particles are more likely to be in the entangled state. As $T \to \infty$ they are more likely to be in the same state.