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Section 9: Density Matrices & 2-level atom

- First pass of Midterms back & talk about them
- Density Matrices
  - some properties & Discussion
- ~~Relaxation~~ Thermal population.
- 2-level atom
  - spontaneous emission
- comment about wigner-weisskopf

Questions?

Density Matrices.

For a pure state, a state whose evolution is governed by the unitary operator (like $U = e^{-i\frac{Ht}{\hbar}}$) can be written as $\rho = |\psi\rangle\langle\psi|$

The diagonals of a pure state are the probabilities in those states $\rho_{ii} = P(i)$.

This means for any observable $\hat{A}$ I can find $\langle A\rangle_\psi$ from $\langle\psi|A|\psi\rangle$ or alternatively $Tr(\rho A)$.

Remember $Tr(\rho) = \sum_i \langle\phi_i|\rho_{ii}|\phi_i\rangle \approx \sum \rho_{ii}$ (general)

↑ diagonal elements

So if $|\psi\rangle = \sum_i c_i|\phi_i\rangle$

then $Tr(\rho A) = \sum_i \langle\phi_i|\psi\rangle\langle\psi|A|\phi_i\rangle$

$= c_i^*(c_i A_i) = \boxed{|c_i^2| A_i}$

$= \boxed{P_i A_i}$

General properties of ρ

⇒ 1) $\rho \geq 0$

2) $\rho^\dagger = \rho$

3) $Tr(\rho) = 1$

4) $\rho^2 = \rho$ ⇒ pure state only!

So what are mixed states ? pure states?

Pure states, in short, can always be written from one $|\psi\rangle\langle\psi|$. A mixed state cannot.

So, ex: if $|\psi\rangle = a|A\rangle + b|B\rangle$

$$\rho = |\psi\rangle\langle\psi| = |a|^2|A\rangle\langle A| + ab^*|A\rangle\langle B| + a^*b|B\rangle\langle A| + |b|^2|B\rangle\langle B|$$

Is this a pure state?

well clearly $\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \rho$

so yes.

We could have also actually taken

$$\rho^2 = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}\begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix} = \begin{pmatrix} (|a|^2)^2 + ab^*a^*b & |a|^2ab^* + ab^*|b|^2 \\ a^*b|a|^2 + |b|^2a^*b & |a^*b|^2 + (|b|^2)^2 \end{pmatrix}$$

$$= \begin{pmatrix} |a|^2|a|^2 + |a|^2|b|^2 & |a|^2ab^* + ab^*|b|^2 \\ |a|^2a^*b + |b|^2a^*b & |a|^2|b|^2 + |b|^2|b|^2 \end{pmatrix}$$

Remember $|b|^2 + |a|^2 = 1$

$$\Rightarrow \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix} = \rho$$

Another way to see this is to remember that if $|\psi\rangle$ is some vector in my 2-D Hilbert space I could find the orthogonal vector $|\phi\rangle$ where $\langle\phi|\psi\rangle = 0$

$$|\phi\rangle = b^*|A\rangle - a^*|B\rangle$$

Then it is clear in the basis of $|\chi\rangle, |\phi\rangle$ that

$|\chi\rangle\langle\chi|$ is a pure state! $\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ so $\rho^2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \rho$ ✓

What about $\rho = F|\chi\rangle\langle\chi| + G|\phi\rangle\langle\phi|$

$\rho = \begin{pmatrix} F & 0 \\ 0 & G \end{pmatrix}$? $\rho^2 = \begin{pmatrix} F^2 & 0 \\ 0 & G^2 \end{pmatrix} \neq \rho$

if $F \neq 0$? $G \neq 0$

Remember $x^2 < x$ for all $x < 1$

Hence $F^2 + G^2 \neq 1$

Basically this is just a statement that ρ of $|\chi\rangle\langle\chi| + |\phi\rangle\langle\phi|$ cannot be written in the form of $|\psi\rangle\langle\psi|$ no matter how I try to decompose $|\psi\rangle$ in terms of $|A\rangle$ & $|B\rangle$

Spin System

This can really be a very powerful statement about correlations within a system and is very important for QM.

Let's consider our favorite example from QM.

a spin-½ system.

$|\chi\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{i}{\sqrt{2}}|\downarrow\rangle$

$\rho = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$.

$\rho = |\chi\rangle\langle\chi|$

$S_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ℏ

$S_y = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}$ ℏ

$S_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ ℏ

Let's consider then measuring $\langle S_x\rangle, \langle S_y\rangle, \langle S_z\rangle$

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For our pure state,

$$\langle S_x \rangle = Tr(S_x \rho) = Tr\left[\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1/2&1/2\\1/2&1/2\end{pmatrix}\right] = Tr\left[\begin{pmatrix}1/2&1/2\\1/2&1/2\end{pmatrix}\right] = 1$$

$$\langle S_y \rangle = Tr(S_y \rho) = Tr\left[\begin{pmatrix}0&-i\\+i&0\end{pmatrix}\begin{pmatrix}1/2&1/2\\1/2&1/2\end{pmatrix}\right] = Tr\left[\begin{pmatrix}-i/2&-i/2\\+i/2&+i/2\end{pmatrix}\right] = 0$$

$$\langle S_z \rangle = Tr(S_z \rho) = Tr\left[\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}1/2&1/2\\1/2&1/2\end{pmatrix}\right] = Tr\left[\begin{pmatrix}1/2&1/2\\-1/2&-1/2\end{pmatrix}\right] = 0$$

Not here that on what this is telling us is that the state we started w/ $\left(|\psi\rangle = (|\uparrow\rangle + |\downarrow\rangle)\frac{1}{\sqrt{2}}\right)$ looks Completely mixed in the base we wrote it down in (mixed as in 50% $|\uparrow\rangle$ & 50% $|\downarrow\rangle$) Our measurements along z & y just see a 50/50 split, but $\langle S_x \rangle = 1$. Which makes sense! Since $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ is also sometimes written $|\rightarrow\rangle$ or it is the eigenstate of the $\hat{S}_x$, With a pure state we can rotate our eyes through the different bases and realize something special about it. The $|\uparrow\rangle$ & $|\downarrow\rangle$ are required to be correlated in such a way that a measurement along $\hat{x}$ gives the answer 1 every time!

What if we had a mixed state?

$$\rho = \tfrac{1}{2}|\uparrow\rangle\langle\uparrow| + \tfrac{1}{2}|\downarrow\rangle\langle\downarrow| = \begin{pmatrix}1/2&0\\0&1/2\end{pmatrix}$$

$$\langle S_x \rangle = Tr(S_x \rho) = Tr\left[\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1/2&0\\0&1/2\end{pmatrix}\right] = Tr\left[\begin{pmatrix}0&1/2\\1/2&0\end{pmatrix}\right] = 0$$

$$\langle S_y \rangle = Tr(S_y \rho) = Tr\left[\begin{pmatrix}0&-i\\+i&0\end{pmatrix}\begin{pmatrix}1/2&0\\0&1/2\end{pmatrix}\right] = Tr\left[\begin{pmatrix}0&-i/2\\+i/2&0\end{pmatrix}\right] = 0$$

$$\langle S_z \rangle = Tr(S_z \rho) = Tr\left[\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}1/2&0\\0&1/2\end{pmatrix}\right] = Tr\left[\begin{pmatrix}1/2&0\\0&-1/2\end{pmatrix}\right] = 0$$

Mixed in every basis!!

Importantly, the mixedness introduced by writing our function down as $\rho = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$ is not removable.

[illegible]

This is also another reason why I was saying last week one should be careful when calculating the dynamics of a quantum system. Even if all the dynamics in my system come from a unitary operator, my system might be initialized in a way such that I don't start off w/ the coherences (ρ_{ij}) term nuked.

Ex. Thermal dist.

My initial state of the two-level system might be given by $\rho = \begin{pmatrix} \frac{e^{-\frac{E_1}{k_B T}}}{Z} & 0 \\ 0 & \frac{e^{-\frac{E_2}{k_B T}}}{Z} \end{pmatrix}$

$P_{11} = e^{-E_1/k_B T}/Z$

$P_{22} = e^{-E_2/k_B T}/Z$

$Z = \sum_i e^{-E_i/k_B T}$

To find $\rho(t)$ I would still calculate.

$\rho(t) = U(t)\rho U^\dagger(t) \Rightarrow P_{11} e^{i\hat{H}t/\hbar}|1\rangle\langle 1| e^{-i\hat{H}t/\hbar} + P_{22} e^{i\hat{H}t/\hbar}|2\rangle\langle 2| e^{-i\hat{H}t/\hbar}$

This will look different compared to starting w/

a $|\psi\rangle = \sqrt{P_{11}}|1\rangle + e^{i\phi}\sqrt{P_{22}}|2\rangle$!

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Show some code for this system.

Spontaneous Emission / Entangled Pairs

There was another comment made in class about how if we know many particles, but ignore the information about one, we introduce this measurable mixedness. For this we need to think of more than one particle.

$$\Rightarrow |\Psi\rangle = |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$$

The way we "trace out" one of these spins is to "measure" it.

Partial Trace

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_A\rangle|\uparrow_B\rangle + |\downarrow_A\rangle|\downarrow_B\rangle\right) \Rightarrow \rho_{AB} = \frac{1}{2}\begin{bmatrix} |\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\uparrow\uparrow\rangle\langle\downarrow\downarrow| \\ + |\downarrow\downarrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow| \end{bmatrix}$$

$$\rho_B = \mathrm{Tr}_A(\rho_{AB}) = \sum_A \langle\uparrow_A|\rho_{AB}|\uparrow_A\rangle =$$

$$\frac{1}{2}\langle\uparrow_A|\left(\begin{array}{l} |\uparrow\rangle_A|\uparrow\rangle_B\langle\uparrow|_A\langle\uparrow|_B + |\uparrow\rangle_A|\uparrow\rangle_B\langle\downarrow_B|\langle\downarrow_B| \\ + |\downarrow\rangle_A|\downarrow\rangle_B\langle\uparrow|_A\langle\uparrow|_B + |\downarrow\rangle_A|\downarrow\rangle_B\langle\downarrow|_A\langle\downarrow|_B \end{array}\right)|\uparrow_A\rangle$$

$$+ \frac{1}{2}\langle\downarrow_A|\left(\begin{array}{l} |\uparrow_A\rangle|\uparrow_B\rangle\langle\uparrow_A|\langle\uparrow_B| + |\uparrow\rangle_A|\uparrow_B\rangle\langle\downarrow_A|\langle\downarrow_B| \\ |\downarrow_A\rangle|\downarrow\rangle_B\langle\uparrow_A|\langle\uparrow|_B + |\downarrow\rangle_A|\downarrow\rangle_B\langle\downarrow|_A\langle\downarrow_B| \end{array}\right)|\downarrow_A\rangle$$

$$= \frac{1}{2}|\uparrow_B\rangle\langle\uparrow_B| + \frac{1}{2}|\downarrow_B\rangle\langle\downarrow_B|$$

completely mixed!! all coherences gone.

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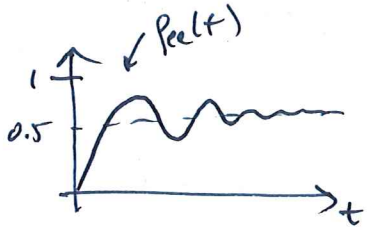
Now imagine instead of $\uparrow$ & $\downarrow$ spins entangled we have an atom emit photons. Our two states are $|e,0\rangle$ & $|g,1\rangle$ (# of photons)

In reality one always traces over the photon when it leaves. This makes the spontaneous emission an incoherent effect! (unlike the Rabi oscillations we saw before). Since the density matrices naturally incorporate this feature, the equations we saw in class

Density Matrices

$$\dot{\rho}_{gg} = \frac{i\Omega}{2}\rho_{ge} - \frac{i\Omega}{2}\rho_{eg} + \gamma\rho_{ee}$$
$$\dot{\rho}_{ee} = \frac{i\Omega}{2}\rho_{eg} - \frac{i\Omega}{2}\rho_{ge} - \gamma\rho_{ee}$$
$$\dot{\rho}_{ge} = +i\delta\rho_{ge} - \frac{i\Omega}{2}(\rho_{gg} - \rho_{ee}) - \frac{\gamma}{2}\rho_{ge}$$
$$\dot{\rho}_{eg} = -i\delta\rho_{eg} + \frac{i\Omega}{2}(\rho_{gg} - \rho_{ee}) - \frac{\gamma}{2}\rho_{eg}$$



Monte Carlo Version

Available for many atoms & eq.