22 Sept. 2005

Density matrix and the optical Bloch equations

Prologue: pure states and mixed states

Anything that can be represented as a wavefunction, as a state vector, something whose evolution is governed by Schrödinger's eqn., is a pure state.

e.g. for a 2-state atom the most general state:

$$c_g|g\rangle + c_e|e\rangle \quad \text{where } c_g, c_e \text{ are complex and } |c_g|^2 + |c_e|^2 = 1$$

is a pure state.

a specific example of a pure state could be:

$$\frac{1}{\sqrt{2}}\left(|g\rangle + e^{-i\omega_0 t}|e\rangle\right)$$

If we measure whether an atom prepared in such a state is in $|g\rangle$ or $|e\rangle$ we will find 50% after many repetitions on identically prepared states.

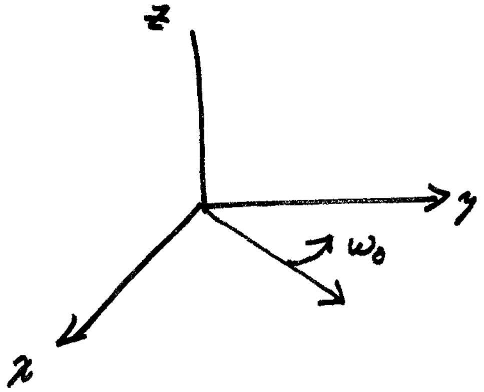
what is a mixed state?

consider an oven at $k_B T \gg \hbar \omega_0$, with a gas of 2-level atoms inside, emitting a beam of atoms. Each level is equally populated, so, if one measures whether an atom is $|e\rangle$ or $|g\rangle$, get 50% in many measurements of these identically prepared atoms

but this is a mixed state! – how is it different from the pure state?

$$|\psi_{pure}\rangle = \frac{1}{\sqrt{2}}\left(|g\rangle + e^{-i\omega_0 t}|e\rangle\right)$$

If we think of $|g\rangle = |\downarrow\rangle$ and $|e\rangle = |\uparrow\rangle$ this is a state with a spin rotating in the x-y plane.



If we measure the x-component of the spin at some time after many identical preparations, we will get a value

$$\langle S_x(t)\rangle \sim \cos\omega_0 t$$

If we do that same repeated measurement on the mixed state, we get

$$\langle S_x(+)\rangle = 0$$

It is as if for each identical preparation of the mixed state we get

$$\frac{1}{\sqrt{2}}\left(|g\rangle + e^{-i\omega_0 t}\cdot e^{i\phi_j}\,|e\rangle\right)$$

where ϕ_j is random in spite of identical preparation.

Such mixed states cannot be represented by wave functions, but <u>require</u> a density matrix.

Pure states may also be represented by a density matrix, but they may be.

for a pure state $|\psi\rangle$ the density operator is

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

the matrix representing such an operator for some orthonormal basis set $\{|i\rangle\}$ is

$$\rho_{ij} = \langle i|\psi\rangle\langle\psi|j\rangle$$

some examples: $|\psi\rangle = |g\rangle$

$$\rho = \begin{array}{c c} & \begin{array}{cc} g & e \end{array} \\ \begin{array}{c} g \\ e \end{array} & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{array}$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|g\rangle + e^{-i\omega_0 t}|e\rangle\right)$$

$$\rho = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & e^{i\omega_0 t} \\ e^{-i\omega_0 t} & 1 \end{pmatrix}$$

$$|\psi\rangle = c_g|g\rangle + c_e|e\rangle$$

$$\rho = \begin{pmatrix} |c_g|^2 & c_g c_e^* \\ c_g^* c_e & |c_e|^2 \end{pmatrix}$$

this is a Hermitian matrix, it can be diagonalized with real eigenvalues, and when diagonalized always has the form

$$\rho_{\text{diag, pure}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and pure state density matrix, diagonalized has <u>one</u> diagonal element. the eigenvector is the pure state.

Trace of an operator:

$$\mathrm{Tr}(\hat{\mathcal{O}}) = \sum_n \langle n|\hat{\mathcal{O}}|n\rangle$$ where $|n\rangle$ represents any orthonormal basis

this is independent of the basis

It is easy to show $\mathrm{Tr}(\rho\hat{\mathcal{O}}) = \langle\hat{\mathcal{O}}\rangle$:

$$\mathrm{Tr}(\hat{\rho}\hat{\mathcal{O}}) = \mathrm{Tr}(|\psi\rangle\langle\psi|\hat{\mathcal{O}}) = \sum_n \langle n|\psi\rangle\langle\psi|\mathcal{O}|n\rangle =$$

$$\sum_n \langle\psi|\hat{\mathcal{O}}|n\rangle\langle n|\psi\rangle = \langle\psi|\mathcal{O}|\psi\rangle \quad \text{Q.E.D.}$$

It follows that $\mathrm{Tr}(\rho) = 1$

It is also obvious for a pure state the $\rho^2 = \rho$

so $\mathrm{Tr}\,\rho^2 = 1$.

That was all for pure states. For mixed states,

think of the density matrix as representing a mixture of pure states $|\psi_i\rangle$, with probabilities P_i such that $\sum P_i = 1$

then $$\rho_{\text{mixed}} = \sum_i P_i\, |\psi_i\rangle\langle\psi_i|$$

if the $|\psi_i\rangle$ are chosen as basis states, this is diagonal as for pure states, it is easy to show that

$$\mathrm{Tr}(\rho\hat{\mathcal{O}}) = \langle\mathcal{O}\rangle$$

as for a pure state.

$\mathrm{Tr}(\rho) = 1$ and ρ is Hermitian

__but__ $\rho \neq \rho^2$ and $\mathrm{Tr}\,\rho^2 \neq 1$ for a mixed state

$\mathrm{Tr}\,\rho^2 = 1 \Rightarrow$ pure state

$\mathrm{Tr}\,\rho^2 < 1 \Rightarrow$ mixed state

let's see this explicitly for a pure state and a mixed state

the most general pure ρ is:

$$\rho = \begin{pmatrix} |c_g|^2 & c_g c_e^* \\ c_g^* c_e & |c_e|^2 \end{pmatrix}$$

$$\rho^2 = \begin{pmatrix} c_g^2 & c_g c_e^* \\ c_g^* c_e & c_e^2 \end{pmatrix} \begin{pmatrix} c_g^2 & c_g c_e^* \\ c_g^* c_e & c_e^2 \end{pmatrix} =$$

$$\begin{pmatrix} |c_g^2|^2 + c_g c_e^* c_g^* c_e & |c_g|^2 c_g c_e^* + |c_e|^2 c_g c_e^* \\ c_g^* c_e (c_g^2 + c_e^2) & |c_g|^2 |c_e|^2 + |c_e^2| |c_e|^2 \end{pmatrix} =$$

$$\begin{pmatrix} |c_g^*|^2 |c_g|^2 + |c_g|^2 |c_e|^2 & c_g c_e^* (|c_g|^2 + |c_e|^2) \\ c_g^* c_e & |c_e|^2 (c_e^2 + c_g^2) \end{pmatrix} =$$

$$\begin{pmatrix} |c_g|^2 & c_g c_e^* \\ c_g^* c_e & |c_e|^2 \end{pmatrix} = \rho$$

and $\mathrm{Tr}(\rho^2) = T(\rho) = |c_g|^2 + |c_e|^2 = 1$

for the mixed state given by

$$\rho = \begin{pmatrix} |C_g|^2 & 0 \\ 0 & |C_e|^2 \end{pmatrix}$$

$$\rho^2 = \begin{pmatrix} |C_g|^2 & 0 \\ 0 & |C_e|^2 \end{pmatrix} \begin{pmatrix} |C_g|^2 & 0 \\ 0 & |C_e|^2 \end{pmatrix} = \begin{pmatrix} |C_g|^2 |C_g|^2 & 0 \\ 0 & |C_e|^2 |C_e|^2 \end{pmatrix}$$

$$\rho^2 = \begin{pmatrix} |C_g|^4 & 0 \\ 0 & |C_e|^4 \end{pmatrix} \neq \rho$$ unless $|C_g|^2$ or $|C_e|^2 = 1$

$T(\rho^2) < 1$ unless $|C_g|^2$ or $|C_e|^2 = 1$

What is the equation of motion for the density matrix ?

Schrod. Eq: $i\hbar \frac{\partial}{\partial t} |\psi_i\rangle = \mathcal{H} |\psi_i\rangle$ or, equivelantly

$$-i\hbar \frac{\partial}{\partial t} \langle \psi_i | = \langle \psi_i | \mathcal{H}$$

$$\rho = \sum P_i |\psi_i\rangle\langle\psi_i|$$

$$\frac{\partial}{\partial t}\rho = \sum P_i \left(\frac{\partial}{\partial t}|\psi_i\rangle\langle\psi_i| + |\psi_i\rangle\frac{\partial}{\partial t}\langle\psi_i|\right)$$

$$= \sum P_i \left(\frac{1}{i\hbar}\mathcal{H}|\psi_i\rangle\langle\psi_i| + |\psi_i\rangle\frac{1}{-i\hbar}\langle\psi_i|\mathcal{H}\right)$$

$$= \frac{1}{i\hbar}\sum P_i \left(\mathcal{H}|\psi_i\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi_i|\mathcal{H}\right)$$

$$\frac{\partial}{\partial t}\rho = \frac{-i}{\hbar}\left[\mathcal{H}, \rho\right]$$

this is the von Neuman Equation

N.B. This is *not* related to the Heisenberg picture equation of motion for an *operator*:

$$\frac{\partial}{\partial t}\hat{O} = \frac{i}{\hbar}\left[\mathcal{H}, \hat{O}\right]$$

ρ is in the *schrodinger* picture

$\rho = \sum P_i |\psi_i\rangle\langle\psi_i|$ where the Ψ_i are functions of time

We described how to get a mixed density matrix, e.g. from an oven providing a thermal mixture. Here is another way:

consider a pure state of a quantum system consisting of 2 subsystems, 1 and 2. These might be 2 particles or they might be an atom and the electromagnetic field.

A general pure state of this combined system is

$$|\psi\rangle_{12} = \sum_{n,m} c_{nm} |n\rangle_1 |m\rangle_2$$

where $\sum_{nm} c_{nm}^2 = 1$

the density matrix for this pure state is

$$\rho = |\psi\rangle\langle\psi| = \sum_{n,m} \sum_{n',m'} c_{nm} c_{n'm'}^* |n\rangle_1 |m\rangle_2 \langle m'|_2 \langle n'|_1$$

the matrix representation has nm rows and collumns.

Now, let us say that we want to consider only system 1. We may have an operator $\mathcal{O}$ that acts only on system 1, and we want

$$\langle \mathcal{O} \rangle = \mathrm{Tr}(\rho \mathcal{O})$$

$$\mathrm{Tr}\left(\rho\hat{O}\right) = \sum_{n,m} \langle n|_1 \langle m|_2\, \rho\hat{O}\, |m\rangle_1 |n\rangle_1$$

where n, m span 1, 2

$$= \sum_n \langle n|_1 \sum_m \langle m|_2\, \rho\, |m\rangle_2\, \hat{O}\,|n\rangle_1$$

(because $\hat{O}$ only operates on 1)

$$= \sum_n \langle n|_1\, \mathrm{Tr}_{(2)}(\rho)\hat{O}\,|n\rangle_1$$

define $\mathrm{Tr}_{(2)}\,\rho \equiv \sigma$, the reduced density matrix of system 1

than $\langle O\rangle = \mathrm{Tr}_1\, \sigma\hat{O}$

and $\mathrm{Tr}_{(2)}\,\rho \equiv \sum_m \langle m|_2\, \rho\, |m\rangle_2$ is the partial trace of ρ over system 2

explicitly $\sigma = \sum_{n,n',m} c_{nm}\, c^*_{n'm}\; |n\rangle_1\langle n'|_1$

this may be a mixEd state, although ρ was a pure state take as an example the entangled state

$$|\psi\rangle_{12} = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right)$$

each system, 1 + 2, has 2 basis vectors $|\uparrow\rangle$ + $|\downarrow\rangle$ and the combined system is spanned by 2×2 vectors:

$$\underset{a}{|\uparrow\rangle_1|\uparrow\rangle_2},\quad \underset{b}{|\downarrow\rangle_1|\downarrow\rangle_2},\quad \underset{c}{|\uparrow\rangle_1|\downarrow\rangle_2},\quad \underset{d}{|\downarrow\rangle_1|\uparrow\rangle_2}$$

$$\rho = |\psi\rangle\langle\psi| = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array}\!\!\begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \left(\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{array}\right) \end{array}\left(\frac{1}{2}\right)$$

, a pure state

now, trace over system 2 :

$$\sigma_1 = \frac{1}{2}\sum_{\uparrow,\downarrow_2} \langle 2|\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right)\left(\langle\uparrow|_1\langle\downarrow|_2 + \langle\downarrow|_1\langle\uparrow_2|\right)|2\rangle$$

$$= \frac{1}{2}\left(|\downarrow\rangle_1\langle\downarrow_1| + |\uparrow\rangle_1\langle\uparrow|_1\right)$$

$$\sigma_1 = \begin{array}{c} \\ \downarrow \\ \uparrow \end{array}\!\!\begin{array}{c} \begin{array}{cc} \downarrow & \uparrow \end{array} \\ \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right) \end{array}\left(\frac{1}{2}\right)$$

obviously, a mixed state

take as another example a ~~[illegible]~~ separable state:

$$|\psi\rangle_{12} = \frac{1}{2}\left(|\uparrow\rangle_1 + |\downarrow\rangle_1\right)\left(|\uparrow\rangle_2 + |\downarrow\rangle_2\right)$$

$$= \frac{1}{2}\left(|\uparrow\rangle_1|\uparrow\rangle_2 + |\downarrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2 + |\uparrow\rangle_1|\downarrow\rangle_2\right)$$

$$\rho = \begin{array}{c c} & \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{array}{c} a \\ b \\ c \\ d \end{array} & \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \end{array} \left(\frac{1}{4}\right)$$, a pure state

and ~~[illegible]~~

$$\sigma_1 = \frac{1}{4}\sum_{\uparrow\downarrow_2} \langle 2|\left(|\uparrow\rangle_1 + |\downarrow\rangle_1\right)\left(|\uparrow\rangle_2 + |\downarrow\rangle_2\right)\left(\langle\uparrow|_1 + \langle\downarrow|_1\right)\left(\langle\uparrow|_2 + \langle\downarrow|_2\right)|2\rangle$$

$$\sigma_1 = \frac{1}{2}\begin{array}{c} \begin{array}{cc} \downarrow & \uparrow \end{array} \\ \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{array}$$ a pure state

for 2 entangled systems, tracing over one system leaves the reduced density matrix mixed

for separable system, tracing leaves the state pure.

Our immediate reason for this discussion of the reduced density matrix and mixed states is the context of a 2-level atom as system 1, coupled to the electromagnetic field as system 2.

We can treat the applied field classically (at least if it has lots of photons), but the spontaneous emission photons are quantum, and we will trace over them to get the reduced density matrix for the atom.

In fact we will not do that here rigorously but only phenomenologically, introducing terms into the equations for σ that make it mixed.

Aside: If the atom radiates not into free space, with its infinity of modes, but into a single mode of a cavity, we don't have to trace over the field, and we can treat the coupled system. This is cavity QED.