Density Matrices

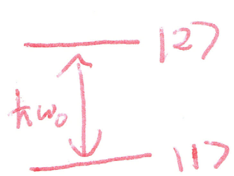
We'll need to use a density matrix formalism to describe systems where we don't measure everything. This can ~~include ensembles~~ be used to describe the evolution of "open" quantum systems that interact with an environment, which we don't measure directly.

- Also useful for describing ~~the~~ single-particle properties of an ensemble of particles

$$\rho_{ens} = \sum_i w_i |\psi_i\rangle\langle\psi_i|$$, where $|\psi_i\rangle$ are different possible states in the ensemble, with weights (probabilities) w_i

Examples of ensembles

a single "spin" (two-level system)



$$|\psi\rangle = a e^{i\omega_0 t/2} |1\rangle + b e^{-i\omega_0 t/2} |2\rangle$$

$$\rho = |\psi\rangle\langle\psi|$$

$$\rho = \begin{pmatrix} |a|^2 & a b^* e^{-i\omega_0 t/2} \\ a^* b^* e^{+i\omega_0 t/2} & |b|^2 \end{pmatrix}$$

for

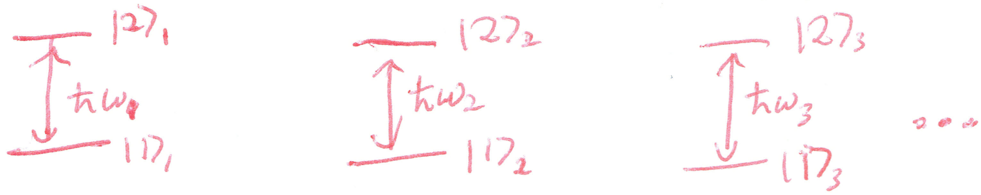
$$|\psi\rangle = \cos\tfrac{\theta}{2}|1\rangle + \sin\tfrac{\theta}{2} e^{i\varphi}|2\rangle$$

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \cos^2\frac{\theta}{2} & \sin\frac{\theta}{2}\cos\frac{\theta}{2} e^{i\varphi} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2} e^{-i\varphi} & \sin^2\frac{\theta}{2} \end{pmatrix}$$

② examples

a collection of independent spins (e.g., separate realizations of expts w/ a single spin, or independent spins from a single experiment)

(a) many "spins" w/ different Larmor frequencies (as for a spatially varying field or slowly drifting, ~~shot~~ shot-to-shot, field



$|\psi_1\rangle = a e^{i\omega t/2}|1\rangle + b e^{-i\omega t/2}|2\rangle$ . . .

$|\psi_3\rangle = a e^{i\omega_3 t/2}|1\rangle + b e^{-i\omega_3 t/2}|2\rangle$ . . .

$\Longrightarrow$ dephasing

(b) bunch of spins w/ same Larmor freq., but prepared in different states → i.e., spread over Bloch sphere

$|\psi_1\rangle = a_1|1\rangle + b_1|2\rangle$ $\qquad$ $|\psi_2\rangle = a_2|1\rangle + b_2|2\rangle$

③ The density matrix for an ensemble (of spin-$\frac{1}{2}$'s)

$$|\psi_i\rangle = a_i|1\rangle + b_i|2\rangle = \cos\frac{\theta_i}{2}|1\rangle + \sin\frac{\theta_i}{2}e^{i\varphi_i}|2\rangle$$

$$\rho_{ens} = \frac{1}{N}\sum_{i=1}^{N}|\psi_i\rangle\langle\psi_i| = \frac{1}{N}\sum_{i=1}^{N}\begin{pmatrix}\cos^2\frac{\theta_i}{2} & \sin\frac{\theta_i}{2}\cos\frac{\theta_i}{2}e^{i\varphi_i} \\ \sin\frac{\theta_i}{2}\cos\frac{\theta_i}{2}e^{-i\varphi_i} & \sin^2\frac{\theta_i}{2}\end{pmatrix}$$

for a random distribution of θ_i, φ_i

in the limit $N \to \infty$ (many spins or many realizations)

$$\rho_{ens} = \frac{1}{4\pi}\int d\Omega \begin{pmatrix}\cos^2\frac{\theta}{2} & \sin\theta\cos\theta\, e^{i\varphi} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\varphi} & \sin^2\frac{\theta}{2}\end{pmatrix}$$

$$\int \sin^2\frac{\theta}{2}\,d\theta = \int \cos^2\frac{\theta}{2}\,d\theta = \frac{1}{2}$$, φ-values average to give vanishing off-diagonals.

$$\rho_{ens}^{random} = \begin{pmatrix}1/2 & 0 \\ 0 & 1/2\end{pmatrix}$$

off-diagonal terms go to zero → incoherent ensemble

④ some terminology

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}$$

"coherences" "populations"

[$\rho = \rho^{\dagger}$ self-adjoint

[positive - non-negative eigenvalues

[$\mathrm{tr}(\rho) = 1$

for a pure quantum state (one we can represent on the unit Bloch sphere)

$$\rho^2 = \rho$$

ex $|\psi_a\rangle = |1\rangle \qquad \rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ (trivially pure)

or $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle + i|2\rangle\right) \qquad \rho = \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$

"mixed states" $\rho^2 \neq \rho$ - no longer a pure quantum state; reduced, but non-zero coherences

classical states - coherences are <u>zero</u>

5 expectation values - some observable A

$$\boxed{\langle A \rangle = \mathrm{tr}(\rho A)} = \mathrm{tr}(A\rho)$$

example $|\psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ $\quad \rho = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

$$\langle \sigma_x \rangle = \mathrm{tr}\left[\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] = \mathrm{tr}\left[\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}\right] = 1$$

$$\langle \sigma_z \rangle = \mathrm{tr}\left[\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] = 0$$

$$\langle \sigma_y \rangle = 0$$

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for the mixed state $\quad \rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$$\langle \sigma_x \rangle = \mathrm{tr}\left[\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] = 0 = \langle \sigma_z \rangle = \langle \sigma_y \rangle$$

⑥ What about multiparticle states?

$$|\psi\rangle_{ab} = \frac{1}{\sqrt{2}}\left(|1\rangle_a|1\rangle_b + |2\rangle_a|2\rangle_b\right)$$

entangled "Bell" state

$$\rho_{ab} = \begin{array}{c|cccc} & |1\rangle|1\rangle & |1,2\rangle & |2,1\rangle & |2,2\rangle \\ \hline |1,1\rangle & & & & \\ |1,2\rangle & & \left(\begin{matrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{matrix}\right) & & \\ |2,1\rangle & & & & \\ |2,2\rangle & & & & \end{array}$$

What if we only measure the properties of particle a? What density matr[ix] describes ~~[illegible]~~ the outcome of this incomplete measurem[ent]

reduced density matrix

$$\rho^a = \mathrm{tr}_b(\rho_{ab})$$

the reduced density matrix ρ^a is found by a "partial trace" over b ["trace over" particle b –

$$\boxed{\rho^a = \sum_{i,j,\mu} a^*_{j,\mu} a_{i\mu} |i\rangle_a {}_a\langle j|}$$

for $|\psi\rangle_{ab} = \sum_{i,\mu} a_{i\mu} |i\rangle_a |\mu\rangle_b$

$$\rho^a_{11} = \cancel{\ldots}\ |a_{11}|^2 + |a_{12}|^2$$

$$\rho^a_{12} = \cancel{\ldots}\ a^*_{21}a_{11} + a^*_{22}a$$

$$\rho^a_{21} = a^*_{11}a_{21} + a^*_{12}a_{22}$$

$$\rho^a_{22} = |a_{21}|^2 + |a_{22}|^2$$

for this entangled state

$$\rho^a = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

← maximally mixed!

⑦ For any state $|\Psi\rangle$ involving correlations of the measurement outcomes for particles a and b, tracing over b [i.e. not observing the properties of this particle, even if you could in principle], then ~~the~~ coherent information about particle a is lost.

The partial trace accounts for this. Incoherent sum of populations / coherences for the particle / degree of freedom we care about, weighted by the probabilities to find the other, unobserved particle/DoF in some given state

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Measurement outcome on part a of $|\Psi_{ab}\rangle$, ignoring b

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Let's say M is an observable for system a, such that

$$M|m\rangle_a = m|m\rangle_a$$

~~such~~, which we can measure w/ some device

To describe the outcome of measurement on the product state

$|\Psi_{ab}\rangle^{prod} = |m\rangle_a |\phi\rangle_b$, we should find that a related observable $\tilde{M}$ gives $\tilde{M}|\Psi_{ab}\rangle^{prod} = m|\Psi_{ab}\rangle^{prod}$

this is satisfied for $\tilde{M} = M \otimes \mathbb{1}_b$

$\hat{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

(8) This works for general state $|\Psi_{ab}\rangle$ described by ρ_{ab},

where

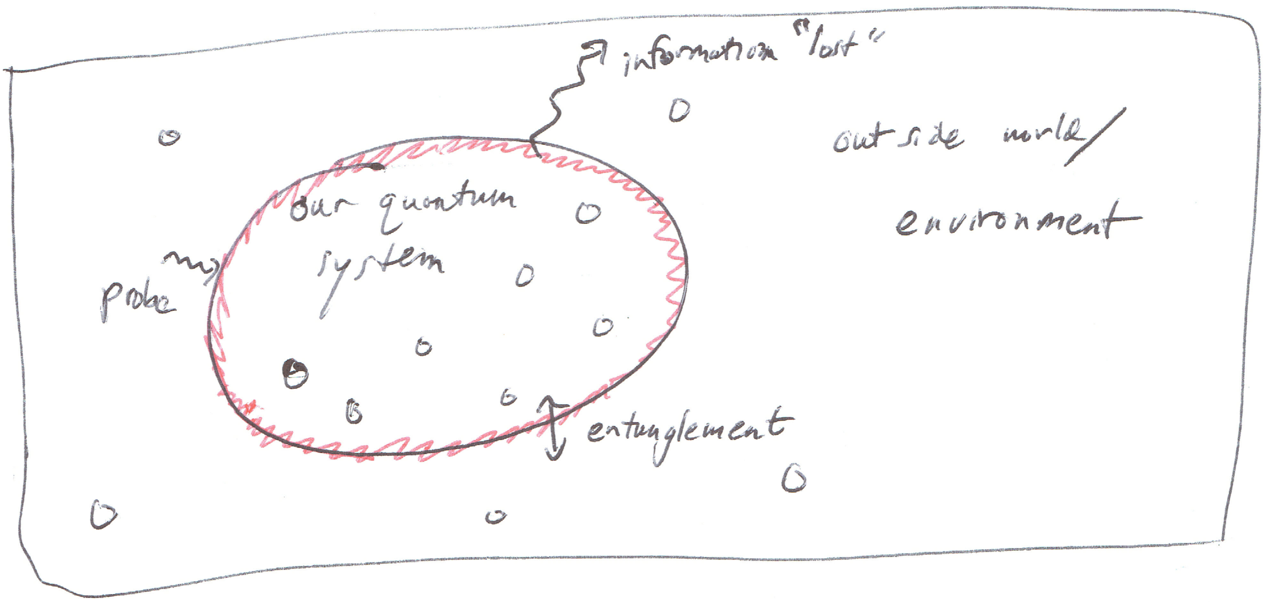
$$\mathrm{tr}(\tilde{M}\rho_{ab}) = \mathrm{tr}(M\rho^a)$$

$$\hookrightarrow \mathrm{tr}\left[(M \otimes \mathbb{I}_b)\rho_{ab}\right]$$

satisfied for

$$\rho^a = \mathrm{tr}_b(\rho_{ab})$$

The physical picture behind decoherence [as we currently understand it]



We're assuming that we can keep track of all of the particles / degrees of freedom within "our quantum system" (red circle). If we draw our inner, red circle large enough, i.e. measure everything in the universe, then we just see unitary evolution, entanglement, w/ no loss of coherence [i.e. incoherent, classical dynam[ics] emerges from purely quantum evolution

9 Goal of quantum computing / quantum technologies, preserve coherence by decoupling our system from the environment, and do this for larger and larger system sizes.

So, the physically relevant density matrix for our system will be a trace of $\rho_{universe}$ over the total outside environment.

to make a highly coherent quantum system, one can

- choose some DOF that couples weakly to the environment
- work hard to isolate it from the environment
- "shape" the environment w/ which it interacts
- monitor + use feedback to stabilize quantum system