Tuesday, April 2, 2024

Monte Carlo Wavefunctions – Quantum Trajectories

The "Schrodinger equation" for a 2-level atom in a laser field with spontaneous emission is

$$i\hbar \frac{d}{dt}\begin{pmatrix} C_g \\ C_e \end{pmatrix} = \hbar \begin{pmatrix} \delta/2 & \Omega/2 \\ \Omega^*/2 & -\delta/2 \end{pmatrix} - \begin{pmatrix} 0 \\ -i\hbar \frac{\gamma}{2} C_e \end{pmatrix}$$

$$= \hbar \begin{pmatrix} \delta/2 & \Omega/2 \\ \Omega^*/2 & -\delta/2 - i\frac{\gamma}{2} \end{pmatrix} \begin{pmatrix} C_g \\ C_e \end{pmatrix}$$

effectively, $H = \hbar \begin{pmatrix} \delta/2 & \Omega/2 \\ \Omega^*/2 & \delta/2 - i\gamma/2 \end{pmatrix}$

↑ non-Hermitian

↳ does not conserve probability

(complex eigenenergies)

↳ time evolution: $e^{-i\left(\frac{iE_e}{\hbar}\right)t} = e^{\pm\frac{E_e}{\hbar}}$

How do the states evolve in time?

Before a photon is emitted :

$$|\Psi_0(t)\rangle = \left[C_g(t)|g\rangle_a |N+1\rangle_\ell + C_e(t)|e\rangle_a |N\rangle_\ell \right] \otimes \underbrace{|0\rangle}_{\substack{\text{all other}\\ \text{vacuum photon states}}}$$

$C_g(t)$ & $C_e(t)$ are given by the previous "Schrodinger" equation.

After a photon is emitted at time $t = t_\gamma$, then

$$|\Psi_1(t=t_\gamma)\rangle = |g\rangle \otimes \Big[\sum_{k,\varepsilon} \alpha_{k,\varepsilon} \, |k, \varepsilon, 1\rangle \Big]$$

all possible "1" photon states

photon polarization

momentum

accounts for dipole spatial emission distribution

Actually, the system (atom + laser + universe) could be in a superposition of these 2 states:
(leaked photon not yet detected)

$$|\Psi(t)\rangle = \underbrace{\sqrt{1-\beta^2}}_{\text{for short times}} \underbrace{|\Psi_0(t)\rangle}_{\text{no photon emitted}} + \beta \underbrace{|\Psi_1(t)\rangle}_{\substack{\text{1 photon leaks into an infinite}\\ \text{superposition of photon momentum states}}}$$

Loss of probability from H ends up here

$$\beta = \underbrace{\sqrt{\gamma |C_e|^2 dt}}_{\text{for short times}}$$

Environment Detector

But we are not dealing with a closed system, but an open quantum system. The "leaked photon" could be detected at any moment by the environment [environment is like a giant detector].

Let's assume that the "environment detector" is 100% efficient and makes a measurement in a time dt immediately after a photon leaks out $\longrightarrow$ wavefunction collapses

"photon not emitted state"

keeps evolving as before, but needs to be renormalized, since system is definitely here.

Immediately after collapse:

$$|\psi(t+dt)\rangle = \begin{cases} |\psi_0(t+dt)\rangle \text{ with probability } p = 1-\beta^2 \\ \text{or} \\ |\psi_1(t+dt)\rangle = |g\rangle \underbrace{|k,\varepsilon,1\rangle} \text{ with probability } p=\beta^2 \end{cases}$$

photon collapses to some k, ε state, but we don't pay attention to it.

$\hookrightarrow$ process repeats $\longrightarrow$ propagate a time dt again.

This story suggests the following algorithm for calculating the time evolution of the "atom + laser + universe/environment detector" system ---- though we only pay attention to the atomic state.

Step 1: at time $= t$ the state of the system is

$$|\psi(t)\rangle = |\psi_0(t)\rangle$$
$$= c_g(t)|g\rangle + c_e(t)|e\rangle$$

step 2: at time $= t + dt$ we have 2 possible trajectories for the wavefunction

re-normalization

$$|\psi(t+dt)\rangle = \begin{cases} \text{case A}: \dfrac{1}{\sqrt{1-dp}}\left[c_g(t+dt)|g\rangle + c_e(t+dt)|e\rangle\right] \text{ with probability } 1-dp \\ \text{OR} \\ \text{case B}: |g\rangle \text{ with probability } dp \end{cases}$$

$$\text{with } dp = \gamma |c_e|^2 dt = \beta^2$$

How do you pick between case A & case B ?

↳ "flip a coin" : choose a random number $\varepsilon \in [0,1]$

↳ $\begin{cases} \text{if } \varepsilon > dp \Rightarrow |\psi(t+dt)\rangle = |\text{case A}\rangle \\ \text{if } \varepsilon < dp \Rightarrow |\psi(t+dt)\rangle = |\text{case B}\rangle = |g\rangle \end{cases}$

Condition on dt: $dt = \Delta t \ll \dfrac{1}{\Omega}, \dfrac{1}{\gamma}, \dfrac{1}{\delta}$

not infinitesimal (though that would be ideal)

⚠ Random number generator must work well for very small number ie. $\varepsilon \simeq 0$.

Electronic structure of Alkali Atoms

(I) Fine structure Hamiltonian (i.e. includes spin-orbit coupling)

$$H_0 = \frac{P^2}{2m_e} \underbrace{- \frac{e^2}{R}}_{V(R)} + H_{LS}$$

with $H_{LS} = -\vec{\mu}_e \cdot \vec{B}'$

$\vec{\mu}_e$: $\frac{e}{m_e}\vec{S}$

$\vec{B}'$: effective magnetic field seen by the electron because it is moving through an electric field. [in frame of e^-, "relativistic" effect]

$$\vec{B}' = -\frac{1}{c^2}\vec{v}_e \times \vec{E}$$

$\vec{v}_e = \frac{\vec{P}}{m_e}$ $\qquad$ $\vec{E}$: $-\frac{1}{e}\frac{1}{r}\frac{dV}{dr}\vec{r}$ $\qquad$ $\vec{p} \times \vec{r} = -\vec{L}$

Thus $H_{LS} = \frac{1}{2}\frac{e^2}{m_e^2 c^2}\frac{1}{R^3}\vec{L}\cdot\vec{S} = E_{LS}\,\vec{L}\cdot\vec{S}$

$\frac{1}{2}$: due to thomas precession ↳ rotating relativistic frame effect

$$= \frac{E_{LS}}{2}\left(\vec{J}^2 - \vec{L}^2 - \vec{S}^2\right)$$

$$= \frac{E_{LS}}{2}\left[J(J+1) - L(L+1) - S(S+1)\right]$$

Recall:
$\vec{J} = \vec{L} + \vec{S}$
$\vec{J}^2 = \vec{L}^2 + \vec{S}^2 + 2\vec{L}\cdot\vec{S}$

Possible values for J: $J = L+S,\ L+S-1, \ldots, |L-S|$

Example: for $L=1$, $S=1/2 \Rightarrow J = 3/2$ or $1/2$