Lecture IV

Solution of SE for spin $\frac{1}{2}$ in ia representation

The interaction representation consists of expanding the state $|\psi(t)\rangle$ in terms of the eigenstates $|e\rangle, |g\rangle$ of the Hamiltonian H_0, including their known time dependence $e^{-iH_0t/\hbar}$ due to H_0. That means we write here

$$|\psi(t)\rangle = a_e(t)\,|e\rangle\, e^{-i\omega_0 t/2} + a_g(t)\,|g\rangle\, e^{i\omega_0 t/2}$$

Substituting this into the SE,

$$H = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_R e^{-i\omega t} \\ \omega_R e^{i\omega t} & -\omega_0 \end{pmatrix}$$

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = (H_0 + H_1)|\psi(t)\rangle$$

then results in the eqs of motion for the coefficients

$$i\,\dot{a}_e = \frac{\omega_R}{2} e^{i(\omega_0-\omega)t}\, a_g$$

$$i\,\dot{a}_g = \frac{\omega_R}{2} e^{-i(\omega_0-\omega)t}\, a_e$$

where we have used the matrix form of the Hamiltonian, p. 43 $\quad \delta = \omega - \omega_0$

$$i\,\dot{a}_g = \frac{\omega_R}{2} e^{i\delta t}\, a_e$$

$$i\,\dot{a}_e = \frac{\omega_R}{2} e^{-i\delta t}\, a_g$$

The explicit time dependence can be eliminated by the substitution

$$b_g = e^{-i\delta t/2} a_g$$
$$b_e = e^{i\delta t/2} a_e$$

As you will show in the problem set, this leads to solutions for b_g given by

$$b_g(t) = e^{i\Omega_R t/2} B_1 + e^{-i\Omega_R t/2} B_2$$
$$b_e(t) = \frac{\omega_R}{\delta - \Omega_R} e^{i\Omega_R t/2} B_1 + \frac{\omega_R}{\delta + \Omega_R} e^{-i\Omega_R t/2} B_2$$

with two constants that are determined by the initial conditions.

For $a_g = 1$ we find

$$|a_e(t)|^2 = \frac{\omega_R^2}{\Omega_R^2} \sin^2 \frac{\Omega_R t}{2} ,$$

as already derived from the fact that the expectation value for the magnetic moment obeys the classical equation.

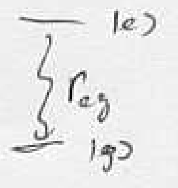
Decoherence processes, mixed states, density matrix

The purely Hamiltonian evolution, as described by the SE, leaves the system in a pure state. However, often we have to deal with incoherent processes such as the uncontrolled loss or addition of atoms, or other perturbations that change the system evolution in an uncontrollable way. If the incoherent process is merely a (state-dependent) loss of atoms to a third state

then we can describe the system still by a Hamiltonian with complex eigenenergies

$E_{g,e} \to E_{g,e} + i\,\frac{\Gamma_{g,e\,f}}{2}$ The decay of the norm $\langle\psi|\psi\rangle$ corresponds to decay out of the $|g\rangle, |e\rangle$ system

However, other processes, such as spontaneous decay $|e\rangle \to |g\rangle$



loss of coherence (well-defined phase relationship) between $|e\rangle$ and $|g\rangle$ due to uncontrolled level shifts (e.g. collisions, uncontrolled B-field fluctuations) cannot be dealt with within the Hamiltonian approach, and require the density matrix formalism.

<u>Density operator</u>

The density operator formalism is necessary when the preparation process does not prepare a single quantum state $|\psi\rangle$, but a statistical mixture of quantum states $|\psi_i\rangle$ with probabilities p_i. The density operator is the projection operator for that statistical mixture, or ensemble average,

$$\hat{\rho} = \sum p_i \, |\psi_i\rangle\langle\psi_i| =: \overline{|\psi\rangle\langle\psi|}$$

From the SE it follows that the Hamiltonian evolution of the density operator is governed by

$$i\hbar\dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]$$

In the presence of damping and decay processes there are additional terms, and the time evolution is governed by a so-called Master equation.

The expectation value of any operator is given by

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

The expectation value of the unity operator must be 1,

$$\mathrm{Tr}(\hat{\rho}) = 1$$

The expectation value of $\hat{\rho}$, $\mathrm{Tr}(\hat{\rho}^2)$, is unity for a pure state, and <1 for a mixed state.

In any basis $\{|n\rangle\}$, $\hat{\rho}$ is specified in terms of its matrix elements

$$\rho_{n'n} := \langle n'|\hat{\rho}|n\rangle,$$

and the expectation value of any operator can be written as

$$\langle \hat{O} \rangle = Tr(\hat{O}\hat{\rho}) = \sum_n \langle n|\hat{O}\hat{\rho}|n\rangle = \sum_{n,n'} \langle n|\hat{O}|n'\rangle\langle n'|\hat{\rho}|n\rangle$$

$$\langle O \rangle = \sum_{n,n'} O_{nn'} \rho_{n'n} \qquad \text{with} \qquad O_{nn'} := \langle n|\hat{O}|n'\rangle$$

The diagonal elements of the density matrix ($\rho_{n'n}$) are called the probabilities (since ρ_{nn} is the probability to find the system in state n),

the off-diagonal elements are called coherences ($\rho_{n'n}$ is the coherence between states n' and n)

If we write $\rho_{n'n} = A_{n'n} e^{i\phi_{n'n}}$ with A, ϕ real

then $\phi_{n'n}$ is the phase between states n' and n,

while $A \leq \sqrt{\rho_{nn}\rho_{n'n'}}$. The coherence is maximum

when $A = \sqrt{\rho_{nn}\rho_{n'n'}}$.

probabilities coherences

$$\hat{\rho} = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \cdot \\ \rho_{21} & \rho_{22} & \rho_{23} & \vdots \\ \rho_{31} & \rho_{32} & \rho_{33} & \\ & \cdots & & \ddots \end{pmatrix} \qquad \rho_{n'n} = \rho^*_{nn'}$$

Density matrix for a two-level system and Bloch vector

We parametrize the two-level Hamiltonian from p. 43 slightly differently

$$H = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_R e^{-i\omega t} \\ \omega_R e^{i\omega t} & -\omega_0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & V_1 - iV_2 \\ V_1 + iV_2 & -\omega_0 \end{pmatrix}$$

$$H = \frac{\hbar}{2}\left(V_1 \hat{\sigma}_x + V_2 \hat{\sigma}_y + \omega_0 \hat{\sigma}_z \right)$$

and the density matrix as well

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} =: \frac{1}{2}\begin{pmatrix} r_0 + r_3 & r_1 - ir_2 \\ r_1 + ir_2 & r_0 - r_3 \end{pmatrix} = \frac{1}{2}\left(r_0 \hat{\mathbb{1}} + r_1 \hat{\sigma}_x + r_2 \hat{\sigma}_y + r_3 \hat{\sigma}_z \right)$$

In the problem set you will show that the Hamiltonian evolution of the density matrix

$$i\hbar \dot{\rho} = [H, \rho]$$

implies the equation of motion

$$\frac{d\vec{r}}{dt} = \vec{\omega} \times \vec{r}$$

for the vectors $\vec{r} = (r_1, r_2, r_3)$ and $\vec{\omega} = (V_1, V_2, \omega_0)$

This slightly generalizes our previous result:

For a pure state using the Heisenberg eqs. of motion we had shown that the spin $\frac{1}{2}$, and the corresponding magnetic moment obey

$$\frac{d}{dt}\vec{S} = \vec{\omega} \times \vec{S}$$

The above generalizes this result to mixed states with $|r_1|^2 + |r_2|^2 < 1$, i.e. for ensemble averages that have less than the maximum possible magnetic moment.

Note that Hamiltonian evolution does not change the purity of a state: A pure state always remains pure, no matter how violently it is rotated, and a mixed state retains its degree of mixedness ($\mathrm{tr}\,\rho^2(t) = \mathrm{const.}$) Here we can check this explicitly by noting that $\mathrm{tr}\,\rho^2 = \frac{1}{2}(r_0^2 + r_1^2 + r_2^2 + r_3^2) = \frac{1}{2}(r_0^2 + |\vec{r}|^2)$ since $\dot{\vec{r}} \perp \vec{r}$, the length of $\vec{r}$ does not change, and hence $\mathrm{tr}\,\rho^2$ is constant in time.

End-of-chapter review questions (PRS).