PC3130 W11L1 AY24

Tuesday, 29 October 2024 9:55 am

5 Nov - Tut 6 due

7 Nov - Project due 23:59

No lecture on 31 Oct

Final exam

- closed book, but you can bring in an A4 sheet written on both sides.
- Calculators not needed
- Strictly follow instructions
- 3 questions; 2 worth 25 marks, 1 worth 50 marks.
- Nov 19 - Dec 1. — away. (Nov 19 - am ok)

W10L1 weak field Zeeman effect

We showed that

$$E^{(1)}_{n j m_j l s} = \frac{eB}{2m} \langle n j m_j l s | L_z + g_e S_z | n j m_j l s \rangle \quad (*)$$

(Degeneracies: for different m_j & l but same n & j (s is fixed; $s = \frac{1}{2}$) same E)

Today, we evaluate (*).

Use $g_e = 2$. $L_z + g_e S_z \approx L_z + 2S_z = J_z + S_z$

$$\langle n j m_j l s | J_z | n j m_j l s \rangle = \hbar m_j$$

$$E^{(1)}_{n j m_j l s} = \frac{eB}{2m} \Big(\hbar m_j + \underbrace{\langle n j m_j l s | S_z | n j m_j l s \rangle}_{(**)} \Big)$$

J_z

$\vec{J}^2 \quad \vec{L}^2 \quad \vec{S}^2$

To evaluate (**), we use the projection theorem.

For any vector operator $\vec{T}$,

$$\langle j m_j' | \vec{T} | j m_j \rangle = \frac{1}{\underbrace{\hbar^2 j(j+1)}_{\text{"}J^2\text{"}}} \langle j m_j' | (\vec{T}\cdot\vec{J})\vec{J} | j m_j \rangle$$

$$\approx \left(\vec{T}\cdot\frac{\vec{J}}{|\vec{J}|}\right)\frac{\vec{J}}{|\vec{J}|}$$

Projection of $\vec{T}$ onto $\vec{J}$.

$\vec{S}$ is a vector operator.

$\leftarrow$ vector operator

so $\langle n j m_j l s | \vec{S} | n j m_j l s \rangle$

$$= \frac{1}{\hbar^2 j(j+1)} \langle n j m_j l s | (\vec{S}\cdot\vec{J})\vec{J} | n j m_j l s \rangle$$

$$= \frac{1}{\hbar^2 j(j+1)} \langle n\, j\, m_j\, l s | \underbrace{(\vec{S}\cdot\vec{J})}_{\text{scalar operator}} \underset{\substack{\uparrow \\ \text{vector operator}}}{\vec{J}} | n\, j\, m_j\, l s \rangle$$

$$\langle n\, j\, m_j\, l\, s | S_z | n\, j\, m_j\, l\, s \rangle$$

$$= \frac{1}{\hbar^2 j(j+1)} \langle n\, j\, m_j\, l\, s | (\vec{S}\cdot\vec{J})\, J_z | n\, j\, m_j\, l\, s \rangle$$

$$= \frac{\hbar m_j}{\hbar^2 j(j+1)} \langle n\, \underline{j}\, m_j\, \underline{l}\, \underline{s} | (\vec{S}\cdot\vec{J}) | n\, j\, m_j\, l\, s \rangle$$

Write $\vec{S}\cdot\vec{J}$ in terms of $\vec{S}^2, \vec{J}^2, \vec{L}^2$.

last time: $\vec{J} = \vec{L} + \vec{S}$

$$\vec{J}^2 = (\vec{L} + \vec{S})^2 = \vec{L}^2 + \vec{S}^2 + 2\vec{L}\cdot\vec{S}$$

($\vec{L}$ & $\vec{S}$ commute)

$$\vec{L}\cdot\vec{S} = \frac{1}{2}(\vec{J}^2 - \vec{L}^2 - \vec{S}^2)$$

$$\vec{L} = \vec{J} - \vec{S}$$

$$\vec{L}^2 = (\vec{J} - \vec{S})^2 = \vec{J}^2 + \vec{S}^2 - 2\vec{S}\cdot\vec{J} \quad ([\vec{S}, \vec{J}] = 0)$$

$$\vec{S}\cdot\vec{J} = \frac{1}{2}(\vec{J}^2 + \vec{S}^2 - \vec{L}^2)$$

So $\langle n\, j\, m_j\, l s | (\vec{S}\cdot\vec{J}) | n\, j\, m_j\, l s \rangle$

$$= \frac{1}{2} \langle n\, j\, m_j\, l\, s | \vec{J}^2 + \vec{S}^2 - \vec{L}^2 | n\, j\, m_j\, l\, s \rangle$$

$$= \frac{1}{2} \left(\hbar^2 j(j+1) + \hbar^2 s(s+1) - \hbar^2 l(l+1) \right) \quad (s = \tfrac{1}{2})$$

This gives

$$E^{(1)}_{n j m_j l s} = \underbrace{\left(\frac{e\hbar}{2m_e}\right)}_{\mu_B} B\, m_j \underbrace{\left(\frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)} \right)}_{g_J \text{ Landé g-factor}}$$

$$= \mu_B\, g_J\, m_j\, B$$

Eg $B = 0.01\,T$ $\quad$ ($\mu_B \sim 10^{-5}\, eV/T$)

$n = 3$, $\quad$ $s = \frac{1}{2}$

p states $l = 1$

p states $l=1$

$j = 3/2,\ 1/2$

For $j = 3/2$, $g_J = \frac{3}{2} + \frac{\frac{1}{2}(\frac{1}{2}+1) - 1(1+1)}{2 \cdot \frac{3}{2}(\frac{3}{2}+1)} = \frac{4}{3}$

$$E^{(1)} = \mu_B g_J m_j B$$
$$= m_j \times 7.70 \times 10^{-7}\ \text{eV}$$
$$= \begin{cases} 1.16 \times 10^{-6}\ \text{eV} & m_j = 3/2 \\ 3.85 \times 10^{-7}\ \text{eV} & m_j = 1/2 \\ -3.85 \times 10^{-7}\ \text{eV} & m_j = -1/2 \\ -1.16 \times 10^{-6}\ \text{eV} & m_j = -3/2 \end{cases}$$

Time-dependent perturbation theory

$$H(t) = H_0 + V(t)$$

H_0: time-independent

$V(t)$: small perturbation. may be time-dependent eg transient EM field.

Earlier time-independent perturbation theory.
- Stationary states, energy eigenvalues } How they depend on V.

Now: Time-dependent Hamiltonians do not have stationary states.

To answer: 1) What is the time evolution of the wavefunction?

2) If the system is originally in a stationary state of H_0, the time-dependent perturbation can result in transitions to different eigenstates of H_0. What are the probabilities of these transitions?

Time-evolution / Quantum dynamics

Schrödinger representation.

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$ – time-dependent Schrödinger's

equations.

We introduce an operator $U(t, t_0)$

where $|\psi(t)\rangle = \underbrace{U(t, t_0)}_{}|\psi(t_0)\rangle$; $U(t_0, t_0) = \mathbb{1}$.

time-development
or time-evolution
or Dyson operator.

$U(t, t_0)$ is unitary — preserves inner products.

What is U?

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle \quad \text{— (1)}$$

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle \quad \text{— (2)}$$

Sub. (2) in (1):

$$i\hbar \frac{\partial U}{\partial t}(t, t_0) = H(t)\,U(t, t_0) \quad \text{— (3)}$$

Time-independent H: $U(t, t_0) = \exp\left(-\frac{i}{\hbar}H(t-t_0)\right)$, $U(t_0, t_0) = \mathbb{1}$.

Time-dependent H:

Rewrite (3):
$(t \to t')$

$$i\hbar \frac{\partial}{\partial t'}U(t', t_0) = H(t')\,U(t', t_0)$$

$\int_{t'=t_0}^{t'=t} dt'$ on both sides:

$$i\hbar \left[U(t', t_0)\right]_{t_0}^{t} = \int_{t_0}^{t} dt'\, H(t')\,U(t', t_0)$$

$$i\hbar\left(U(t, t_0) - 1\right) = dt'\, H(t')\,U(t', t_0)$$

$$\boxed{U(t, t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, H(t')\,U(t', t_0)}$$

$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$

In general, not easy to solve this exactly.

What can we do?

We have $U(t,t_0)$ in the integral on the RHS.

Substitute in the RHS Eg. $U(t_0,t_0)=\mathbb{1}$ as a starting point.

$$\underbrace{U(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} H(t')\,\mathbb{1}\,dt'}_{\text{Sub in RHS.}} \quad \text{— 1st approx.}$$

$$U(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} H(t')\,\underbrace{U(t',t_0)}_{\mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t'} H(t'')\,dt''}\,dt' \quad \text{— 2nd approx.}$$

$$\boxed{\text{Is this reasonable?}}$$

This will be reasonable if we know that higher order corrections are smaller / we can reach convergence.

<u>2nd approx</u>:

$$U(t,t_0) = \underbrace{\mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} H(t')\,dt'}_{\text{1st approx.}} + \underbrace{\left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} H(t') \int_{t_0}^{t'} H(t'')\,dt''\,dt'}_{\text{Is this necessarily smaller than } -\frac{i}{\hbar}\int_{t_0}^{t} H(t')\,dt' \text{ ?}} - (t)$$

No.

Therefore, this is <u>NOT</u> a reasonable approach.

What if, instead of H in (t), we have the perturbation, V?

(Recall Taylor series:

$|x-x_0| \ll 1$

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + \underbrace{\frac{f''(x_0)}{2!}(x-x_0)^2}_{\text{smaller than } f'(x_0)(x-x_0)} + \mathcal{O}((x-x_0)^3)$$

If $|x-x_0| = 0.1$

If $|x-x_0| = 2$

$|x-x_0|^2 = 4$

If $|x-x_0| = 0.1$
$|x-x_0|^2 = 0.01$
$|x-x_0|^3 = 0.001$

If $|x-x_0| = 2$
$|x-x_0|^2 = 4$
$|x-x_0|^3 = 8$

Final result of time-dependent perturbation theory:

To 2nd order in V, ("small")

$$\hat{U}_I(t,t_0) = \underbrace{\mathbb{1}}_{\text{zeroth order term}} + \underbrace{\frac{1}{i\hbar}\int_{t_0}^{t} \hat{V}_I(t_1)\,dt_1}_{\text{1st order corrections}} + \underbrace{\left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} \hat{V}_I(t_1)\int_{t_0}^{t_1} \hat{V}_I(t_2)\,dt_2\,dt_1}_{\text{2nd order correction.}}$$

(smaller than 1st order correction)

(c.f. $i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}(t)\,\hat{U}(t,t_0)$)

$\hat{U} \to \hat{U}_I$
$\hat{H} \to \hat{V}_I$

$$i\hbar\frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \hat{V}_I(t)\,\hat{U}_I(t,t_0) \quad \text{— } (\dagger\dagger)$$

$$\hat{U}_I(t,t_0) = \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t} \hat{V}_I(t_1)\,\hat{U}_I(t_1,t_0)\,dt_1$$

What is $\hat{U}_I(t,t_0)$?
What is $\hat{V}_I(t,t_0)$?
How do we get $(\dagger\dagger)$?
"I" stands for "interaction" in what we call the "interaction picture".

Earlier, we used the "Schrödinger picture":

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)\,|\psi(t)\rangle.$$

Let's 1st bring up the "Heisenberg picture":

- States are fixed (time-independent)

Quantum evolution is equivalently expressed as transformations of observables.

Expectation value of an arbitrary observable at time t:

Schrödinger picture: $\langle\psi(t)|\,\hat{O}(t)\,|\psi(t)\rangle$

Heisenberg picture: $\langle\psi(t_0)|\,\hat{O}_H(t)\,|\psi(t_0)\rangle$

Heisenberg picture : $\langle \psi(t_0) | \hat{O}_H(t) | \psi(t_0) \rangle$

Representations / pictures must be equivalent.

So $\langle \psi(t_0) | \hat{O}_H(t) | \psi(t_0) \rangle = \langle \psi(t) | \hat{O}(t) | \psi(t) \rangle$

We can use $|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle$

RHS $= \langle \psi(t_0) | \hat{U}^{\dagger}(t,t_0) \hat{O}(t) \hat{U}(t,t_0) | \psi(t_0) \rangle$

$=$ LHS for any $|\psi(t_0)\rangle$

$\Rightarrow \quad \hat{O}_H(t) = \hat{U}^{\dagger}(t,t_0)\, \hat{O}(t)\, \hat{U}(t,t_0)$.

Interaction picture

$$\hat{H}(t) = \underset{\text{time-indep}}{\hat{H}_0} + \underset{\text{small perturbation.}}{\hat{V}(t)}$$

We write

$$\hat{U}(t,t_0) = \underbrace{\hat{U}_0(t,t_0)}_{\substack{\text{time-evolution}\\\text{operator}\\\text{for } H_0}} \underbrace{\hat{U}_I(t,t_0)}_{\substack{\text{correction due}\\\text{to the perturbation.}}} \quad -(1)$$

Goal: Find out more about $\hat{U}_I(t,t_0)$.

We know: $\hat{U}_0(t,t_0)$ obeys

$$i\hbar \frac{\partial}{\partial t} \hat{U}_0(t,t_0) = \hat{H}_0 \hat{U}_0(t,t_0).$$

$$\hat{U}_0(t,t_0) = \exp\left(-\frac{i}{\hbar} \hat{H}_0 (t-t_0)\right)$$

What is $i\hbar \frac{\partial}{\partial t} \hat{U}_I(t,t_0)$?

From (1), we can write $\hat{U}_I(t,t_0) = \hat{U}_0^{\dagger}(t,t_0)\, \hat{U}(t,t_0)$

(since $\underset{\text{unitary}}{\hat{U}_0^{\dagger}(t,t_0)\hat{U}_0(t,t_0) = \mathbb{1}}$)

$i\hbar \frac{\partial}{\partial t} \hat{U}_I(t,t_0)$

$= i\hbar \left(\frac{\partial}{\partial t} \hat{U}_0^{\dagger}(t,t_0)\right) \hat{U}(t,t_0) + i\hbar\, \hat{U}_0^{\dagger}(t,t_0) \left(\frac{\partial}{\partial t} \hat{U}(t,t_0)\right)$

$i\hbar \frac{\partial}{\partial t} \hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0)$ — definition.

$i\hbar \frac{\partial}{\partial t} \hat{U}_0(t,t_0) = \hat{H}_0 \hat{U}_0(t,t_0)$ — definition.

∂t

$$-i\hbar \frac{\partial}{\partial t} \hat{U}_0^\dagger(t, t_0) = \hat{U}_0^\dagger(t, t_0)\, \hat{H}_0^\dagger = \hat{U}_0^\dagger(t, t_0)\, H_0$$

(since $\hat{H}_0^\dagger = H_0$ Hermitian)