Introductory Remarks

1) Name: Daniel Chapman — Official TA for Phys 402
2) As you may already know, Dr. Anlage is out of town until Monday
3) I am giving second of three guest lectures
4) Friday likely will be Dr. Orozco
5) Homework 6 is still due Friday — I will be there at the end to pick up
6) Exam 1 will be returned Monday. Dr. Anlage wants to see them before they are returned, and all grading questions should go to him
7) I will have extended office hours this week from 3:00pm to 5:30pm, at Phys 4110, on Thursday
8) Any Questions?

Then let's begin...

Today's Lecture: Time-Dependent Perturbation Theory

Past Lectures: Until now, we have been ~~worried about~~ dealing with steady-state systems. We have looked at the main solvable systems — the particle in a box, the harmonic oscillator, and the hydrogen atom. We have also seen the effects of small, position-dependent perturbations in the potentials of such systems. And we have taken a glimpse into the field of atomic physics. But many questions remain.

<u>Motivation</u>: One such question — How to deal with the effects of outside, short-time interactions with these systems. Perhaps ~~the~~ electron inside a hydrogen atom is hit by a photon. Such interactions cannot be modelled with our current time-independent perturbation theory. But many of the lessons learned can still be adapted. We only require a look at the full time-dependent equations

1) $$\mathcal{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

The full time-dependent Schrödinger equation

If $\mathcal{H} = H^o_\bullet$ is independent of time, the technique of separation of variables can be used to "pull out" the time dependence

2) $$\Psi^o_n(r,t) = \psi^o_n(r)\, g^o_n(t), \text{ where then}$$

3) $$g_n(t) = e^{-iE_nt/\hbar} \text{ solves the time-dependent piece,}$$

$$E_n g(t) = i\hbar \frac{dg(t)}{dt}$$

and the time-independent piece ~~is solved by~~ must then solve

4) $$H^o(r)\,\psi^o_n(r) = E_n \psi^o_n(r)$$

However, if then an extra, time-dependent piece is added to the Hamiltonian, $\mathcal{H} = H^o(r) + H'(r,t)$, separation of variables can no longer be used

We can still attempt to look at what changes though.

$$H^o_\bullet \Psi(r,t) + H'\Psi(r,t) = i\hbar \frac{\partial \Psi(r,t)}{\partial t}$$

$$\Psi = \Psi^o + \Psi^D \quad \Rightarrow \quad \text{(next page)}$$

$$\underbrace{H^0\Psi^0}\ + H^0\Psi^D + H'\Psi^0 + H'\Psi^D = \underbrace{i\hbar\frac{\partial\Psi^0}{\partial t}} + i\hbar\frac{\partial\Psi^D}{\partial t}$$

Satisfy the original Schrödinger equation

$$\Rightarrow H^0\Psi^D + H'\Psi^0 + H'\Psi^D = i\hbar\frac{\partial\Psi^D}{\partial t}$$

From the completeness postulate of QM, any wavefunction can be represented as a sum of "basis" wavefunctions — that is,

$$\Psi_n^D(\vec{r},t) = \sum_\ell a^D_{n\ell}(t)\Psi^0_\ell(\vec{r},t) \Rightarrow \frac{\partial\Psi^D}{\partial t} = \sum_\ell\Big(\dot{a}^D_{n\ell}(t)\Psi^0_\ell(\vec{r},t)$$
$$+ a^D_{n\ell}(t)\frac{\partial}{\partial t}\Psi^0_\ell(\vec{r},t)\Big)$$

This means $\sum_\ell\Big(H^0 a^D_{n\ell}(t)\Psi_\ell^0(\vec{r},t) + H'\Psi_n^0(\vec{r},t) + H'(\vec{r},t)\,a^D_{n\ell}(t)\Psi_\ell^0(\vec{r},t)\Big)$

$$= \sum_\ell \dot{a}^D_{n\ell}(t)\,i\hbar\,\Psi_\ell^0(\vec{r},t) + \sum_\ell a^D_{n\ell}(t)\frac{\partial}{\partial t}i\hbar\,\Psi_\ell^0(\vec{r},t)\Big)\Big)$$

Since $H^0(\vec{r})$ does not depend on t, the order of H^0 and $a^D_{n\ell}$ does not matter, and then $\sum_\ell a^D_{n\ell}(t)\,H^0(\vec{r})\Psi_\ell^0(\vec{r},t) = \sum_\ell a^D_{n\ell}(t)\frac{\partial(i\hbar\Psi_\ell^0)}{\partial t}$

So Finally, $\sum_\ell H'(\vec{r},t)\left(\delta_{n\ell} + a^D_{n\ell}(t)\right)\Psi_\ell^0(\vec{r},t) = \sum_\ell i\hbar\,\dot{a}^D_{n\ell}(t)\,\Psi_\ell^0(\vec{r},t)$

Next, we can multiply both sides from the left with Ψ_j^{*0}, and integrate over all space.

$$\int\Psi_j^{*0}\sum_\ell H'(\vec{r},t)\left(\delta_{n\ell} + a^D_{n\ell}(t)\right)\Psi_\ell^0(\vec{r},t)\,d^3r = \sum_\ell i\hbar\,\dot{a}^D_{n\ell}(t)\underbrace{\int d^3r\,\Psi_j^{*0}\Psi_\ell^0}_{=\delta_{j\ell}}$$

$$= i\hbar\,\dot{a}^D_{nj}(t)$$

Typically, this is a very difficult differential equation to solve. There are some tools that can be used, however.

For instance, imagine now being able to control the strength of H' via a variable, λ.

$$H'(r,t) \rightarrow \lambda H'(r,t)$$

The wavefunction difference, Ψ^D need not be linear in λ, but instead can include extra powers of λ

$$\Psi^D \Rightarrow \lambda\Psi^{(1)} + \lambda^2\Psi^{(2)} + \lambda^3\Psi^{(3)} + \dots$$

This directly translates down to $a^D_{n\ell}$

$$a^D_{n\ell} \Rightarrow \lambda a^{(1)}_{n\ell} + \lambda^2 a^{(2)}_{n\ell} + \lambda^3 a^{(3)}_{n\ell} + \dots$$
$$\dot{a}^D_{n\ell} \Rightarrow \lambda \dot{a}^{(1)}_{n\ell} + \lambda^2 \dot{a}^{(2)}_{n\ell} + \lambda^3 \dot{a}^{(3)}_{n\ell} + \dots$$

We can then collect powers of λ in our differential equation

$$\lambda: \int \Psi_j^{*0} \sum_\ell H' \delta_{n\ell} \Psi^0_\ell(\vec{r},t)\, d^3r = i\hbar\, \dot{a}^{(1)}_{nj}(t) \quad \Rightarrow a^{(1)}_{nj}(t) = \int dt \left(\int d^3r\, \Psi_j^{*0} H' \Psi^0_n \right.$$

$$\lambda^2: \int \Psi_j^{*0} \sum_\ell H' a^{(1)}_{n\ell} \Psi^0_\ell\, d^3r = i\hbar\, \dot{a}^{(2)}_{nj}(t) \quad \Rightarrow a^{(2)}_{n\ell}(t)$$

So each successive equation can let you solve directly for the next term in the series. By assuming $\lambda H'$ is small compared to H^0, one can then terminate the series at λ^n to give an nth order approx.

Two level Systems:

If we deal with an original H^0 with only two states, $H^0\psi_a = E_a\psi_a$ and $H^0\psi_b = E_b\psi_b$, the situation simplifies dramatically.

~~Wlog, we can assume at~~ At time 0, say the solution begins in state a. Then the perturbation begins, and at time T, we want to calculate what the probability a measurement will find the system in state b.

$$\psi^0(\vec{r}) = \Psi^0(\vec{r},0) = a_a(0)\psi_a + c_b(0)\psi_b, \text{ with } |a_a(0)|^2 + |a_b(0)|^2 = 1$$

$$\Psi^0(\vec{r},t) = a_a(t)\psi_a + a_b(t)\psi_b = a_a(0)e^{-iE_at/\hbar}\psi_a + a_b(0)e^{-iE_bt/\hbar}\psi_b$$

So in the absence of a perturbation, the probability the state is in state a is $|a_a(t)|^2 = |a_a(0)|^2$, and similarly for state b

In our case, $a_a(0) = 1$ and $a_b(0) = 0$

Now, let us assume we have a small, time-dependent perturbation between $t=0$ and $t=T$

To first order, then we can solve for the transition amplitude: $a^{(1)}_{a\to b}(T) = -\frac{i}{\hbar}\int_0^T dt \int \Psi_b^{*0} H' \Psi_a^0 d^3r = -\frac{i}{\hbar}\int_0^T dt\, e^{[i(E_b^0 - E_a^0)t/\hbar]} \int d^3r\, \psi_b^*(r) H'(r,t)\, \psi_a(r)$

the combination $\frac{E_b^0 - E_a^0}{\hbar} \equiv \omega_0$ is called the "transition frequency"

This analysis can be continued then to second order, and each successive order

7 minute break after first part, then informal discussion period – show the slides on the projector & talk about them plus homework