

PHY456H1F: Quantum Mechanics II. Lecture 8 (Taught by Prof J.E. Sipe). Time dependent perturbation (cont.)

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Contents

1 Disclaimer.	1
2 Time dependent perturbation.	1
3 Sudden perturbations.	2
3.1 Example: Harmonic oscillator.	4
4 Adiabatic perturbations.	5

1. Disclaimer.

Peeter's lecture notes from class. May not be entirely coherent.

2. Time dependent perturbation.

We'd gotten as far as calculating

$$c_m^{(1)}(\infty) = \frac{1}{i\hbar} \boldsymbol{\mu}_{ms} \cdot \mathbf{E}(\omega_{ms}) \quad (1)$$

where

$$\mathbf{E}(t) = \int \frac{d\omega}{2\pi} \mathbf{E}(\omega) e^{-i\omega t}, \quad (2)$$

and

$$\omega_{ms} = \frac{E_m - E_s}{\hbar}. \quad (3)$$

Graphically, these frequencies are illustrated in figure (1)

The probability for a transition from m to s is therefore

$$\rho_{m \rightarrow s} = \left| c_m^{(1)}(\infty) \right|^2 = \frac{1}{\hbar^2} \left| \boldsymbol{\mu}_{ms} \cdot \mathbf{E}(\omega_{ms}) \right|^2 \quad (4)$$

Recall that because the electric field is real we had

$$|\mathbf{E}(\omega)|^2 = |\mathbf{E}(-\omega)|^2. \quad (5)$$

"Positive frequencies" :
 absorption

— $\omega_{ms} > 0$
 — m
 — s

— $\omega_{ms} < 0$
 —

"Negative frequencies" :
 stimulated emission

Figure 1: Positive and negative frequencies.

Suppose that we have a wave pulse, where our field magnitude is perhaps of the form

$$E(t) = e^{-t^2/T^2} \cos(\omega_0 t), \tag{6}$$

as illustrated with $\omega = 10, T = 1$ in figure (2).

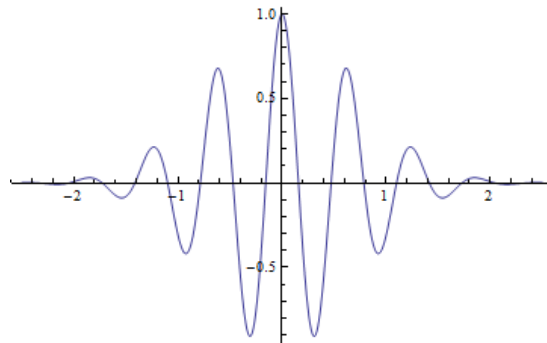


Figure 2: Gaussian wave packet

We expect this to have a two lobe Fourier spectrum, with the lobes centered at $\omega = \pm 10$, and width proportional to $1/T$.

For reference, as calculated using **Mathematica** this Fourier transform is

$$E(\omega) = \frac{e^{-\frac{1}{4}T^2(\omega_0+\omega)^2}}{2\sqrt{\frac{2}{T^2}}} + \frac{e^{\omega_0 T^2 \omega - \frac{1}{4}T^2(\omega_0+\omega)^2}}{2\sqrt{\frac{2}{T^2}}} \tag{7}$$

This is illustrated, again for $\omega_0 = 10, and T = 1$, in figure (3)

where we see the expected Gaussian result, since the Fourier transform of a Gaussian is a Gaussian.

FIXME: not sure what the point of this was?

3. Sudden perturbations.

Given our wave equation

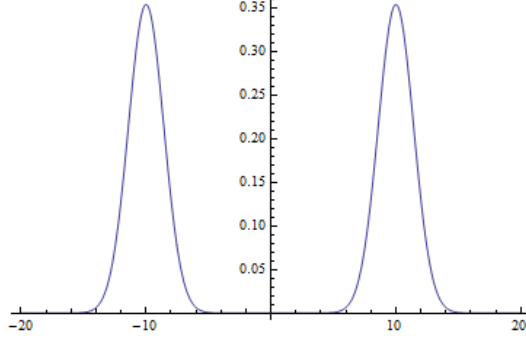


Figure 3: FTgaussianWavePacket

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (8)$$

and a sudden perturbation in the Hamiltonian, as illustrated in figure (4)

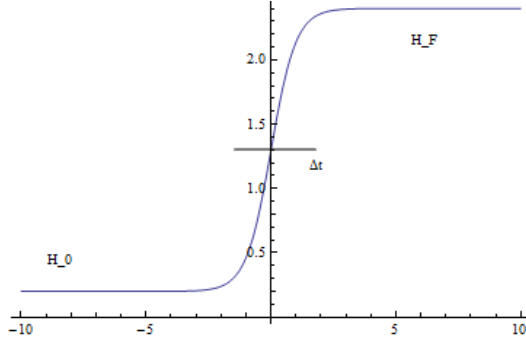


Figure 4: Sudden step Hamiltonian.

Consider H_0 and H_F fixed, and decrease $\Delta t \rightarrow 0$. We can formally integrate [8](#)

$$\frac{d}{dt} |\psi(t)\rangle = \frac{1}{i\hbar} H(t) |\psi(t)\rangle \quad (9)$$

For

$$|\psi(t)\rangle - |\psi(t_0)\rangle = \frac{1}{i\hbar} \int_{t_0}^t H(t') |\psi(t')\rangle dt'. \quad (10)$$

While this is an exact solution, it is also not terribly useful since we don't know $|\psi(t)\rangle$. However, we can select the small interval Δt , and write

$$|\psi(\Delta t/2)\rangle = |\psi(-\Delta t/2)\rangle + \frac{1}{i\hbar} \int_{t_0}^t H(t') |\psi(t')\rangle dt'. \quad (11)$$

Note that we could use the integral kernel iteration technique here and substitute $|\psi(t')\rangle = |\psi(-\Delta t/2)\rangle$ and then develop this, to generate a power series with $(\Delta t/2)^k$ dependence. However, we note that [11](#) is still an exact relation, and if $\Delta t \rightarrow 0$, with the integration limits narrowing (provided $H(t')$ is well behaved) we are left with just

$$|\psi(\Delta t/2)\rangle = |\psi(-\Delta t/2)\rangle \quad (12)$$

Or

$$|\psi_{\text{after}}\rangle = |\psi_{\text{before}}\rangle, \quad (13)$$

provided that we change the Hamiltonian fast enough. On the surface there appears to be no consequences, but there are some very serious ones!

3.1. Example: Harmonic oscillator.

Consider our harmonic oscillator Hamiltonian, with

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 X^2 \quad (14)$$

$$H_F = \frac{p^2}{2m} + \frac{1}{2}m\omega_F^2 X^2 \quad (15)$$

Here $\omega_0 \rightarrow \omega_F$ continuously, but very quickly. In effect, we have tightened the spring constant. Note that there are cases in linear optics when you can actually do exactly that.

Imagine that $|\psi_{\text{before}}\rangle$ is in the ground state of the harmonic oscillator as in figure (5)

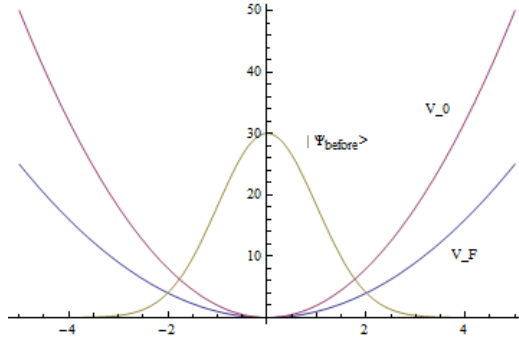


Figure 5: Harmonic oscillator sudden Hamiltonian perturbation.

and we suddenly change the Hamiltonian with potential $V_0 \rightarrow V_F$ (weakening the “spring”). Professor Sipe gives us a graphical demo of this, by impersonating a constrained wavefunction with his arms, doing weak chicken-flapping of them. Now with the potential weakened, he wiggles and flaps his arms with more freedom and somewhat chaotically. His “wave function” arms are now bouncing around in the new limiting potential (initially over doing it and then bouncing back).

We had in this case the exact relation

$$H_0|\psi_0^{(0)}\rangle = \frac{1}{2}\hbar\omega_0|\psi_0^{(0)}\rangle \quad (16)$$

but we also have

$$|\psi_{\text{after}}\rangle = |\psi_{\text{before}}\rangle = |\psi_0^{(0)}\rangle \quad (17)$$

and

$$H_F|\psi_n^{(f)}\rangle = \frac{1}{2}\hbar\omega_F \left(n + \frac{1}{2} \right) |\psi_n^{(f)}\rangle \quad (18)$$

So

$$\begin{aligned}
 |\psi_{\text{after}}\rangle &= |\psi_0^{(0)}\rangle \\
 &= \sum_n |\psi_n^{(f)}\rangle \underbrace{\langle \psi_n^{(f)} | \psi_0^{(0)} \rangle}_{c_n} \\
 &= \sum_n c_n |\psi_n^{(f)}\rangle
 \end{aligned}$$

and at later times

$$\begin{aligned}
 |\psi(t)^{(f)}\rangle &= |\psi_0^{(0)}\rangle \\
 &= \sum_n c_n e^{i\omega_n^{(f)}t} |\psi_n^{(f)}\rangle,
 \end{aligned}$$

whereas

$$|\psi(t)^{(o)}\rangle = e^{i\omega_0^{(0)}t} |\psi_0^{(0)}\rangle,$$

So, while the wave functions may be exactly the same after such a sudden change in Hamiltonian, the dynamics of the situation change for all future times, since we now have a wavefunction that has a different set of components in the basis for the new Hamiltonian. In particular, the evolution of the wave function is now significantly more complex.

FIXME: plot an example of this.

4. Adiabatic perturbations.

This is treated in §17.5.2 of the text [1].

FIXME: what does Adiabatic mean in this context. The usage in class sounds like it was just “really slow and gradual”, yet this has a definition “Of, relating to, or being a reversible thermodynamic process that occurs without gain or loss of heat and without a change in entropy”.

This is the reverse case, and we now vary the Hamiltonian $H(t)$ very slowly.

$$\frac{d}{dt} |\psi(t)\rangle = \frac{1}{i\hbar} H(t) |\psi(t)\rangle \quad (19)$$

We first consider only non-degenerate states, and at $t = 0$ write

$$H(0) = H_0, \quad (20)$$

and

$$H_0 |\psi_s^{(0)}\rangle = E_s^{(0)} |\psi_s^{(0)}\rangle \quad (21)$$

Imagine that at each time t we can find the “instantaneous” energy eigenstates

$$H(t) |\hat{\psi}_s(t)\rangle = E_s(t) |\hat{\psi}_s(t)\rangle \quad (22)$$

These states do not satisfy Schrödinger’s equation, but are simply solutions to the eigen problem. Our standard strategy in perturbation is based on analysis of

$$|\psi(t)\rangle = \sum_n c_n(t) e^{-i\omega_n^{(0)}t} |\psi_n^{(0)}\rangle, \quad (23)$$

Here instead

$$|\psi(t)\rangle = \sum_n b_n(t) |\hat{\psi}_n(t)\rangle, \quad (24)$$

we will expand, not using our initial basis, but instead using the instantaneous kets. Plugging into Schrödinger's equation we have

$$\begin{aligned} H(t)|\psi(t)\rangle &= H(t) \sum_n b_n(t) |\hat{\psi}_n(t)\rangle \\ &= \sum_n b_n(t) E_n(t) |\hat{\psi}_n(t)\rangle \end{aligned}$$

This was complicated before with matrix elements all over the place. Now it is easy, however, the time derivative becomes harder. Doing that we find

$$\begin{aligned} i\hbar \frac{d}{dt} |\psi(t)\rangle &= i\hbar \frac{d}{dt} \sum_n b_n(t) |\hat{\psi}_n(t)\rangle \\ &= i\hbar \sum_n \frac{db_n(t)}{dt} |\hat{\psi}_n(t)\rangle + \sum_n b_n(t) \frac{d}{dt} |\hat{\psi}_n(t)\rangle \\ &= \sum_n b_n(t) E_n(t) |\hat{\psi}_n(t)\rangle \end{aligned}$$

We bra $\langle \hat{\psi}_m(t) |$ into this

$$i\hbar \sum_n \frac{db_n(t)}{dt} \langle \hat{\psi}_m(t) | \hat{\psi}_n(t) \rangle + \sum_n b_n(t) \langle \hat{\psi}_m(t) | \frac{d}{dt} | \hat{\psi}_n(t) \rangle = \sum_n b_n(t) E_n(t) \langle \hat{\psi}_m(t) | \hat{\psi}_n(t) \rangle, \quad (25)$$

and find

$$i\hbar \frac{db_m(t)}{dt} + \sum_n b_n(t) \langle \hat{\psi}_m(t) | \frac{d}{dt} | \hat{\psi}_n(t) \rangle = b_m(t) E_m(t) \quad (26)$$

If the Hamiltonian is changed very very slowly in time, we can imagine that $|\hat{\psi}_n(t)\rangle'$ is also changing very very slowly, but we are not quite there yet. Let's first split our sum of bra and ket products

$$\sum_n b_n(t) \langle \hat{\psi}_m(t) | \frac{d}{dt} | \hat{\psi}_n(t) \rangle \quad (27)$$

into $n \neq m$ and $n = m$ terms. Looking at just the $n = m$ term

$$\langle \hat{\psi}_m(t) | \frac{d}{dt} | \hat{\psi}_m(t) \rangle \quad (28)$$

we note

$$\begin{aligned}
0 &= \frac{d}{dt} \langle \hat{\psi}_m(t) | \hat{\psi}_n(t) \rangle \\
&= \left(\frac{d}{dt} \langle \hat{\psi}_m(t) | \right) | \hat{\psi}_m(t) \rangle \\
&+ \langle \hat{\psi}_m(t) | \frac{d}{dt} | \hat{\psi}_m(t) \rangle
\end{aligned}$$

Something plus its complex conjugate equals 0

$$a + ib + (a + ib)^* = 2a = 0 \implies a = 0, \quad (29)$$

so $\langle \hat{\psi}_m(t) | \frac{d}{dt} | \hat{\psi}_m(t) \rangle$ must be purely imaginary. We write

$$\langle \hat{\psi}_m(t) | \frac{d}{dt} | \hat{\psi}_m(t) \rangle = -i\Gamma_s(t), \quad (30)$$

where Γ_s is real.

References

- [1] BR Desai. *Quantum mechanics with basic field theory*. Cambridge University Press, 2009. 4