PHY662, Spring 2004, Apr. 6, 2004

6th April 2004

1 Miscellaneous

1. Reading: Continue Shankar Ch. 18 for time-dependent perturbation theory, electromagnetism, also Griffiths Ch. 9 (though it is a bit simplified, especially as it sticks to two-level systems at first). Skip higher order perturbation theory in Shankar and read up to “Field Quantization” (p. 506 in the second edition) by Tuesday, April 13. We will spend four more lectures on time-dependent perturbation theory, then two weeks on scattering.
2. Office hours will start at 4:00 on Wednesday for this week and next. This week’s and next week’s homework are due on Thursdays.

2 Fermi’s Golden rule

For $H' = V(\vec{r})e^{-i\omega t}$, the transition *rate* from $i \to f$ is

$$\Gamma \approx \frac{2\pi}{\hbar}|\langle f|V(\vec{r},\omega)|i\rangle|^2\delta(E_f - E_i - \hbar\omega)\,.$$

In this form, the δ-function has been pulled out for convolving with $\rho(\omega)$ and the perturbation is taken to be of the form $V(\vec{r},\omega)e^{-i\omega t}$.
Reminders:

- This can be applied to $V = V(r)\cos(\omega t)$ by writing the $\cos()$ as the sum of two $\exp()$.
- The $\delta()$ results from integration over perturbation time T in the limit $T \to \infty$. Handling the δ-function can require careful application.
- *What are the units in this formula?*

3 Examples

Fermi's golden rule allows one to compute real transition rates for real atoms. To do so, we will need to build up some background with electromagnetism as applied in quantum mechanics. Before we do that, let us apply this rule using two examples.

3.1 Harmonic oscillator subject to a distribution of frequencies

Suppose you have a charged particle in a 1D harmonic oscillator with frequency ω_0. You modify the potential by applying a classical electric field $\mathcal{E}(t)$ that is uniform in space and that behaves like "white noise" over time. At any given instant t, the change in potential is $-q\mathcal{E}(t)X$. White noise has the property that the Fourier component at each frequency is uniform. Writing $\mathcal{E}(t) = \int_0^\infty d\omega\, E_0 \cos(\omega t)\rho_0$ gives

$$V'(t) = q\mathcal{E}(t)X = \int_0^\infty d\omega\, qXE_0\rho_0 \cos(\omega t)\,,$$

where it is understood that there is a randomness between the frequencies that makes the perturbation incoherent (one could add a random phase to each ωt). For a $\cos(\omega t)$ perturbation, Fermi's golden rule then gives the transition rate from the ground state to the first excited state at a given frequency as

$$\Gamma_\omega = \frac{\pi}{2\hbar}|\langle f|qXE_0|\rangle|^2[\delta(E_f - E_i - \hbar\omega) + \delta(E_f - E_i + \hbar\omega)]\,.$$

Since $E_f = E_1 > E_0 = E_i$ and we are integrating over positive frequency, the second δ-function can be dropped. Notice that the matrix element is independent of ω. Summing over ω gives

$$\begin{aligned}
\Gamma_{0\to 1} &= \frac{\pi}{2\hbar}|\langle 1|qXE_0|0\rangle|^2 \int_0^\infty d\omega\, \rho_0 \delta(E_1 - E_0 - \hbar\omega) \\
&= \frac{\pi}{2\hbar^2}|\langle 1|qXE_0|0\rangle|^2 \rho_0 \\
&= \frac{\pi q^2 E_0^2}{2\hbar^2}|\langle 1|\left(\frac{2\hbar}{m\omega_0}\right)^{1/2}(a + a^\dagger)|0\rangle|^2\rho_0 \\
&= \frac{\pi q^2 E_0^2 \rho_0}{m\omega_0\hbar}\,.
\end{aligned}$$

(Let us check the units to help us believe that the calculation was properly done.)

3.2 2D particle in a box with a δ-function potential

Consider a particle confined to 2D motion. The particle can be considered to be confined to a 2D box of linear size L and area L^2, centered at the origin ($-L/2 \le x, y \le L/2$). One could take $\psi = 0$ at the boundaries, but it is much more convenient to take $\psi(\vec{r} + mL\hat{x} + nL\hat{y}) = \psi(\vec{r})$ for integer m, n. This gives periodic or "toroidal" boundary conditions. In the end, we hope (this is not always the case) that the exact boundary conditions do not matter.

Taking these boundary conditions quantizes the energy and momenta of the free particle. The eigenstates $\psi_{\vec{k}}(\vec{r}) = L^{-1}e^{i\vec{k}\cdot\vec{r}}$have momenta $\vec{p} = \hbar\vec{k}$, with $\vec{k} = (k_x, k_y) = \frac{2\pi}{L}(n_x, n_y)$ and energy $E_{n_x,n_y} = \frac{\hbar^2 k^2}{2m}$.

Suppose that the particle is not quite free, but that there is a "weak" potential of the form $V(\vec{r}) = g\delta^{(2}(\vec{r})$. *What are the units of g (V has the units of energy)? This is a zero-frequency ($\omega = 0$) perturbation.*

Let the particle initially be in an unperturbed eigenstate, say $\vec{k}_i \parallel \hat{x}$. This is *not* an eigenstate of the perturbed Hamiltonian. One way to study the effect of the perturbation is to ask the question "What is the rate for a transition to another momentum eigenstate?".

This can be answered using Fermi's golden rule. Let $\vec{k}_f$ be the momentum of the final state. Then

$$\Gamma_{\vec{k}\to\vec{k}'} = \frac{2\pi}{\hbar}|\langle f|V|i\rangle|^2\delta(E_f - E_i)\,.$$

The matrix element is straightforward,

$$\langle f|V|i\rangle = \int_{L^2} d^2r\,\frac{e^{-i\vec{k}_f\cdot\vec{r}}}{L}g\delta^{(2)}(\vec{r})\frac{e^{i\vec{k}_i\cdot\vec{r}}}{L} = gL^{-2}\,.$$

So the only thing to do is to incorporate the δ-function, which requires a little care.

Here, the perturbing frequency is precisely defined ($\omega = 0$), so we look to the density of states for guidance. That is, there is a density $\rho(E)$ that needs to be summed or integrated over together with the δ-function.

For large L, we approximate the sum over final states by an integral.

Given a "volume" element $d^2\vec{k}$ in $\vec{k}$-space, the number of states in that volume element is

$$\left(\frac{L}{2\pi}\right)^2 d^2\vec{k} = \left(\frac{L}{2\pi}\right)^2 k\,d\theta dk\,,$$

where we have gone to polar coordinates since the final states will have constant $k = |\vec{k}|$. [Draw picture here!]

The δ-function is over E, though, so we change coordinates again,

$$\begin{aligned} E &= \frac{\hbar^2 k^2}{2m} \\ dE &= \frac{\hbar^2 k}{m}\,dk \end{aligned}$$

so the number of states in an angle θ and energy range dE is

$$\left(\frac{L}{2\pi}\right)^2 k\,d\theta dk = \left(\frac{L}{2\pi}\right)^2 \frac{m}{\hbar^2}\,d\theta dE\,.$$

The total rate of transitions out of $|i\rangle$ to any final state $\vec{k}_f$ is then

$$\begin{aligned}
\sum_{\vec{k}_f} \Gamma_{\vec{k}_i \to \vec{k}_f} &= \frac{2\pi}{\hbar} g^2 L^{-4} \sum_{\vec{k}_f} \delta(E_f - E_i) \\
&= \frac{2\pi g^2 L^{-4}}{\hbar} \int_0^\infty dE_f \int_0^{2\pi} d\theta \left(\frac{L}{2\pi}\right)^2 \frac{m}{\hbar^2} \delta(E_f - E_i) \\
&= \frac{g^2 m}{\hbar^3 L^2} \qquad \text{UNITS?} \,.
\end{aligned}$$

4 Electromagnetism

[See Shankar for Maxwell's equation and this discussion.]
The highlights are: rewriting the electromagnetic field using the potentials $\vec{A}$ and ϕ,

$$\begin{aligned}
\vec{B} &= \nabla \times \vec{A} \\
\vec{E} &= -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \nabla \phi \,;
\end{aligned}$$

the choice of Coulomb gauge for the "free electromagnetic field" (where sources density $\rho = 0$ and current $\vec{j} = 0$)

$$\begin{aligned}
\nabla \cdot \vec{A} &= 0 \\
\phi &= 0 \,;
\end{aligned}$$

and the equations of motion for $\vec{A}$ in the Coulomb gauge

$$\nabla^2 \vec{A} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = 0 \,.$$

These equations give that waves in $\vec{A}$ travel at speed c and that plane wave solutions for $\vec{A}$ are of the form

$$\vec{A} = \vec{A}_0 \cos(\vec{k} \cdot \vec{r} - \omega t)$$

with the important resulting condition (transverse waves)

$$\vec{k} \cdot \vec{A}_0 = 0 \,.$$

The resulting $\vec{E}$ and $\vec{B}$ fields have equal magnitude and the energy density is

$$u = \frac{1}{8\pi}(|\vec{E}|^2 + |\vec{B}|^2) \,.$$

Note on units: $\frac{e^2}{r}$ has the units of energy, so e has the units of $\sqrt{\mathrm{E} \cdot \mathrm{L}}$. For $r = \frac{\hbar^2}{me^2} = 0.0529\,\mathrm{nm}$ (the Bohr radius), $\frac{e^2}{r}$ has the value $13.6\,\mathrm{eV}$ as a Rydberg is $13.6\,\mathrm{eV}$ and $\langle V \rangle = -2\langle H \rangle$. So $e^2 = 13.6 \times 0.0529\,\mathrm{eV} \cdot \mathrm{nm} = 0.72\,\mathrm{eV} \cdot \mathrm{nm}$ (mixing up CGS and SI units in a controlled way).

4.1 Potentials in quantum theory

Shankar works using path integrals. This is important and I suggest you read it, but we are not focusing on path integrals this term. Remember that the Hamiltonian for a charged particle in only an electromagnetic potential is

$$\frac{\hbar^2}{2m}\left(\vec{p}-\frac{q}{c}\vec{A}\right)^2+q\phi\,.$$

Let's rederive the conservation of current using this Hamiltonian.