Physics 512 **Winter 2003**

Homework Set #10 – Solutions

1. This is based on Sakurai, Chapter 5, Problem 28. A hydrogen atom is initially in its ground state ($1s$). At time $t=0$ we turn on a spatially uniform electric field as follows:
$$\vec{E}(t) = \begin{cases} 0 & t<0 \\ \mathcal{E}_0 e^{-t/\tau}\hat{z} & t\geq 0 \end{cases}$$

   a) Using first-order time dependent perturbation theory, compute the probability for the atom to be found in each of the three $2p$ states at time $t \gg \tau$. You need not evaluate the radial integrals, but perform all other integrations.

   This electric field corresponds to a potential
$$V = -e\mathcal{E}_0 z e^{-t/\tau}$$
   Thus we calculate
$$\begin{aligned} A_{k\leftarrow s} &= -\frac{i}{\hbar}\int_0^t e^{i\omega_{ks}t'}\langle k(-e)\mathcal{E}_0 z e^{-t'/\tau}|s\rangle\,dt' \\ &= \frac{ie\mathcal{E}_0}{\hbar}\int_0^t e^{(i\omega_{ks}-1/\tau)t'}\langle k|z|s\rangle\,dt' \\ &= \frac{ie\mathcal{E}_0}{\hbar}\frac{e^{(i\omega_{ks}-1/\tau)t}-1}{i\omega_{ks}-1/\tau}\langle k|z|s\rangle \end{aligned}$$
   The transition probability is given by
$$P_{k\leftarrow s} = |A_{k\leftarrow s}|^2 = \frac{e^2\mathcal{E}_0^2}{\hbar^2}\frac{1-2e^{-t/\tau}\cos\omega_{ks}t + e^{-2t/\tau}}{\omega_{ks}^2+1/\tau^2}|\langle k|z|s\rangle|^2$$
   For $t \gg \tau$, the decaying exponentials may be dropped, and we find
$$P_{k\leftarrow s}(t\gg\tau) = \frac{e^2\mathcal{E}_0^2}{\hbar^2}\frac{|\langle k|z|s\rangle|^2}{\omega_{ks}^2+1/\tau^2} \tag{1}$$
   which is independent of time t.

   We now note that this matrix element corresponds to a dipole transition, with corresponding selection rule $\Delta\ell=\pm1$. Furthermore, in terms of spherical tensors, $z = r\cos\theta = \sqrt{\frac{4\pi}{3}}rY_1^0(\theta,\phi)$, which is an $m=0$ component of a spherical vector. As a result, we furthermore have a selection rule $\delta m = 0$. So the only possible transition from the $1s$ state is to the $m=0$ $2p$ state, ie $|100\rangle \to |210\rangle$. In this case, the relevant hydrogen wavefunctions are
$$\begin{aligned} \psi_{100} &= \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0} \\ \psi_{210} &= \left(\frac{1}{2\pi a_0^3}\right)^{1/2}\frac{r}{4a_0}e^{-r/2a_0}\cos\theta \end{aligned}$$

Thus

$$\begin{aligned}
\langle 210|z|100\rangle &= \frac{1}{\sqrt{2}\pi a_0^3}\int\Big(\frac{r}{4a_0}e^{-r/2a_0}\cos\theta\Big)r\cos\theta\Big(e^{-r/a_0}\Big)\,r^2\sin\theta\,dr\,d\theta\,d\phi\\
&= \frac{2\pi}{4\sqrt{2}\pi a_0^4}\int_0^\infty r^4e^{-3r/2a_0}\,dr\int_0^\pi\cos^2\theta\sin\theta\,d\theta\\
&= \frac{1}{3\sqrt{2}a_0^4}\int_0^\infty r^4e^{-3r/2a_0}\,dr
\end{aligned}$$

Although the problem does not require it, this radial integral is not too difficult to evaluate. We find

$$\langle 210|z|100\rangle = \frac{128\sqrt{2}}{243}a_0$$

On dimensional grounds, this is a reasonable result, since $\langle z\rangle$ *has to give a length, and the Bohr radius* a_0 *is what governs the size of the hydrogen atom. This may now be substituted into* (1) *to obtain the transition probability*

$$P_{|210\rangle\leftarrow|100\rangle}(t\gg\tau) = \left(\frac{8}{9}\right)^5\frac{e^2\mathcal{E}_0^2a_0^2}{\hbar^2}\frac{1}{\omega_{ks}^2+1/\tau^2}$$

where $\hbar\omega_{ks} = E_{210}-E_{100} = -E_0/2^2+E_0 = \frac{3}{4}E_0$ *(with* $E_0 = 13.6\,\mathrm{eV}$*).*

b) What would happen if instead the atom was in the $2s$ state to begin with?

Since we have the selection rules $\delta\ell=\pm1$ *and* $\delta m = 0$*, transitions to the* $1s$ *state would be forbidden. However it would still be possible to end up in the* $2p$ $|210\rangle$ *state. Note, however, that in this case,* $\omega_{ks}\approx 0$*, so the probability would behave as*

$$P(t\gg\tau)\approx\frac{e^2\mathcal{E}_0^2\tau^2}{\hbar^2}|\langle 210|z|200\rangle|^2$$

where a calculation indicates $\langle 210|z|200\rangle = -3a_0$*. Note, however, that this expression may be large for large* τ*, and thus must be handled with care. This mixing between the* $2s$ *and* $2p$ *state is similar to that which happens for the linear Stark effect, where degenerate time independent perturbation theory was required.*

2. Consider a two-photon transition from an initial state of angular momentum $\ell_1 = 0$ to a lower energy intermediate state of angular momentum $\ell_2 = 1$ to the ground state of the system with angular momentum $\ell_3 = 0$. Both photons are emitted via electric dipole transitions.

a) Using second order time-dependent perturbation theory, show that the amplitude for this transition is proportional to $\hat\epsilon_1\cdot\hat\epsilon_2$ where $\hat\epsilon_1$ and $\hat\epsilon_2$ are the polarization vectors of the two photons (ignore identical particle effects).

The second order transition amplitude is given by

$$A = \left(-\frac{i}{\hbar}\right)^2\sum_n\int_0^t\int_0^{t'}e^{i\omega_{kn}t'}e^{i\omega_{ns}t''}\langle k|V|n\rangle\langle n|V|s\rangle\,dt''\,dt'$$

However all we are interested in is how this amplitude depends on the polarization of the two photons. Hence we only need to consider the matrix elements $\langle k|V|n\rangle\langle n|V|s\rangle$. Furthermore, in the dipole approximation, the interaction matrix element has the form

$$\langle k|\vec{p}\cdot\hat{\epsilon}_2|n\rangle\langle n|\vec{p}\cdot\hat{\epsilon}_1|s\rangle$$

where each photon is associated with its own polarization. Since dipole transitions obey a selection rule $\delta\ell = \pm 1$, it is useful to highlight the angular momentum states. Thus we ignore all quantum numbers of the states except for the angular momentum values $|\ell m\rangle$. The matrix element of interest is then

$$\mathcal{M} = \sum_{m=-1}^{1}\langle 00|\vec{p}\cdot\hat{\epsilon}_2|1m\rangle\langle 1m|\vec{p}\cdot\hat{\epsilon}_1|00\rangle = \sum_{i,j}\hat{\epsilon}_1^j\hat{\epsilon}_2^i\sum_{m=-1}^{1}\langle 00|p^i|1m\rangle\langle 1m|p^j|00\rangle$$

Now we can note that the sum over intermediate states $|1m\rangle$ is complete in the subspace we are interested in (since we specify in principle what the intermediate state is) to get

$$\mathcal{M}\sim\sum_{i,j}\hat{\epsilon}_1^j\hat{\epsilon}_2^i\langle 00|p^ip^j|00\rangle$$

While the intermediate states are complete in this particular $\ell = 1$ subspace, they are not necessarily complete in the full Hilbert space. Thus although we can say that $\mathcal{M}$ is proportional as above, we would not be able to compute the actual constant of proportionality using this method. In any case, we proceed by noting that since the cartesian tensor operator p^ip^j is placed between $\ell = 0$ states, only the $\ell = 0$ component of the tensor contributes to a non-vanishing result. Using the decomposition

$$p^ip^j = \tfrac{1}{3}\delta^{ij}\vec{p}\cdot\vec{p}+\cdots$$

we find

$$\mathcal{M}\sim\hat{\epsilon}_1\cdot\hat{\epsilon}_2\langle 00|p^2|00\rangle\sim\hat{\epsilon}_1\cdot\hat{\epsilon}_2$$

Alternatively, we may avoid any arguments about completeness by using $\vec{p}\cdot\hat{\epsilon} = \sum_q(-)^q p_q\hat{\epsilon}_{-q}$ to rewrite $\mathcal{M}$ in terms of spherical-tensor operators

$$\mathcal{M} = \sum_{q_1,q_2}(-)^{q_1+q_2}\hat{\epsilon}_1^{-q_2}\hat{\epsilon}_2^{-q_1}\sum_{m=-1}^{1}\langle 00|p_{q_1}|1m\rangle\langle 1m|p_{q_2}|00\rangle$$

With the Δm selection rule for spherical tensor matrix elements, this becomes

$$\begin{aligned}\mathcal{M} = {} & \hat{\epsilon}_1^{+1}\hat{\epsilon}_2^{-1}\langle 00|p_1|1-1\rangle\langle 1-1|p_{-1}|00\rangle + \hat{\epsilon}_1^0\hat{\epsilon}_2^0\langle 00|p_0|10\rangle\langle 10|p_0|00\rangle \\ & + \hat{\epsilon}_1^{-1}\hat{\epsilon}_2^{+1}\langle 00|p_{-1}|11\rangle\langle 11|p_1|00\rangle\end{aligned}$$

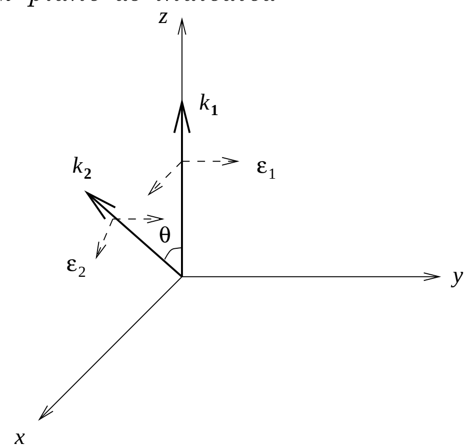
Now, one can appeal to the Wigner-Eckart theorem to show that all three terms are related to appropriate reduced matrix elements (the first element of each term *is related to the Clebsch-Gordan combination* 1×1*, while the second is related to the trivial combination* 0×1*). The result is*

$$\begin{aligned}\mathcal{M} &= \tfrac{1}{\sqrt{3}}[\hat{\epsilon}_1^{+1}\hat{\epsilon}_2^{-1} - \hat{\epsilon}_1^{0}\hat{\epsilon}_2^{0} + \hat{\epsilon}_1^{-1}\hat{\epsilon}_2^{+1}]\langle\gamma 0||p||\beta 1\rangle\langle\beta 1||p||\alpha 0\rangle \\ &= -\tfrac{1}{\sqrt{3}}\hat{\epsilon}_1\cdot\hat{\epsilon}_2\langle\gamma 0||p||\beta 1\rangle\langle\beta 1||p||\alpha 0\rangle\end{aligned}$$

where α*,* β *and* γ *denote the additional quantum numbers of the initial, intermediate and final states. In either approach, the result is that the amplitude is proportional to* $\hat{\epsilon}_1\cdot\hat{\epsilon}_2$*.*

b) Averaging over photon polarizations, show that the probability distribution for the angle θ between the two photons has the form $P(\theta) \sim 1 + \cos^2\theta$.

Since we are only concerned about the relative angle θ *between the two photons, we may assume one photon* ($\vec{k}_1$) *is emitted along the* $+\hat{z}$ *axis and the other* ($\vec{k}_2$) *in the* $x - z$ *plane as indicated*



Each photon may have two orthogonal polarization states. Since we will average over polarizations, we may take any set of convenient (but orthonormal) polarizations for each photon. We choose

$$\begin{aligned}\hat{\epsilon}_1^{(a)} &= \hat{x}, \qquad \hat{\epsilon}_1^{(b)} = \hat{y} \\ \hat{\epsilon}_2^{(a)} &= \hat{y}, \qquad \hat{\epsilon}_2^{(b)} = \hat{x}\cos\theta - \hat{z}\sin\theta\end{aligned}$$

Since the probability is proportional to the amplitude squared, we average

$$\begin{aligned}P(\theta) \sim \mathcal{M}^2 \sim \overline{(\hat{\epsilon}_1\cdot\hat{\epsilon}_2)^2} &= \tfrac{1}{4}\big[(\hat{x}\cdot\hat{y})^2 + (\hat{x}\cdot(\hat{x}\cos\theta - \hat{z}\sin\theta))^2 + (\hat{y}\cdot\hat{y})^2 \\ &\qquad + (\hat{y}\cdot(\hat{x}\cos\theta - \hat{z}\sin\theta))^2\big] \\ &= \tfrac{1}{4}(1 + \cos^2\theta)\end{aligned}$$

3. A hydrogen atom initially in its ground state is exposed to a harmonic perturbation:

$$\vec{E}(t) = \mathcal{E}_0\cos(\omega t)\hat{z} \qquad t \geq 0$$

Calculate the rate of ionization of the atom as a function of ω.

We use Fermi's Golden Rule for harmonic perturbations

$$w = \frac{2\pi}{\hbar} |\langle k|V^\dagger|s\rangle|^2 \rho(E_k)\Big|_{E_k \approx E_s + \hbar\omega}$$

where the perturbation is given by

$$V(t) = Ve^{i\omega t} + V^\dagger e^{-i\omega t}$$

The given electric field in the $\hat{z}$ *direction corresponds to a linear electric potential* $\phi(t) = -\mathcal{E}_0 z \cos(\omega t)$. *Multiplying by the (negative) charge of the electron gives the potential energy*

$$V(t) = e\mathcal{E}_0 z \cos(\omega t) = \tfrac{1}{2} e\mathcal{E}_0 z (e^{i\omega t} + e^{-i\omega t})$$

Therefore we need to calculate the matrix element of V *where*

$$V = V^\dagger = \tfrac{1}{2} e\mathcal{E}_0 z$$

The initial state of the atom is given by the 1s *wavefunction*

$$\psi_{100}(r) = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

while for the final (ionized) electron state, we may take a plane wave

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}}$$

Note that, for normalization, we have placed the ionized electron into a box with periodic boundary conditions. Thus the matrix element is

$$\langle k|V^\dagger|s\rangle = \tfrac{1}{2} e\mathcal{E}_0 \langle k|z|s\rangle = \frac{e\mathcal{E}_0}{2\sqrt{\pi L^3 a_0^3}} \int e^{-i\vec{k}\cdot\vec{r}} z e^{-r/a_0}\, d^3\vec{r}$$

This integral is easier to perform when the plane wave state is decomposed in terms of spherical waves. Recall (eg from scattering theory) that

$$e^{i\vec{k}\cdot\vec{r}} = \sum_l (2l+1) i^l j_l(kr) P_l(\hat{k}\cdot\hat{r}) = 4\pi \sum_{l,m} i^l j_l(kr) Y_l^m(\hat{k})^* Y_l^m(\hat{r})$$

Hence

$$\langle k|V^\dagger|s\rangle = \frac{2e\mathcal{E}_0 \pi^{1/2}}{(La_0)^{3/2}} \sum_{l,m} (-i)^l Y_l^m(\hat{k}) \int j_l(kr) Y_l^m(\hat{r})^* (r\cos\theta) e^{-r/a_0}\, r^2 dr d\Omega$$

Since $z = r\cos\theta$ is the $m = 0$ component of a vector operator, and since we start from the 1s state, the Wigner-Eckart selection rules indicates that the final state can only have $l = 1$, $m = 0$. Thus

$$\begin{aligned}
\langle k|V^\dagger|s\rangle &= -\frac{2ie\mathcal{E}_0\pi^{1/2}}{(La_0)^{3/2}}Y_1^0(\hat{k})\int j_1(kr)e^{-r/a_0}\,r^3dr\int Y_1^0(\hat{r})^*\cos\theta\,d\Omega \\
&= -\frac{3ie\mathcal{E}_0\cos\theta_k}{2\pi^{1/2}(La_0)^{3/2}}\int j_1(kr)e^{-r/a_0}\,r^3dr\int\cos^2\theta\,d\Omega \\
&= -\frac{2ie\mathcal{E}_0\pi^{1/2}\cos\theta_k}{(La_0)^{3/2}}\int_0^\infty j_1(kr)e^{-r/a_0}\,r^3dr
\end{aligned}$$

The integral may be performed using the explicit form of the spherical Bessel function

$$\begin{aligned}
\int_0^\infty j_1(kr)e^{-r/a_0}\,r^3dr &= k^{-4}\int_0^\infty j_1(z)e^{-z/(ka_0)}z^3dz \\
&= k^{-4}\int_0^\infty\left(\frac{\sin z}{z^2}-\frac{\cos z}{z}\right)e^{-z/(ka_0)}z^3dz \\
&= -k^{-4}\mathrm{Re}\int_0^\infty(iz+z^2)e^{iz}e^{-z/(ka_0)}\,dz \\
&= -k^{-4}\mathrm{Re}\int_0^\infty(iz+z^2)e^{(i-1/(ka_0))z}\,dz \\
&= -k^{-4}\mathrm{Re}\left(\frac{i}{(i-1/(ka_0))^2}-\frac{2}{(i-1/(ka_0))^3}\right) \\
&= k^{-4}\mathrm{Re}\,\frac{3+i/(ka_0)}{(i-1/(ka_0))^3} = k^{-4}\frac{8(ka_0)^5}{((ka_0)^2+1)^3}
\end{aligned}$$

As a result, we have

$$\langle k|V^\dagger|s\rangle = -\frac{16ie\mathcal{E}_0\pi^{1/2}\cos\theta_k}{k^4(La_0)^{3/2}}\frac{(ka_0)^5}{((ka_0)^2+1)^3}$$

Finally, this matrix element must be squared and combined with the density of states

$$\rho(E_k) = \frac{m^{3/2}E_k^{1/2}L^3}{\sqrt{2}\pi^2\hbar^3}\frac{d\Omega}{4\pi}$$

(for plane wave electrons in three dimensions). The result is

$$\begin{aligned}
w &= \frac{2\pi}{\hbar}\frac{256e^2\mathcal{E}_0^2\pi\cos^2\theta_k}{k^8L^3a_0^3}\frac{(ka_0)^{10}}{((ka_0)^2+1)^6}\frac{m^{3/2}E_k^{1/2}L^3}{\sqrt{2}\pi^2\hbar^3}\frac{d\Omega}{4\pi} \\
&= \frac{256me^2\mathcal{E}_0^2}{\hbar^3k^4}\frac{(ka_0)^7}{((ka_0)^2+1)^6}\frac{\cos^2\theta_k\,d\Omega}{4\pi}
\end{aligned}$$

More properly, this is the differential rate dw for emission of an electron into a solid angle $d\Omega$ (at an angle θ_k from the $\hat{z}$ axis). This $\cos^2\theta_k$ behavior is standard for a dipole. Integrating over all angles then gives a total ionization rate of

$$w = \frac{256\mathcal{E}_0^2}{3\hbar k^3}\frac{(ka_0)^6}{((ka_0)^2+1)^6}$$

where

$$E_k = \frac{\hbar^2 k^2}{2m} = \hbar\omega - E_0 \qquad\qquad (E_0 = 13.6\,\mathrm{eV})$$

and we have also made use of the relation $a_0 = \hbar^2/me^2$. Note that typically $ka_0 \ll 1$, in which case the ionization rate is proportional to $k^3 \sim E_k^{3/2}$

$$w \approx \frac{256\mathcal{E}_0^2 a_0^6}{3\hbar}k^3$$

4. Given two distinguishable spin-1 particles with vanishing orbital angular momenta, one can form states of total angular momentum $j = 0$, 1 and 2. Now suppose the two particles are identical. What restrictions do we get? What about two spin-2 particles? What is the general rule for allowed values of j? [See Sakurai, Chapter 6, Problem 2].

   For spin-1, it is easy to see that the Clebsch-Gordan combinations are symmetric for $j = 0$ and 2, and antisymmetric for $j = 1$. Since spin-1 particles are bosons, and since the spatial wavefunction is symmetric (due to vanishing orbital angular momentum), only the symmetric spin combinations are allowed. Hence only states of $j = 0$ or 2 are allowed for the combination of two identical spin-1 particles. Similarly, only states of total $j = 0$, 2, or 4 are allowed for two identical spin-2 particles.

   In general, we note the following symmetry property of Clebsch-Gordan coefficients under interchange

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 JM\rangle = (-)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 JM\rangle$$

   For identical particles, with $j_1 = j_2 = s$, this reads

$$\langle ss m_1 m_2 | ss JM\rangle = (-)^{J-2s}\langle ss m_2 m_1 | ss JM\rangle$$

   Thus interchanging both particles ($m_1 \leftrightarrow m_2$) is symmetric for $J - 2s$ even and antisymmetric for $J - 2s$ odd. Hence for identical bosons (s integer), only even J combinations are allowed, while for identical fermions (s half-integer) antisymmetry also demands that only even J combinations are allowed. This results in a simple rule that combinations of any two identical particles with vanishing orbital angular momenta can only result in even J. Note that for integer spin this result is closely related to the symmetry properties of the spherical harmonics.