

PHYS30201 Advanced Quantum Mechanics: Examples 5

In all questions below referring to a spherical finite square well, the potential is given by $V(r) = -V_0$ for $r < a$ and $V(r) = 0$ for $r > a$. We also define $b = 2mV_0/\hbar^2$, which has units of inverse length squared; note that here, contrary to in lectures, definitions are such that b is positive for a well. We use $k = \sqrt{2mE}/\hbar$ and $k' = \sqrt{2m(V_0 + E)}/\hbar$ to denote wavenumbers outside and inside the well respectively; if $E < 0$ we use $\kappa = -ik = \sqrt{2m|E|}/\hbar$.

34. Verify that all the transitions you drew for question 27 are in fact consistent with the electric dipole selection rules.

List the allowed decays of the $4f_{5/2}$ and $4p_{3/2}$ states of hydrogen.

Discuss the allowed transitions between all the states of helium with the electronic configurations $1s^2$, $1s2s$, $1s2p$ and $1s3d$, assuming exact LS coupling. Which decays can take place due to the fact that LS coupling is not exact?

35. (Challenge question) In this question you will calculate the cross section for the electric field of an EM wave of a given frequency to liberate an electron from the ground state of hydrogen—an example of the photoelectric effect. We will take the final state to be a completely free electron in a plane wave state $|\mathbf{k}_f\rangle$, ignoring the fact that in reality it still feels the Coulomb attraction of the proton—we expect this will be a reasonable approximation if the energy of the photon is much greater than the ionisation energy. (Not too large though, as we will continue to use the electric dipole approximation.) See Shankar if you get stuck at any point.

The *cross section* for absorption is defined as the rate of energy absorbed from the field divided by the energy flux. Starting from Fermi's golden rule for monochromatic radiation, show that the cross section is

$$\sigma = \frac{\hbar\omega R_{1s \rightarrow \mathbf{k}_f}}{\frac{1}{2}c\epsilon_0 \mathcal{E}^2} = 4\pi^2 \hbar\omega\alpha |\langle \mathbf{k}_f | \boldsymbol{\epsilon} \cdot \mathbf{r} | 100 \rangle|^2 \delta(E_f - E_0 - \hbar\omega)$$

where E_0 is the energy of the $1s$ state, and check that it has units of area. Verify that $\hat{p}_i = \frac{m}{i\hbar} [\hat{x}_i, \hat{H}_0]$ and so $\omega_{fi} \langle \mathbf{k}_f | \boldsymbol{\epsilon} \cdot \mathbf{r} | 100 \rangle = -\frac{i}{m} \langle \mathbf{k}_f | \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}} | 100 \rangle$ (this trick makes the matrix element easier to evaluate though it isn't essential). Show that

$$\langle \mathbf{k}_f | \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}} | 100 \rangle = 8\hbar \sqrt{\frac{\pi a_0^3}{V}} \frac{\boldsymbol{\epsilon} \cdot \mathbf{k}_f}{(1 + k_f^2 a_0^2)^2}.$$

(Hint - take the z -axis to lie along \mathbf{k}_f in order to do the angle integration; the $1/\sqrt{V}$, where V is the volume of the large box we are working in, comes from normalising $|\mathbf{k}_f\rangle$.) Hence write down the cross section and describe the angular distribution of the emitted electron.

Finally integrate over all values of \mathbf{k}_f using the density of states for a non-relativistic particle, to get the total cross section

$$\sigma_t = \frac{256a_0^2\alpha}{3} \frac{k_f^3 a_0^3}{(1 + k_f^2 a_0^2)^5}.$$

36. Show that, in the Born approximation, the scattering amplitude for a spherical finite square well of depth V_0 and radius a is

$$f(k, \theta) = -\frac{b}{q^3} (\sin aq - aq \cos aq)$$

where $q = 2k \sin(\theta/2)$ and θ is the scattering angle. Hence show that at low energies ($ak \ll 1$) the total cross section is approximately $4\pi a^2 (ba^2)^2/9$.

37. Show that the condition for a spherical finite square well to have an s -wave bound states of energy E is given by the solutions of the equation $\sqrt{b - (k')^2} = -k' \cot k'a$. (Hint: it is easiest to solve the equivalent one-dimensional problem, but if you want to work in 3D for practice, the wave function outside the well will have the form $\exp(-\kappa r)/r$.)

Hence verify that the condition for zero-energy s -wave bound states is $a\sqrt{b} = (2n - 1)\pi/2$, for positive integer n .

38. Show that the $l = 0$ phase shift for a spherical finite square well is given by $\delta_0 = -ak + \arctan(k \tan(ak')/k')$.

Show that (unless $\tan(ak')$ happens to be very large) the s -wave cross section at zero energy is given by $\sigma_0(k = 0) = 4\pi(a - \tan(a\sqrt{b})/\sqrt{b})^2$

Hence show that at low energies and for shallow wells ($ak \ll 1$ and $a\sqrt{b} \ll 1$), σ_0 agrees with the Born approximation.

Verify that if the well has a zero-energy bound state, the low-energy phase shift is $\delta_0 = \pi/2 - ak/2 + \mathcal{O}(k^2)$. (This is the only exception to the rule that the phase-shift at the origin is a multiple of π . It requires careful treatment of limits as $k \rightarrow 0$; work in terms of $\cot(\delta_0 + ka)$.)

39. Though low-energy s -wave scattering is usually strong, for particular values of b it vanishes because $\delta_0 = \pi$. Show that the condition can be expressed as $\tan k'a = k'a$ ($k'a$ not being small). Sketch the wave function with and without the potential in this case. This is the Ramsauer-Townsend effect, which has been observed in electron scattering from rare-gas atoms.

40. (Challenge question) Consider p -wave scattering from a spherical finite square well. Sketch the well and find the highest value of ka for which a quasi-bound state might exist.

Show that the condition for a well to have a zero-energy bound state of angular momentum $l > 0$ is $j_{l-1}(a\sqrt{b}) = 0$. (You will find useful the relation $f'_l(z) = f_{l-1} - (l-1)f_l/z$, where f_l stands for j_l , n_l , or any linear combination of the two, which is true for $l > 0$. In addition the combination $h_l^{(1)}(kr) \equiv j_l(kr) + in_l(kr)$ is exponentially decaying for $k = i\kappa$.)

Show that for $l = 1$, there are zero-energy bound states for $b = (n\pi/a)^2$, for non-negative integer n .

If b is just below one of these critical values, ie $b = (n\pi/a)^2 - db$, there will be a quasi-bound state at $k = k_r \equiv \sqrt{db/3}$, and in its vicinity we can write

$$\delta_1(k) = -ka + \arctan\left(\frac{adb}{9(k_r - k)}\right).$$

You are not required to prove this, but check it numerically for some $db \ll 1$ and a range of values of k in the vicinity of k_r against the exact answer

$$\delta_1(k) = -ka + \operatorname{arccot}\left[\frac{1 + (\frac{k}{k'})^2(ak' \cot(ak') - 1)}{ak}\right]$$

Show that such a form gives a Breit-Wigner cross section as a function of energy and identify the lifetime Γ . (It is useful to note that $e^{i\delta} \sin \delta = (\cot \delta - i)^{-1}$.)