1 Square Well in Three Dimensions

1)

The potential is spherically symmetric which makes the Hamiltonian rotationally invariant. Therefore it commutes with all components L_i of the angular momentum and any analytic function of these. Since L_i's do not commute with each other we will chose the z-component L_z and total angular momentum $\vec{L}^2$. The corresponding quantum numbers are $m\hbar$ and $l(l+1)\hbar^2$ with l being a non negative integer and $m = -l, -l+1 \ldots l-1, l$ taking $2l+1$ different values. The angular part of the wave function is a spherical harmonic $Y_m^l(\phi, \theta)$. Also the potential commutes with the parity operator, but the spherical harmonics are already eigenstates of that.

2)

Assuming that the wave function on which it operates is of the form $\psi(r, \phi, \theta)$ one can in principle express r, ϕ and θ in terms of x, y and z and express the $\vec{\nabla}^2$ appearing in the Hamiltonian with derivatives of the spherical coordinates. There are many ways to make the algebra more efficient but the net result is:

$$\vec{\nabla}^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

One can similarly show that the total angular momentum operator can be expressed in spherical coordinates as:

$$\vec{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

which depends only on ϕ and θ and is proportional to the angular part of $\vec{\nabla}^2$. Putting it all together the Hamiltonian in spherical coordinates reads:

$$H = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\vec{L}^2}{2mr^2} + U(r)$$

Considering the Schroedinger equation for a wave function of the form $\psi(r, \phi, \theta) = R(r)F(\phi, \theta)$ and dividing by $\frac{\psi}{r^2}$ will give:

$$-\frac{\hbar^2}{2m}\frac{1}{R(r)}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R(r) + r^2(U(r) - E) = \frac{1}{F(\phi,\theta)}\frac{\vec{L}^2F(\phi,\theta)}{2m}$$

This is separation of variables. The right side only depends on the angles and the left side on the radial component and both of them must be a constant. If the angular part of the wave function $F(\phi, \theta)$ is chosen to diagonalize $\vec{L}^2$ then this constant is $\frac{\hbar^2}{2m}l(l+1)$ and the radial part satisfies the equation:

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R(r) + \left[U(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right]R(r) = ER(r)$$

The angular part is chosen to be a spherical Harmonic. The radial equation can be transformed in a Schroedinger like form if we use:

$$\chi(r) = rR(r)$$

so that $\chi(r)$ satisfies:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\chi(r) + \left[U(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right]\chi(r) = E\chi(r)$$

3)

To solve the radial Schroedinger equation for $E < 0$ we define

$$\begin{aligned} k^2 &= \frac{2m}{\hbar^2}(E - U_0) > 0 \\ \kappa^2 &= \frac{2m}{\hbar^2}|E| \end{aligned}$$

In a bound state the particle must exist somewhere around the center of the potential and it cannot escape to infinity. This means that $\int d\vec{x}^3 |\psi|^2$ must be finite. Expressing this in spherical coordinates and remembering that the integral over the angles is finite because the interval is finite, we get the constraint that:

$$\int_0^\infty drr^2 |R(r)|^2 = \int_0^\infty dr\, |\chi(r)|^2$$

is finite and therefore $\chi(r) \to 0$ as $r \to \infty$. In this case both the potential and the angular momentum term vanish and therefore

$$\chi(r) \to e^{-\kappa r}$$

At $r = a$ the wave-function and its derivative must both be continuous. Also at the origin $R(r)$ remains finite which makes $\chi(r)$ zero. More specifically only the angular momentum term contributes and

$$\chi(r) \to r^{l+1}$$

For $r < a$ the radial part will have an oscillatory behavior with wavelength k and for $r > a$ it will decay with length $1/\kappa$. To be more explicit we consider the two cases:

1. $r < a$ the radial equation reads:

$$-\frac{\partial^2}{\partial r^2}\chi(r) + \left[-k^2 + \frac{l(l+1)}{r^2}\right]\chi(r) = 0$$

   which is the free particle equation with solution $\chi(r) = krj_l(kr)$ (check lecture notes), where $j_l(x)$ is the spherical Bessel function. The other solution, the spherical Neumann function $n_l(r)$, diverges are the origin so it is ignored.

2. $r > a$ the radial equation reads:

$$-\frac{\partial^2}{\partial r^2}\chi(r) + \left[\kappa^2 + \frac{l(l+1)}{r^2}\right]\chi(r) = 0$$

The general solution of this equation is

$$\chi(r) = \kappa r h_l(i\kappa r)$$

with $h_l(i\kappa r) = j_l(i\kappa r) + i n_l(i\kappa r)$ being the Hankel function which behaves as $r^{-1}e^{-\kappa r}$ at infinity. Any other linear combination will diverge at infinity.

Finally for the radial part of the wave-function:

$$R(r) = \begin{cases} A j_l(kr) & r < a \\ B h_l(i\kappa r) & r > a \end{cases}$$

Continuity of the wave-function and its derivative implies that the logarithmic derivative at $r = a$ is continues which gives the quantization condition:

$$k\frac{j_l'(ka)}{j_l(ka)} = \kappa\frac{h_l'(\kappa a)}{h_l(\kappa a)}$$

The constants A and B are connected via the continuity condition:

$$A j_l(ka) = B h_l(i\kappa a)$$

Finally the wave function can be parametrized as follows:

$$\psi(r,\phi,\theta) = C \times \begin{cases} h_l(i\kappa a) j_l(kr) Y_m^l(\phi,\theta) & r < a \\ j_l(ka) h_l(i\kappa r) Y_m^l(\phi,\theta) & r > a \end{cases}$$

where C is some normalization constant.

4)

The s and p levels have total angular momentum $l = 0$ and $l = 1$ respectively. We will the corresponding spherical Bessel and Neumann function:

$$\begin{aligned} j_0(x) &= \frac{\sin x}{x} \\ n_0(x) &= -\frac{\cos x}{x} \\ j_1(x) &= \frac{1}{x}\left(\frac{\sin x}{x} - \cos x\right) \\ n_1(x) &= -\frac{1}{x}\left(\frac{\cos x}{x} + \sin x\right) \end{aligned}$$

From this we derive:

$$
\begin{aligned}
h_0(ix) &= -\frac{e^{-x}}{x} \\
h_1(ix) &= i\frac{e^{-x}}{x}\left(\frac{1}{x}+1\right)
\end{aligned}
$$

In the case $l=0$ the quantization condition becomes:

$$\cot ka = -\frac{\kappa a}{ka}$$

To proceed we note that:

$$a^2k^2 + a^2\kappa^2 = \frac{2ma^2}{\hbar^2}\,|U_0|$$

If we define $y=\kappa a$ and $x=ka$ then they lie on a circle with radium $\rho^2=\frac{2ma^2}{\hbar^2}|U_0|$. We can then parametrize them as $y=\rho\cos q$ and $x=\rho\sin q$ where $0<q<\frac{\pi}{2}$ so that they are both positive. The quantization condition will then become:

$$
\begin{aligned}
\cot(\rho\sin q) &= -\cot q \Rightarrow \\
\rho\sin q &= n\pi - q
\end{aligned}
$$

where n is an integer. Remember here that q takes only values in the interval $[0,\pi/2]$ in which $\sin q$ rises from 0 to 1 and the left side drops linearly from $n\pi$ to $n\pi-\pi/2$. Since $\sin q$ is positive, only $n>0$ can give a solution. If $\rho<\pi/2$ we can have no solution. At $\rho=\pi/2$ we get the first solution at $q=\pi/2$ which corresponds to $\kappa=0$ and $ka=\rho$, that is zero energy. As ρ increases this solution shifts to lower energies until $\rho=3\pi/2$ in which case we get a second solution. A new solution is added every time $\rho=n\pi-\pi/2$ for $n>0$. In other words the number of solutions is the floor function of

$$n_s = round\left(\frac{a\sqrt{2m\,|U_0|}}{\pi\hbar}\right)$$

The argument has to be at least $1/2$ to have at least one solution.

Now lets consider the $l=1$ case. The quantization condition becomes:

$$\frac{\cot ka}{ka} - \frac{1}{k^2a^2} = \frac{1}{\kappa^2a^2} + \frac{1}{\kappa a}$$

The right side is positive and decreasing with κ. The left side is decreasing but at $ka=n\pi$ it jumps from minus to plus infinity. For $n=0$ however it is a constant $-1/3$. Both k and κ run from 0 to ρ and they are correlated. As a function of k the right side goes from the value $\rho^{-2}+\rho^{-1}$ when $k=0$ to infinity at $k=\rho$. Clearly if $\rho<\pi$ there is no solution. At $\rho=\pi^+$ the first p state enters the system. Generally at $\rho = n\pi$ a new state enters. The number of p states is then given by:

$$n_p = floor\left(\frac{a\sqrt{2m\,|U_0|}}{\pi\hbar}\right)$$

The degeneracy of all these states is equal to $2l+1$ that is it comes from the rotational symmetry. Remember that in the Hydrogen atom it is n^2 because of an "accidental" degeneracy. This is particular to the Hydrogen atom and cannot be generalized.

To generalize for all momenta we note that in order to obtain the critical values of U_0 for which a new state enters the system it suffices to set $E = 0$ in the quantization condition. Now lets consider the logarithmic derivative for $r > a$ and $\kappa \to 0$. Close to zero the neuman part of the hankel function which behaves like x^{-l-1} dominates and the logarithmic derivative is just $-(l+1)/r$. If we take that to the other side we find that the critical values of the potential are defined by:

$$\frac{d}{dx}\left(x^{l+1} j_l(x)\right) = 0$$

where $x = ka$. For example for $l = 0$ this will give us $\cos x = 0$ and for $l = 1$ it gives $x \sin x = 0$ which for $x > 0$ gives us $\sin x$.

5)

The states $1s$ and $2s$ correspond to the two first states with $l = 0$. These states are not degenerate and for them to exist

$$\frac{a\sqrt{2m\,|U_0|}}{\pi\hbar} > \frac{3}{2}$$

The spherical harmonic $Y_0^0 = \frac{1}{\sqrt{4\pi}}$ is just a constant. The only difference between the two states is the value of the energy which determines κ and k. The wave function is given by:

$$\begin{aligned}
\psi_{n,s}(r,\phi,\theta) &= C_{n,s} \times \begin{cases} h_0(i\kappa_{n,s}a) j_0(k_{n,s}r) & r < a \\ j_0(k_{n,s}a) h_0(i\kappa_{n,s}r) & r > a \end{cases} \\
&= C_{n,s} \times \begin{cases} \frac{e^{-\kappa a}}{\kappa a} \frac{\sin kr}{kr} & r < a \\ \frac{\sin ka}{ka} \frac{e^{-\kappa r}}{\kappa r} & r > a \end{cases}
\end{aligned}$$

where is the last expressions both k and κ still depend on n.

The state $2p$ is the first p states and can only exist if

$$\frac{a\sqrt{2m\,|U_0|}}{\pi\hbar} > 1$$

which means that it has lower energy than $2s$. There are actually three such states with the same energy differing by the quantum number m. The spherical harmonic is:

$$Y_m^{l=1}(\phi,\theta) = \begin{cases} -\frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{i\phi}\sin\theta & m=1 \\ \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta & m=0 \\ \frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{-i\phi}\sin\theta & m=-1 \end{cases}$$

And the wave function is given by:

$$\begin{aligned} \psi_{n,p,m}(r,\phi,\theta) &= C_{n,p}Y_m^1(\phi,\theta) \times \begin{cases} h_1(i\kappa_{n,s}a)j_1(k_{n,s}r) & r<a \\ j_1(k_{n,s}a)h_1(i\kappa_{n,s}r) & r>a \end{cases} \\ &= C_{n,p}Y_m^1(\phi,\theta) \times \begin{cases} \frac{e^{-\kappa a}}{\kappa a}\left(\frac{1}{\kappa a}+1\right)\frac{1}{kr}\left(\frac{\sin kr}{kr}-\cos kr\right) & r<a \\ \frac{1}{ka}\left(\frac{\sin ka}{ka}-\cos ka\right)\frac{e^{-\kappa r}}{\kappa r}\left(\frac{1}{\kappa r}+1\right) & r>a \end{cases} \end{aligned}$$

In the notation NL where $L = s, p, d, f \ldots$ is the total angular momentum and the first index N is a label denoting the total number of nodes in the wave function (plus one). Therefore for the p states which already have one angular node always start with $N = 2$. Similarly the d states that have at least 2 angular nodes start with $N = 3$. The general state starts with $N = l + 1$ so that the number of radial nodes is $N - L$.

6)

It is rewarding to express the wave function using the absolute value and the argument:

$$\psi = ue^{iz}$$

where u and z are both real functions. With a bit of algebra one gets:

$$\frac{1}{2i}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right) = |\psi|^2\,\vec{\nabla}z$$

The first term can be identified as the density and the second is the phase gradient which is what gives rise to the current. Notice that if the wave function is real (or has constant phase) the current must be zero. This is the case for $m = 0$. Therefore both s states and one of the p states will have zero current. In the two $m = \pm 1$ states belonging to the $2p$ triplet, $z = m\phi$ and

$$\vec{\nabla}z = \hat{e}_\phi \frac{m}{r\sin\theta}$$

Therefore if there is any current this will be an azimuthal one:

$$J_\phi = \frac{m\hbar}{M}\int drrR^2(r)\int d\phi d\theta\left|Y_m^l(\phi,\theta)\right|^2$$

The integrand is positive and the current is non zero and proportional to L_z. This result can be generalized: all $m \neq 0$ states have a non zero azimuthal current proportional to L_z.

2 A diatomic molecule in 3D

1)

The Hamiltonian of the problem is:

$$H = \frac{\vec{p_1}^2}{2m_1} + \frac{\vec{p_2}^2}{2m_2} + \frac{1}{2}m\omega^2\left(\vec{r_1} - \vec{r_2}\right)^2$$

We will consider the canonical transformation:

$$\begin{aligned}
\vec{r} &= \vec{r_1} - \vec{r_2} \\
\vec{R} &= \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{M} \\
\frac{\vec{p}}{\mu} &= \frac{\vec{p}_1}{m_1} - \frac{\vec{p}_2}{m_2} \\
\vec{P} &= \vec{p}_1 + \vec{p}_2
\end{aligned}$$

where $M = m_1 + m_2$ is the total and $\mu^{-1} = m_1^{-1} + m_2^{-1}$ the reduced mass. This transformation just expressed the coordinates with respect to the center of mass, but in the Hamiltonian language this is expressed as a canonical transformation. One can easily verify that this is a canonical transformation with the pairs of independent variables being $\vec{r}, \vec{p}$ and $\vec{R}, \vec{P}$. The capitalized quantities correspond to the center of mass and the small quantities are the relative ones. Inverting this transformation and replacing it in the Hamiltonian will give after some algebra:

$$H = \frac{\vec{P}^2}{2M} + \frac{\vec{p}^2}{2\mu} + \frac{1}{2}m\omega^2\vec{r}^2$$

We see that that $\vec{P}$ is a constant of motion. The total wave function can be expressed as:

$$\Psi(\vec{R}, \vec{r}) = e^{i\vec{K}\cdot\vec{R}}\psi(\vec{r})$$

something that one can show with the separation of the center of mass and relative variables and then diagonalizing trivially the center of mass part. The total energy is:

$$E_{tot} = \frac{\hbar^2\vec{K}^2}{2M} + E$$

where the second term comes from the relative part of the hamiltonian. The relative Hamiltonian $H_{rel} = \frac{\vec{p}^2}{2\mu} + \frac{1}{2}k\vec{r}^2$ is rotationally invariant and thus commutes with all L_i and therefore $\vec{L}^2$. This means that the angular part can be chosen to be a spherical harmonic.

$$\psi(\vec{r}) = \frac{\chi(r)}{r}Y^l_m(\phi, \theta)$$

2)

This algebra has been performed for part 2 of problem 1. The resulting radial equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\chi(r) + \left[\frac{1}{2}m\omega^2 r^2 + \frac{\hbar^2 l(l+1)}{2mr^2}\right]\chi(r) = E\chi(r)$$

The easiest path to make this dimensionless is to set:

$$\hbar = m = \omega = 1$$

To restore the original units one has to remember that $\hbar\omega$ has the units of energy and $\sqrt{\frac{\hbar}{m\omega}}$ has units of distance. Using the natural system of units is equivalent to defining:

$$\begin{aligned} E' &= \frac{E}{\hbar\omega} \\ r' &= \sqrt{\frac{m\omega}{\hbar}}r \end{aligned}$$

and then ignore the primes. After the rescaling we get:

$$-\frac{\partial^2}{\partial r^2}\chi(r) + \left[r^2 + \frac{l(l+1)}{r^2} - 2E\right]\chi(r) = 0$$

3)

At the limit $r \to 0$ only the angular momentum part contributes to the potential and the equation becomes:

$$-\frac{\partial^2}{\partial r^2}\chi(r) + \frac{l(l+1)}{r^2}\chi(r) = 0$$

The general solution is of the form r^{s+1} where s satisfies:

$$s(s+1) = l(l+1)$$

from the two solutions $s = l$ and $s = -1 - l$ the latter diverges at the origin. Therefore $\chi(r) \to r^{l+1}$.

On the other hand at $r \to \infty$ the radial equation becomes:

$$-\frac{\partial^2}{\partial r^2}\chi(r) + r^2\chi(r) = 0$$

Lets insert $e^{-\lambda r^2/2}$ and see if the dominant terms cancel. The dominant term of the second derivative is obtained by applying the derivative on the exponential both times (to makes sure that you do not reduce the order by applying it on some r) and it is therefore

$$\frac{\partial^2}{\partial r^2}\chi(r) \to \lambda^2 r^2 e^{-\lambda r^2}$$

For the two terms to cancel one needs $\lambda = 1$ and therefore $\chi(r) \to e^{-r^2/2}$ as $r \to \infty$.

4)

It is tedious but straightforward to evaluate the second derivative. The resulting equation is:

$$zw''(x) + (\gamma - z)w'(z) - aw(z) = 0$$

which is the confluent hyper-geometric series with parameters:

$$\begin{aligned} \gamma &= l + \frac{3}{2} \\ a &= \frac{\gamma - E}{2} \end{aligned}$$

5)

The solution that does not diverge at the origin is the confluent hyper-geometric function $F(a, \gamma, z)$. Unless the series terminates this will become $w(z) \to e^z$ which results in a wave function that diverges at infinity like r^{l+1} (the exponentials cancel). This is in contradiction to the boundary condition we derived in part 3. The series has to terminate which means that $F(a, \gamma, z)$ is just a polynomial of some degree n. For this to happen the $n+1$ coefficient must be zero. The termination condition is controlled only by the numerator and therefore:

$$a + n = 0$$

For example for $n = 0$ it suffices that $a = 0$ for $n = 1$ $a + 1 = 0$ as one can see from the series expansion of $F(a, \gamma, z)$. From this we obtain the energy:

$$E = \hbar\omega\left(\frac{3}{2} + 2n + l\right)$$

where the energy unit has been restored. In this expression the degree n of the polynomial can be any non negative integer and same applies to the total angular momentum quantum number.

For a particular n and l there is a degeneracy because of L_z which is equal to $2l + 1$. There can be additional degeneracy involving different l and n because the energy depends on the combination $2n + l$.

The ground state is obtained for $n = l = 0$ with energy $E = 3\hbar\omega/2$. This is not degenerate and $w(z) = 1$ and the corresponding spherical harmonic is also a constant. The wave function is then:

$$\psi_{000}(r) = Ae^{-r^2/2}$$

The first excited energy level is for $n = 0$ and $l = 1$. It is a triplet with $m = 0, \pm 1$ with energy $E = 5\hbar\omega/2$. Again $w(z) = 1$ and the angular part is a spherical harmonic $Y^1_m(\phi, \theta)$. The wave function is:

$$\psi_{01m}(r, \phi, \theta) = Are^{-r^2/2}Y^1_m(\phi, \theta)$$

The second excited energy level has $2n+l = 2$. and energy $E = 7\hbar\omega/2$. This means that either $l = 2$ and $n = 0$ or $l = 0$ and $n = 1$. The total degeneracy is 6. The corresponding wave function are:

$$\begin{aligned}
\psi_{02m}(r, \phi, \theta) &= Ar^2 e^{-r^2/2} Y^2_m(\phi, \theta) \\
\psi_{100}(r, \phi, \theta) &= A\left(1 - \frac{2}{3}r^2\right) e^{-r^2/2}
\end{aligned}$$

The third excited energy level has $2n+l = 3$ energy $E = 9\hbar\omega/2$ and therefore $n = 0$ and $l = 3$ or $n = 1$ and $l = 1$. The total degeneracy is 10, the energy is and the corresponding wave functions are:

$$\begin{aligned}
\psi_{03m}(r, \phi, \theta) &= Ar^3 e^{-r^2/2} Y^3_m(\phi, \theta) \\
\psi_{11m}(r, \phi, \theta) &= A\left(1 - \frac{2}{3}r^2\right) re^{-r^2/2} Y^3_m(\phi, \theta)
\end{aligned}$$

6)

In Cartesian coordinates the problem is separated in three independent 1D harmonic oscillators, one for each direction. Each quantum state is characterized by three quantum numbers (n_x, n_y, n_z) and the total energy is given by

$$E = \hbar\omega(\frac{3}{2} + n_x + n_y + n_z)$$

The quantum numbers can take any non negative integer value and for each oscillator all states are non degenerate. The wave function is

$$\psi(\vec{r}) = \phi_{n_x}(x)\phi_{n_y}(x)\phi_{n_z}(x)$$

where $\phi_n(x_i) = A_n e^{-x_i^2/2} H_n(x_i)$ is the 1D harmonic oscillator wave function. The first 4 Hermite polynomials are:

$$\begin{aligned}
H_0(x) &= 1 \\
H_1(x) &= 2x \\
H_2(x) &= 4x^2 - 2 \\
H_3(x) &= -12x\left(1 - \frac{2}{3}x^2\right)
\end{aligned}$$

The first energy levels are

1. $(0,0,0)$ non degenerate with energy $E = 3\hbar\omega/2$ and wave function $e^{-r^2/2}$
2. $(1,0,0)$ (and all permutations) with degeneracy 3, energy $E = 5\hbar\omega/2$ and wave function $x_i e^{-r^2/2}$
3. $(1,1,0)$ and $(2,0,0)$ (and all permutations with degeneracy 3+3=6, energy $E = 7\hbar\omega/2$
4. $(1,1,1)$, $(2,1,0)$ and $(3,0,0)$ with degeneracy 1+6+3=10, energy $E = 9\hbar\omega/2$

Although it is a bit tedious to demonstrate the rule is that the states in spherical coordinates can always be written as linear combinations of the states in Cartesian coordinates belonging to the same degeneracy space. For example one can see that the ground states where there is no degeneracy match completely. For the first excited state we use the fact that:

$$Y_m^{l=1}(\phi,\theta) = \begin{cases} -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\frac{x+iy}{r} & m=1 \\ \frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{z}{r} & m=0 \\ \frac{1}{2}\sqrt{\frac{3}{2\pi}}\frac{x-iy}{r} & m=-1 \end{cases}$$

which implies that each spherical harmonic is written as a linear combination of x_i/r so that $\psi_{01m}(r,\phi,\theta) = Are^{-r^2/2}Y_m^1(\phi,\theta)$ is just a linear combination of the eigen-states expressed in Cartesian coordinates.

3 Scattering from a Short Range Potential

1)

One way is to follow the Greens method as described explicitly in the lecture notes.

2)

Since the potential is short range then the integrand is appreciable in a small region around the origin and therefore we can assume that $\vec{r}'$ is small. For $\vec{r}$ much larger than the range of the potential we can write:

$$|\vec{r} - \vec{r}'| \approx r\left(1 - \frac{\vec{r}\cdot\vec{r}'}{r^2}\right) = r - \hat{r}\cdot\vec{r}'$$

so that

$$\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \approx \frac{e^{ikr}}{r}e^{-ik\hat{r}\cdot\vec{r}'}$$

Note that we Taylor expanded the exponent but not the denominator. The reason for this is that we typically assume that the incoming wavelength is of the same order of magnitude as the range of the potential which means that small variations of $\vec{r}'$ can induce important phase changes even though the distance $|\vec{r}-\vec{r}'|$ does not change much. In other words we treat $k\vec{r}'$ as zero order. (Note: you should always justify your approximations).

Under this approximation the eigenstates can be written:

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{M}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3\vec{r}' e^{-ik\hat{r}\cdot\vec{r}'}U(\vec{r}')\psi_{\vec{k}}(\vec{r}')$$

which has the advertised form.

3)

We remember that the current is proportional to the phase gradient and we evaluate it for the incoming and the outgoing wave. For the incoming wave it is equal to:

$$\vec{J} = \frac{\hbar}{m}\vec{k}$$

For the outgoing wave only the radial current is of interest. Since the phase is kr this is equal to:

$$J_r = \frac{\hbar k}{m}\frac{1}{r^2}\left|f(\hat{r})\right|^2 = J\frac{1}{r^2}\left|f(\hat{r})\right|^2$$

The number of particles per unit of time that go through a base of a solid angle $d\Omega$ at some distance r is $Jd\sigma = r^2 J_r d\Omega$. The last formula means that $d\sigma$ is an area such that when multiplied with the flux it will give the number of particles that were scattered within a solid angle. This is the exact definition of the cross section.

4)

If the potential is rotationally invariant there are only two directions in the problem $\hat{r}$ and $\hat{k}$ and their relative orientation is the only source of angular dependence for any quantity in the system. This is equivalent to saying that with no loss of generality that $\hat{k}$ is along the $\hat{z}$ axis so that $\vec{k}\cdot\vec{r} = kr\cos\theta$ and also that $\vec{r}$ is on the xz plane ($\phi = 0$) so that ϕ does not appear explicitly in the equation any more. This means that $\psi(\vec{r})$ for which we need to solve this equation must also be ϕ independent. Since the incoming wave only depends on θ also $f(\hat{r}) = f(\theta)$. In this case the amplitude can be expanded with respect to Legend re polynomials (or spherical Harmonics for $m = 0$).

In this symmetry the most general solution to the Schroedinger equation can be written as:

$$\psi(r,\theta) = \sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta)\frac{S_l h_l(kr) + h_l^*(kr)}{2}$$

which is a sum of the partial waves with the Radial part $R_l(r)$ written as a linear combination of two Hankel functions. In the particular case that $S_l = 1$ the above sum is equal to a plane wave which is the $U_0 = 0$ case.

If we assume elastic collisions then the potential cannot be a source or sink of particles. This means that the radial current from all partial waves must be zero:

$$R_l^*(r)\partial_r R_l(r) = R_l(r)\partial_r R_l^*(r)$$

This is equivalent

$$\Im R_l^*(r)\partial_r R_l(r) = 0 = |S_l|^2 h_l^* h_l' + h_l h_l^{*\prime}$$

and from this we deduce that S_l is just a phase:

$$S_l = e^{2i\delta_l}$$

The phase of S_l measures the difference in the phase of the plane waves with and without potential. Now lets write the eigen function as follows:

$$\psi(r,\theta) = e^{ikr\cos\theta} + \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) \frac{e^{2i\delta_l} - 1}{2i} i h_l(kr)$$

where we reconstructed the plane wave.

For large r the hankel function take the asymptotic form:

$$h_l(x) \approx \frac{1}{x} e^{i(x-(l+1)\frac{\pi}{2})} = \frac{e^{ix}}{ix} i^{-l}$$

Using this asymptotic form one gets:

$$\psi(r,\theta) = e^{ikr\cos\theta} + \frac{e^{ikr}}{kr} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) e^{i\delta_l} \sin\delta_l$$

from which we get the scattering amplitude:

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) e^{i\delta_l} \sin\delta_l$$

5)

To simplify notation a bit we will temporarily define:

$$g_l = e^{i\delta_l} \sin\delta_l$$

The total cross section is given by integrating the result of part 2:

$$\sigma = \int d\Omega\, |f(\hat{r})|^2 = \frac{1}{k^2} \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (2l+1)(2l'+1) g_l g_{l'}^* 2\pi \int_0^{\pi} d\theta \sin\theta P_l(\cos\theta) P_{l'}(\cos\theta)$$

were we use that the Legendre polynomials are real functions.

$$\begin{aligned}
\int_0^\pi d\theta \sin\theta P_l(\cos\theta)P_{l'}(\cos\theta) &= \int_{-1}^1 dx P_l(x)P_{l'}(x) \\
&= \frac{2}{2l+1}\delta_{ll'}
\end{aligned}$$

Substituting gives:

$$\begin{aligned}
\sigma &= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)g_l g_{l'}\frac{1}{2l+1}\delta_{ll'} \\
&= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l
\end{aligned}$$

It is interesting to note that because $P_l(1) = 1$ the total cross section is:

$$\sigma = \frac{4\pi}{k}\Im f(0)$$

and so it satisfies the optical theorem. Actually, the conservation of probability, from which the optical theorem stems, has already been used in the derivation of the scattering amplitude (part 4). One could also start from the optical theorem and derive the expansion of $f(\theta)$ in legendre polynomials.

6)

The spherical Bessel functions satisfy:

$$j_l(z) = \sqrt{\frac{\pi}{2z}}J_{l+1/2}(z)$$

1. Attractive potential well.

$$\begin{aligned}
\delta_l &= \frac{2Mk|U_0|}{\hbar^2}\int_0^{r_0} dr r^2 j_l^2(kr) \\
&= \frac{2M|U_0|}{\hbar^2 k^2}\int_0^{kr_0} dz z^2 \frac{\pi}{2z}J_{l+1/2}^2(z) \\
&= \frac{\pi M|U_0|}{2\hbar^2 k^2}J_{l+3/2}^2(kr_0) \\
&= \frac{|U_0|\, kr_0}{2E_k}j_{l+1}^2(kr_0)
\end{aligned}$$

2. Yukawa potential

$$\begin{aligned}
\delta_l &= -\frac{2MkU_0}{\hbar^2\kappa}\int_0^\infty dr r e^{-\kappa r}j_l^2(kr) \\
&= -\frac{2MU_0}{\hbar^2 k\kappa}\int_0^\infty dz z e^{-z\kappa/k}\frac{\pi}{2z}J_{l+1/2}^2(z) \\
&= -\frac{MU_0}{\hbar^2 k\kappa}P_l\left(1+\frac{\kappa^2}{2k^2}\right)
\end{aligned}$$

7)

Born approximation:

$$f_{\vec{k}}(\hat{r}) = -\frac{M}{2\pi\hbar^2}\int d^3\vec{r}' e^{i\left(\vec{k}-\vec{k}'\right)\cdot\vec{r}'}U(r')$$

This is essentially the Fourier transform of the Yukawa potential $\tilde{U}\left(\vec{k}-\vec{k}'\right)$. Lets consider just the integral:

$$\tilde{U}\left(\vec{k}\right) = \int d^3\vec{r}' e^{i\vec{k}\cdot\vec{r}'}U(r')$$

We can use spherical coordinates such that $\vec{k}$ is along the z direction. We note that there is no ϕ dependence in the integrand. Also since the potential does not have any characteristic direction the integral should only depend the the magnitude of $\vec{k}$. Therefore:

$$\begin{aligned}
\tilde{U}(q) &= 2\pi\int_0^\infty drr^2U(r)\int_0^\pi d\theta\sin\theta e^{iqr\cos\theta} \\
&= 4\pi\int_0^\infty drr^2\frac{U_0e^{-\kappa r}}{\kappa r}\frac{\sin qr}{qr} \\
&= \frac{4\pi U_0}{\kappa q}\int_0^\infty dre^{-\kappa r}\sin qr = \frac{4\pi U_0}{\kappa}\frac{1}{\kappa^2+q^2}
\end{aligned}$$

Since $\left|\vec{k}\right| = \left|\vec{k}'\right| = k$ we have

$$q^2 = \left(\vec{k}-\vec{k}'\right)^2 = 2k^2 - 2k^2\cos\theta = \left(2k\sin\frac{\theta}{2}\right)^2$$

From this we can determine the scattering amplitude:

$$\begin{aligned}
f_{\vec{k}}(\hat{r}) &= -\frac{2MU_0}{\kappa\hbar^2}\frac{1}{\kappa^2+q^2} \\
&= -\frac{U_0}{\kappa}\left(\frac{\hbar^2\kappa^2}{2M} + 4E_k\sin^2\frac{\theta}{2}\right)^{-1}
\end{aligned}$$

The differential cross section is then:

$$\frac{d\sigma}{d\Omega} = |f(\hat{r})|^2 = \frac{U_0^2}{\kappa^2}\left(\frac{\hbar^2\kappa^2}{2M} + 4E_k\sin^2\frac{\theta}{2}\right)^{-2}$$

Although we cannot really apply this method in the original Coulomb potential (which is long range) we can consider it to be the limit of the $Yukawa$ potential for $\kappa \to 0$ with $U_0/\kappa \to Ze^2$. In this case we get

$$\frac{d\sigma}{d\Omega} = |f(\hat{r})|^2 = \frac{Z^2e^4}{16E_k^2\sin^4\frac{\theta}{2}}$$

which the the classical scattering formula.