Solutions - HW5

PHYS 457 - Winter 2024

January 2024

1 Problem 1

(a)

To compute $\langle r \rangle, \langle r^2 \rangle$ we use

$$\begin{aligned}\langle r^m \rangle &= \int d\boldsymbol{r}\, r^m |\psi_{nlm}(\boldsymbol{r})|^2 \\ &= \int_0^\infty dr\, r^2\, r^m |R(\boldsymbol{r})|^2 \int d\phi\, d\theta\, \sin\theta\, |Y_{lm}(\theta,\phi)|^2 \\ &= \int_0^\infty dr\, r^{m+2} |R(\boldsymbol{r})|^2,\end{aligned} \tag{1}$$

where $m = 1, 2$, $R(r)$ is the radial part of the wavefunction, and $Y_{lm}(\theta,\phi)$ is the spherical harmonic with indices (lm). In the second line we have used the fact that the spherical harmonics are normalized, i.e. $\int d\phi\, d\theta\, \sin\theta |Y_{lm}|^2 = 1$. The (unnnormalized) radial wavefunction for the hydrogen atom is given by

$$R(r) = \frac{u(r)}{r}, \quad u(\rho) = \rho^{l+1} e^{-\rho/2} F(\rho), \tag{2}$$

where $\rho = r\sqrt{8\mu|E_n|}/\hbar$ and $E_n = -\mu e^4/2\hbar^2 n^2 = -e^2/a_0 n^2$ [see, for example, Eq. (10.21) of Townsend[1]] where $a_0 = \hbar^2/\mu e^2$ is the Bohr radius. $F(\rho)$ is given by the series

$$F(\rho) = \sum_{k=0}^{k_{\max}} c_k \rho^k, \tag{3}$$

where $k_{\max} = \lambda - l - 1 = n - l - 1$ (the second equality defines the quantum number n) and $\lambda = e^2\sqrt{\mu/2|E_n|\hbar^2}$. We consider the case $l = n-1$, which implies $k_{\max} = 0$ and therefore $F(\rho) = 1$. The radial part of the wavefunction is then

$$R(r) = \frac{u(r)}{r} = \beta^{l+1} r^l e^{-\beta r/2}, \tag{4}$$

where we defined $\beta \equiv \sqrt{8\mu|E|}/\hbar$ to avoid clutter. The expectation values $\langle r^m \rangle$ is then given by

$$\langle r^m \rangle = \frac{\int_0^\infty dr\, r^{m+2}|R(r)|^2}{\int_0^\infty dr\, r^2 |R(r)|^2} = \frac{\int_0^\infty dr\, r^{2(l+1)+m} e^{-\beta r}}{\int_0^\infty dr\, r^{2(l+1)} e^{-\beta r}}, \tag{5}$$

where the denominator ensures the normalization of $R(r)$. We perform a change of variables $u = \beta r$ to rewrite the equation above as

$$\langle r^m \rangle = \frac{\beta^{-(2l+2+m)}}{\beta^{-2(l+1)}} \frac{\int_0^\infty du\, u^{2l+m} e^{-u}}{\int_0^\infty dr\, u^{2l} e^{-u}}. \tag{6}$$

[1] Recall that his textbook uses Gaussian units.

Using the definition of the Gamma function

$$\Gamma(z+1) = \int_0^\infty dz\, u^z e^{-u} = z!, \tag{7}$$

where the second equality is satisfied when z is a positive integer. Considering that l and m are integers and using $n = l + 1$, we obtain

$$\langle r^m \rangle = \beta^{-m} \frac{(2n+m)!}{(2n)!} \implies \langle r \rangle = \frac{\hbar}{\sqrt{8\mu|E_n|}}(2n+1), \quad \langle r^2 \rangle = \frac{\hbar^2}{8\mu|E_n|}(2n+2)(2n+1). \tag{8}$$

Using $E_n = -e^2/n^2 a_0$, we have

$$\boxed{\langle r \rangle = \frac{a_0}{2} n(2n+1)}, \quad \boxed{\langle r^2 \rangle = \frac{a_0^2}{4} n^2 (2n+2)(2n+1)}. \tag{9}$$

The uncertainty principle is then

$$\Delta r = \frac{a_0}{2}\sqrt{[n^2(2n+2)(2n+1)] - [n(2n+1)]^2} = \frac{a_0}{2} n\sqrt{2n+1} \tag{10}$$

Using the definition of the Bohr radius $a_0 = \hbar^2/\mu e^2$ (again, using Gaussian units) we can write

$$\boxed{\Delta r = \frac{a_0}{2} n\sqrt{2n+1}} \tag{11}$$

(b)

To obtain a relationship between E_n and $\langle r \rangle$, we first use Eq. (8) to solve for n and then use $E = -e^2/n^2 a_0$. We have

$$\langle r \rangle = \frac{\hbar}{\sqrt{8\mu|E_n|}}(2n+1) = \sqrt{\frac{\hbar^2 a_0}{8\mu e^2}} n(2n+1) = \frac{a_0}{2} n(2n+1). \tag{12}$$

We solve this using Mathematica (see Appendix) to obtain two solutions and only consider the one that is positive:

$$n = \frac{1}{4\sqrt{a_0}}\left(-\sqrt{a_0} + \sqrt{16\langle r \rangle + a_0}\right). \tag{13}$$

The energy is then given by

$$\boxed{E_n = -\frac{16e^2}{\left(\sqrt{16\langle r \rangle + a_0} - \sqrt{a_0}\right)^2}}. \tag{14}$$

(c)

From the first equation in (9), we can see that for large n we have $\langle r \rangle \approx a_0 n^2$. This implies that the energy is $E_n = -e^2/n^2 a_0 \approx -e^2/\langle r \rangle$. This is what our classical intuition would tell us as it is the one given by the Coulomb potential. In Fig. 1 we plot the exact energy and $E_n = -e^2/\langle r \rangle$ to confirm this.

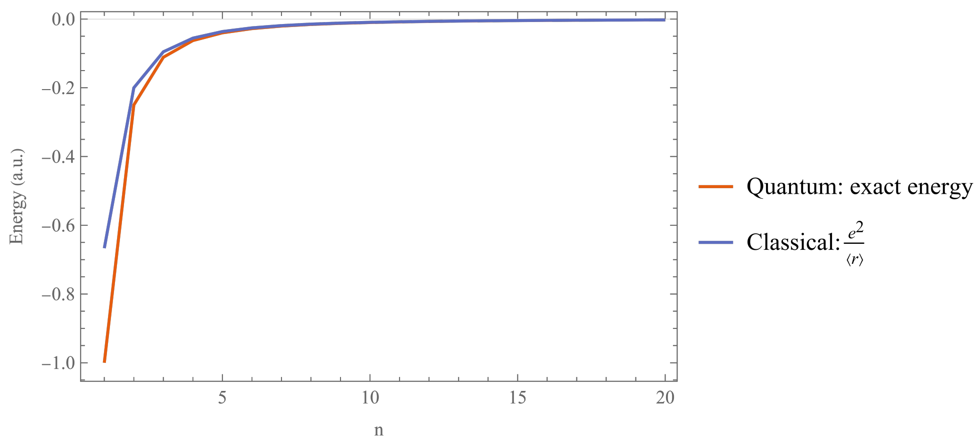


Figure 1: Comparison between classically expected energy and eigenenergies of the Hydrogen atom.

2 Problem 2

(a)

The Hamiltonian for the 3D harmonic oscillator is given by

$$H = \frac{\boldsymbol{p}^2}{2\mu} + \frac{1}{2\mu}\mu\omega^2\boldsymbol{r}^2, \tag{1}$$

where $\boldsymbol{r} = (r_x, r_y, r_z)$. The general differential equation for $u(r) = rR(r)$ (where $R(r)$ is the radial part of the solution to the Schrodinger equation) is given by Eq. (10.4) Townsend:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right]u(r) = Eu(r). \tag{2}$$

In our case, we have $V(r) = \mu\omega^2\boldsymbol{r}^2/2$, so the equation above takes the form

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + \frac{1}{2}\mu\omega^2 r^2\right]u(r) = Eu(r). \tag{3}$$

If we divide both sides by $\hbar\omega/2$ and use $\lambda = 2E/\hbar\omega$, we obtain

$$\left[-\frac{\hbar}{\omega\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar}{\omega\mu r^2} + \frac{1}{\hbar}\mu\omega r^2\right]u(r) = \lambda u(r). \tag{4}$$

Now, we use $\rho = r\sqrt{\mu\omega/\hbar} \implies r = \rho\sqrt{\hbar/\omega\mu}$, $\frac{du}{dr} = \frac{du}{d\rho}\frac{d\rho}{dr} = \sqrt{\mu\omega/\hbar}\frac{du}{d\rho} \implies \frac{d^2u}{dr^2} = \frac{\mu\omega}{\hbar}\frac{d^2u}{d\rho^2}$, which gives

$$\left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} + \rho^2\right]u = \lambda u \implies \boxed{\frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2}u - \rho^2 u = -\lambda u}. \tag{5}$$

(b)

Similar to the hydrogen atom, we can look at the asymptotic behaviour of the differential equation. For $\rho \to 0$ we have

$$\frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2} \implies u \sim A\rho^{l+1} + B\rho^{-l}. \tag{6}$$

The second term blows up as $\rho \to 0$ so we expect that at small ρ our solution behaves as $\rho \sim \rho^{l+1}$. Then, we look at the behaviour of the differential equation as $\rho \to \infty$. In this case, the dominant terms are

$$\frac{d^2u}{d\rho^2} = \rho^2 u \tag{7}$$

We can see that $u \sim e^{-\rho^2/2}$ satisfy this equation for large ρ as we have

$$\frac{d^2}{d\rho^2}\left(e^{-\rho^2/2}\right) = \frac{d}{d\rho}\left(-e^{-\rho^2/2}\rho\right) = -e^{\rho^2/2} + e^{-\rho^2/2}\rho^2 \overset{\rho\gg 1}{\approx} \rho^2 e^{-\rho^2/2}. \tag{8}$$

satisfying Eq. (7). Therefore, it makes sense to look at solutions of the form

$$u(\rho) = \rho^{l+1} e^{-\rho^2/2} f(\rho). \tag{9}$$

(c)

Our first goal is to insert Eq. (9) into our differential Eq. (5) hoping to obtain an easier equation for $F(\rho)$. The result is (we have used *Mathematica*, see Appendix)

$$(\lambda - 2l - 3)\rho f(\rho) + 2(l + 1 - \rho^2) f'(\rho) + \rho f''(\rho) = 0. \tag{10}$$

We now write $f(\rho)$ (and its derivatives) as a series

$$f(\rho) = \sum_{n=0}^{\infty} c_n \rho^n, \tag{11}$$

$$f'(\rho) = \sum_{n=0}^{\infty} c_n\, n\, \rho^{n-1} \tag{12}$$

$$f''(\rho) = \sum_{n=0}^{\infty} c_n\, n(n-1)\, \rho^{n-2} \tag{13}$$

We then insert the equations above into Eq. (10), we get

$$\begin{aligned} 0 &= \sum_{n=0}^{\infty} \left[(\lambda - 2l - 3)c_n \rho^{n+1} + 2(l+1)c_n n \rho^{n-1} - 2c_n n \rho^{n+1} + c_n n(n-1)\rho^{n-1}\right] \\ &= \sum_{n=0}^{\infty} \left[(\lambda - 2l - 3 - 2n)c_n \rho^{n+1} + (2l + 1 + n)c_n n \rho^{n-1}\right] \end{aligned} \tag{14}$$

We want to have the same power of ρ in the sum so that we have a coefficient that has to vanish for every value of ρ. To do this we change the index $n \to n-2$ in the first sum. This means that we would need to start our sum at $n = 2$. Hence, we can write the equation above as

$$\sum_{n=0}^{1} (2l + 1 + n)c_n n \rho^{n-1} + \sum_{n=2}^{\infty} \left[c_{n-2}(\lambda - 2l - 2n + 1) + c_n(2l + n + 1)n\right] \rho^{n-1} = 0 \tag{15}$$

For the equation above to vanish for any ρ, we need both summations to vanish independently (as they involve different powers of ρ). The first term is

$$(2l + 2)c_1 = 0 \implies c_1 = 0. \tag{16}$$

From the second term, we obtain the recurrence relation

$$c_n = \frac{\lambda - 2l - 2n + 1}{(2l + n + 1)n} c_{n-2} \implies c_{n+2} = \frac{\lambda - 2l - 2n - 3}{(2l + n + 3)(n + 2)} c_n \tag{17}$$

Since the series must terminate, we obtain that for a maximum value for $n-2$, we should have $\lambda - 2l - 2n + 1$. Since λ, n are integers, λ must be an integer. We recall that $\lambda = 2E/\hbar\omega$ which means the energy must be an integer of $\hbar\omega$. Above, we have rewritten the recurrence relation in terms of c_n because we can then identify the maximum n such that $c_n \neq 0$. This n satisfies

$$\lambda = \frac{2E}{\hbar\omega} = 2l + 2n + 3,\ n = 0, 2, 4, \ldots \implies E = \hbar\omega\left(2n_r + l + \frac{3}{2}\right),\ n_r = 0, 1, 2 \ldots, \tag{18}$$

which agrees with Eq. (10.95) from the textbook.

3 Problem 3

(a)

The Hamiltonian of a particle in a 2D harmonic oscillator is

$$H = \frac{p_x^2}{2\mu} + \frac{1}{2}\mu\omega^2 x^2 + \frac{p_y^2}{2\mu} + \frac{1}{2}\mu\omega^2 y^2. \tag{1}$$

Similar to the 1D harmonic oscillator, we define the ladder operators as

$$a_1 = \sqrt{\frac{\mu\omega}{2\hbar}}\left(x + \frac{i}{\mu\omega}p_x\right), \quad a_2 = \sqrt{\frac{\mu\omega}{2\hbar}}\left(y + \frac{i}{\mu\omega}p_y\right). \tag{2}$$

The operators $a_1^\dagger, a_2^\dagger$ are the Hermitian conjugate of the operators above. With these definitions, we have

$$\begin{aligned}
\hbar\omega\left(a_1^\dagger a_1 + a_2^\dagger a_2\right) &= \frac{\mu\omega^2}{2}\left(x^2 + \frac{p_x^2}{m^2\omega^2} + \frac{i}{\mu\omega}[x, p_x] + x \to y\right) \\
&= \frac{\mu\omega^2}{2}x^2 + \frac{p_x^2}{2m} - \hbar\omega + x \to y \\
&= \frac{\mu\omega^2}{2}x^2 + \frac{p_x^2}{2m} - \frac{1}{2}\hbar\omega + \frac{\mu\omega^2}{2}y^2 + \frac{p_y^2}{2m} - \frac{1}{2}\hbar\omega.
\end{aligned} \tag{3}$$

Above, the notation $x \to y$ indicates that we have the same term but substituting x with y. Comparing with H, we note that

$$H = \hbar\omega(a_1^\dagger a_1 + a_2^\dagger a_2 + 1). \tag{4}$$

The commutation relations between the ladder operators are

$$[a_1, a_1^\dagger] = \frac{\mu\omega}{2\hbar}\left(\cancelto{0}{[x,x]} - \frac{i}{\mu\omega}[x, p_x] + \frac{i}{\mu\omega}[p_x, x] + \frac{1}{\mu^2\omega^2}\cancelto{0}{[p_x,p_x]}\right) = 1. \tag{5}$$

Any commutator between ladder operators of different indices commute because they involve the position and momentum operators in different directions. This means $[a_1, a_2] = [a_1^\dagger, a_2^\dagger] = [a_1^\dagger, a_2] = 0$. Then, we have

$$[H, a_1^\dagger] = \hbar\omega[a_1^\dagger a_1, a_1^\dagger] = \hbar\omega\left(a_1^\dagger[a_1, a_1^\dagger] + [a_1^\dagger, a_1^\dagger]a_2\right) = \hbar\omega a_1^\dagger. \tag{6}$$

This means that if $|\psi\rangle$ is an eigenstate of H: $H|\psi\rangle = E_\psi|\psi\rangle$, then

$$Ha^\dagger|\psi\rangle = (\hbar\omega a^\dagger + a^\dagger H)|\psi\rangle = (E_\psi + \hbar\omega)a_1^\dagger|\psi\rangle. \tag{7}$$

The equaiton above implies that if $|\psi\rangle$ is an eigenstate of H with energy E_ψ, then $a_1^\dagger|\psi\rangle$ is also an eigenstate with energy $E_\psi + \hbar\omega$. Since the Hamiltonian is symmetric under $x \leftrightarrow y$ we conclude that we have the same story with $a_2^\dagger$. Then, we can define the ground state $|0\rangle$ as the state that is annihilated by both a_1, a_2: $a_1|0\rangle = a_2|0\rangle = 0$. We can then create the *excitations* (states with energy above the ground state) by acting with the operators $a_1^\dagger, a_2^\dagger$ on the ground state $|0\rangle$. By this procedure, we obtain the states $\sim (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}|0\rangle$ which have energy $(n_1 + n_2 + 1)\hbar\omega$.

(b)

Using Eq. (2) (and their Hermitian conjugates) we can write the position and momentum operators as

$$x = \sqrt{\frac{\hbar}{2\mu\omega}}\left(a_1^\dagger + a_1\right), \quad p_x = i\sqrt{\frac{\mu\omega\hbar}{2}}\left(a_1^\dagger - a_1\right), \tag{8}$$

and similar for y. Then, we have

$$
\begin{aligned}
L_z &= xp_y - yp_x \\
&= i\frac{\hbar}{2}\left[\left(a_1^\dagger a_2^\dagger - a_1^\dagger a_2 + a_1 a_2^\dagger - a_1 a_2\right) - (1 \leftrightarrow 2)\right] \\
&= i\frac{\hbar}{2}\left[\left(-a_1^\dagger a_2 + a_1 a_2^\dagger\right) - (1 \leftrightarrow 2)\right] \\
&= i\frac{\hbar}{2}\left[\left(-a_1^\dagger a_2 + a_1 a_2^\dagger\right) - \left(-a_2^\dagger a_1 + a_2 a_1^\dagger\right)\right] \\
&= i\hbar\left(a_2^\dagger a_1 - a_1^\dagger a_2\right).
\end{aligned}
\tag{9}
$$

Our Hamiltonian has rotational symmetry over the z-axis. Since L_z is the generator of rotations along this axis, we expect $[H, L_z] = 0$. The commutator is

$$
\begin{aligned}
[H, L_z] &= i\hbar^2\left([a_1^\dagger a_1 + a_2^\dagger a_2, (a_2^\dagger a_1 - a_1^\dagger a_2)]\right) \\
&= i\hbar^2\left([a_1^\dagger a_1, a_2^\dagger a_1] - [a_1^\dagger a_1, a_1^\dagger a_2] + [a_2^\dagger a_2, a_2^\dagger a_1] - [a_2^\dagger a_2, a_1^\dagger a_2]\right)
\end{aligned}
\tag{10}
$$

We already know that $[a_1^\dagger a_1, a_1^\dagger] = a_1^\dagger$ [see Eq. (6)] (similarly for $1 \to 2$). Taking the Hermitian conjugate of the commutator we have

$$
[a_1^\dagger a_1, a_1^\dagger]^\dagger = [a_1, a_1^\dagger a_1] = a_1 \implies [a_1^\dagger a_1, a_1] = -a_1. \tag{11}
$$

The equation above is useful to compute each commutator of the second line in Eq. (10), we have

$$
[a_1^\dagger a_1, a_2^\dagger a_1] = [a_1^\dagger a_1, a_1]a_2^\dagger = -a_1 a_2^\dagger \tag{12}
$$

$$
[a_1^\dagger a_1, a_1^\dagger a_2] = [a_1^\dagger a_1, a_1^\dagger]a_2 = a_1^\dagger a_2 \tag{13}
$$

$$
[a_2^\dagger a_2, a_2^\dagger a_1] = a_2^\dagger a_1 \tag{14}
$$

$$
[a_2^\dagger a_2, a_1^\dagger a_2] = -a_1^\dagger a_2. \tag{15}
$$

Then, Eq. (10) becomes

$$
[H, L_z] = i\hbar(-a_1 a_2^\dagger - a_1^\dagger a_2 + a_2^\dagger a_1 + a_1^\dagger a_2) = 0. \tag{16}
$$

(c)

We have four states with $E = 2\hbar\omega$: $\{(1,0),(0,1)\}$, where the indices in the parenthesis indicate (n_x, n_y). We can obtain the matrix elements in this subspace by computing the action of L_z on the states in this manifold:

$$
L_z |1,0\rangle \propto |0,1\rangle \tag{17}
$$

$$
L_z |0,1\rangle \propto -|1,0\rangle \tag{18}
$$

We then have the matrix

$$
PL_zP = i\hbar\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \hbar\sigma_z, \tag{19}
$$

where P is the projection operator into the subspace of states with energy $2\hbar\omega$ and σ_z is the third Pauli matrix. Then, our eigenstates are the eigenvectors of σ_z, given by

$$
|e_1\rangle \propto i\,|1,0\rangle + |0,1\rangle \tag{20}
$$

$$
|e_2\rangle \propto |1,0\rangle - i\,|0,1\rangle \tag{21}
$$

Appendix

Problem 1b

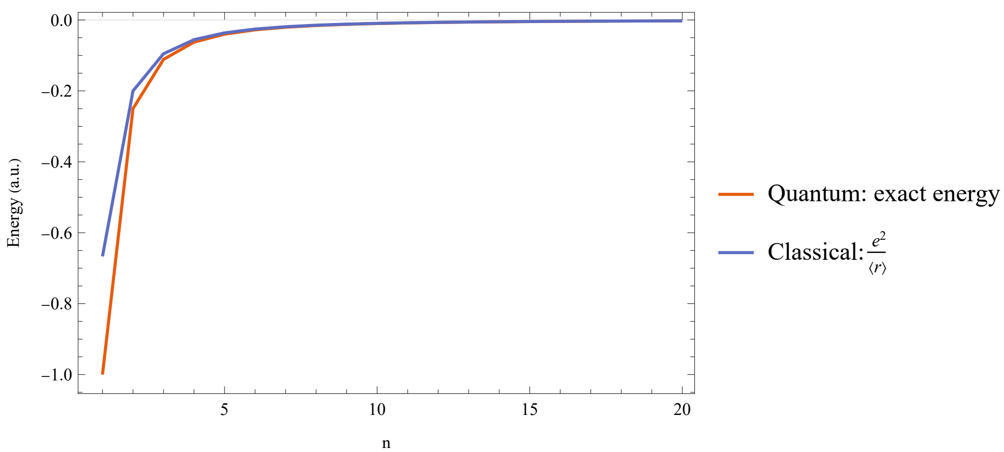
In[5]:=
```
Solve[r == (a0 / 2) n (2 n + 1), n] // Simplify
```

Out[5]=

$$\left\{\left\{n \to -\frac{1}{4} - \frac{\sqrt{a0 + 16\,r}}{4\,\sqrt{a0}}\right\}, \left\{n \to \frac{1}{4}\left(-1 + \frac{\sqrt{a0 + 16\,r}}{\sqrt{a0}}\right)\right\}\right\}$$

In[50]:=
```
ListLinePlot[Table[{-1/(n^2), -2/(n (2 n + 1))}, {n, 1, 20}] // Transpose, PlotRange → All,
 PlotTheme → "Scientific", PlotLegends → {"Quantum: exact energy", "Classical: e^2/⟨r⟩"},
 FrameLabel → {"n", "Energy (a.u.)"}]
```

Out[50]=



In[52]:=
```
(*Export["C:\\Users\\Ivan\\Desktop\\figure1.png",
 %,Background→None,ImageResolution→1000]*)
```

Problem 2c

Write u(ρ)

In[•]:=
```
u[ρ] := ρ^(l + 1) Exp[-ρ^2 / 2] f[ρ]; u[ρ]
```

Out[•]=

$$e^{-\frac{\rho^2}{2}}\,\rho^{1+l}\,f[\rho]$$

Insert u(ρ) in our differential equation to obtain the simplified equation for F(ρ)

In[•]:=
```
D[u[ρ], {ρ, 2}] - (l (l + 1))/ρ^2 u[ρ] - ρ^2 u[ρ] + λ u[ρ] // FullSimplify
```

Out[•]=

$$e^{-\frac{\rho^2}{2}}\,\rho^{l}\left((-3 - 2\,l + \lambda)\,\rho\,f[\rho] + 2\left(1 + l - \rho^2\right) f'[\rho] + \rho\,f''[\rho]\right)$$

The above result should be equal to zero as we have passed all the terms to one side. Therefore, we can cancel the factor of $e^{-\frac{\rho^2}{2}} \rho^1$.