PHY 303, I-Semester 2023/24, Assignment 6 solution

(1) Angular momentum and commutators [8pts]:

(a) Consider the three dimensional Gaussian wavepacket given in Eq. (4.15) of the lecture, with $\mathbf{r}_0 = [x_0, 0, 0]^T$ and $\mathbf{k}_0 = [0, k_0, 0]^T$. Make a sketch of the probability density for $\sigma \ll x_0$ and describe the state of the particle in terms of physics. Then find the expectation value of the angular momentum and discuss. *Hint: Make extensive use of symmetries to avoid most of the integrations that pop up.* Why does this result make sense?

Solution: The 3D Gaussian wavepacket required is given by

$$\phi(x, y, z) = \frac{\exp(ik_0 y) \exp\left(-\frac{y^2}{2\sigma^2}\right) \exp\left(-\frac{z^2}{2\sigma^2}\right) \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right)}{(\pi\sigma^2)^{3/4}} \tag{1}$$

It looks like a fuzzy ball centered at $[x_0, 0, 0]$ in Cartesian coordinates, see Fig. 1. The

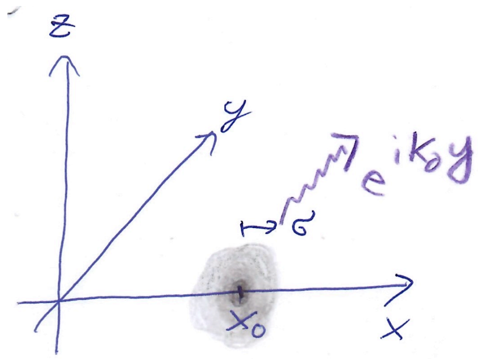

Figure 1: 3D Gaussian wavepacket. We attempted to draw a transparent grey sphere, the darkness of which corresponds to probability density. We also indicated the plane wave component of the wavefunction $\sim \exp(iky)$ in violet.

state of the particle is one localised near the 3D location $\mathbf{r}_0 = [x_0, 0, 0]^T$ as shown, up to a position uncertainty σ, which is the same in each of the three cartesian direction. The particle has a non-zero momentum expectation value only in the y-direction, thus in time this wavepacket would move along the y-direction with momentum $\hbar k_0$ while it's the probability density remains Gaussian but in time spreads out along all three directions (x,y,z).

To find the expectation value of angular momentum,

$$\langle \hat{\mathbf{L}} \rangle = \int dx \int dy \int dz \phi^*(x, y, z) \hat{\mathbf{L}}\, \phi(x, y, z) \tag{2}$$

first realise that this is a vector hence we have to calculate each cartesian component *separately, inserting*

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right),$$
$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right),$$
$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right), \tag{3}$$

which ultimately gives us 6 terms to calculate.

Luckily, we can spot that most of them are zero, even before doing any integrations. Consider for example

$$\phi^*(x,y,z)\hat{L}_x\,\phi(x,y,z) = (-i\hbar)\phi^*(x,y,z)\left[y\left(-\frac{z}{2\sigma^2} - z\frac{\partial}{\partial y}\right),\right]\phi(x,y,z) \tag{4}$$

where we have already evaluated the (easy) $\frac{\partial}{\partial z}$ *derivative. Since we can do the 3 integrations over* x, y, z *in any order we like, let us do the* z *one first. Now we see that the 3D integration for both terms will contain a contribution*

$$\int_{-\infty}^{\infty} dz\, z\exp\left(-\frac{z^2}{\sigma^2}\right) = 0, \tag{5}$$

in which we are integrating an anti-symmetric integrand over a symmetric interval, hence this vanishes by symmetry. We thus directly saw that $\langle\hat{L}_x\rangle = 0$*. The exact same steps yield* $\langle\hat{L}_y\rangle = 0$*, again looking at derivatives and integrations wrt.* z *first.*

For $\langle\hat{L}_z\rangle$ *these arguments do not work, since the wavefunction is not a simple Gaussian centered on zero in terms of either* x *or* y*, which are the axis that appear on the RHS of* $\hat{L}_z$*. We evaluate the complete action of* $\hat{L}_z$ *acting on the wavefuntion*

$$\phi^*(\mathbf{r})\hat{L}_z\phi(\mathbf{r}) = \frac{(\hbar k_0 + i\hbar y/\sigma)xe^{-\frac{(x-x_0)^2}{\sigma^2} - \frac{y^2}{\sigma^2} - \frac{z^2}{\sigma^2}}}{\pi^{3/2}\sigma^3} - \frac{i\hbar(x-x_0)ye^{-\frac{(x-x_0)^2}{\sigma^2} - \frac{y^2}{\sigma^2} - \frac{z^2}{\sigma^2}}}{\pi^{3/2}\sigma^5} \tag{6}$$

where we have used the product rule for the first fraction. When integrating over all space, we can use $\int_{-\infty^\infty} dy\, ye^{-y^2/\sigma^2} = 0$ *by symmetry, which sets all terms to zero with get multiplied by the imaginary unit* i*, which is good, since we need the end result to be real.*

We are left with

$$\langle\hat{L}\rangle_z = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdydz\, \frac{\hbar k_0 xe^{-\frac{(x-x_0)^2}{\sigma^2} - \frac{y^2}{\sigma^2} - \frac{z^2}{\sigma^2}}}{\pi^{3/2}\sigma^3} \tag{7}$$

where we can use the normalisation condition for the 1D Gaussian, e.g. $\frac{1}{(\sqrt{\pi}\sigma)}\int dy\; e^{-\frac{y^2}{\sigma^2}} = 1$ *to trivially sort out the* y *and* z *integrations. For the remaining* x *integration we make the substitution* $\tilde{x} = x - x_0$*, thus*

$$\langle\hat{L}\rangle_z = \int_{-\infty}^{\infty} dx\, \frac{\hbar k_0 xe^{-\frac{(x-x_0)^2}{\sigma^2}}}{\pi^{1/2}\sigma} = \int_{-\infty}^{\infty} d\tilde{x}\, \frac{\hbar k_0(\tilde{x}+x_0)e^{-\frac{\tilde{x}^2}{\sigma^2}}}{\pi^{1/2}\sigma}. \tag{8}$$

Yet again the first integrand $\sim \tilde{x}$ gives an integral that vanished by symmetry, and for the term $\sim x_0$ we use the above normalisation of a 1D Gaussian to finally find:

$$\langle \hat{L} \rangle_z = \hbar k_0 x_0 \tag{9}$$

This is roughly what we would expect, given the particle is "mostly at position $[x_0, 0, 0]^T$" (up to an uncertainty σ) and "mostly moving with momentum $\mathbf{p} = [0, \hbar k_0, 0]^T$ (up to an uncertainty $\sim 1/\sigma$). Using the classical relation for angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p} = [0, 0, \hbar k_0 x_0]^T$.

More rigorously we have found that <u>in this case</u> $\langle \hat{L} \rangle = \langle \mathbf{r} \rangle \times \langle \mathbf{p} \rangle$, but note that this will <u>not be always the case</u>.

(b) *Consider an eigenstate of the TISE with a spherically symmetric potential. Show explicitly (with integrations) that in any eigenstate $\langle \hat{\mathbf{r}} \rangle = 0$ and $\langle \hat{\mathbf{p}} \rangle = 0$ and then argue why we could have known this without calculation.*

The TISE of a spherically symmetric potential $V(r)$ can be solved by seperation of variables,and by solving the radial and angular equation independently:

$$sin(\theta)\frac{\partial}{\partial\theta}\left(sin(\theta)\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -l(l+1)sin(\theta)^2 Y, \tag{10}$$

$$\frac{d}{dr}(r^2\frac{dR}{dr}) - \frac{2mr^2}{\hbar^2}\left[V(r) - E\right] = l(l+1)R, \tag{11}$$

where the eigenstate of the TISE is given as $\Psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$. Note that $Y(\theta, \phi)$ has a parity of -1^l, thus $Y(\theta, \phi)^* Y(\theta, \phi)$ is always even. To calculate the expectations $\langle \hat{\boldsymbol{r}} \rangle = [\langle \hat{\boldsymbol{x}} \rangle, \langle \hat{\boldsymbol{y}} \rangle, \langle \hat{\boldsymbol{z}} \rangle]^T$ where $x = r \sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$. Thus:

$$\begin{aligned}
\langle x \rangle &= \int |\Psi|^2 r \sin\theta\cos\phi d^3\boldsymbol{r} = \int_0^\infty R(r)^2 r^3 dr \int_0^\pi \sin^2\theta P_m^l(\theta)^* P_m^l(\theta) d\theta \underbrace{\int_0^{2\pi} \cos\phi d\phi}_{=0} = 0 \\
\langle y \rangle &= \int |\Psi|^2 r \sin\theta\cos\phi d^3\boldsymbol{r} = \int_0^\infty R(r)^2 r^3 dr \int_0^\pi \sin^2\theta P_m^l(\theta)^* P_m^l(\theta) d\theta \underbrace{\int_0^{2\pi} \sin\phi d\phi}_{=0} = 0 \\
\langle z \rangle &= \int |\Psi|^2 r \cos\theta d^3\boldsymbol{r} = \int_0^\infty R(r)^2 r^3 dr \underbrace{\int_0^\pi \sin\theta\cos\theta P_m^l(\theta)^* P_m^l(\theta) d\theta}_{=0} \int_0^{2\pi} d\phi = 0
\end{aligned} \tag{12}$$

For the expectation values of momentum, we apply the momentum operator in spherical polar coordinates onto the wavefunction (see Eq. (4.35))

$$-i\hbar\boldsymbol{\nabla} = -i\hbar\left[\mathbf{e}_r\frac{\partial}{\partial r} + \mathbf{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta} + \mathbf{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\right] \tag{13}$$

and then perform integrations similar to the ones above again, with the same results, that also $\langle \hat{\mathbf{p}} \rangle = 0$.

We can use similar arguments as for assignment 3 Q1b to see this without integrations (but using symmetries): The potential is symmetric under reflections through the origin $V(\mathbf{r}) = V(-\mathbf{r})$*, due to which you can show that the wavefunction must be symmetric or antisymmetric under any such reflection* $\phi(\mathbf{r}) = \pm\phi(-\mathbf{r})$*. You can use this property to show that both* $\langle \mathbf{r} \rangle$ *and* $\langle \mathbf{p} \rangle$ *must be zero, and we will do that more formally at the beginning of QM-II.*

(c) *Show the commutators [3 pts]*

$$\left[\hat{\mathbf{L}}^2, \hat{L}_n\right] = 0, \tag{14}$$

$$\left[\hat{L}_z, \hat{L}_\pm\right] = \pm\hbar\hat{L}_\pm, \tag{15}$$

$$\left[\hat{\mathbf{L}}^2, \hat{L}_\pm\right] = 0. \tag{16}$$

and show that

$$\hat{\mathbf{L}}^2 = \hat{L}_\pm\hat{L}_\mp + \hat{L}_z^2 \mp \hbar\hat{L}_z. \tag{17}$$

Solution:

$$\begin{aligned}
\left[\hat{\mathbf{L}}^2, \hat{L}_x\right] &= \underbrace{\left[\hat{L}_x^2, \hat{L}_x\right]}_{\equiv 0} + \left[\hat{L}_y^2, \hat{L}_x\right] + \left[\hat{L}_z^2, \hat{L}_x\right] \\
&= \hat{L}_y\left[\hat{L}_y, \hat{L}_x\right] + \left[\hat{L}_y, \hat{L}_x\right]\hat{L}_y + \hat{L}_z\left[\hat{L}_z, \hat{L}_x\right] + \left[\hat{L}_z, \hat{L}_x\right]\hat{L}_z \\
&= -\imath\hbar\hat{L}_y\hat{L}_z - \imath\hbar\hat{L}_z\hat{L}_y + \imath\hbar\hat{L}_z\hat{L}_y + \imath\hbar\hat{L}_y\hat{L}_z \\
&\implies \left[\hat{\mathbf{L}}^2, \hat{L}_x\right] = 0
\end{aligned} \tag{18}$$

The same can be proven for $\hat{L}_{y,z}$.
To prove $\left[\hat{L}_z, \hat{L}_\pm\right] = \pm\hbar\hat{L}_\pm$ *let us use the definition* $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ *[Eq. (4.58)] of the ladder operators. Then*

$$\begin{aligned}
\left[\hat{L}_z, \hat{L}_\pm\right] &= \left[\hat{L}_z, \hat{L}_x \pm i\hat{L}_y\right] \\
&= \left[\hat{L}_z, \hat{L}_x\right] \pm i\left[\hat{L}_z, \hat{L}_y\right] \\
&= i\hbar\hat{L}_y \pm i\left(-i\hbar\hat{L}_x\right) \\
&= \pm\hbar\left(\hat{L}_x \pm i\hat{L}_y\right) \\
&\implies \left[\hat{L}_z, \hat{L}_\pm\right] = \pm\hbar\hat{L}_\pm
\end{aligned} \tag{19}$$

To prove $\left[\hat{\mathbf{L}}^2, \hat{L}_\pm\right] = 0$

$$\begin{aligned}
\left[\hat{\mathbf{L}}^2, \hat{L}_\pm\right] &= \left[\hat{\mathbf{L}}^2, \hat{L}_x \pm \hat{L}_y\right] \\
&= \underbrace{\left[\hat{\mathbf{L}}^2, \hat{L}_x\right]}_{\equiv 0} \pm \underbrace{\left[\hat{\mathbf{L}}^2, \hat{L}_y\right]}_{\equiv 0} \\
\implies & \left[\hat{\mathbf{L}}^2, \hat{L}_\pm\right] = 0
\end{aligned} \tag{20}$$

One could also show that

$$\begin{aligned}
\hat{L}_\pm \hat{L}_\mp &= \hat{L}_x^2 + \hat{L}_y^2 \mp i\left[\hat{L}_x, \hat{L}_y\right] \\
&= \hat{L}_x^2 + \hat{L}_y^2 \pm \hbar \hat{L}_z
\end{aligned}$$

Thus,

$$\hat{\mathbf{L}}^2 = \hat{L}_\pm \hat{L}_\mp + \hat{L}_z^2 \mp \hbar \hat{L}_z \tag{21}$$

(d) *Suppose that* $\left[\hat{A}, \hat{B}\right] = c \in \mathbb{C}$ *is just a number. Consider a function* $f(x)$ *with convergent Taylor series and its derivative* $f'(x) = df(x)/dx$. *Show that* $\left[f(\hat{A}), \hat{B}\right] = cf'(\hat{A})$.

Solution :Before attempting the solution for a general function f(x), it is easier to show that $\left[\hat{A}, \hat{B}^n\right] = n\hat{B}^{n-1}\left[\hat{A}, \hat{B}\right]$

$$\begin{aligned}
\left[\hat{A}, \hat{B}^n\right] &= \hat{B}^{n-1}\left[\hat{A}, \hat{B}\right] + \left[\hat{A}, \hat{B}^{n-1}\right]\hat{B} \\
&= \hat{B}^{n-1}\left[\hat{A}, \hat{B}\right] + \hat{B}^{n-2}\left[\hat{A}, \hat{B}\right]\hat{B} + \left[\hat{A}, \hat{B}^{n-2}\right]\hat{B}^2 \\
\implies & \left[\hat{A}, \hat{B}^n\right] = \sum_{i=0}^{n-1} \hat{B}^{n-i-1}\left[\hat{A}, B\right]\hat{B}^i
\end{aligned} \tag{22}$$

To show that

$$\left[f(\hat{A}), \hat{B}\right] = f'(\hat{A})\left[\hat{A}, \hat{B}\right], \tag{23}$$

From Taylor series expansion $f(A) = f(0) + A\frac{f'(0)}{1!} + A^2\frac{f''(0)}{2!} + \ldots\ldots$

$$
\begin{aligned}
&\big[f(\hat{A}),\hat{B}\big] = -\big[\hat{B}, f(0) + \hat{A}\frac{f'(0)}{1!} + \hat{A}^2\frac{f''(0)}{2!} + ...\big] \\
&= -\big[\hat{B}, f(0)\big] - \big[\hat{B}, \hat{A}\frac{f'(0)}{1!}\big] - \big[\hat{B}, \hat{A}^2\frac{f''(0)}{2!}\big] - .... \\
&\textit{using } (22), \ \textit{we get} \\
&= -\big[\hat{B},\hat{A}\big]f'(0) + 2\hat{A}\big[\hat{B},\hat{A}\big]\frac{f''(0)}{2!} + 3\hat{A}^2\big[\hat{B},\hat{A}\big]\frac{f'''(0)}{3!} + ... \\
&= -\left[f'(0) + A\frac{f''(0)}{1!} + A^2\frac{f''(0)}{2!} + ...\right]\big[\hat{B},\hat{A}\big] \\
&\implies \big[f(\hat{A}),\hat{B}\big] = f'(\hat{A})\big[\hat{A},\hat{B}\big]
\end{aligned} \tag{24}
$$

(2) Two-dimensional Harmonic oscillator in polar coordinates [10pts]: Consider the isotropic quantum harmonic oscillator in two dimensions using planar polar coordinates.

(a) Convert the Hamiltonian from cartesian coordinates:

$$
\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2), \tag{25}
$$

to planar polar coordinates $r = \sqrt{x^2 + y^2}$, $\varphi = \operatorname{atan2}(y, x)$.

Solution: The isotropic two-dimensional quantum harmonic oscillator Hamiltonian in cartesian coordinates is given by:

$$
\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + m\omega^2\frac{1}{2}(x^2 + y^2). \tag{26}
$$

To find the Laplacian in 2D in terms of polar coordinate let we start with $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$. *The Cartesian coordinates are related to polar coordinates by* $x = r\cos\varphi, y = r\sin\varphi$ *and the reverse relations are given by* $r = \sqrt{x^2 + y^2}$ *and* $\varphi = \tan^{-1}\left(\frac{y}{x}\right)$.
Also $\frac{\partial r}{\partial x} = \frac{x}{\sqrt{x^2+y^2}} = \cos\varphi$ *and* $\frac{\partial \varphi}{\partial x} = -\frac{y}{x^2+y^2} = -\frac{\sin\varphi}{r}$.
Using the chain rule, we know that:

$$
\frac{\partial u}{\partial x} = \frac{\partial u}{\partial r}\cdot\frac{\partial r}{\partial x} + \frac{\partial u}{\partial \varphi}\cdot\frac{\partial \varphi}{\partial x} = \cos\varphi\frac{\partial u}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial u}{\partial \varphi}
$$

We also observe that

$$\frac{\partial}{\partial x} = \cos\varphi\frac{\partial}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial}{\partial\varphi} \quad and \quad \frac{\partial}{\partial y} = \sin\varphi\frac{\partial}{\partial r} + \frac{\cos\varphi}{r}\frac{\partial}{\partial\varphi}$$

Hence we can write

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) = \left(\cos\varphi\frac{\partial}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial}{\partial\varphi}\right)\left(\cos\varphi\frac{\partial u}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial u}{\partial\varphi}\right) \\ &= \cos^2\varphi\frac{\partial^2 u}{\partial r^2} - 2\sin\varphi\cos\varphi\frac{1}{r}\frac{\partial^2 u}{\partial r\partial\varphi} + \sin^2\varphi\frac{1}{r^2}\frac{\partial^2 u}{\partial\varphi^2} + \sin^2\varphi\frac{1}{r}\frac{\partial u}{\partial r} + 2\sin\varphi\cos\varphi\frac{1}{r^2}\frac{\partial u}{\partial\varphi}\end{aligned} \tag{27}$$

Similarly, we also observe that,

$$\frac{\partial^2 u}{\partial y^2} = \sin^2\varphi\frac{\partial^2 u}{\partial r^2} + 2\sin\varphi\cos\varphi\frac{1}{r}\frac{\partial^2 u}{\partial r\partial\varphi} + \cos^2\varphi\frac{1}{r^2}\frac{\partial^2 u}{\partial\varphi^2} + \cos^2\varphi\frac{1}{r}\frac{\partial u}{\partial r} - 2\sin\varphi\cos\varphi\frac{1}{r^2}\frac{\partial u}{\partial\varphi} \tag{28}$$

Adding the two expressions, we finally get the transformed equation,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial\varphi^2} \tag{29}$$

Thus, we can rewrite the Hamiltonian in polar coordinates as

$$\hat{H} = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right) + \frac{m\omega^2}{2}r^2. \tag{30}$$

(b) With the Ansatz $\phi_{n\ell}(r,\varphi) = \Phi_{n\ell}(r)A_\ell(\varphi)$, use separation of variables to split the TISE into an angular and a radial part. Solve the angular equation, using techniques and boundary conditions similar to what you learnt regarding angular momentum states in 3D. Discuss how one would go about solving the radial equation schematically (you do not have to solve it).

Solution: Starting with TISE and inserting the product Ansatz we have

$$\begin{aligned}&\hat{H}\phi_{n\ell}(r,\varphi) = E_{n\ell}\phi_{n\ell}(r,\varphi) \\ &\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right)\phi_{n\ell}(r,\varphi) + \frac{m\omega^2}{2}r^2\phi_{n\ell}(r,\varphi) = E_{n\ell}\phi_{n\ell}(r,\varphi) \\ &\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right)\phi_{n\ell}(r,\varphi) + \frac{m\omega^2}{2}r^2\phi_{n\ell}(r,\varphi) - E_{n\ell}\phi_{n\ell}(r,\varphi) = \frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial\varphi^2}\phi_{n\ell}(r,\varphi) \\ &\Rightarrow -\frac{r^2}{\Phi_{n\ell}(r)}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right) + \frac{2m}{\hbar^2}\left(\frac{m\omega^2}{2}r^4 - r^2E_{n\ell}\right) = \frac{1}{A_\ell(\varphi)}\frac{\partial^2}{\partial\varphi^2}A_\ell(\varphi) = const = -\mu^2\,(say)\end{aligned} \tag{31}$$

from this we get angular Schrödinger equation which gives us the solution

$$\begin{aligned}
&\frac{\partial^2}{\partial\varphi^2} A_\ell(\varphi) = -\mu^2 A_\ell(\varphi) \\
\Rightarrow &A_\ell(\varphi) = \exp(-i\mu\varphi).
\end{aligned} \tag{32}$$

Since the coordinate φ is periodic over $[02\pi]$ and the wavefunction must be continuous, we require that $A_\ell(\varphi = 0) = A_\ell(\varphi = 2\pi)$, which implies that μ must be an integer.

The radial Schrödinger equation is more complex:

$$\begin{aligned}
&-r^2\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right) + \frac{2m}{\hbar^2}\left(\frac{m\omega^2}{2} r^4 - r^2 E_{n\ell}\right)\Phi_{n\ell}(r) = -\mu^2 \Phi_{n\ell}(r) \\
\Rightarrow &\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{m^2\omega^2}{\hbar^2} r^2 + \frac{2mE_{n\ell}}{\hbar^2}\right)\Phi_{n\ell}(r) = \frac{\mu^2}{r^2}\Phi_{n\ell}(r)
\end{aligned} \tag{33}$$

Proceeding with the usual program (as done in the lecture for the harmonic oscillator or the Hydrogen atom), we could first inspect the limiting case $r \to \infty$ in equation (33), which gives:

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{m^2\omega^2}{\hbar^2} r^2\right)\Phi_{n\ell}(r) = 0 \tag{34}$$

and subsequently $r \to 0$, yielding

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{\mu^2}{r^2}\right)\Phi_{n\ell}(r) = 0. \tag{35}$$

Using solutions in these limiting cases, one could make a refined Ansatz in the hope to transform the complete equation Eq. (33) into a neater one. However since both limiting cases already give rise to special functions in their solution, we shall avoid the discussion here.

Alternatively one can just solve Eq. (33) on a computer. If you are interested you can surely find the discussion of their analytical solution online.

(3) Two-dimensional Harmonic oscillator in the Schrödinger and Heisenberg pictures [10pts]:

(a) Write down all eigenstates and eigenenergies of the Hamiltonian (25) by adapting the discussion of section 4.1.1.

Solution: The 2D TISE with inserted potential reads

$$E\phi(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}m\omega^2\left(x^2 + y^2\right)\right)\phi(\mathbf{r}) \tag{36}$$

Since we can write this as a sum of x, y terms, we make the usual factorisation Ansatz $\phi(\mathbf{r}) = \phi_{n_x}(x)\phi_{n_y}(y)$. Inserting this into (36) *and reshuffling terms, we can write this as*

$$E\phi_{n_x}(x)\phi_{n_y}(y) = \left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2\right)\phi_{n_x}(x)\right]\phi_{n_y}(y) + \left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega^2y^2\right)\phi_{n_y}(y)\right]\phi_{n_x}(x) \tag{37}$$

We can now move all the x-dependent pieces on the LHS and y dependent ones on the RHS and then conclude that LHS $= C =$ RHS using separation of variables (see section 1.6.5.):

$$\frac{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2\right)\phi_{n_x}(x)}{\phi_{n_x}(x)} = \text{const} = E - \frac{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega^2y^2\right)\phi_{n_y}(y)}{\phi_{n_y}(y)} \tag{38}$$

we finally reach two separate TISEs for each dimension:

$$E_{n_x}\phi_{n_x}(x) = (-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \underbrace{\frac{1}{2}m\omega^2x^2}_{\equiv V_x(x)})\phi_{n_x}(x) \tag{39}$$

$$E_{n_y}\phi_{n_y}(y) = (-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \underbrace{\frac{1}{2}mw^2y^2}_{\equiv V_y(y)})\phi_{n_y}(y) \tag{40}$$

such that $E = E_{n_z} + E_{n_y}$. Eq.(39) and Eq.(40) are the TISE of the harmonic oscillator, hence we know that $\phi_{n_x}(x)$ and $\phi_{n_y}(y)$ are the usual $1D$ eigenfunctions of the harmonic oscillator. Altogether our $2D$ eigenstates are thus

$$\phi(\mathbf{r}) = \phi_{n_x}(x)\phi_{n_y}(y), \tag{41}$$

with two discrete indices n_x and n_y. Equation for the energy along x and y :

$$E_{n_x} = \left(n_x + \frac{1}{2}\right)\hbar\omega, \tag{42}$$

$$E_{n_y} = \left(n_y + \frac{1}{2}\right)\hbar\omega \tag{43}$$

The total energy is $E = E_{n_x} + E_{n_y}$

(b) Consider the initial state

$$\Psi(x, y, t=0) = \frac{1}{2}\big[\phi_0(x) + \phi_1(x)\big]\big[\phi_0(y) + i\phi_1(y)\big]. \tag{44}$$

[OR SUCH, adjust to get circular motion] Visualise this state (e.g. with `mathematica`) and discuss its physical meaning. Then find the time evolution of $\langle \hat{\mathbf{r}} \rangle$ in the Schrödinger picture and interpret/discuss the result.

Solution: The state at time t is given by

$$|\,\Psi(t)\,\rangle = \frac{1}{2}\big[e^{-iE_0t}|\,\phi_0^x\,\rangle + e^{-iE_1t}|\,\phi_1^x\,\rangle\big]\big[e^{-iE_0t}|\,\phi_0^y\,\rangle + ie^{-iE_1t}|\,\phi_1^y\,\rangle\big]. \tag{45}$$

From this, to calculate

$$\langle\,\psi(t)\,|\hat{\mathbf{r}}|\,\psi(t)\,\rangle = \langle\,\psi(t)\,|x\hat{i} + y\hat{j}|\,\psi(t)\,\rangle \tag{46}$$

Evaluating both terms independently

$$\begin{aligned}
&\langle\,\psi(t)\,|x|\,\psi(t)\,\rangle \\
=&\frac{1}{4}\big[\langle\,\phi_0^x\,|e^{iE_0t} + \langle\,\phi_1^x\,|e^{iE_1t}\big]\big[\langle\,\phi_0^y\,|e^{iE_0t} - i\langle\,\phi_1^y\,|e^{iE_1t}\big]x \\
&\big[e^{-iE_0t}|\,\phi_0^x\,\rangle + e^{-iE_1t}|\,\phi_1^x\,\rangle\big]\big[e^{-iE_0t}|\,\phi_0^y\,\rangle + ie^{-iE_1t}|\,\phi_1^y\,\rangle\big] \\
=&\frac{1}{2}\big[\langle\,\phi_0^x\,|x|\,\phi_1^x\,\rangle e^{i(E_0-E_1)t} + \langle\,\phi_1^x\,|x|\,\phi_0^x\,\rangle e^{i(E_1-E_0)t}\big] \\
=&\frac{1}{2}\big[\frac{\sigma}{\sqrt{2}}e^{i(E_0-E_1)t} + \frac{\sigma}{\sqrt{2}}e^{i(E_1-E_0)t}\big] \\
=&\frac{\sigma}{\sqrt{2}}\cos{(E_1-E_0)t}
\end{aligned} \tag{47}$$

$$\begin{aligned}
&\langle\,\psi(t)\,|y|\,\psi(t)\,\rangle \\
=&\frac{1}{4}\big[\langle\,\phi_0^x\,|e^{iE_0t} + \langle\,\phi_1^x\,|e^{iE_1t}\big]\big[\langle\,\phi_0^y\,|e^{iE_0t} - i\langle\,\phi_1^y\,|e^{iE_1t}\big]y \\
&\big[e^{-iE_0t}|\,\phi_0^x\,\rangle + e^{-iE_1t}|\,\phi_1^x\,\rangle\big]\big[e^{-iE_0t}|\,\phi_0^y\,\rangle + ie^{-iE_1t}|\,\phi_1^y\,\rangle\big] \\
=&\frac{i}{2}\big[\langle\,\phi_0^y\,|y|\,\phi_1^y\,\rangle e^{i(E_0-E_1)t} - \langle\,\phi_1^y\,|y|\,\phi_0^y\,\rangle e^{i(E_1-E_0)t}\big] \\
=&\frac{i}{2}\big[\frac{\sigma}{\sqrt{2}}e^{i(E_0-E_1)t} - \frac{\sigma}{\sqrt{2}}e^{i(E_1-E_0)t}\big] \\
=&\frac{\sigma}{\sqrt{2}}\sin{(E_1-E_0)t}
\end{aligned} \tag{48}$$

combinedly we see

$$\langle\,\psi(t)\,|\hat{\mathbf{r}}|\,\psi(t)\,\rangle = \frac{\sigma}{\sqrt{2}}\big[\cos{(E_1-E_0)t}\hat{i} + \sin{(E_1-E_0)t}\hat{j}\big] \tag{49}$$

(c) Now, let us reproduce these results in the Heisenberg picture. Start by finding the Heisenberg equations of motion for operators $\hat{x}_H(t)$, $\hat{y}_H(t)$, $\hat{p}_{xH}(t)$, $\hat{p}_{yH}(t)$.

Solution: Using $\left[\hat{x}_k, \hat{x}_\ell\right] = 0$, $\left[\hat{p}_k, \hat{p}_\ell\right] = 0$ *and* $\left[\hat{x}_k, \hat{p}_\ell\right] = i\hbar\delta_{k\ell}$, *where* $k, \ell \in \{x, y\}$ *here, we find:*

$$i\hbar\dot{\hat{x}}_H(t) = \left[\hat{x}_H, \hat{H}\right] = i\hbar\left[\hat{x}_H, \frac{\hat{p}_x^2}{2m}\right] \overset{Eq.\ (3.46)}{=} i\hbar\frac{2\hat{p}_x}{2m}\left[\hat{x}_H, p_x^2\right] = i\hbar\frac{\hat{p}_x}{/}m \tag{50}$$

hence

$$\dot{\hat{x}}_H(t) = \frac{\hat{p}_{xH}(t)}{m}, \tag{51}$$

$$\dot{\hat{y}}_H(t) = \frac{\hat{p}_{yH}(t)}{m}, \tag{52}$$

$$\dot{\hat{p}}_{xH}(t) = -m\omega^2\hat{x}_H(t), \tag{53}$$

$$\dot{\hat{p}}_{yH}(t) = -m\omega^2\hat{y}_H(t), \tag{54}$$

where the other three equations follow similarly. We see that these take exactly the same form as the classical Hamilton's equations (see PHY305) for the same problem.

(d) Solve those, to find a solution for the time-dependent operators in terms of operators at time $t = 0$. *Hint: To solve differential equations involving operators, pretend they are not operators initially, then confirm the solution holds also if they are, possibly worrying about commutators.*

Solution: Since Eq. (51)-Eq. (54) take the same form as the classical equations, we solve them in the same way. Differentiating Eq. (51) wrt. time again and inserting Eq. (53) and similarly for the x-equations we reach

$$\ddot{\hat{x}}_H(t) = -\omega^2\hat{x}_H(t), \tag{55}$$

$$\ddot{\hat{y}}_H(t) = -\omega^2\hat{y}_H(t), \tag{56}$$

from which we write

$$\hat{x}_H(t) = \hat{x}_H(0)\cos(\omega t) + \frac{1}{m\omega}\hat{p}_H(0)\sin(\omega t),$$

$$\hat{y}_H(t) = \hat{y}_H(0)\cos(\omega t) + \frac{1}{m\omega}\hat{p}_H(0)\sin(\omega t). \tag{57}$$

The prefactor of the sine terms follows by inserting the expression into e.g. Eq. (51) and looking at $t = 0$.

(e) Recalculate $\langle \hat{\mathbf{r}} \rangle$ in the Heisenberg picture and confirm your result from (c).

Solution: We find $\langle \hat{\mathbf{r}} \rangle$ now by taking the expectation value of the time-dependent operators in Eq. (57) in the time-independent initial state Eq. (44). We find

$$\langle \Psi | \hat{x}_H(t) | \Psi \rangle = \langle \Psi | \hat{x}_H(0) | \Psi \rangle \cos(\omega t) + \frac{1}{m\omega} \langle \Psi | \hat{p}_H(0) | \Psi \rangle \sin(\omega t) \tag{58}$$

Then we use that $\langle \phi_n | x | \phi_n \rangle = 0$ and $\langle \phi_n | p_x | \phi_n \rangle = 0$ by symmetry, where ϕ_n are the 1D oscillator eigenstates. Hence

$$\begin{aligned}
\langle \Psi | \hat{x}_H(0) | \Psi \rangle &= \frac{1}{\sqrt{2}} (\langle \phi_0 | + \langle \phi_1 |) \hat{x}_H(0) \frac{1}{\sqrt{2}} (| \phi_0 \rangle + | \phi_1 \rangle) \\
&= \frac{1}{2} (\langle \phi_0 | \hat{x}_H(0) | \phi_1 \rangle + cc.) \\
&= \frac{1}{2} \left(\int_{-\infty}^{\infty} dx \, x \, \phi_0^*(x) \phi_1(x) + cc \right) \\
&= \frac{1}{2} \left(\frac{1}{(2\pi\sigma^2)^{1/2}} \underbrace{\int_{-\infty}^{\infty} dx \, x \, 2 \frac{x}{\sigma} e^{-\frac{x^2}{\sigma^2}}}_{=\sqrt{\pi}\sigma^2} + cc \right) = \frac{\sigma}{\sqrt{2}}
\end{aligned} \tag{59}$$

In the first line we had split off the y-dependent part such that it is normalised to one, and since no operator depends on y, the integration over y gives trivially one. Similarly

$$\langle \Psi | \hat{p}_{xH}(0) | \Psi \rangle = \frac{1}{2} \left(-i\hbar \underbrace{\int_{-\infty}^{\infty} dx \, \phi_0^*(x) \frac{\partial}{\partial x} \phi_1(x)}_{=1/(\sqrt{2}\sigma)} + cc \right) = 0, \tag{60}$$

vanishing due to the "+cc", and we can show $\langle \Psi | \hat{y}_H(0) | \Psi \rangle = 0$ and $\langle \Psi | \hat{p}_{yH}(0) | \Psi \rangle = \frac{1}{\sqrt{2}\sigma}$. Using $\sigma = \sqrt{\hbar/(m\omega)}$ we can again write the total result as

$$\langle \hat{\mathbf{r}} \rangle = \frac{\sigma}{\sqrt{2}} \begin{pmatrix} \cos(\omega t) \\ \sin(\omega t) \end{pmatrix} \tag{61}$$

*describing circular motion. See **anim.gif** provided, for the corresponding evolution of the probability density.*

Note that you only know how to take expectation values of the operator at time $t = 0$, e.g. $\hat{x}_H(0)$ in a state such as Eq. (44). It would be wrong to write e.g. $\langle \Psi | \hat{x}_H(t) | \Psi \rangle = \int dx \, \Psi^*(x) x \Psi(x)$ directly, you first need to find an equation such as Eq. (57) and then use $\langle \Psi | \hat{x}_H(0) | \Psi \rangle = \int dx \, \Psi^*(x) x \Psi(x)$, which is correct.

(4) Circular Hydrogen states: [**10pts**] The code `Assignment6_program_draft_v1.nb` can setup all electronic eigenfunctions of the Hydrogen atom.

(a) Visualise the probability density, and the complex phase in what is called a "circular Rydberg state" $n = 10$, $l = 9$, $m = 9$ using smartly chosen 2D or 1D cuts through those.

Solution: First we inspect the density and phase of the wavefunction in the xy-plane only, as shown in Fig. 2. We see that the density is only significant in a circular shaped orbit at a roughly fixed distance. Along that circle, the phase varies with a constant phase gradient (indicating a constant probability current along the circular path). To see this in a bit more detail, we can plot a 1D cut through the density along the x axis as shown in Fig. 3. The probability density almost looks like a Gaussian centered on the target radius (but only almost). When going away from the xy plane (i.e. along the angle θ), we see that the nonvanishing density region extends a little away from the xy plane, but becomes very small there. We could explore further and confirm that the electron really only is likely to be found in close proximity to the xy-plane.

(b) Calculate the probability current density in that state. With all information together, discuss the corresponding physical state of the electron.

Solution: The probability current vector in 3-D is given as

$$\begin{aligned}
\hat{\boldsymbol{J}} &= \frac{i\hbar}{2m}\left(\Psi\boldsymbol{\nabla}\Psi^* - \Psi^*\boldsymbol{\nabla}\Psi\right) = J_r\mathbf{e}_r + J_\theta\mathbf{e}_\theta + J_\phi\mathbf{e}_\phi, \text{ with} \\
J_r &= \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial r} - \Psi^*\frac{\partial\Psi}{\partial r}\right) \\
J_\theta &= \frac{i\hbar}{2mr}\left(\Psi\frac{\partial\Psi^*}{\partial\theta} - \Psi^*\frac{\partial\Psi}{\partial\theta}\right) \\
J_\phi &= \frac{i\hbar}{2mr\sin\theta}\left(\Psi\frac{\partial\Psi^*}{\partial\phi} - \Psi^*\frac{\partial\Psi}{\partial\phi}\right),
\end{aligned} \tag{62}$$

where we have used Eq. (4.35) of the lecture.

We can chose to calculate these using mathematica, see `Assignment6_program_solution_v4.nb`. There we see that the probability current density indicates a probability flux moving in a circle, since only J_ϕ is nonzero, while $J_\theta = J_r = 0$.

Together with the angular momentum in this state pointing very closely to the positive z-axis, everything reminds us of a classical particle orbiting in a circle, such that at all times $\mathbf{r} \times \mathbf{p} \approx L\mathbf{e}_z$. Note, however that it still is a steady state, so no charge or current density changes at any time, and the electron already is "everywhere on the circle" at all times. Nonetheless the picture of it orbiting the nucleus in the clockwise or counterclockwise direction is quite appropriate.

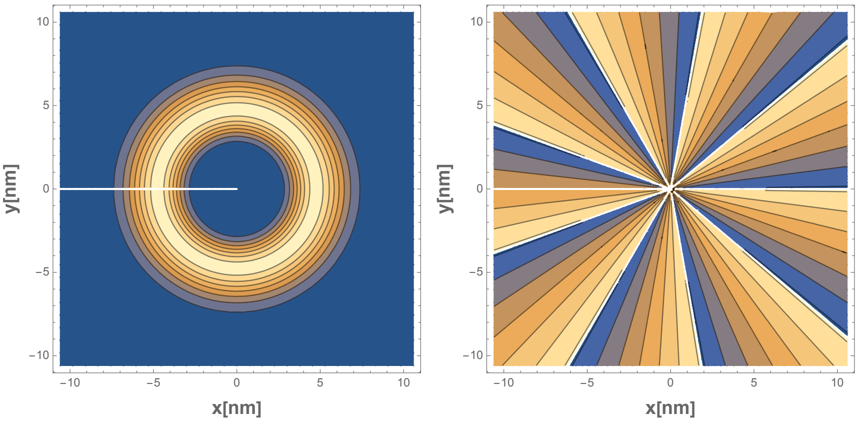

Figure 2: (left) Electron position probability density $|\phi_{n\ell m}(x, y, 0)|^2$ in the $z = 0$ plane (bright yellow = high, blue = zero). (right) Complex phase of the wavefunction $\arg[\phi_{n\ell m}] \sim e^{im\varphi}$ in the $z = 0$ plane (bright yellow 0, blue 2π). .

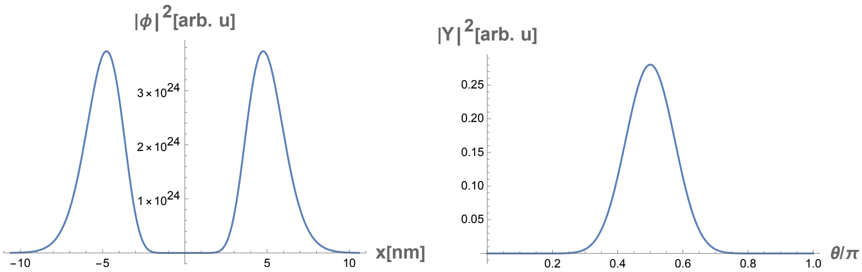

Figure 3: (left) The same as left panel in Fig. 2, but concentrating on a 1D cut along x. (right) Probability density $|\phi_{n\ell m}(R, \theta, 0)|^2$ along the polar angle θ using spherical polar coordinates, with R fixed to the central radius of the ring visible in Fig. 2.

(c) Discuss the corresponding charge and current density in this state (without calculation), their time-dependences, and finally how you can reconcile all earlier results in this question with a stable atom.

Solution: The charge density would be $\rho(\mathbf{r}) = -e|\phi|^2$, where we have multiplied the position probability density of the electron with its charge. Since ϕ is a stationary state, nothing changes. Similarly, we can obtain the current density by multiplying the probability current with the electron charge. Also that does not change. Since Maxwell's equations require either of these quantities to change for the emission of radiation, the atom can remain stable in such an orbit within a classical picture of electro-magnetism. When quantising the electro-magnetic field, you shall see that this is no longer the case, which gives rise to spontaneous decay. Nonetheless, circular Rydberg states can be very long lived, up to seconds!