# PHY 303, I-Semester 2023/24, Tutorial 6 solution

**Stage 1** **(Atoms in a waveguide)** At very low temperatures, it is possible to trap atoms in a laser-beam through a technique called optical trapping. Assuming a laser beam that is axially symmetric around the z-axis as shown below, we can approximately write the potential as:

$$V(\mathbf{r}) = \frac{1}{2} m\omega_\perp^2 \left(x^2 + y^2\right). \tag{1}$$

(note that it does not depend on $z$).

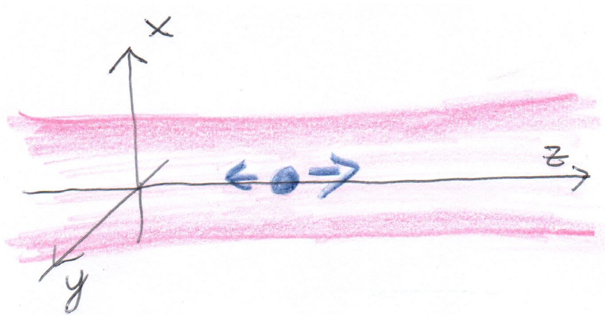


Figure 1: The atom (blue) is attracted to high laser intensity (pink), which drops with $r = \sqrt{x^2 + y^2}$, thus the laser beam along the $z$ axis forms a waveguide for the atom, in which it can move freely along $z$ (arrows).

(a) Adapt the discussion of week8, section 4.1.1. to this scenario: What are the three one-dimensional TISEs which are equivalent to the 3D one? What form do the eigenstates take? Which quantum numbers control them and what do they physically imply. Give an equation for the energy.
*Solution: The 3D TISE with inserted potential reads*

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

*Since we can write this as a sum of x,y,z terms, we make the usual factorisation Ansatz* $\phi(\mathbf{r}) = \phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z)$*. Inserting this into (2) and reshuffling terms, we can write this as*

$$\begin{aligned} E\phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z) = &\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega_\perp^2 x^2\right)\phi_{n_x}(x)\right]\phi_{n_y}(y)\phi_{n_z}(z) \\ &+ \left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2} m\omega_\perp^2 y^2\right)\phi_{n_y}(y)\right]\phi_{n_x}(x)\phi_{n_z}(z) \\ &+ \left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\right)\phi_{n_z}(z)\right]\phi_{n_x}(x)\phi_{n_y}(y). \end{aligned} \tag{3}$$

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

$$\frac{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega_\perp^2 x^2\right)\phi_{n_x}(x)}{\phi_{n_x}(x)} = const = E - \frac{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\frac{1}{2}m\omega_\perp^2 y^2\right)\phi_{n_y}(y)}{\phi_{n_y}(y)} - \frac{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\right)\phi_{n_z}(z)}{\phi_{n_z}(z)}. \tag{4}$$

*Doing the same again to separate the y and the z dependence, we finally reach three separate TISEs for each dimension:*

$$E_{n_x}\phi_{n_x}(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\underbrace{\frac{1}{2}m\omega_\perp^2 x^2}_{\equiv V_x(x)}\right)\phi_{n_x}(x) \tag{5}$$

$$E_{n_y}\phi_{n_y}(y) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\underbrace{\frac{1}{2}mw_\perp^2 y^2}_{\equiv V_y(y)}\right)\phi_{n_y}(y) \tag{6}$$

$$E_{n_z}\phi_{n_z}(z) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}+\underbrace{0}_{=V_z(z)}\right)\phi_{n_z}(z) \tag{7}$$

*such that $E = E_{n_x} + E_{n_y} + E_{n_z}$. Eq.5 and Eq. 6 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. We can thus use the discussion of section 2.1. to write the eigenstates of Eq. (7) as*

$$\phi_{k_z(z)} = \mathcal{N}e^{ik_z z}, \tag{8}$$

*where $k_z^2 = \frac{2mE}{\hbar^2}$. Alltogether our 3D eigenstates are thus*

$$\phi(\mathbf{r}) = \mathcal{N}e^{ik_z z}\phi_{n_x}(x)\phi_{n_y}(y), \tag{9}$$

*with two discrete indices $n_x$ and $n_y$ and one continuous one (wavenumber) $k_z$. Equation for the energy along x and y:*

$$E_{n_x} = \left(n_x+\frac{1}{2}\right)\hbar\omega_\perp,$$
$$E_{n_y} = \left(n_y+\frac{1}{2}\right)\hbar\omega_\perp$$

*Equation for the energy along along z:*

$$E_{n_z} = \frac{\hbar^2 k_z^2}{2m}$$

(b) Now consider only states for which the energy difference $\Delta E$ to the ground-state is $\Delta E \ll \hbar\omega_\perp$, which subset of states from (a) does this condition select?
*Solution: As per energy equation found in (a)*

$$E = \left(n_x + \frac{1}{2}\right)\hbar\omega + \left(n_y + \frac{1}{2}\right)\hbar\omega + \frac{\hbar^2 k_z^2}{2m}$$

*so the ground state (lowest energy state) has $n_x = 0$, $n_y = 0$ and $k_z = 0$. The condition given thus prohibits $n_x > 0$ or $n_y > 0$, only $n_x = n_y = 0$ is possible. Additionally $\frac{\hbar^2 k_z^2}{2m} \ll \hbar\omega_\perp$, which constrains $k_z$. Inserting the explicit harmonic oscillator wavefunctions thus yields*

$$\phi_{k_z}(\mathbf{r}) = \mathcal{N} e^{-\frac{x^2}{2\sigma_\perp^2}} e^{-\frac{y^2}{2\sigma_\perp^2}} e^{ik_z z} \tag{10}$$

*with $\sigma_\perp = \sqrt{\hbar/(m\omega_\perp)}$.*

(c) Suppose you want to describe an atom in this waveguide, localized near a position $z = z_0$ in the waveguide and moving with a velocity $v_z$ in the z-direction. Which 3D wavefunction would describe such an atom?
*Solution: A 3D gaussian would describe such an atom moving along z with width $\sigma_z$ centered on $z_0$ given by*

$$\Phi(\mathbf{r}) = \frac{1}{(\pi\sigma_\perp^2)1/4} e^{-\frac{x^2}{2\sigma_\perp^2}} \frac{1}{(\pi\sigma_\perp^2)1/4} e^{-\frac{y^2}{2\sigma_\perp^2}} \frac{1}{(\pi\sigma_z^2)1/4} e^{-\frac{(z-z_0)^2}{2}\sigma_z^2} e^{-ik_z(z-z_0)}, \tag{11}$$

*where $k_z = mv_z/\hbar$ and we have taken our known normalisation constants for Gaussian wavefunctions or the oscillator ground-state. Note that we can construct this as a wavepacket out of planewaves in the z-direction (10) exactly as we did in week 5 (just multiplying everything with the transverse oscillator ground-state in the x and y directions).*

(d) Rewrite the 3D expectation value of the operator for the gravitational potential energy $V_{\text{grav}}$ in a state such as what you found in (c). Lets consider two cases

(i) $V_{\text{grav}}(\mathbf{r}) = mgz$ (direction of gravity along z), (12)

(ii) $V_{\text{grav}}(\mathbf{r}) = mgx$ (direction of gravity along x). (13)

You do not need to do any non-trivial 1D integrations. *Hint: Trivial means the answer is 0 or 1.*
*Solution: (i) The 3D expectation value is* $E_{pot} = \int d^3\mathbf{r}\ \Phi^*(\mathbf{r})V_{grav}(\mathbf{r})\Phi(\mathbf{r})$ *into which we have to insert* $\Phi(\mathbf{r})$ *from Eq. (11). This starts off as*

$$E_{pot} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz$$
$$\left[\frac{1}{(\pi\sigma_\perp^2)^{1/4}} e^{-\frac{x^2}{2\sigma_\perp^2}} \frac{1}{(\pi\sigma_\perp^2)^{1/4}} e^{-\frac{y^2}{2\sigma_\perp^2}} \frac{1}{(\pi\sigma_z^2)^{1/4}} e^{-\frac{(z-z_0)^2}{2}\sigma_z^2} e^{ik_z(z-z_0)}\right] mgz$$
$$\times \left[\frac{1}{(\pi\sigma_\perp^2)^{1/4}} e^{-\frac{x^2}{2\sigma_\perp^2}} \frac{1}{(\pi\sigma_\perp^2)^{1/4}} e^{-\frac{y^2}{2\sigma_\perp^2}} \frac{1}{(\pi\sigma_z^2)^{1/4}} e^{-\frac{(z-z_0)^2}{2}\sigma_z^2} e^{ik_z(z-z_0)}\right] \tag{14}$$

*Luckily we can factor this into individual integration involving only a single cartesian coordinate*

$$E_{pot} = \underbrace{\left[\int_{-\infty}^{\infty} dx \frac{1}{(\pi\sigma_\perp^2)^{1/2}} e^{-\frac{x^2}{\sigma_\perp^2}}\right]}_{=\int dx|\phi_0(x)|^2=1} \underbrace{\left[\int_{-\infty}^{\infty} dy \frac{1}{(\pi\sigma_\perp^2)^{1/2}} e^{-\frac{y^2}{\sigma_\perp^2}}\right]}_{=\int dy|\phi_0(y)|^2=1} \left[\int_{-\infty}^{\infty} dz \frac{1}{(\pi\sigma_\perp^2)^{1/2}} e^{-\frac{z^2}{\sigma_z^2}} mgz\right] \tag{15}$$

*In the line above, we see that the* $x$ *and* $y$ *integration just give one as shown, due to the normalisation of the oscillator ground-states in the* $x$ *and* $y$ *direction. Thus in the end we reach*

$$\langle V_{grav}(\mathbf{r})\rangle = \int_{-\infty}^{\infty} dz\ mgz \left[\frac{1}{(\pi\sigma_\perp^2)^{1/2}} e^{-(z-z_0)^2/\sigma_z^2}\right], \tag{16}$$

*which for very small* $\sigma_z$ *will be approximately* $mgz_0$ *(imagine the Gaussian approaches a delta-function or make a drawing).*
*Following similar steps for the potential (ii) we end up with*

$$E_{pot} = \left[\int_{-\infty}^{\infty} dx \frac{1}{(\pi\sigma_\perp^2)^{1/2}} e^{-\frac{x^2}{\sigma_\perp^2}} mgx\right] \underbrace{\left[\int_{-\infty}^{\infty} dy \frac{1}{(\pi\sigma_\perp^2)^{1/2}} e^{-\frac{y^2}{\sigma_\perp^2}}\right]}_{=\int dy|\phi_0(y)|^2=1} \underbrace{\left[\int_{-\infty}^{\infty} dz \frac{1}{(\pi\sigma_\perp^2)^{1/2}} e^{-\frac{z^2}{\sigma_z^2}}\right]}_{=1}$$
$$= \left[\int_{-\infty}^{\infty} dx \frac{1}{(\pi\sigma_\perp^2)^{1/2}} e^{-\frac{x^2}{\sigma_\perp^2}} mgx\right] \tag{17}$$

*The last remaining integral is zero since the integrand is odd, hence now* $E_{pot} = 0$.

### Stage 2 (Angular momentum)

(i) How can you prove in quantum mechanics that angular momentum is conserved if the potential is spherically symmetric?

*Solution: We can see that the Hamiltonian commutes with (all three components of) the Angular momentum operator* $\hat{\mathbf{L}}$. *Hence angular momentum is conserved according to Eq. (3.50). The easiest way to see the initial statement, is to re-write the Hamiltonian in terms of the square of the Angular momentum operator as in Eq. (4.37), and then use Eq. (4.24)*

(ii) Is angular momentum also conserved if the potential is not spherically symmetric? Why/why not?
*Solution: No. Since then we cannot write the Hamiltonian such that it only depends on* $\hat{\mathbf{L}}^2$, *and* $\left[\hat{L}_k, \hat{L}_k\right]$ *may be nonzero.*

(iii) Show the commutator

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z. \tag{18}$$

Do this once based on your knowledge of the commutators of $\hat{r}_k$ and $\hat{p}_\ell$, and once from the definitions via partial derivatives applied onto a testfunction.

*Solution: We have that*

$$\begin{aligned}
\hat{L}_x &= -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \\
\hat{L}_y &= -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \\
\hat{L}_z &= -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).
\end{aligned} \tag{19}$$

*Hence applying the commutator onto a testfunction* $\psi(\mathbf{r})$ *gives*

$$\begin{aligned}
\left[\hat{L}_x, \hat{L}_y\right]\psi(\mathbf{r}) &= (-i\hbar)^2\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) - \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\right]\psi(\mathbf{r}) \\
&= \textit{From here on, use the product rule}
\end{aligned} \tag{20}$$

*Doing that, we arrive at*

$$\begin{aligned}
\left[\hat{L}_x, \hat{L}_y\right]\psi(\mathbf{r}) &= (-i\hbar)^2\left(y\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial y}\right)\psi(\mathbf{r}) \\
&= i\hbar\hat{L}_z\psi(\mathbf{r})
\end{aligned}$$

*Since this is true for* <u>*any*</u> *testfunction, we conclude the operator identity* $\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z$.
*If we directly want to use the known commutation relation* $\left[x_k, p_m\right] = i\hbar\delta_{km}$ *between position and momentum operators, we start instead with the definitions*

$$\begin{aligned}
L_x &= yp_z - zp_y \\
L_y &= zp_x - xp_z.
\end{aligned} \tag{21}$$

*Then we can write*

$$
\begin{aligned}
\left[\hat{L}_x, \hat{L}_y\right] &= [yp_z - zp_y, zp_x - xp_z] \\
&\overset{\text{commutator bi-linear}}{=} [yp_z, zp_x] - [yp_z, xp_x] - [zp_y, zp_x] + [zp_y, xp_z] \\
&\overset{\text{Eq. (3.41)}}{=} y\,[p_z, z]\,p_x + z\,[y, p_x]\,p_z - y\,[p_z, x]\,p_x - x\,[y, p_x]\,p_z \\
&\quad - z\,[p_y, z]\,p_x - z\,[z, p_x]\,p_y + z\,[p_y, x]\,p_z + x\,[z, p_z]\,p_y \\
&= (i\hbar)(-yp_x + xp_y) \\
&= i\hbar\hat{L}_z
\end{aligned}
$$

*In the third equality there would be twice as many terms after applying (3.41), but haven't written any such as* $\left[x_k, x_m\right]$ *that are more obviously zero.*

**Stage 3 (Pictures of time dependence)**

(i) Convince yourself that for time-independent Hamiltonian, $|\,\Psi(t)\,\rangle = \hat{U}(t)|\,\Psi(0)\,\rangle$ solves the TDSE. Here $\hat{U}(t) = \exp\left[-i\hat{H}t/\hbar\right]$ is the time-evolution operator or propagator. Discuss what is meant by exponential of an operator and how we could possible find this in practice.

(ii) Write the time-dependence of a generic expectation value $\langle\,\Psi(t)\,|\hat{O}|\,\Psi(t)\,\rangle$ and thus convince yourself that instead of assuming a time-dependent states and time-independent operator, we could also work with a time-independent state and time-dependent Operator. Which is that operator?

*Solution: See lecture section 3.9.1.*

**Stage 4 (Three-dimensional wavefunctions)** Consider a radially symmetric problem, such that an eigenstate of the Hamiltonian takes the form $\phi(\mathbf{r}) = R(r)Y(\theta, \varphi)$.

(i) Why do we know that the eigenstates takes this form?
*Solution: Since we know that for a radially symmetric problem* $\left[\hat{H}, \hat{L}^2\right] = \left[\hat{H}, \hat{L}_z\right] = 0$*, we know that eigenfunctions are simultaneously eigenfunctions of the Hamiltonian as well as* $\hat{\mathbf{L}}^2$ *and* $\hat{L}_z$*. In week 10 we had derived that such eigenfunctions can be written of the form above, in particular that the* $Y(\theta, \varphi)$ *separately are the eigenfunctions of* $\hat{\mathbf{L}}^2$ *and* $\hat{L}_z$*.*

(ii) Suppose the particle carries a charge $q$. Then the operator for its electric dipole is

$$\hat{\mathbf{d}} = q\hat{\mathbf{r}}. \tag{22}$$

How can you find the expectation value of this dipole? What integration(s) do you have to do? *Hint: You can actually find the answer without any*

*nasty integrations, but the idea here is to write all the steps converting the 3D integration into separate 1D ones, and only then "see" the answer.*
*Solution: The expectation value involves a 3D integration again and its result is a 3D vector:*

$$\begin{aligned}
\langle\, \hat{\mathbf{d}}\, \rangle &= \int d^3\mathbf{r}\;\; \phi^*(\mathbf{r})\hat{\mathbf{d}}\phi(\mathbf{r}) \\
&= q \iiint dr d\theta d\varphi\; r^2 \sin\theta \Bigg[ \begin{pmatrix} r\sin\theta\sin\varphi \\ r\sin\theta\cos\varphi \\ r\cos\theta \end{pmatrix} R(r)^2 Y^*_{l,m}(\theta,\varphi) Y_{l,m}(\theta,\varphi) \Bigg] \\
&\equiv \begin{pmatrix} d_x \\ d_y \\ d_z \end{pmatrix} \qquad (23)
\end{aligned}$$

*I the end we thus find that $\langle \mathbf{d} \rangle = 0$. Let us write $d_x$ tidies up by integration variables*

$$d_x = q \left[ \int_0^\infty dr\; r^2 R(r)^2 \right] \left[ \int_0^\pi d\theta \sin^2\theta \mathcal{N}^2 P_\ell^m(\cos\theta) \right] \left[ \int_0^{2\pi} d\varphi \sin\varphi \right] \quad (24)$$

*We have used that $|Y|^2$ is independent of $\varphi$ [see Eq. (4.51)], and written the shorthand $\mathcal{N}$ for the normalisation factor and phase factor of spherical Harmonnics. We can easily do the $\varphi$ integration, which gives zero, hence $d_x = 0$. Similarly $d_y = 0$. For $d_z$ it is the $\theta$ integration that gives zero (exercise).*
*A shorter way to see this, is to realize that all Hydrogen states have a definite parity. That means that $\phi(\mathbf{r}) = \pm\phi(-\mathbf{r})$. To convince yourself of that, note that in spherical polar coordinates $\mathbf{r} \to -\mathbf{r}$ implies $r \to r$ (unchanged), $\theta \to \pi - \theta$ and $\varphi \to \varphi - \pi$. We have that $Y_\ell^m(\theta,\varphi) \sim e^{im\varphi} P_\ell^m(\cos\theta)$. Since $\cos\theta \to -\cos\theta$ under the above parity transformation, and $e^{im\varphi} \to e^{im\varphi}e^{-im\pi}$ we finally see that $Y_\ell^m(\theta,\varphi) \to Y_\ell^m(\theta,\varphi)(-1)^{|m|}(-1)^o$, where $o$ is the order of the associated Legendre function (note these are either even or odd).*
*Why does this help us? Because $\phi(\mathbf{r}) = \pm\phi(-\mathbf{r})$ implies $|\phi(\mathbf{r})|^2 = +|\phi(-\mathbf{r})|^2$. We thus directly see that $\langle\, \hat{\mathbf{d}}\, \rangle = \int d^3\mathbf{r}\;\; \phi^*(\mathbf{r})\hat{\mathbf{d}}\phi(\mathbf{r}) = 0$, since each piece of the integration at $\mathbf{r}$ is cancelled by the one at $-\mathbf{r}$.*
*The physical meaning of all of this, is that Hydrogen in an eigenstate <u>does not have</u> a permanent dipole moment.*