Oppgave 1

a. With \( \hat{H} = \hat{K} + V = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \), we can write Schrödinger’s time-independent equation on the form

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = [E - V(x)]\psi(x) \quad \text{that is,} \quad \frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} [V(x) - E].
\]

(i) In \textit{classically allowed regions} (where \( E > V(x) \)), we see that the curvature \( \frac{d^2 \psi}{dx^2} \) is negative when \( \psi \) is positive (and vice versa). This means that \( \psi \) must \textit{curve towards} the \( x \)-axis. Examples:

(ii) In \textit{classically forbidden regions} (where \( E < V(x) \)), the curvature has the same sign as \( \psi \). \( \psi \) then will \textit{curve away} from the axis. Examples:

For one-dimensional potentials \( V(x) \) the energy levels are non-degenerate, with only one eigenstate \( \psi_n(x) \) for each energy level \( E_n \). (The degeneracy is \( g_n = 1 \).) When the potential is symmetric (with respect to the origin \( x = 0 \)), the parity operator will commute with the Hamiltonian, and it is possible to show that \( \psi_n \) is also an eigenfunction of the parity operator, with parity \( +1 \) (\( \psi_n \) symmetric) or \( -1 \) (\( \psi_n \) antisymmetric). One also finds that the ground state is symmetric, the first excited state is antisymmetric, the second excited state is symmetric, and so on.

b. For \( x > a \), the time-independent Schrödinger equation,

\[
\psi'' = \frac{2m}{\hbar^2} [V(x) - E]\psi = \frac{2m}{\hbar^2} (V_0 - E)\psi \equiv \kappa^2 \psi,
\]

has the general solution

\[
\psi(x) = Ce^{-\kappa x} + De^{+\kappa x}.\]

Since the last term diverges in the limit \( x \to \infty \), we have to choose \( D = 0 \) to get an acceptable solution. Thus,

\[
\psi(x) = Ce^{-\kappa x} \quad \text{for} \quad x > a, \quad \text{with} \quad \kappa \equiv \frac{1}{\hbar} \sqrt{2m(V_0 - E)}, \quad \text{q.e.d.}
\]
The penetration depth may be defined as the depth at which $|\psi|^2$ is reduced by a factor $1/e$:

$$|e^{-\kappa_{p.d.}}|^2 = e^{-1} \quad \implies \quad l_{p.d.} = \frac{1}{2\kappa_i}.$$  

**c.** When the number $N$ of bound states is large ($\gg 1$), the energies $E_1$ and $E_2$ of the ground state and the first excited state will be much smaller than $V_0$. Therefore,

$$\kappa_i = \frac{1}{\hbar} \sqrt{2m(V_0 - E_i)} \approx \frac{1}{\hbar} \sqrt{2mV_0} \quad \text{for } i = 1, 2.$$  

Since $8mV_0a^2/\hbar^2 \approx \pi^2 N^2$, we find that

$$\frac{l_{p.d.}}{a} = \frac{1}{2\kappa_i a} \approx \sqrt{\frac{\hbar^2}{8mV_0a^2}} \approx \frac{1}{\pi N} \ll 1,$$

showing that the penetration depths for $\psi_1$ and $\psi_2$ are almost equal and much smaller than $a$.

Inside the well, the two solutions behave as $\psi_1 = A_1 \cos k_1 x$ and $\psi_2 = A_2 \sin k_2 x$. Since the penetration depths are small, we see from the figure that $k_1 \cdot 2a \approx \pi$ and $k_2 \cdot 2a \approx 2\pi$. Thus the energies are only a little bit lower than the corresponding energies for a box with width $2a$:

$$E_1 = \frac{\hbar^2 k_1^2}{2m} \approx \frac{\pi^2 \hbar^2}{8ma^2} \quad \text{and} \quad E_2 = 4 \frac{\hbar^2 k_2^2}{2m} \approx \frac{\pi^2 \hbar^2}{2ma^2} \approx 4E_1, \quad \text{q.e.d.}$$  

**d.** When $b$ is small compared to $l_{p.d.}$, we have

$$\frac{\kappa_i b}{2} = 2\kappa_i \frac{b}{4} = \frac{b}{l_{p.d.}} \ll 1, \quad i = 1, 2.$$  

Then the solutions for the region $-\frac{1}{2}b < x < \frac{1}{2}b$,

$$\psi_1 = B_1(e^{\kappa_1 x} + e^{-\kappa_1 x}) \quad \text{and} \quad \psi_2 = B_2(e^{\kappa_2 x} - e^{-\kappa_2 x}),$$

will not curve very much over the interval $-\frac{1}{2}b < x < \frac{1}{2}b$, even less than shown in the figure, which exaggerates the effect:
We then understand that the wave number $k_1$ and hence the energy $E_1$ will be slightly larger than for the case $b = 0$. We also see that $k_2$ and $E_2$ will be slightly smaller than for $b = 0$.

e. When $b$ is large compared to $l_{p.d.}$, on the other hand, the two wave functions are strongly suppressed in the barrier region in the middle, and $\psi_1$ and $\psi_2$ in the well regions are very similar to the ground state for an isolated well of width $a$:

![Diagram of two wave functions with $\psi_1$ and $\psi_2$]

Here, we see that the two wave numbers are almost equal, both being approximately equal to $k_2$ for the case $b = 0$. Thus the two energy levels are almost degenerate, $E_1$ of course being slightly smaller than $E_2$:

$$E_2 \approx E_1 \approx \frac{\pi^2 \hbar^2}{2ma^2}.$$  

**Oppgave 2**

a. From the formula for the current density we find for region III ($x > L$):

$$j_{III} = \mathcal{R}e \left[ t^* e^{-ikx} \frac{\hbar}{im} \frac{d}{dx} t e^{ikx} \right] = \frac{\hbar k}{m} |t|^2.$$  

Similarly, with $\psi_i = \exp(i kx)$ alone, or $\psi_r = r \exp(-i kx)$ alone, we would find

$$j_i = \frac{\hbar k}{m} \cdot 1 \quad \text{and} \quad j_r = -\frac{\hbar k}{m} |r|^2,$$  

respectively. With $\psi_I = \exp(i k x) + r \exp(-i k x)$, we find

$$j_I = \mathcal{R}e \left[ \left( e^{-ikx} + r^* e^{ikx} \right) \frac{\hbar k}{m} \left( e^{ikx} - re^{-ikx} \right) \right]$$

$$= \frac{\hbar k}{m} \left[ 1 - |r|^2 + \mathcal{R}e \left( r^* e^{2ikx} - re^{-2ikx} \right) \right]$$

$$= j_i + j_r, \quad \text{q.e.d.},$$  

since the underbraced quantity is purely imaginary.

b. For a stationary state, the probability current density (and the probability density) are time-independent. Then there can be no accumulation of probability anywhere, and
since we are here dealing with a one-dimensional problem, the current density has to be constant, not only in time but also along the \( x \)-direction. Thus

\[
j_I = j_{II} = j_{III}.
\]

This means that \( j_i = -j_r + j_{III} = |j_r| + j_{III} \). Our interpretation is that the incoming probability current is divided into a reflected current and a transmitted current, and that the transmission and reflection probabilities are

\[
T = \frac{j_{III}}{j_i} = |t|^2 \quad \text{and} \quad R = \frac{|j_r|}{j_i} = |r|^2,
\]

respectively.

c. With

\[
k^2 = 2mE/\hbar^2, \quad q^2 = 2m(E - V_0)/\hbar^2 \quad \text{and} \quad k^2 - q^2 = 2m(E - E + V_0)/\hbar^2 = 2mV_0/\hbar^2;
\]

we have

\[
T = \frac{|t|^2} = \frac{4k^2q^2}{4k^2q^2 \cos^2 qL + (k^2 + q^2)^2 \sin^2 qL} = \frac{4k^2q^2}{4E(E - V_0)} \cdot \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2 qL}, \quad \text{q.e.d.}
\]

In the limit \( E/|V_0| \to \infty \), we have

\[
T = \lim_{E/|V_0| \to \infty} \frac{1}{1 + \frac{V_0^2}{4E(E - V_0)} \sin^2 qL} = 1,
\]

in accordance with classical mechanics (which states that transmission takes place whenever \( E > V_0 \)). For finite values of \( E/V_0 \ (> 1) \), we see that the transmission probability \( T \) is smaller than 1, contrary to the classical result. However, there are exceptions: For values of \( E \) and \( V_0 \) such that

\[
qL = \frac{L}{\hbar} \sqrt{2m(E - V_0)} = n\pi, \quad n = 1, 2, \ldots,
\]

we get complete transmission also quantum mechanically. Since \( q = 2\pi/\lambda_{II} \), we see that \( T \) equals 1 whenever the width \( L \) of the barrier or well is an integer multiple of \( \frac{1}{2} \lambda_{II} \), where \( \lambda_{II} \) is the wavelength in region II. (We are here supposing that \( E > V_0 \).)

d. With \( a = 2\pi a_0 \) and \( k \approx \pi/a = 1/2a_0 \), we have an energy that is smaller than the height \( V_0 \) of the barrier,

\[
E = \frac{\hbar^2 k^2}{2m_e} \approx \frac{\hbar^2}{8m_e a_0^2} < V_0 = \frac{5\hbar^2 k^2}{8m_e a_0^2}.
\]

In the formula for \( T \) we must then replace \( q \) by \( ik \), where

\[
k = \sqrt{\frac{2m_e V_0}{\hbar^2} - \frac{2m_e E}{\hbar^2}} = \frac{1}{a_0}.
\]
With $\sin^2 qL = [\sin(i\kappa L)]^2 = -\sinh^2(\kappa L)$, we then have a (tunneling) transmission probability

$$T = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2(\kappa L)}.$$ 

Since $\kappa L = \frac{1}{a_0} \cdot 5a_0 = 5$ is rather large, we have approximately

$$\sinh^2(\kappa L) \approx \frac{1}{4} \left( e^{\kappa L} - e^{-\kappa L} \right)^2 \approx \frac{1}{4} e^{2\kappa L} \gg 1.$$ 

This means that the second term in the denominator is much larger than the first one. Thus

$$T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2L\kappa},$$ 

which is much smaller than 1. With $E/V_0 = 1/5$ we find

$$T = \frac{64}{25} e^{-10} = 1.16 \times 10^{-4}.$$ 

To estimate the “lifetime” $\tau$, we must find the semiclassical velocity and collision frequency of the particle. The velocity is of typical “atomic” size:

$$v = \sqrt{2E/m_e} = \frac{\hbar}{2m_e a_0} = \frac{e^2}{4\pi e_0 \hbar c} = \frac{1}{2} \alpha c.$$ 

This gives a collision frequency

$$\nu = \frac{v}{2a} = \frac{\alpha c}{8\pi a_0} = 1.65 \times 10^{15} \text{s}^{-1},$$

and a time

$$t_1 = \frac{1}{\nu} = 6.07 \times 10^{-16} \text{s}$$

between each collision. The probability to find the particle “still in jail” at time $t$ then is $(1 - T)^t/t_1$. This means that the “lifetime” $\tau$ is given by

$$(1 - T)^{\tau/t_1} = 1/e \quad \implies \quad \tau = \frac{t_1}{T} = 5.22 \times 10^{-12} \text{s}.$$ 

**Oppgave 3**

a. The existence of a simultaneous set of eigenfunctions of a set of operators requires that the operators commute among themselves. In the present case we have for example:

$$[\hat{H}, \hat{L}^2] = 0 = [\hat{H}, \hat{L}_z] = [\hat{L}^2, \hat{L}_z].$$ 

The “magnetic” quantum number $m_l$ is restricted to the values $0, \pm 1, \pm 2, \ldots, \pm l$. This means that there are $2l + 1$ spherical harmonics for a given value of the quantum number $l$.

The magnetic quantum number $m_l$ does not enter the radial equation, which determines the energies. Therefore, the energy eigenvalues $(E_{nl})$ in this problem can be characterized by the quantum numbers $n$ and $l$, and each of these levels will have a degeneracy $2l + 1$, which is typical for a spherically symmetric potential.
Since the wave function $\psi$ must be zero for $r > a$, where the potential is infinite, we must have $u_{nl}(a) = 0$ to get a continuous wave function, just as for the one-dimensional box.

Using the normalized spherical harmonics, we have from the normalization condition:

$$1 = \int |\psi_{nlm}|^2 d^3r = \int |Y_{lm}|^2 d\Omega \int_0^a [R_{nl}(r)]^2 r^2 dr = 1 \cdot \int_0^a [u_{nl}(r)]^2 dr, \quad \text{q.e.d.},$$

when we work with real radial functions.

b. We see that the radial equation has “one-dimensional form”, and for $l = 0$ we have

$$\frac{d^2u}{dr^2} = -\frac{2mE}{\hbar^2} u = -k^2 u, \quad \text{with} \quad E \equiv \frac{\hbar^2 k^2}{2m} \quad \text{and} \quad u(0) = u(a) = 0,$$

that is, an ordinary box of width $a$. The general solution is

$$u = A \sin kr + B \cos kr,$$

where the condition $u(0) = 0$ gives $B = 0$, and the condition $u(a) = 0$ gives $ka = n\pi$, or $k_{n0} = n\pi/a$, with $n = 1, 2, 3, \ldots$. We get a normalized solution ($\int_0^a [u_{n0}(r)]^2 dr = 1$) by choosing $A = \sqrt{2/a}$. The energies and the complete solutions for the $s$-waves then are

$$E_{n0} = \frac{\hbar^2 k_{n0}^2}{2m} = \frac{\hbar^2 n^2}{2ma^2} n^2 = n^2 E_{10} \quad \text{and} \quad \psi_{n00} = \frac{u_{n0}}{r} \ Y_{00} = \frac{1}{\sqrt{2\pi a}} \frac{\sin(n\pi r/a)}{r}, \quad n = 1, 2, \ldots.$$

c. The figure shows the effective potential, which in this case consists only of the centrifugal barrier $\frac{\hbar^2 l(l+1)}{2mr^2}$, for $l = 1$ and $l = 2$.

We note that the centrifugal barrier is proportional to $l(l+1)$ and makes the well more shallow and also more narrow for increasing $l$. Based on this we must expect that the energies for a given number $n$ of nodes increase in the order of increasing $l$:

$$E_{n0} < E_{n1} < E_{n2} < \cdots.$$

We also expect the energy to increase when the number of nodes increases for a fixed $l$:

$$E_{11} < E_{21} < E_{31} < \cdots,$$

as we have already verified for the $s$-waves. This is because an increasing number of nodes means increasing curvature and increasing kinetic energy.

From this kind of reasoning, we expect the ground state to be an $s$-wave, with no zeros except those for $r = 0$ and $r = a$, that is, $\psi_{100}$. 
d. With $kr = x$ we have for small $r$:

$$u_a = \sin \frac{kr}{kr} - \cos kr = x^{-1}(x - x^3/3! + O(x^5)) \quad (1 - x^2/2! + O(x^4)) = x^2/3 - O(x^4),$$

$$u_b = -\cos \frac{kr}{kr} - \sin kr = -x^{-1}(1 - x^2/2! + O(x^4)) - (x - x^3/3! + O(x^5)) = -1/x - x/2 + O(x^3).$$

Only $u_a$ behaves as $(kr)^{l+1} \propto x^{l+1}$ for small $r$, which is acceptable, while $u_b$ behaves unacceptably for small $r$ and can not be normalized.

Since $u_a$ is a solution of the radial equation and behaves as it should for small $r$, it only remains to require that $u(a) = 0$:

$$l = 1 : \quad u(a) = \sin \frac{ka}{ka} - \cos ka = 0 \quad \Rightarrow \quad \tan ka = ka, \quad \text{q.e.d.}$$

e. In c, we concluded that the ground state must correspond to $nl = (1, 0)$, and $u_{10} \propto \sin(k_{10}r)$, with

$$k_{10} = \frac{\pi}{a} \quad \text{and} \quad E_{10} = \frac{\hbar^2 k_{10}^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2}.$$ 

Based on the discussion in c, we must expect that the first excited level corresponds either to $nl = 1, 1$ or $nl = 2, 0$. In the latter case we have already found the energy:

$$nl = 20 : \quad k_{20} = \frac{2\pi}{a} = 2k_{10} \quad \Rightarrow \quad E_{20} = 4E_{10}.$$ 

To find the energy of the states $\psi_{11m} = r^{-1}u_{11}Y_{1m}$, corresponding to $nl = 1, 1$, we must find the smallest value of $k$ which gives $u_a$ a zero at $x = a$;

$$\left. \sin \frac{kr}{kr} - \cos kr \right|_{r=a} = 0 \quad \Rightarrow \quad \frac{\sin ka}{ka} - \cos ka = 0,$$

corresponding to the condition $\tan ka = ka$. To find this $k$-value it would be instructive to plot $x^{-1}\sin x - \cos x$ as a function of $x$ (see the Comment below). However, it is fairly easy to locate the first zero using the calculator. We already know that this function is positive for small $x$, starting out as $x^2/3$. For $x = \pi$ it is still positive (=1). For $x = 2\pi$ it is equal to $-1$, so the first zero is somewhere between $\pi$ and $2\pi$. Using the calculator, it is fairly easy to find that the first zero occurs for $x = ka = 4.4934$, corresponding to $k_{11} = 4.4934/a = \frac{\pi}{a} \cdot \frac{4.4934}{\pi} = 1.4303k_{10}$, and $E_{11} = (1.4303)^2E_{10} = 2.046E_{10}$, which is lower than $E_{20}$. Thus the first excited level is $E_{11}$ (for $n = 1$ and $l = 1$), with the wave functions

$$\psi_{11m} = C r^{-1} \left( \sin \frac{k_{11}r}{k_{11}r} - \cos k_{11}r \right) Y_{1m}, \quad m = 0, \pm 1.$$ 

Comment: The dashed curve in the figure below shows

$$u_{11}(r) = C \left( \sin \frac{k_{11}r}{k_{11}r} - \cos k_{11}r \right)$$
(plotted with the “$E_{11}$-line” as axis). Note that $u_{11}$ has a turning point where the “$E_{11}$-line” crosses the centrifugal barrier for $l = 1$. Also shown is the “$E_{12}$-line” ($n = 1$, $l = 2$), which is in fact the second excited level (with energy $E_{12} \approx 3.366 E_{10}$), and the corresponding function $u_{12}$, which turns out to be

$$u_{12} = \left( \frac{3}{(k_{12}r)^2} - 1 \right) \sin(k_{12}r) - \frac{3}{k_{12}r} \cos(k_{12}r).$$

In addition we see that the s-waves $u_{10}$ and $u_{20}$ are ordinary box curves. We also observe that $u_{20}$ corresponds to the third excited level.