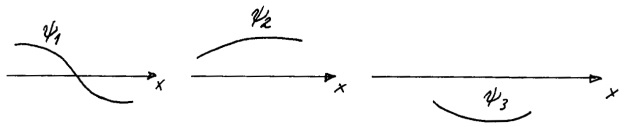
Løsningsforslag
Eksamen 18. desember 2003
TFY4250 Atom- og molekylfysikk og FY2045 Innføring i kvantemekanikk

Oppgave 1

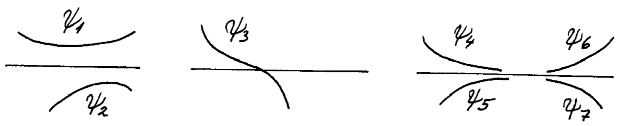
a. With $\hat{H} = \hat{K} + V = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$, we can write Schrödinger's time-independent equation on the form

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

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



(ii) In *classically forbidden regions* (where $E < V(x)$), the curvature has the same sign as ψ. ψ then will *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 operatotor will commute with the Hamiltonian, and it is possible to show that ψ_n is also an eigenfunction of the parity operator, with parity $+1$ (ψ_n symmetric) or -1 (ψ_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

$$\psi(x) = C\,e^{-\kappa x} + D\,e^{+\kappa x}.$$

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

$$\psi(x) = C\,e^{-\kappa x} \qquad \text{for} \qquad x > a, \quad \text{with} \quad \kappa \equiv \frac{1}{\hbar}\sqrt{2m(V_0 - E)}, \quad \text{q.e.d.}$$

The penetration depth may be defined as the depth at which $|\psi|^2$ is reduced by a factor $1/e$:

$$|e^{-\kappa l_{\text{p.d.}}}|^2 = e^{-1} \qquad \Longrightarrow \qquad l_{\text{p.d.}} = \frac{1}{2\kappa}.$$

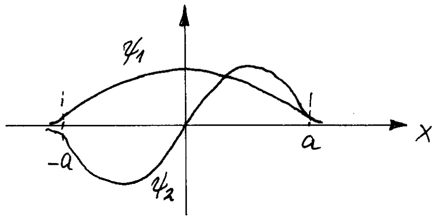
<u>**c.**</u> When the number N of bound states is large ($>> 1$), the energies E_1 and E_2 of the ground state and the first excited state will be much smaller than V_0. Therefore,

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

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

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

showing that the penetration depths for ψ_1 and ψ_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 $2a$:

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

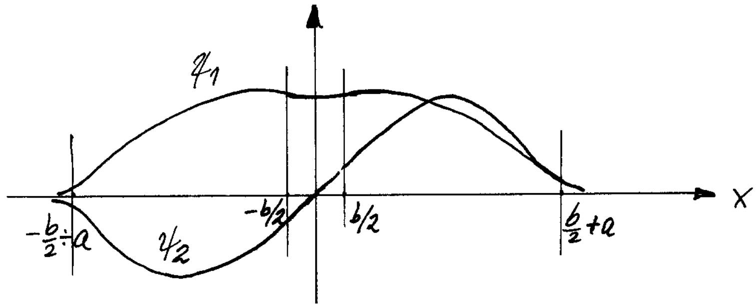
<u>**d.**</u> When b is small compared to $l_{\text{p.d.}}$, we have

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

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

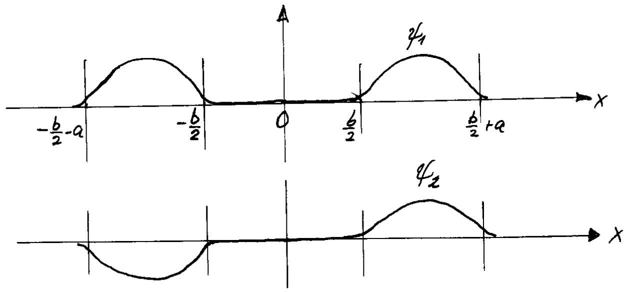
$$\psi_1 = B_1(e^{\kappa_1 x} + e^{-\kappa_1 x}) \quad \text{and} \quad \psi_2 = B_2(e^{\kappa_2 x} - e^{-\kappa_2 x}),$$

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 $l_{\text{p.d.}}$, on the other hand, the two wave functions are strongly suppressed in the barrier region in the middle, and ψ_1 and ψ_2 in the well regions are very similar to the ground state for an isolated well of width a:



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:

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

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 $\psi_i = \exp(ikx)$ alone, or $\psi_r = r\exp(-ikx)$ alone, we would find

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

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

$$\begin{aligned} j_I &= \mathcal{R}e\left[\left(e^{-ikx} + r^* e^{ikx}\right)\frac{\hbar k}{m}\left(e^{ikx} - re^{-ikx}\right)\right] \\ &= \frac{\hbar k}{m}\left[1 - |r|^2 + \mathcal{R}e\,\underbrace{\left(r^* e^{2ikx} - re^{-2ikx}\right)}\right] \\ &= j_i + j_r, \quad \text{q.e.d.,} \end{aligned}$$

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

$$T = \frac{j_{III}}{j_i} = |t|^2 \qquad \text{and} \qquad R = \frac{|j_r|}{j_i} = |r|^2,$$

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

$$\begin{aligned} T &= |t|^2 = \frac{4k^2q^2}{4k^2q^2\cos^2 qL + (k^2+q^2)^2\sin^2 qL} = \frac{4k^2q^2}{4k^2q^2 + (k^2-q^2)^2\sin^2 qL} \\ &= \frac{4E(E-V_0)}{4E(E-V_0) + V_0^2\sin^2 qL}, \quad \text{q.e.d.} \end{aligned}$$

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

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

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 λ_{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 $i\kappa$, where

$$\kappa = \sqrt{\frac{2m_e V_0}{\hbar^2} - \frac{2m_e E}{\hbar^2}} = \frac{1}{a_0}.$$

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

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

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" τ, we must find the semiclassical velocity and collision frequency of the particle. The velocity is of typical "atomic" size:

$$v = \sqrt{2E/m_e} = \frac{\hbar}{2m_e a_0} = \frac{e^2}{4\pi\epsilon_0 \hbar c} \frac{c}{2} = \tfrac{1}{2}\alpha c.$$

This gives a collision frequency

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

and a time

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

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" τ is given by

$$(1 - T)^{\tau/t_1} = 1/e \qquad \Longrightarrow \qquad \tau = \frac{t_1}{T} = 5.22 \times 10^{-12} \mathrm{s}.$$

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:

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

The "magnetic" quantum number m_l is restricted to the values $0, \pm 1, \pm 2, ..., \pm l$. 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 ψ 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:

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

when we work with real radial functions.

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

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

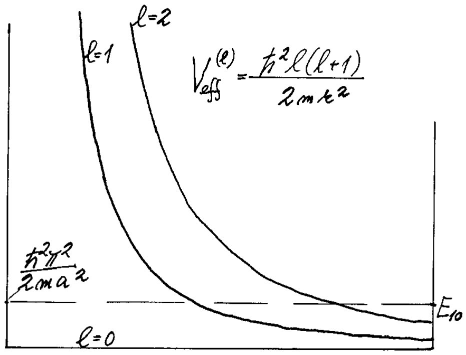
that is, an ordinary box of width a. The general solution is

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

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 $n = 1, 2, 3, \cdots$. 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

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

c. The figure shows the effective potential, which in this case consists only of the centrifugal barrier $\hbar^2 l(l+1)/2mr^2$, 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, ψ_{100}.

d. With $kr = x$ we have for small r:

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

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

Only u_a behaves as $(kr)^{l+1} \propto r^{l+1} = r^2$ 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 $u(a) = 0$:

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

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

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

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:

$$nl = 20: \qquad k_{20} = \frac{2\pi}{a} = \underline{2k_{10}} \qquad \Longrightarrow \qquad E_{20} = 4E_{10}.$$

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 $x = a$;

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

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 π and 2π. Using the calculator, it is fairly easy to find that the first zero occurs for $x = ka = 4.4934$, corresponding to

$$k_{11} = \frac{4.4934}{a} = \frac{\pi}{a}\,\frac{4.4934}{\pi} = 1.4303\, k_{10}, \qquad \text{and} \qquad E_{11} = (1.4303)^2 E_{10} = 2.046\, E_{10},$$

which is lower than E_{20}. Thus the first excited level is E_{11} (for $n = 1$ and $l = 1$), with the wave functions

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

Comment: The dashed curve in the figure below shows

$$u_{11}(r) = C\left(\frac{\sin k_{11} r}{k_{11} r} - \cos k_{11} r\right)$$

(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.