

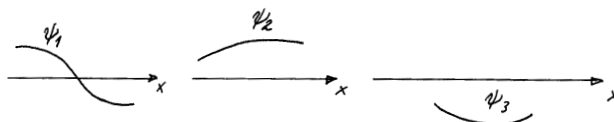
Løsningsforslag
Eksamen 18. desember 2003
TFY4250 Atom- og molekylfysikk og
FY2045 Innføring i kvantemekanikk

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

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

(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 operator 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 $x \rightarrow \infty$, we have to choose $D = 0$ to get an acceptable solution. Thus,

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

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

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

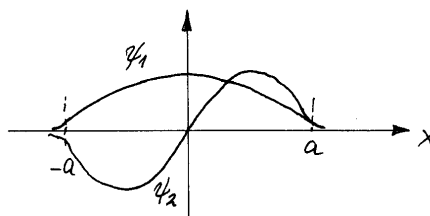
c. When the number N of bound states is large ($\gg 1$), the energies E_1 and E_2 of the ground state and the first excited state will be much smaller than V_0 . Therefore,

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

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

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

showing that the penetration depths for 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 $2a$:

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

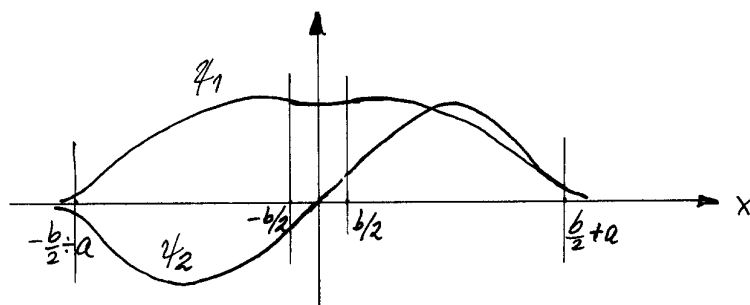
d. When b is small compared to $l_{\text{p.d.}}$, we have

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

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

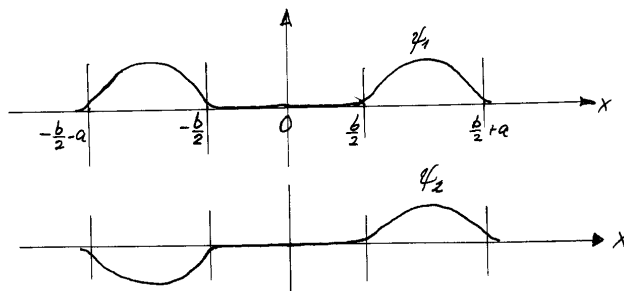
$$\psi_1 = B_1(e^{\kappa_1 x} + e^{-\kappa_1 x}) \quad \text{and} \quad \psi_2 = B_2(e^{\kappa_2 x} - e^{-\kappa_2 x}),$$

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 $l_{\text{p.d.}}$, 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 :

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

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

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

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

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

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

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

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

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

In the limit $E/|V_0| \rightarrow \infty$, we have

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

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

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

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

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

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

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

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” τ 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:

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

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

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

when we work with real radial functions.

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

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

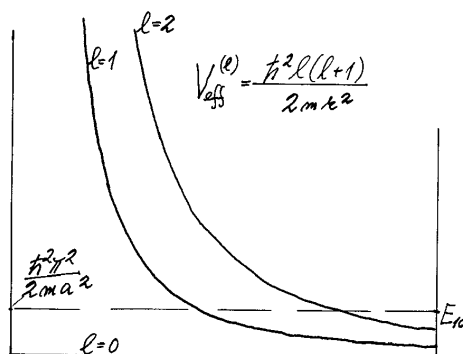
that is, an ordinary box of width a . The general solution is

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

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

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

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 :

$$E_{n0} < E_{n1} < E_{n2} < \dots$$

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

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

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 $u(a) = 0$:

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

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:

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

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 $x = a$;

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

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

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

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

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

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.

