UNIVERSITY OF OSLO
FACULTY OF MATHEMATICS AND NATURAL SCIENCES

Solution to exam in: FYS3110, Quantum mechanics

Day of exam: Dec. 2. 2013

Permitted material: Approved calculator, D.J. Griffiths: "Introduction to Quantum Mechanics", the printed notes: "Time evolution of states in quantum mechanics", "Symmetry and degeneracy" and "WKB connection formulae", one handwritten A4-sheet(2 pages) with your own notes, and K. Rottmann: "Matematisk formelsamling"

Problem 1

1.1 The angular dependence of the energy eigenfunctions are given by the spherical harmonics $Y_l^m(\theta,\phi)$. (This follows from the rotational symmetry of the Hamiltonian which ensures that the only operator angular dependence comes from the Laplacian which operation on the angles is according to L^2. The spherical harmonics are eigenfunctions of L^2.)

1.2 The energies in a central symmetric problem depend only on the quantum numbers n and l. They cannot depend on the quantum number m of L_z because of rotational invariance. Therefore, for $F = 0$, all levels with angular momentum l are $2l + 1$-fold degenerate because m goes from $-l$ to l. A weak perturbation can thus be dealt with using degenerate perturbation theory where the first order energy correction is found by diagonalizing the perturbation within the degenerate subspace. Since the perturbation here is proportional to L_z^2 the good states are the spherical harmonics themselves and the energy corrections become $\langle lm|gFL_z^2/\hbar^2|lm\rangle = gFm^2$. Thus states with different $|m|$ will split. The $m = 0$ states will not be affected and will not be degenerate in the presence of F. The other levels with $m \neq 0$ will be two-fold degenerate in the presence of F corresponding to $\pm m$. Fig. 1 shows the energy vs. F for a few energy levels. One cannot from the information given in this problem know the energies at $F = 0$, so they are chosen arbitrarily in the figure.

1.3 The Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

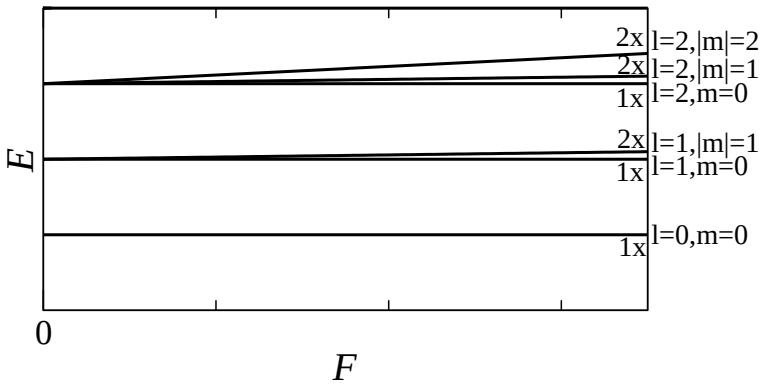

Figure 1: Energy vs. F for a few energy levels.

Separating out the radial part $R(r)$ as $\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi)$ and using the expression for the Laplacian in spherical coordinates

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}L^2$$

where we have identified the angular part with the operator $-L^2/\hbar^2$. we get

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2}l(l+1)\right]R(r) + V(r)R(r) = ER(r)$$

where we have used the fact that Y_l^m are eigenfunctions for L^2 with eigenvalue $\hbar^2 l(l+1)$. This equation (multiplied by $\frac{2mr^2}{\hbar^2}$) is given in Griffiths section 4.1.3 and is also an acceptable starting point for doing this problem. Now set $R(r) = u(r)/r$. Then

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\frac{u}{r} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r} - u\right) = \frac{1}{r}\frac{\partial^2 u}{\partial r^2}$$

Thus

$$\begin{aligned} -\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}u - \frac{l(l+1)}{r^2}\frac{u}{r}\right] + V(r)\frac{u}{r} &= E\frac{u}{r} \\ -\frac{\hbar^2}{2m}\frac{\partial^2 u(r)}{\partial r^2} + \frac{\hbar^2 l(l+1)}{2mr^2}u(r) + V(r)u(r) &= Eu(r) \end{aligned}$$

which is the form of a 1D Schrödinger equation with an effective one dimensional potential

$$\underline{V_{1d}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}}$$

and the 1d wavefunction $u(r)$ is related to the 3D radial part as

$$\underline{u(r) = rR(r) \quad \text{or} \quad R(r) = u(r)/r}$$

1.4 For $l = 0$ there is no centrifugal barrier, and so the effective 1D potential is

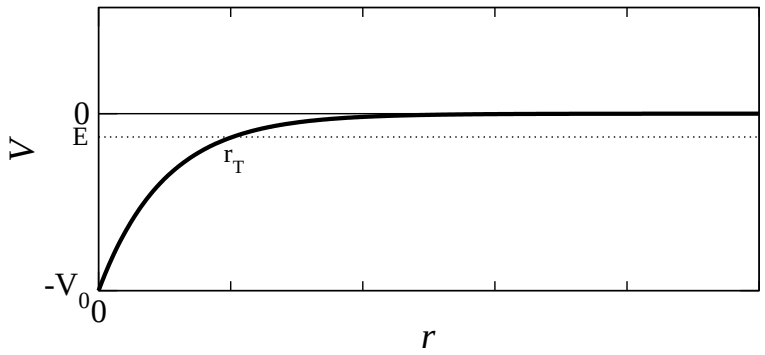

Figure 2: V(r) (problem 1.4)

just $V(r)$ which is shown in Fig. 2. For large r the WKB-wave function must be falling off exponentially for $E < 0$. The connection formula for an upward sloping potential gives then the following form for the WKB wave function in the region where $E > V$.

$$u(r) = \frac{2D}{\sqrt{p(r)}} \sin(\int_r^{r_T} dr' p(r') + \pi/4)$$

where $p(r) = \sqrt{2m(E - V(r))}$ and r_T is the classical turning point where $E = V(r_T)$. The 1D wavefunction $u(r) = rR(r)$ must be 0 at $r = 0$ which gives the following condition

$$0 = \frac{2D}{\sqrt{p(0)}} \sin(\int_0^{r_T} dr' p(r') + \pi/4)$$

which implies that

$$\int_0^{r_T} \sqrt{2m(E - V(r))} = (n - 1/4)\pi\hbar \qquad n \in 1, 2, 3, \ldots$$

The energy of the lowest bound state becomes bigger as V_0 decreases. The limiting case is when V_0 reaches a minimum value where the energy of the lowest bound state becomes 0. For V_0 values smaller than this, the potential does not allow a bound state. Thus we can find the limit where the potential no longer admits a bound state by setting $E = 0$. The turning point r_T goes to infinity as E approaches 0 from below. Thus we need to solve

$$\int_0^{\infty} \sqrt{-2mV(r)} = (n - 1/4)\pi\hbar$$

for $n = 1$. The integral is simple: $\int_0^\infty dr\sqrt{2mV(r)} = \int_0^\infty \sqrt{2mV_0}e^{-\alpha r/2} = \sqrt{2mV_0}\frac{2}{\alpha}$ which gives

$$\sqrt{2mV_0}\frac{2}{\alpha} = (1 - 1/4)\pi\hbar$$

or

$$V_0 = \frac{\alpha^2\hbar^2}{8m}(3/4)^2\pi^2 = \underline{\frac{9\pi^2}{128}\frac{\alpha^2\hbar^2}{m}} \approx 0.69\frac{\alpha^2\hbar^2}{m}$$

This WKB-result is quite close to the exact answer which is $V_0 = \frac{x_1^2}{8}\frac{\alpha^2\hbar^2}{m} \approx 0.72290\frac{\alpha^2\hbar^2}{m}$. ($x_1$ is the first zero of the Bessel function $J_0(x)$).

Problem 2.

2.1 Lets denote the state where particle 1 is in the one-particle energy eigenstate n_1 and particle 2 is in the one-particle energy eigenstate n_2 for $|n_1, n_2\rangle$. The energy of this state is $E_{n_1,n_2} = \hbar\omega(n_1 + 1/2 + n_2 + 1/2) = \hbar\omega\,(n_1 + n_2 + 1)$ For distinguishable particles, there is no symmetry requirement. Therefore the three lowest energy level with corresponding degeneracies are

energy	degeneracy	states
$\hbar\omega$	1	$\|00\rangle$
$2\hbar\omega$	2	$\|10\rangle, \|01\rangle$
$3\hbar\omega$	3	$\|20\rangle, \|02\rangle, \|11\rangle$

2.2 When the particles are identical spin-1 bosons the state must be symmetric under the interchange of both particle coordinates and their spins. For two spin-1 particles there are altogether $3 \times 3 = 9$ different spin states which have the same energy because the Hamiltonian does not depend on spins. The spin states need to be written such that they are either antisymmetric or symmetric under the interchange of the two particles. The Clebsch-Gordan table for combining two spin-1's (last page of problem set, table 1×1) reveals that there are 3 antisymmetric (in the notation (S, m_S): $(1, 0)$, $(1, \pm 1)$) and 6 symmetric combinations ($(2, \pm 2)$, $(2, \pm 1)$, $(2, 0)$ and $(0, 0)$). The (anti)symmetric spin states must be combined with (anti)symmetric spatial states in order to make a fully symmetric state. The ground state $|00\rangle$ is symmetric. Combining this with the symmetric spin states one then finds a degeneracy of 6. For the first excited level one can construct both antisymmetric and symmetric spatial parts. Combining them with their respective

spin parts give $6 + 3 = 9$ states. For the third level the states $|20\rangle$ and $|02\rangle$ can be put together in both antisymmetric and a symmetric combinations giving also 9 states, and in addition the state $|11\rangle$ is fully symmetric which adds 6 states. Therefore

energy	degeneracy	states
$\hbar\omega$	6	$\|00\rangle\|\chi_+\rangle$
$2\hbar\omega$	9	$(\|10\rangle \pm \|01\rangle)\,\|\chi_\pm\rangle$
$3\hbar\omega$	15	$(\|20\rangle \pm \|02\rangle)\,\|\chi_\pm\rangle, \|11\rangle\|\chi_+\rangle$

2.3 The unperturbed ground state is non-degenerate, thus

$$\begin{aligned} E' &= \langle 00|H_{int}|00\rangle = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \psi_0^*(x_1)\psi_0^*(x_2) g\delta(x_1 - x_2)\psi_0(x_1)\psi_0(x_2) \\ &= g\int_{-\infty}^{\infty} dx_1 |\psi_0(x_1)|^4 = g\frac{m\omega}{\pi\hbar}\int_{-\infty}^{\infty} dx e^{-2m\omega x^2/\hbar} \\ &= g\frac{m\omega}{\pi\hbar}\left(\frac{\hbar}{2m\omega}\right)^{1/2} \underbrace{\int_{-\infty}^{\infty}\left(\frac{2m\omega}{\hbar}\right)^{1/2} dx e^{-(\sqrt{2m\omega/\hbar}x)^2}}_{\sqrt{\pi}} = \underline{\frac{g}{\sqrt{2\pi}}\left(\frac{m\omega}{\hbar}\right)^{1/2}} \\ &= \hbar\omega\frac{g}{\hbar\omega}\sqrt{\frac{m\omega}{2\pi\hbar}} \end{aligned}$$

where we have used the ground state wave function for the 1D harmonic oscillator $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$.

2.4 The Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 + \frac{1}{2}m\omega^2 x_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + \frac{1}{2}m\omega^2 x_2^2 + g\delta(x_1 - x_2)$$

The trial wavefunction is normalized, so the variational energy is

$$E_{trial} = \frac{2b}{\pi}\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 e^{-b(x_1^2+x_2^2)} H e^{-b(x_1^2+x_2^2)}$$

Writing this out in details gives

$$\begin{aligned}
E_{trial} &= \left(\frac{2b}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}dx_1 e^{-bx_1^2}\left(-\frac{\hbar^2}{2m}\nabla_1^2+\frac{1}{2}m\omega^2x_1^2\right)e^{-bx_1^2}\times\underbrace{\left(\frac{2b}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}dx_2e^{-2bx_2^2}}_{1}\\
&+\left(\frac{2b}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}e^{-bx_2^2}\left(-\frac{\hbar^2}{2m}\nabla_2^2+\frac{1}{2}m\omega^2x_2^2\right)e^{-bx_2^2}\times\underbrace{\left(\frac{2b}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}dx_1e^{-2bx_1^2}}_{1}\\
&+g\frac{2b}{\pi}\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2e^{-b(x_1^2+x_2^2)}\delta(x_1-x_2)e^{-b(x_1^2+x_2^2)}\\
&= 2\left(\frac{2b}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}dxe^{-bx^2}\left(-\frac{\hbar^2}{2m}\nabla^2+\frac{1}{2}m\omega^2x^2\right)e^{-bx^2}+g\frac{2b}{\pi}\underbrace{\int_{-\infty}^{\infty}dxe^{-4bx^2}}_{(\pi/4b)^{1/2}}\\
&= \underline{2\left(\frac{\hbar^2b}{2m}+\frac{m\omega^2}{8b}\right)+g\left(\frac{b}{\pi}\right)^{1/2}}
\end{aligned}$$

This expression is not easily minimized analytically. However for large g the problem simplifies.

For large g the last term forces b to be a small value in order to minimize the expression. For small values of b the second term is much bigger than the the first term. Thus we can neglect the first term in comparison with the second. That is

$$E_{trial}\approx\frac{m\omega^2}{4b}+g\left(\frac{b}{\pi}\right)^{1/2}$$

Seeking the minimum by differentiating, we obtain

$$\frac{\partial E_{trial}}{\partial b}=-\frac{m\omega^2}{4b^2}+g\frac{1}{2\sqrt{b\pi}}=0\implies b=g^{-2/3}\left(\frac{\pi m^2\omega^4}{4}\right)^{1/3}$$

Inserting this into the expression for the trial energy

$$\begin{aligned}
E_{trial,min} &\approx \frac{m\omega^2}{4}g^{2/3}\left(\frac{4}{\pi m^2\omega^4}\right)^{1/3}+\frac{g}{\sqrt{\pi}}g^{-1/3}\left(\frac{\pi m^2\omega^4}{4}\right)^{1/6}\\
&= g^{2/3}\left(\left(\frac{m\omega^2}{8\cdot 2\pi}\right)^{1/3}+\underbrace{\left(\frac{\pi m^2\omega^4}{4\pi^3}\right)^{1/6}}_{\left(\frac{m\omega^2}{2\pi}\right)^{1/3}}\right)=\underline{g^{2/3}\frac{3}{2}\left(\frac{m\omega^2}{2\pi}\right)^{1/3}}
\end{aligned}$$

This can be written in a more transparent form by introducing the dimensionless coupling $\tilde{g}=(g/\hbar\omega)(m\omega/\hbar)^{1/2}$ which gives

$$E_{trial,min}=\hbar\omega\ \tilde{g}^{2/3}\frac{3}{2}\left(\frac{1}{2\pi}\right)^{1/3}$$

2.5 Alternative b) and d) have the lowest trial energy for large g. This is because the interaction energy is minimized (it is zero) in these wavefunctions:

$$g\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2|x_1-x_2|\delta(x_1-x_2)e^{-2b(x_1^2+x_2^2)}=0$$

and

$$g\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2(x_1-x_2)\delta(x_1-x_2)e^{-2b(x_1^2+x_2^2)}=0.$$

Since this is a system of bosons one can argue that d) is ruled out as a candidate for the ground state wavefunction as it is antisymmetric under the interchange of the bosons while b) is permissible as it is symmetric. Nevertheless d) gives *exactly* the same variational energy as b). The reason is that with this hard-core interaction potential in one dimension the particles cannot physically change places. Therefore the distinction between bosons and fermions does not matter. Full credit will be given for realizing that *b*) and *d*) have the lowest energy as they minimize the interaction energy. No deduction will be made if one rules out *d*) by arguing that it describes fermions.

Doing the calculations (not required for credit) give the following variational energies

$$\begin{aligned}
E_a &= \frac{\hbar^2}{2m}4b+\frac{1}{2}m\omega^2\frac{1}{b}+g\sqrt{\frac{b}{\pi}}\\
E_b &= \frac{\hbar^2}{2m}4b+\frac{1}{2}m\omega^2\frac{1}{b}\\
E_c &= \frac{\hbar^2}{2m}4b+\frac{1}{2}m\omega^2\frac{1}{b}+g\sqrt{\frac{b}{\pi}}\\
E_d &= \frac{\hbar^2}{2m}4b+\frac{1}{2}m\omega^2\frac{1}{b}
\end{aligned}$$

Minimizing the trial energy E_b (or E_d) gives $b=m\omega/2\hbar$ and a minimum variational energy of $E_{b,min}=E_{d,min}=2\hbar\omega$ which coincides with the first excited energy level of the system without the interaction g. Comparing to the trial energy obtained in 2.4

$$E_{2.4}=\frac{\hbar^2}{2m}2b+\frac{1}{2}m\omega^2\frac{1}{2b}+g\left(\frac{b}{\pi}\right)^{1/2}$$

and the fact that $E_{2.4}\sim g^{2/3}$ for large g, one sees that $E_{b,min}=E_{d,min}$ are smaller for large values of g. In fact for $g\to\infty$ the wavefunction b) with $b=m\omega/2\hbar$ is the exact ground state wavefunction of the two-particle system.

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