UNIVERSITY OF OSLO
FACULTY OF MATHEMATICS AND NATURAL SCIENCES

Solution to exam in: FYS3110, Quantum mechanics

Day of exam: Nov. 30. 2015

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".

Two dimensional harmonic oscillator

a)

$$H^0\psi(r,\phi) = E\psi(r,\phi)$$

$$e^{ik\phi}\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f(r)}{\partial r}\right)-\frac{k^2 f(r)}{r^2}\right)+\frac{1}{2}m\omega^2 r^2 f(r)\right] = Ee^{ik\phi}f(r)$$

$$\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}-\frac{k^2}{r^2}\right)+\frac{1}{2}m\omega^2 r^2\right] f(r) = Ef(r)$$

Single-valuedness under rotation by 2π: $\psi(r,\phi+2\pi)=\psi(r,\phi) \implies e^{ik2\pi}=1 \implies \underline{k\in\mathcal{Z}}$.

b)

$$L_z\psi(r,\phi) = L_z f(r)e^{ik\phi} = -i\hbar f(r)\frac{\partial}{\partial\phi}e^{ik\phi} = \hbar k f(r)e^{ik\phi} = \hbar k\ \psi(r,\phi)$$

Eigenvalues: $\underline{\hbar k}$.

c)

$$H^0 = \hbar\omega\left(a_x^\dagger a_x+\frac{1}{2}+a_y^\dagger a_y+\frac{1}{2}\right) = \underline{\hbar\omega\left(a_x^\dagger a_x+a_y^\dagger a_y+1\right)}$$

No further justifications are needed. The three lowest energy levels, their degeneracy and states:

Energy	deg.	states
$\hbar\omega$	1	$\|00\rangle$
$2\hbar\omega$	2	$\|10\rangle$,$\|01\rangle$
$3\hbar\omega$	3	$\|20\rangle$,$\|02\rangle$,$\|11\rangle$

d) We use $x = \sqrt{\frac{\hbar}{2m\omega}}\left(a_x^\dagger + a_x\right)$ and $p_x = i\sqrt{\frac{\hbar m\omega}{2}}\left(a_x^\dagger - a_x\right)$ and similar for y and p_y in terms of the y ladder operators. We get

$$\begin{aligned} L_z &= xp_y - yp_x \\ &= \frac{\hbar}{2} i\left[\left(a_x^\dagger + a_x\right)\left(a_y^\dagger - a_y\right) - \left(a_y^\dagger + a_y\right)\left(a_x^\dagger - a_x\right)\right] \\ &= \underline{i\hbar\left(a_x a_y^\dagger - a_x^\dagger a_y\right)} \end{aligned}$$

Lowest energy level: $L_z|00\rangle = 0, \implies k = 0$, and $H^0|00\rangle = \hbar\omega|00\rangle \implies E = \hbar\omega$. Thus $|00\rangle$ is simultaneously an eigenket of both L_z and H^0. For states in the first excited level we have $L_z|10\rangle = i\hbar|01\rangle$ and $L_z|01\rangle = -i\hbar|10\rangle$. Multiplying the second equation with i and adding and subtracting the equations we see that the normalized eigenstates of L_z are $\frac{1}{\sqrt{2}}\left(|10\rangle \pm i|01\rangle\right)$ with eigenvalues $k = \pm\hbar$. Both $|10\rangle$ and $|01\rangle$ are eigenstates of H^0 with eigenvalue $2\hbar\omega$, thus $\frac{1}{\sqrt{2}}\left(|10\rangle \pm i|01\rangle\right)$ are simultaneous eigenstates for both H^0 and L_z.

e) First order perturbation theory requires the calculation of the matrix elements $w_{mn} = \langle m|H^1|n\rangle$ where m and n label degenerate unperturbed states, $E_m^0 = E_n^0$. If there is no degeneracy, $m = n$. Using the fact that H^0 and H^1 are both hermitian which implies real energies E_m^0 the matrix elements become

$$\begin{aligned} w_{mn} &= \langle m|H^1|n\rangle = \langle m|[H^0, A]|n\rangle = \langle m|H^0 A|n\rangle - \langle m|AH^0|n\rangle \\ &= \langle n|A^\dagger H^0|m\rangle^* - \langle m|AH^0|n\rangle = E_m^{0*}\langle n|A^\dagger|m\rangle^* - E_n^0\langle m|A|n\rangle = E_m^0\langle m|A|n\rangle - E_n^0\langle m|A|n\rangle \\ &= \left(E_m^0 - E_n^0\right)\langle m|A|n\rangle = 0 \end{aligned}$$

So all the w_{mn}s are zero which implies that the first order energy correction is zero. q.e.d. Taking the hermitian conjugate of the equation $H^1 = [H^0, A]$ and using the fact that H^0 and H^1 are hermitian we get $H^1 = A^\dagger H^0 - H^0 A^\dagger = -[H^0, A^\dagger]$. So if $A^\dagger = A$, we get $H^1 = [H^0, A] = -[H^0, A] = -H^1$ which is only true for $H^1 = 0$. Thus A <u>cannot be hermitian</u>, it must be anti-hermitian $A^\dagger = -A$. Note that the commutator of two hermitian operators is always anti-hermitian ($[x, p] = i\hbar$ for instance).

f) $H^1 = g\sqrt{\frac{2m\omega}{\hbar}}x$. Lets try $A \propto p_x$. This term commutes with p_x^2, p_y^2 and y^2. However its commutation with x^2 is non-trivial:

$$\left[x^2, p_x\right] = x^2 p_x - p_x x^2 = x^2 p_x - x p_x x + x p_x x - p_x x^2 = x[x, p_x] + [x, p_x]x = 2i\hbar x$$

which implies

$$\left[H^0, p_x\right] = \frac{1}{2}m\omega^2[x^2, p_x] = im\omega^2\hbar x \implies \left[H^0, \frac{1}{im\omega^2\hbar}g\sqrt{\frac{2m\omega}{\hbar}}p_x\right] = g\sqrt{\frac{2m\omega}{\hbar}}x = H^1$$

Thus

$$\underline{A = \frac{g}{im\hbar\omega^2}\sqrt{\frac{2m\omega}{\hbar}}p_x = -ip_x g\sqrt{\frac{2}{m(\hbar\omega)^3}}}$$

Observe that $A^\dagger = -A$. Another way of writing this is to use ladder operators. With $p_x = i\sqrt{\frac{\hbar m\omega}{2}}\left(a_x^\dagger - a_x\right)$ we get

$$\underline{A = \frac{g}{\hbar\omega}\left(a_x^\dagger - a_x\right).}$$

The first order energy correction to any state is therefore 0. The second order correction can be computed as

$$E_{00}^2 = \sum_{n_x n_y \neq (00)} \frac{|\langle n_x n_y|H^1|00\rangle|^2}{E_{00} - E_{n_x n_y}}$$

The operator $H^1 = g\sqrt{\frac{2m\omega}{\hbar}}x = g\left(a_x^\dagger + a_x\right)$ thus $H^1|00\rangle = g|10\rangle$. Therefore the sum has just a single non-zero term (10), and we get $E_{00}^2 = g^2\frac{1}{\hbar\omega - 2\hbar\omega} = \underline{-\frac{g^2}{\hbar\omega}}$.

g) Set $H = H^0 + H^1$. The trial state is normalized. Therefore the variational principle is $\langle\psi|H|\psi\rangle \geq E_{gs}$. Compute $H|\psi\rangle$ first:

$$\begin{aligned} H\left(\cos\theta|00\rangle + \sin\theta|10\rangle\right) &= \hbar\omega\cos\theta|00\rangle + 2\hbar\omega\sin\theta|10\rangle \\ &\quad + g\cos\theta|10\rangle + g\sin\theta\left(\sqrt{2}|20\rangle + |00\rangle\right) \end{aligned}$$

Then

$$\langle\psi|H|\psi\rangle = \hbar\omega\left(\cos^2\theta + 2\sin^2\theta\right) + g2\sin\theta\cos\theta = \hbar\omega\left(1 + \sin^2\theta\right) + g\sin 2\theta$$

Differentiating this w.r.t. θ gives

$$\hbar\omega 2\sin\theta\cos\theta + g2\cos 2\theta = 0 \implies \tan 2\theta = -2\frac{g}{\hbar\omega}$$

Squaring the identity $\tan 2\theta = \frac{\sin 2\theta}{\sqrt{1-\sin^2 2\theta}}$ we can solve the above equation for $\sin 2\theta$:

$$\frac{\sin^2 2\theta}{1 - \sin^2 2\theta} = 4\left(\frac{g}{\hbar\omega}\right)^2 \implies \sin^2 2\theta = \frac{4\left(\frac{g}{\hbar\omega}\right)^2}{1 + 4\left(\frac{g}{\hbar\omega}\right)^2} \quad \& \quad \cos^2 2\theta = \frac{1}{1 + 4\left(\frac{g}{\hbar\omega}\right)^2}$$

When taking the square roots we need to choose signs such the extremum condition is satisfied, which means that $\sin 2\theta$ and $\cos 2\theta$ must have different signs. To help us select the sign we must also calculate the second derivative to ensure we have a minimum. The 2. derivative condition for a minimum is

$$\frac{d^2\langle\psi|H|\psi\rangle}{d\theta^2} = 2\hbar\omega\cos(2\theta) - 4g\sin(2\theta) > 0$$

which means that $\cos 2\theta > 0$ and $\sin 2\theta < 0$. Therefore

$$\sin 2\theta = -\sqrt{\frac{4\left(\frac{g}{\hbar\omega}\right)^2}{1+4\left(\frac{g}{\hbar\omega}\right)^2}} \quad \& \quad \cos 2\theta = \sqrt{\frac{1}{1+4\left(\frac{g}{\hbar\omega}\right)^2}}$$

We need to express $\sin^2\theta$ in terms of these. This can be done by observing that $\cos 2\theta = \cos^2\theta - \sin^2\theta = 1 - 2\sin^2\theta \implies \sin^2\theta = \frac{1}{2}(1-\cos 2\theta)$. Therefore

$$\begin{aligned}\langle\psi|H|\psi\rangle &= \hbar\omega\left(\frac{3}{2} - \frac{1}{2}\cos 2\theta\right) + g\sin 2\theta = \hbar\omega\left(\frac{3}{2} - \frac{1}{2}\sqrt{\frac{1}{1+4\left(\frac{g}{\hbar\omega}\right)^2}}\right) - g\sqrt{\frac{4\left(\frac{g}{\hbar\omega}\right)^2}{1+4\left(\frac{g}{\hbar\omega}\right)^2}} \\ &= \frac{3}{2}\hbar\omega - \frac{\hbar\omega}{2}\left(1+4\left(\frac{g}{\hbar\omega}\right)^2\right)\sqrt{\frac{1}{1+4\left(\frac{g}{\hbar\omega}\right)^2}} = \underline{\hbar\omega\left(\frac{3}{2} - \frac{1}{2}\sqrt{1+4\left(\frac{g}{\hbar\omega}\right)^2}\right)}\end{aligned}$$

h) The electric field causes an additional term in the Hamiltonian

$$H_E = -qE_0\hat{n}\cdot\vec{r}e^{-t^2/\tau^2}.$$

Initially, before the pulse arrives ($t = -\infty$), the system is in the ground state $|00\rangle$.

First order time-dependent perturbation theory gives then the following probability amplitude for finding the system in one of the states $|f\rangle \in \{|10\rangle, |01\rangle\}$ after the pulse has passed (at $t = \infty$)

$$\begin{aligned}a_f(t\to\infty) &= \frac{1}{i\hbar}\int_{-\infty}^{\infty} dt\langle f|H_E|\psi_i\rangle e^{i\omega t} \\ &= \frac{1}{i\hbar}qE_0\int_{-\infty}^{\infty} dt e^{-t^2/\tau^2+i\omega t}\langle f|x|00\rangle\end{aligned}$$

Since the matrix element $\langle 01|x|00\rangle = 0$ there is a zero probability to find the system in the state $|01\rangle$ after the pulse. The other matrix element is $\langle 10|x|00\rangle = \sqrt{\frac{\hbar}{2m\omega}}$ and the integral over time is

$$\int_{-\infty}^{\infty} dt e^{-t^2/\tau^2+i\omega t} = \int_{-\infty}^{\infty} dt e^{-\left(\frac{t}{\tau}-i\omega\tau/2\right)^2} e^{-\omega^2\tau^2/4} = e^{-\omega^2\tau^2/4}\,\tau\int_{-\infty}^{\infty} du e^{-u^2} = e^{-\omega^2\tau^2/4}\tau\sqrt{\pi}$$

The integral can also be found in Rottmann, Chapter X 3., 52):

$$\int_{-\infty}^{\infty} dx e^{-ax^2+2bx+c} = \sqrt{\frac{\pi}{a}} e^{(b^2-ac)/a}$$

setting $x = t$, $a = 1/\tau^2$, $2b = i\omega$ and $c = 0$ we get the above answer. Therefore the transition amplitude becomes

$$a_{10}(t \to \infty) = \frac{qE_0}{i\hbar} \sqrt{\frac{\hbar}{2m\omega}} \sqrt{\pi} \tau e^{-\omega^2\tau^2/4}$$

and the probability for finding the system in the first excited level after the pulse is

$$\underline{P(t \to \infty) = \frac{\pi}{2} \frac{q^2 E_0^2}{m\hbar\omega} \tau^2 e^{-\omega^2\tau^2/2}}$$

i) Two spin-1/2 fermions. Let us denote the states $|n_{x1} n_{y1}\rangle \otimes |n_{x2} n_{y2}\rangle \otimes |s_1\rangle \otimes |s_2\rangle$ where n_{xj}, n_{yj} are the harmonic oscillator quantum numbers of particle j, and s_j is the z-component of the spin of particle j. Since $b \ll \hbar\omega$ the spin interaction will only give slight energy changes so the lowest energy states are found by putting as many fermions as possible in the lowest oscillator levels. The particles are identical fermions so the state must be antisymmetric under the interchange of both orbital (oscillator) and spin quantum numbers. Ground state:

$$|0\rangle = |00\rangle \otimes |00\rangle \otimes \frac{1}{\sqrt{2}} \left(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle \right)$$

The spin interaction term can be written

$$H_s = \frac{b}{\hbar^2} \vec{S}_1 \cdot \vec{S}_2 = b \frac{1}{2} \left(S_{tot}^2 - S_1^2 - S_2^2 \right) = \frac{b}{2} \left(S(S+1) - 3/2 \right)$$

The spin part of the above state has total spin $S = 0$ as it is the spin singlet thus it is an energy eigenstate with energy $E_0 = 2\hbar\omega - \frac{3}{4}b$ and it is not degenerate.

The next to lowest energy states must have one fermion in an excited level and the other in the $|00\rangle$ state. The first excited single-particle energy level is degenerate so we can choose any basis for it. Here we choose $|10\rangle$ and $|01\rangle$, but we could as well have chosen the eigenstates of L_z gotten in d). One particle in $|00\rangle$ and the other in $|10\rangle$ or $|01\rangle$ gives an

energy $\hbar\omega(1+2) = 3\hbar\omega$. The states are

$$
\begin{aligned}
|1\rangle &= \frac{1}{2}\left(|00\rangle \otimes |10\rangle + |10\rangle \otimes |00\rangle\right) \otimes \left(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle\right) \\
|2\rangle &= \frac{1}{\sqrt{2}}\left(|00\rangle \otimes |10\rangle - |10\rangle \otimes |00\rangle\right) \otimes |\uparrow\rangle \otimes |\uparrow\rangle \\
|3\rangle &= \frac{1}{2}\left(|00\rangle \otimes |10\rangle - |10\rangle \otimes |00\rangle\right) \otimes \left(|\uparrow\rangle \otimes |\downarrow\rangle + |\downarrow\rangle \otimes |\uparrow\rangle\right) \\
|4\rangle &= \frac{1}{\sqrt{2}}\left(|00\rangle \otimes |10\rangle - |10\rangle \otimes |00\rangle\right) \otimes |\downarrow\rangle \otimes |\downarrow\rangle \\
|5\rangle &= \frac{1}{2}\left(|00\rangle \otimes |01\rangle + |01\rangle \otimes |00\rangle\right) \otimes \left(|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle\right) \\
|6\rangle &= \frac{1}{\sqrt{2}}\left(|00\rangle \otimes |01\rangle - |01\rangle \otimes |00\rangle\right) \otimes |\uparrow\rangle \otimes |\uparrow\rangle \\
|7\rangle &= \frac{1}{2}\left(|00\rangle \otimes |01\rangle - |01\rangle \otimes |00\rangle\right) \otimes \left(|\uparrow\rangle \otimes |\downarrow\rangle + |\downarrow\rangle \otimes |\uparrow\rangle\right) \\
|8\rangle &= \frac{1}{\sqrt{2}}\left(|00\rangle \otimes |01\rangle - |01\rangle \otimes |00\rangle\right) \otimes |\downarrow\rangle \otimes |\downarrow\rangle
\end{aligned}
$$

From the spin-spin interaction we know that all spin triplet states gets an additional energy $+\frac{b}{4}$ while the spin singlets are lowered in energy by $-\frac{3b}{4}$. There are 2 singlet states ($|1\rangle$ and $|5\rangle$), thus $E_1 = 3\hbar\omega - \frac{3b}{4}$ has degeneracy 2. There are 6 triplet states, which means that $E_2 = 3\hbar\omega + \frac{b}{4}$ has degeneracy 6.

j) To achieve the lowest energy the oscillator levels must be filled from below under the constraint that the wave function is antisymmetric under interchange of particle labels. An antisymmetric state can be gotten by forming the Slater determinant (not required for credit), which for the case $n = 2$ can be written $det(|00\uparrow\rangle, |00\downarrow\rangle)$. The table lists the single-particle states that goes into the Slater determinant. For degenerate one-particle states the sequence of one-particle states is arbitrary.

n	States	$E_n[\hbar\omega]$	E_n/n $[\hbar\omega]$
1	$\|00\uparrow\rangle$	1	1
2	$\|00\uparrow\rangle, \|00\downarrow\rangle$	2	1
3	$\|00\uparrow\rangle, \|00\downarrow\rangle, \|10\uparrow\rangle$	4	4/3=1.33
4	$\|00\uparrow\rangle, \|00\downarrow\rangle, \|10\uparrow\rangle, \|10\downarrow\rangle$	6	3/2=1.5
5	$\|00\uparrow\rangle, \|00\downarrow\rangle, \|10\uparrow\rangle, \|10\downarrow\rangle, \|01\uparrow\rangle$	8	8/5=1.6
6	$\|00\uparrow\rangle, \|00\downarrow\rangle, \|10\uparrow\rangle, \|10\downarrow\rangle, \|01\uparrow\rangle\ \|01\downarrow\rangle$	10	10/6=1.66
7	$\|00\uparrow\rangle, \|00\downarrow\rangle, \|10\uparrow\rangle, \|10\downarrow\rangle, \|01\uparrow\rangle\ \|01\downarrow\rangle, \|20\uparrow\rangle$	13	13/7=1.86

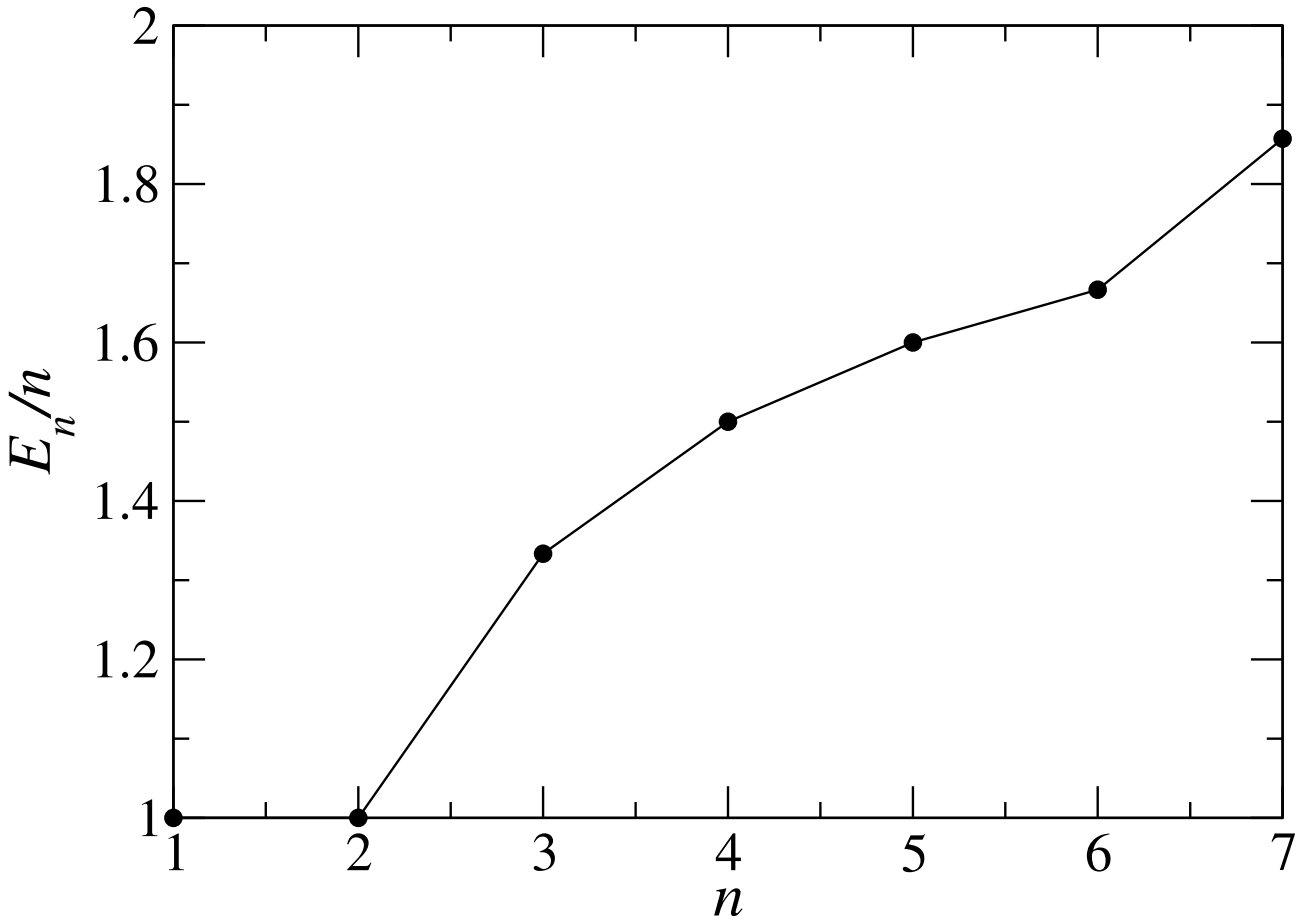

Figure 1: Energy per particle vs. n

A plot of the total energy E_n divided by the number of particles n, right column, is shown in Fig. 1.

We see that the lowest oscillator energy level can take 2 fermions, the next 4, and the third 6, fourth 8 etc. An inert element is an element with its shells completely filled. Therefore an inert element in the 2d world with harmonic oscillator potential instead of Coulomb-potential will be elements where the single-particle energy levels are completely filled. This happens for $\underline{n = 2, 6, 12}, 20, 30, 42, \ldots$ and can be seen in the plot of E_n/n as the last integer before the energy per particle makes a jump.