LULEÅ TEKNISKA UNIVERSITET
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Svar till Sammanställning av tentamensuppgifter Kvant (F0053T).

1. a) S.E. : $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi = E\psi$ lösningen utanför V=0 är $\psi = 0$, i området med V=0 ges lösningen av (efter lite räknande) $\psi_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$ Normeringen $N = \sqrt{\frac{2}{L}}$ fås ur integralen
$N^2 \int_0^L \sin(\frac{n\pi x}{L})\sin(\frac{n\pi x}{L})dx = 1$

   b) Energinivåerna ges av (insättning i S.E. av egenfunktionen) $E_n = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}$ vilket ger att om vidden på lådan halveras så ökar grundtillståndets energi med en faktor 4.

   c) Ortogonaliteten $\int_0^L \sin(\frac{n\pi x}{L})\sin(\frac{m\pi x}{L})dx = \int_0^L \cos(\frac{\pi x}{L}(n-m)) - \cos(\frac{\pi x}{L}(n+m))dx$ = Integralen $\int_0^L \cos(\frac{\pi x}{L}(\text{heltal}))dx = 0$ utom då heltalet råkar vara lika med 0, dvs ψ_m och ψ_n är ortogonala om $m \neq n$.

2. a) $E = \frac{3}{2}k_BT = \frac{1}{2}mv^2$; $v = \sqrt{\frac{3k_BT}{m}} = 134863.88\text{m/s}$, $\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{3mk_BT}} = \frac{6.626\ 10^{-34}}{\sqrt{3\cdot 9.109\ 10^{-31}\ 1.38\ 10^{-23}\ 400}} = 5.39\ 10^{-9}\text{m}$

   b) Uppgiften utgår. Fotonens energi för väte lika system ges av $W_f = W_n - W_m$ där $W_n = -W_HZ^2/n^2$, W_H=13.56 eV. För övergång mellan innersta nivåer ger detta. $W_{f12} = Z^2 13.56(1-\frac{1}{4}) = Z^2\ 10.17 = \frac{hc}{\lambda}$ vilket ger $Z = \sqrt{\frac{6.626\ 10^{-34} 2.998\ 10^{8}}{253\ 10^{-9} 10.17\ 1.602\ 10^{-19}}} = 0.69$ dvs uppgiften felformulerad. Antagandet nm skall vara Å ger Z=2.2 vilket är långt ifrån ett heltal.

3. a) $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$ och randvillkor $\psi(0) = \psi(L) = 0$. Lösningen till SE är på formen $\psi(x) = A\cos(kx) + B\sin(kx)$ med randvillkor ger A=0 och $kL = n\pi$; $k = \frac{n\pi}{L}$ med n=1, 2, 3,.... Detta ger $E_n = \frac{\hbar^2k_n^2}{2m} = \frac{\hbar^2n^2\pi^2}{L^2 2m}$ och $h\nu = E_f = E_2 - E_1 = (4-1)\frac{\hbar^2\pi^2}{L^2 2m}$; $L = \sqrt{\frac{3\pi\hbar}{4m\nu}} = \sqrt{\frac{3\pi 1.055\ 10^{-34}}{49.109\ 10^{-31}\ 2\ 10^{14}}} = 1.168\ 10^{-9}\text{m} = 1.17$ nm.

   b) Kinetiska energin i grundtillståndet ges av $E_1 = \frac{\hbar^2k_1^2}{2m} = \frac{\hbar^2 1^2\pi^2}{L^2 2m} = \frac{1.055^2\ 10^{-68}\pi^2}{1.168^2 10^{-18} 2\ 9.109\ 10^{-31} 1.602\ 10^{-19}} = 0.276$ eV.

4. This is a 2 dimensional problem with a Schrödinger equation (where $V(x,y) = 0$) like

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x,y) - \frac{\hbar^2}{2m}\frac{d^2}{dy^2}\Psi(x,y) = E\Psi(x,y)$$

This equation is separable and the ansatz $\Psi(x,y) = \psi(x) * \psi(y)$ gives the following result

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_x(x) - \frac{\hbar^2}{2m}\frac{d^2}{dy^2}\psi_y(y) = E_x\psi_x(x) + E_y\psi_y(y)$$

ie two independent one dimensional Schrödinger equations one for the variable x and on for y. We therefor solve the one dimensional problem first and after that we construct the two dimensional solution. To find the eigenfunctions we need to solve the Schrödinger equation which is (in the region where $V(x)$ is zero)

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi = E\Psi \ \rightarrow \ \frac{d^2}{dx^2}\Psi + k^2\Psi = 0 \text{ where } k^2 = \frac{2mE}{\hbar^2}$$

Solutions are of the kind:

$$\Psi(x) = A\cos kx + B\sin kx$$

Now we need to take the boundary conditions for the wave function Ψ $\big(\Psi(-\frac{a}{2}) = \Psi(\frac{a}{2}) = 0\big)$ into account.

$$A\cos(-\frac{ka}{2}) + B\sin(-\frac{ka}{2}) = 0 \text{ and } A\cos(\frac{ka}{2}) + B\sin(\frac{ka}{2}) = 0$$

Adding the two conditions gives: $\cos(\frac{ka}{2}) = 0$ and subtracting them gives $\sin(\frac{ka}{2}) = 0$. These two conditions cannot be fulfilled at the same time, so either A or B has to be zero. We start with $A = 0$ and we get the following solution: The normalising constant $B = \sqrt{\frac{2}{a}}$ you get from the condition $\int_{-a/2}^{a/2} \mid \Psi \mid^2 dx = 1$. The condition $\sin(\frac{ka}{2}) = 0$ gives $\frac{ka}{2} = \frac{\pi}{2} * (even - integer)$. The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a}) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 2,4,6,... \tag{1}$$

In a similar way the other function is analysed $(A = 0)$ which gives: The condition $\cos(\frac{ka}{2}) = 0$ gives $\frac{ka}{2} = \frac{\pi}{2} * (odd - integer)$. The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\cos(\frac{n\pi x}{a}) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1,3,5,... \tag{2}$$

The eigenfunctions in the y direction are the same as for the x direction as the potential is similar for this direction. Now we have the eigenfunctions of the one dimensional problem and the solution to the 2 dimensional problem is readily produced. The eigenfunctions are:

$$\Psi_{n,m}(x,y) = \psi_n(x)\cdot\psi_m(y) \text{ eigenenergys } E_{n,m} = E_n + E_m \text{where } n = 1,2,,. \text{ and } m = 1,2, \tag{3}$$

In the area where the potential is infinite the wave function is equal to zero.

An **alternative route** taken by many students has been to present a calculation with the following boundary conditions: Ψ ($\Psi(0) = \Psi(a) = 0$) into account. In this case the solution is for these boundary conditions:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a}) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 2, 3, ... \tag{4}$$

This solution has to be adapted to the boundary conditions related to this exam problem:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}(x+\frac{a}{2})) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 2, 3, ... \tag{5}$$

$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a} + \frac{n\pi}{2}) = \sqrt{\frac{2}{a}}\left(\sin(\frac{n\pi x}{a}) \cdot \cos(\frac{n\pi}{2}) + \cos(\frac{n\pi x}{a}) \cdot \sin(\frac{n\pi}{2})\right)$. We see that we recover the solution in eq (1), (2) and (3) as we let n run from 1 to ∞.

b) The ground state eigenfunction is given by (using eq. (2))

$$\Psi_{n=1,m=1}(x, y) = \psi_1(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}}\cos(\frac{\pi x}{a}) \cdot \sqrt{\frac{2}{a}}\cos(\frac{\pi y}{a}) \tag{6}$$

The next lowest state eigenfunction is given by (using eq. (2) and (1)). Note there are two eigenfunctions with the same energy ($\Psi_{n=1,m=2}(x, y)$) you may use either one of them.

$$\Psi_{n=2,m=1}(x, y) = \psi_2(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}}\sin(2\frac{\pi x}{a}) \cdot \sqrt{\frac{2}{a}}\cos(\frac{\pi y}{a}) \tag{7}$$

Orthogonality is defined as

$$\int_x \int_y \Psi_{n_1,m_1}(x, y)\Psi_{n_2,m_2}(x, y) = \delta_{n_1,n_2}\ \delta_{m_1,m_2} \tag{8}$$

by explicit calculation

$$\int_{x=-a/2}^{a/2}\int_{y=-a/2}^{a/2}\left(\frac{2}{a}\cos(\frac{\pi x}{a}) \cdot \cos(\frac{\pi y}{a})\right)\cdot\left(\frac{2}{a}\sin(2\frac{\pi x}{a}) \cdot \cos(\frac{\pi y}{a})\right) = \text{calculations} = 0 \tag{9}$$

this is a separable integral (in x and y), suggestion do the integral in x first as this will be zero as they belong to different eigenvalues. Thus the calculation ends with a zero as it should.

5. Normering $\int_0^L \psi_n^*(x,t)\psi_n(x,t)dx = 1$ ger $C^2 \int_0^L \sin^2(\frac{n\pi x}{L})dx = 1$ vilket ger $C = \sqrt{\frac{2}{L}}$. Sannolikheten att finna partikeln i ett intervall $dx = 0.001L$ nära $x = L/3$ ges av: $\psi^*\psi dx = \frac{2}{L}\sin(\frac{n\pi\frac{L}{3}}{L})\sin(\frac{n\pi\frac{L}{3}}{L}) \cdot 0.001L = 0.002\sin^2(n\frac{\pi}{3})$.

   Det blir två fall: $= 0.002(\frac{\sqrt{3}}{2}) = 0.0015$ om n=1+3k eller n=2+3k, k=0,1,2,... eller $= 0$ om n=3k, k=1,2,3,...

6. Systemet är preparerat i vågfunktionen $\frac{1}{6}[4\psi_{100}(r) + 3\psi_{211}(r) - \psi_{210}(r) + \sqrt{10}\psi_{21-1}(r)]$. Den är normerad och tex ψ_{210} är väte egenfunktionen med kvanttalen $n = 2$, $l = 1$ och $m_l = 0$.

   a) För väte $E_n = -\frac{13.56}{n^2}$eV ; $< E >= \frac{1}{36}[16\cdot\frac{1}{1^2}+9\cdot\frac{1}{2^2}+1\cdot\frac{1}{2^2}+10\cdot\frac{1}{2^2}](-13.56)$eV = -7.91 eV

   b) $\mathbf{L}^2 = \hbar^2 l(l+1)$; $< L^2 >= \frac{1}{36}[16\cdot 0\cdot 1 + 9\cdot 1\cdot 2 + 1\cdot 1\cdot 2 + 10\cdot 1\cdot 2]\frac{40}{36}\hbar^2$

   c) $L_z = m_l\hbar$; $< L_z >= \frac{1}{36}[16\cdot 0 + 9\cdot 1 + 1\cdot 0 - 10\cdot 1] = -\frac{\hbar}{36}$

7. Se Atkins ed7 Problem 13.1. Den ena gränsen 3281.4 nm är övergång från oändligheten ner till lägsta nivån i serien. Detta ger övergångar ner mot $n_0 = 6$. Det går också att borja i andra ändan av serien 12368 nm. Denna motsvarar en övergång mellan två närliggande nivåer, $n_0 + 1$ ner till n_0. Detta ger också att 12368 nm är mellan n=7 och n=6 dvs $n_0 = 6$. Serien är 12368 nm, 7503 nm, 5908 nm, 5129 nm,... konvergerar mot 3282 nm

8. Visa $\psi = Ae^{ax^2+bx}$ är grundtillståndet. Det går ut på att sätta in ψ i S.E. Skriv om S.E. till

   $\frac{\partial^2}{\partial x^2}\psi = \frac{2m}{\hbar^2}\left(V(x) - E\right)\psi = \left[\frac{mk}{\hbar^2}x^2 - \frac{2mk}{\hbar^2}x_0 x + \frac{mk}{\hbar^2}x_0^2 - \frac{2mE}{\hbar^2}\right]Ae^{ax^2+bx}$

   Bilda derivatorna

   $\frac{\partial}{\partial x}\psi = (2ax+b)Ae^{ax^2+bx}$; $\frac{\partial^2}{\partial x^2}\psi = (4a^2x^2 + 4abx + b^2 + 2a)Ae^{ax^2+bx}$

   vilket ger $4a^2 = \frac{mk}{\hbar^2}$; $a = -\frac{\sqrt{mk}}{2\hbar}$, a måste vara mindre än 0 ty annars ej normerbar vågfunktion. Vidare $-\frac{2mk}{\hbar^2}x_0 = 4ab$ vilket ger $b = \frac{\sqrt{mk}}{\hbar}x_0$. Vidare $\frac{mk}{\hbar^2}x_0^2 - \frac{2mE}{\hbar^2} = b^2 + 2a = \frac{mk}{\hbar^2}x_0^2 - \frac{\sqrt{mk}}{\hbar}$ och detta ger energin $E = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$, dvs grundtillståndets energi och med konstanterna $a = -\frac{\sqrt{mk}}{2\hbar}$ och $b = \frac{\sqrt{mk}}{\hbar}x_0$.

9. Fotonens energi $W_f = W_n - W_m$ där $W_n = -W_H/n^2$, W_H=13.6 eV. Våglängderna för synligt ljus 400 nm < λ < 700 nm, vilket motsvarar 1.77 eV < W_f < 3.1 eV. Prövning ger att synligt ljus kommer från (Balmer serien), m=2 och n=3,4,... vilket ger W_f= 1.89, 2.55, 2.86, 3.12 eV Motsvarande våglängder är λ = 656, 486, 434, 410 nm. (Om m=1 är fotonenergierna för stora och om m=3 är fotonenergierna för små.)

10. a) Lyman serien ges av övergången mellan högre nivåer ner till lägsta nivån_0 ($n_0 = 1$). Den ges $\nu = \frac{1}{\lambda} = R_{Li}(1 - \frac{1}{n^2})$ Serien som ges är för n_1 =2,3 resp 4. Vilket ger $R_{Li} = \frac{4}{3}$ 740747 = 987662.7cm^{-1}, $R_{Li} = \frac{9}{8}$ 877924 = 987664.5cm^{-1}, $R_{Li} = \frac{16}{15}$ 925933 = 987661.9cm^{-1}. Medelvärdet blir R_{Li} = 987663.0cm^{-1}

    b) Gränsvåglängden ges av $\lambda_\infty = \frac{1}{R_{Li}} = \frac{1}{987663.0\ 100} = 1.01249\ 10^{-8}$m = 101.249Å. Motsvarande energi (=jonisationeenergi) blir $E = \frac{hc}{\lambda_\infty} = \frac{6.626\ 10^{-34}\ 2.998\ 10^{8}}{1.6022\ 10^{-19}\ 1.01249\ 10^{-8}} = 122.45$eV

11. Relevant radieldel: $R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}$ Sannolikheten att hitta den mellan r och r+dr ges av $P(r)dr = R_{21}(r)^2r^2dr$ och därmed $P(r) = R_{21}(r)^2r^2$ = konstant r^4e^{-Zr/a_0}. Extremvärden då derivatan = 0. $\frac{dP(r)}{dr} = 4r^3e^{-Zr/a_0} - r^4\frac{Z}{a_0}e^{-Zr/a_0} = r^3(4 - r\frac{Z}{a_0})e^{-Zr/a_0}$. Vilket ger ett maxima för $r = 4a_0$ ($P(0) = P(\infty) = 0$ och $P(r) \geq 0$ alltså ett max).

    Utan yttre fält (elektriska eller magnetiska) beror väte atomens energi enbart på huvudkvanttalet n och inte på banrörelsemängdsmomentkvanttalet l, och ej heller på m_l kvanttalet. Så följande tillstånd har samma energi (se Atkins 6ed sid 353):
    I) 3s med $m_l = 0$, 3p med $m_l = 1$, 3p med $m_l = -1$, 3p med $m_l = 0$.
    II) 4d med $m_l = 1$, 4p med $m_l = 0$, 4p med $m_l = -1$.
    III) 5d med $m_l = 1$, 5p med $m_l = -1$, 5s med $m_l = 0$.

12. Rewrite the wave function in terms of spherical harmonics: (polar coordinates: $x = r\sin\theta\sin\phi$, $z = r\cos\theta$ and hence $zx = r^2\cos\theta\sin\theta(e^{i\phi} + e^{-i\phi})/2$ using the Euler relations) the appropriate spherical harmonics can now be identified and we arrive at

$$\psi(\boldsymbol{r}) = \psi(x,y,z) = N(zx)e^{-r/3a_0} = N\frac{r^2}{2}\sqrt{\frac{8\pi}{15}}(-Y_{2,1} + Y_{2,-1})e^{-r/3a_0}\ . \quad (10)$$

    As all the involved $Y_{l,m}$ have $l = 2$ the probability to get $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$ is one. For the operator L_z we note the two spherical harmonics have the same pre factor (one has -1 and the other has +1 but the absolute value square is the same) ie they will have the same probability. The probability to find $m = 2\hbar$ is 0, for $m = 1\hbar$ is $\frac{1}{2}$, for $m = 0\hbar$ is 0 for $m = -1\hbar$ is $\frac{1}{2}$, and for $m = -2\hbar$ is 0. As all the involved $Y_{l,m}$ have $l = 2$ the probability to get $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$ is one.

b. To calculate the expectation value $< r >$ we need to normalise the given wave function if we wish to do the integral. In order to achieve this in a simple way is to identify the radial wave function. As l is equal to 2 we know that n cannot be equal to 1 or 2 it has to be **larger** or **equal** to 3. By inspection of eq (10) and 2 we find $n = 3$ this function has the correct exponential and the correct power of r (r^2) and hence $R_{3,2}(r) = \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$. We also note that $Y_{2,1}$ and $Y_{2,-1}$ are normalised but the sum $(-Y_{2,1} + Y_{2,-1})$ is not normalised. The sum has to be changed to $(-\frac{1}{\sqrt{2}}Y_{2,1} + \frac{1}{\sqrt{2}}Y_{2,-1})$ in order to be normalised. Note that $R_{3,2}(r)$ contains an r^2 term as also a $e^{-r/3a_0}$ term. The wave function can now be completed to the following normalized wave function (note that we do not need to calculate the constant N as all separate parts of $\psi(r)$ are normalised by them selves)

$$\psi(\boldsymbol{r}) = \psi(x, y, z) = N(zx)e^{-r/3a_0} = R_{3,2}(r)(-\frac{1}{\sqrt{2}}Y_{2,1} + \frac{1}{\sqrt{2}}Y_{2,-1})e^{-r/3a_0}$$

From physics handbook page 292 you find

$$\langle r\rangle = \frac{1}{2}\left[3n^2 - l(l+1)\right]\left(\frac{a_0}{Z}\right) = \frac{1}{2}\left[3\ 3^2 - 2(2+1)\right]\left(\frac{a_0}{1}\right) = \frac{21}{2}a_0 =$$

$$10.5\ \cdot 0.5292\ \text{Å} = 5.56\ \text{Å}.$$

You may also do the integral directly like this:

$$\langle r\rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} d\phi\, d\theta\, dr\, r^2 \sin(\theta)\, r\ \mid R_{3,2}(r)\mid^2 \mid \left(-\frac{1}{\sqrt{2}}Y_{2,1} + \frac{1}{\sqrt{2}}Y_{2,-1}\right)\mid^2\ e^{-2r/3a_0} =$$

$$\int_0^\infty dr\ r^3 \mid R_{3,2}(r)\mid^2 e^{-2r/3a_0} = \frac{21}{2}a_0 = 10.5\ \cdot 0.5292\ \text{Å} = 5.56\ \text{Å}.$$

13. (a) $i\hbar\frac{\partial^2}{\partial t^2}\cos\omega t = -i\hbar\omega\frac{\partial}{\partial t}\sin\omega t = -i\hbar\omega^2\cos\omega t$ **YES**
    (b) $\frac{\partial}{\partial x}e^{ikx} = ike^{ikx}$ **YES**
    (c) $\frac{\partial}{\partial x}e^{-ax^2} = -2axe^{-ax^2}$ **NO**
    (d) $\frac{\partial}{\partial x}\cos kx = -k\sin kx$ **NO**
    (e) $\frac{\partial}{\partial x}kx = k$ **NO**

(f) $\hat{P}\sin(kx) = \sin(-kx) = -\sin(kx)$ **YES**

(g) $-i\hbar\frac{\partial}{\partial z}C(1+z^2) = -i\hbar C(0+2z)$ **NO**

(h) $-\frac{\hbar}{2}\frac{\partial}{\partial z}Ce^{-3z} = -\frac{\hbar}{2}C(-3)e^{-3z} \;\propto\; \psi(z)$ **YES**

(i) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} =?$ This has to be done in some steps. Start by doing this derivative first: $-\frac{\partial^2}{\partial z^2}ze^{-\frac{1}{2}z^2} = -\frac{\partial}{\partial z}(e^{-\frac{1}{2}z^2} - z^2e^{-\frac{1}{2}z^2}) = -(-ze^{-\frac{1}{2}z^2} - 2ze^{-\frac{1}{2}z^2} + z^3e^{-\frac{1}{2}z^2}) = 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}$.
Now you go back to the start: $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} = \frac{C}{2}(z^3e^{-\frac{1}{2}z^2} + 3ze^{-\frac{1}{2}z^2} - z^3e^{-\frac{1}{2}z^2}) = \frac{C}{2}(+3ze^{-\frac{1}{2}z^2}) = \propto\; \psi(z)$ **YES**

14. (a) $\langle H\rangle = \frac{1}{2}0.31 + \frac{2}{12}0.97 + \frac{1}{12}1.81 + \frac{3}{16}3.35 + \frac{1}{16}4.08 = 1.350625 \approx 1.35\text{eV}$.
Uncertainty is defined by: $\langle \Delta H\rangle = \sqrt{\langle H^2\rangle - \langle H\rangle^2}$
$\langle H^2\rangle = \frac{1}{2}(0.31)^2 + \frac{2}{12}(0.97)^2 + \frac{1}{12}(1.81)^2 + \frac{3}{16}(3.35)^2 + \frac{1}{16}(4.08)^2 = 3.622494 \approx 3.62\text{eV}$.
$\langle \Delta H\rangle = \sqrt{3.622494 - 1.350625^2} = 1.341009 \approx 1.34\text{eV}$

(b) The expression is not unique as we only know the probabilities which are the squares of the coefficients. In the evaluation of $\langle H\rangle$ and $\langle H^2\rangle$ only the probabilities are important that's why a different sign $\pm$ is of no importance in this calculation.
One is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \sqrt{\frac{2}{12}}\psi_2(z) + \frac{1}{\sqrt{12}}\psi_3(z) + \frac{\sqrt{3}}{4}\psi_4(z) + \frac{1}{4}\psi_5(z)$.
Another is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) - \sqrt{\frac{2}{12}}\psi_2(z) + \frac{1}{\sqrt{12}}\psi_3(z) + \frac{\sqrt{3}}{4}\psi_4(z) + \frac{1}{4}\psi_5(z)$.

(c) By a factor of 4. (All eigenvalues change by a factor of 4)

15. The eigenfunctions of the infinite square well are (Collection of formulae or in Physics handbook)

$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$ and the eigenenergies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n = 1, 2, 3, ...$

The correction to the eigenenergies due to perturbation is given by:

$E_n^1 =< H_1 >$ where $H_1 = V_0x$ is the deviation in the potential from the infinite squ

$$E_n^1 = \int_0^1 \frac{2V_0x}{1}\sin^2(\frac{n\pi x}{1})dx = \int_0^1 \frac{2V_0x}{2}\left(1-\cos(2n\pi x)\right)\,dx =$$

$$V_0\left[\frac{x^2}{2}\right]_0^1 + V_0\left[x\frac{\sin(2n\pi x)}{2n\pi}\right]_0^1 - V_0\int_0^1 \frac{\sin(2n\pi x)}{2n\pi}dx = \frac{V_0}{2} + 0 - 0 + V_0\left[\frac{\cos(2n\pi x)}{4n^2\pi^2}\right]_0^1 = \frac{V_0}{2}$$

This is the same for all n. The corrections for n=1 and n=2 and n=3 are of intrest giving the same shift in energy to all three $E_n^1 = E_n^0 + \frac{V_0}{2}$.

$$E_n^1 = E_n^0 + \frac{V_0}{2}$$

If the calculation is done for an arbitrary a we get.

$E_n^1 =< H_1 >$ where $H_1 = V_0 \frac{x}{a}$ is the deviation in the potential from the infinite squ

$$E_n^1 = \int_0^a \frac{2V_0 x/a}{a} \sin^2(\frac{n\pi x}{a})dx = \frac{V_0}{a^2}\left[\frac{x^2}{2}\right]_0^a = \frac{V_0}{2}$$ the same result as previously.

16. The eigenfunctions of the infinite square well are (Physics handbook)

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$ and the eigenenergies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ where $n = 1, 2, 3, ...$

The correction to the eigenenergies due to perturbation is given by:

$E_n^1 =< H_1 >$ where H_1 is the deviation in the potential from the infinite square we

$$E_n^1 = \int_0^{a/2} \frac{2\epsilon}{a} \sin^2 \frac{n\pi x}{a} dx = \int_0^{a/2} \frac{2\epsilon}{a2}\left(1 - \cos\frac{2n\pi x}{a}\right) dx = \frac{\epsilon}{a}\left[x - \frac{a}{2n\pi}\sin\frac{2n\pi x}{a}\right]_0^{a/2} =$$

This is the same for all n. The corrections for n=1 and n=2 are of intrest (**answer to a)**).

$$E_1^1 = E_2^1 = \frac{\epsilon}{2} = 0.0465\text{eV}.$$

The two lowest eigenergies are

$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$ $[n = 1]$ $E_1 = 6.02465 \cdot 10^{-20}\text{J} = 0.376028\text{eV}$ and $E_2 = 1.504114$

The new energys for the two lowest levels are:

$E_1^* = 0.376028 + 0.0465 = 0.422528 \approx 0.4225\text{eV}$ and $E_2^* = 1.504114 + 0.0465 = 1.55061$

The case of $\epsilon = 1.09$ eV. This energy is much higher than the groundstate energy of the unperturbed model. You cannot use perturbation here. The model is more like a square well of width $a/2$. The answer of such a perturbation calculation would not give a trustworthy result.

17. The task is to calculate the change of the energy levels (ground state E_0 and first excited state E_1) for a harmonic oscillator due to a perturbation H^1 to the potential.

The two harmonic oscillator eigenfunctions that are of interest are :

$$\psi_0(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}}\, e^{-\frac{1}{2}\alpha^2 x^2} \quad \text{and} \quad \psi_1(x) = \sqrt{\frac{\alpha}{2\sqrt{\pi}}} 2\alpha x\, e^{-\frac{1}{2}\alpha^2 x^2} \quad \text{where} \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}$$

(a) Here we have a perturbation γx^4 where γ is small in some sence. The first integral to calculate (use integration by parts) will be for the change of the ground state energy

$$\langle 0 \mid \gamma x^4 \mid 0\rangle = \int \psi_0^*(x)\gamma x^4 \psi_0(x) dx = \int \frac{\alpha}{\sqrt{\pi}} \gamma x^4\, e^{-\alpha^2 x^2} dx = [\alpha x = y] = \frac{\gamma}{\alpha^4 \sqrt{\pi}} \int y^4\, e$$

where the integral taken separately will be

$$\int_{-\infty}^{\infty} y^4\, e^{-y^2} dy = [-\frac{y^3}{2} e^{-y^2}]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{3y^2}{2} e^{-y^2} = [-\frac{3y^1}{4} e^{-y^2}]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{3}{4} e^{-y^2} = \frac{3}{4}\sqrt{\pi}$$

Hence the shift of the ground state energy will be

$$\langle 0 \mid \gamma x^4 \mid 0\rangle = \frac{\gamma}{\alpha^4\sqrt{\pi}} \frac{3}{4}\sqrt{\pi} = \frac{3\gamma}{4\alpha^4} = \frac{3\gamma}{4}\left(\frac{\hbar}{m\omega}\right)^2$$

The energy of the unperturbed groundstate is $E_0 = \frac{\hbar\omega}{2}$. Hence the energy of the perturbed groundstate is

$$E_0^{\text{perturbed}} = \frac{\hbar\omega}{2} + \frac{3\gamma}{4}\left(\frac{\hbar}{m\omega}\right)^2$$

(b) Here we have a perturbation ϵx where ϵ is small in some sence. The integrals to be calculated are $\langle 0 \mid \epsilon x \mid 0\rangle$ and $\langle 1 \mid \epsilon x \mid 1\rangle$. The squares of both eigenfunctions are even functions and as the perturbation is odd both integrals will be zero.

Hence there is no change in energy to first order.

18. Use the spin matrixes to evaluate the expectation values.

$$< S_x > = \frac{1}{9}(2+i, 2)\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 2-i \\ 2 \end{pmatrix} = \frac{4}{9}\hbar$$

$$< S_y > = \frac{1}{9}(2+i, 2)\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 2-i \\ 2 \end{pmatrix} = \frac{2}{9}\hbar$$

$$< S_z >= \frac{1}{9}(2+i,2)\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 2-i \\ 2 \end{pmatrix} = \frac{1}{18}\hbar$$

If one squares a spin matrix σ_i^2 you will find a result proportional to the unit matrix for all three indecies x, y or z.

$$S_x^2 = \frac{\hbar^2}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

We arrive at:

$$< S_x^2 >=< S_y^2 >=< S_z^2 >= \hbar^2\frac{1}{36}(2+i,2)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 2-i \\ 2 \end{pmatrix} = \frac{1}{4}\hbar^2$$

19. **a**

The spinor is not normalised and we need to do this first:

$$1 = \chi^*\chi = \mid A \mid^2 (2-5i, 3+i)\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \mid A \mid^2 \left(\mid 2+5i \mid^2 + \mid 3-i \mid^2\right) = \mid A \mid^2 (29 +$$

$$\text{and hence : } A = \frac{1}{\sqrt{39}}$$

Note an expectation value is always a real number, never a complex one! Even if you had taken A to be a complex number like $A = \frac{i}{\sqrt{39}}$ it would not change the expectation value as the expectation value below only involves $\mid A \mid^2$.

$$< S_x >= \frac{1}{39}(2-5i, 3+i)\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \frac{1}{39}\hbar$$

$$< S_y >= \frac{1}{39}(2-5i, 3+i)\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = -\frac{17}{39}\hbar$$

$$< S_z >= \frac{1}{39}(2-5i, 3+i)\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \frac{19}{78}\hbar$$

b

Measurement along the x direction means: $S = (1,0,0)\cdot(S_x, S_y, S_z) = S_x$. The idea is to expand the initial spinor χ into the eigenspinors of S_x. So we start to calculate the eigenvalues and eigenspinors to S_x. The spin operator S_x is

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

we find the eigenvalues from the following equation

$$S_n\chi = \lambda\chi \Leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix} \tag{11}$$

We find the eigenvalues from the equation

$$\begin{vmatrix} -\lambda & 1\frac{\hbar}{2} \\ 1\frac{\hbar}{2} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm\frac{\hbar}{2}$$

The eigenspinors to S_x corresponding to the $+\frac{\hbar}{2}$ we get from

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

The two equations above are linearly dependent and one of them is

$$a = b \Leftrightarrow \text{ let } \; b = 1 \; \text{ and hence } \; a = 1$$

This gives the unnormalised spinor

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and after normalisation we have } \; \chi_{x+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

The other eigenspinor χ_{x-} has to be orthogonal to χ_{x+}. An appropriate choice is:

$$\chi_{x-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

This eigenspinor χ_{x-} is orthogonal to the eigenspinor χ_{x+}.

Now we can expand the initial spinor χ in these eigenspinors of S_x.

$$\chi = \frac{1}{\sqrt{39}}\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = b_+\chi_{x+} + b_-\chi_{x-}$$

The coefficient b_+ is given by

$$b_+ = \chi_{x+}^*\chi = \frac{1}{\sqrt{78}}(1 \;\; 1) * \begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \frac{1}{\sqrt{78}}(2+5i+3-i) = \frac{1}{\sqrt{78}}(5+4i)$$

A similar calculation gives b_- :

$$b_- = \chi_{x+}^*\chi = \frac{1}{\sqrt{78}}(1 \quad -1)*\begin{pmatrix} 2+5i \\ 3-i \end{pmatrix} = \frac{1}{\sqrt{78}}(2+5i-3+i) = \frac{1}{\sqrt{78}}(-1+6i)$$

We may now check that $\mid b_+ \mid^2 + \mid b_- \mid^2 = 1$

$$\mid b_+ \mid^2 + \mid b_- \mid^2 = \frac{1}{78}(25+16+1+36) = 1 \quad \text{ok}$$

The probability (to get $+\frac{\hbar}{2}$) is given by $|b_+|^2$.

$$|b_+|^2 = \frac{1}{78}(25+16) = \frac{41}{78} \approx \mathbf{0.526}$$

and (to get $-\frac{\hbar}{2}$) is given by $|b_-|^2$.

$$|b_-|^2 = \frac{1}{78}(1+36) = \frac{37}{78} \approx \mathbf{0.474}$$

You may make the following check for consistency:

$$< S_x >= \left(\frac{41}{78}(\frac{\hbar}{2}) + \frac{37}{78}(-\frac{\hbar}{2})\right) = \frac{1}{39}\hbar$$

The same result as in part **a**.

20. The appropriate spin opperators are

$$S_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } S_z = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

a) For S_z the eigenvalues are $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ and the eigenspinors are for the positive eigenvalue $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and for the negative eigenvalue $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. We have to express the given spinor in terms of the eigenspinors to S_z in the following expansion:

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \frac{1+i}{\sqrt{6}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} + \frac{2}{\sqrt{6}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1+i}{\sqrt{6}}\chi_- + \frac{2}{\sqrt{6}}\chi_+$$

The probabilities are now just the absolute squares of the coefficients in the expansion above.
The probability to get $-\frac{\hbar}{2}$ is $\frac{2}{6} = \frac{1}{3}$

The probability to get $+\frac{\hbar}{2}$ is $\frac{4}{6} = \frac{2}{3}$

b) For S_y we have to do some calculations to find the appropriate eigenspinors. The eigenvalue equation is

$$S_y\chi = \lambda\chi \Leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix} \tag{12}$$

We find the eigenvalues from

$$\begin{vmatrix} -\lambda & -i\frac{\hbar}{2} \\ i\frac{\hbar}{2} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm\frac{\hbar}{2}$$

The eigenspinors to S_y corresponding to the $+\frac{\hbar}{2}$ we get from

$$\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

This gives two identical equations $-ib = a$. Now let $a = 1$ and hence $b = i$. This gives the unnormalised spinor

$$\begin{pmatrix} 1 \\ i \end{pmatrix} \quad \text{and after normalisation we have} \quad \chi_{y+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$$

For the negative eigenvalue we get the $-a = -ib$ and hence the eigen spinor is

$$\chi_{y-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Now we have to express the given spinor in terms of the eigenspinors to S_y:

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix}$$

We make use of the projection by operating from the left with χ_{y+}^*:

$$\chi_{y+}^*\chi = \frac{1}{\sqrt{2}}(1 \quad -i) * \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \frac{2 + -i(1+i)}{\sqrt{12}} = \frac{3-i}{\sqrt{12}}$$

For the other spinor we find (operating from the left with χ_{y-}^*):

$$\chi_{y-}^*\chi = \frac{1}{\sqrt{2}}(1 \quad i) * \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \frac{2 + i(1+i)}{\sqrt{12}} = \frac{1+i}{\sqrt{12}}$$

Now we know how to expand χ in the eigenspinors of S_y

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ 1+i \end{pmatrix} = \frac{3-i}{\sqrt{12}}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} + \frac{1+i}{\sqrt{12}}\cdot\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{3-i}{\sqrt{12}}\cdot\chi_{y+} + \frac{1+i}{\sqrt{12}}\cdot\chi_{y-}$$

The probabilities are now just the absolute squares of the coefficients in the expansion above.

The probability to get $+\frac{\hbar}{2}$ is $\frac{10}{12} = \frac{5}{6}$

The probability to get $-\frac{\hbar}{2}$ is $\frac{2}{12} = \frac{1}{6}$

21.