MN3 Institutionen för teoretisk fysik
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Solutions to Examination in Quantum Mechanics

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Will be also available on `http://www.teorfys.uu.se/~edsjo/kmek/index.html`

1. a) Using the orthonormality of the basis $\{|\psi_n\rangle\}$ it follows

$$A_{mn} = \langle\psi_m|\hat{A}|\psi_n\rangle = a_n\langle\psi_m|\psi_n\rangle = a_n\delta_{mn} \ .$$

b) Since $\hat{A}$ and $\hat{B}$ commute by hyphothesis, We have

$$\hat{A}\hat{B}|\psi_n\rangle = \hat{B}\hat{A}|\psi_n\rangle = a_n\hat{B}|\psi_n\rangle$$

. Then, it is evident that $\hat{B}|\psi_n\rangle$ and $|\psi_n\rangle$ are both eigenfunction of $\hat{A}$ and they have the same eigenvalues. Since we assumed the spectrum of $\hat{A}$ to be not degenerate, this means that

$$\hat{B}|\psi_n\rangle = c_n|\psi_n\rangle$$

where c_n are some complex constants. Thus,

$$B_{mn} = \langle\psi_m|\hat{B}|\psi_n\rangle = c_n\langle\psi_m|\psi_n\rangle = c_n\delta_{mn} \ .$$

c) The unitarity condition, $\hat{U}^\dagger\hat{U} = \mathbf{I}$, gives

$$\left(\mathbf{I} - i\epsilon\hat{F}^\dagger\right)\left(\mathbf{I} + i\epsilon\hat{F}\right) = \mathbf{I} \ ;$$

then, retaining only the terms to first order in ϵ, we have

$$\mathbf{I} - i\epsilon\hat{F}^\dagger + i\epsilon\hat{F} = \mathbf{I}$$

that implies $\hat{F}^\dagger = \hat{F}$.

2. a) For a free particle $\hat{H} = \dfrac{\hat{p}^2}{2m}$, thus

$$\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} = \frac{1}{i\hbar}[\hat{p},\hat{H}] = \frac{1}{2mi\hbar}[\hat{p},\hat{p}^2] = 0$$

and

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = \frac{1}{2mi\hbar}[\hat{x},\hat{p}^2] = \frac{1}{2mi\hbar}2i\hbar\hat{p} = \frac{\hat{p}}{m}$$

where we used $[\hat{x},\hat{p}^2] = \hat{p}[\hat{x},\hat{p}] + [\hat{x},\hat{p}]\hat{p}$ and $[\hat{x},\hat{p}] = i\hbar\mathbf{I}$.

b) If instead $\hat{H} = \dfrac{\hat{p}^2}{2m} + \dfrac{1}{2}m\omega^2\hat{x}^2$ we have

$$\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} = \frac{1}{i\hbar}\left(\frac{1}{2m}[\hat{p},\hat{p}^2] + \frac{1}{2}m\omega^2[\hat{p},\hat{x}^2]\right) = -m\omega^2\hat{x}$$

and

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = \frac{1}{i\hbar}\left(\frac{1}{2m}[\hat{x},\hat{p}^2] + 2i\hbar\hat{p} = \frac{1}{2}m\omega^2[\hat{x},\hat{x}^2]\right) = \frac{\hat{p}}{m} \ .$$

c) $\Delta x^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$ and $\Delta p^2 = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$. Using $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$, $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and the orthonormality of the $|n\rangle$ states, one can show that

$$\langle n|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\langle n|\hat{a}|n\rangle + \langle n|\hat{a}^\dagger|n\rangle \right) = 0$$

and, anagously,

$$\langle n|\hat{p}|n\rangle = -i\sqrt{\frac{m\hbar\omega}{2}} \left(\langle n|\hat{a}|n\rangle - \langle n|\hat{a}^\dagger|n\rangle \right) = 0 \ .$$

Then

$$\Delta x^2 = \langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega} \langle n|\hat{a}\hat{a} + \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}^\dagger|n\rangle = \frac{\hbar}{2m\omega}(2n+1)$$

and

$$\Delta p^2 = \langle n|\hat{p}^2|n\rangle = -\frac{m\hbar\omega}{2} \langle n|\hat{a}\hat{a} - \hat{a}^\dagger\hat{a} - \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}^\dagger|n\rangle = \frac{\hbar m\omega}{2}(2n+1) \ .$$

For the ground state ($n = 0$) we find:

$$\Delta x \Delta p = \frac{\hbar}{2} \ .$$

d) For the $n = 1$ level we readely find

$$\Delta x \Delta p = \frac{3\hbar}{2} \ .$$

3. a) The transmission and reflection coefficients T and R are defined as

$$T = \frac{|j_{\text{trans}}|}{|j_{\text{inc}}|} \qquad R = \frac{|j_{\text{refl}}|}{|j_{\text{inc}}|}$$

where j_{inc}, j_{trans} and j_{refl} are the incoming, transmitted and reflected probability currents respectively.

b)

$$T = \left[1 - \frac{V_0^2 \sin^2(ka)}{4E(E - V_0)} \right]^{-1}$$

where $k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$ (see Brandsen & Joachain 4.4 and your lecture notes for the derivation of this expression). In our case $\sqrt{\frac{V_0 m}{\hbar^2}}$. In order to have $T = 1$ we must have $ka = \pi, \ 2\pi, \ 3\pi....$ The smallest value of a is obtained for $ka = \pi$ from which we get

$$a = \left(\frac{\pi^2\hbar^2}{V_0 m} \right)^{\frac{1}{2}}$$

.

c) Since, increasing E, k also increases, it is evident that the condition $ka = \pi$ requires a to decrease. $T = 1$ when the waves reflected in $x = 0$ interfere destructively with those reflected in $x = a$. Since the DeBroglie wavelength is $\lambda = 2\pi/k$ the condition $ka = n\pi$ implies

$$\frac{a}{\lambda} = \frac{n}{2}$$

where n is an integer number.

d) The limit $m \to \infty$ correspond to the *classical limit*. In a such a limit there is no reflection, hence $T = 1$ and $T = 0$ for every value of a.

4. a) Since our particle is in a central potential it is convenient to rewrite ψ in spherical coordinates

$$\psi(r,\theta,\phi) = \sqrt{\frac{15}{8\pi}}\frac{1}{(2a)^{3/2}}\sin\theta\cos\theta\left(\frac{e^{i\phi}+e^{-i\phi}}{2}\right)e^{-r/2a} \ .$$

Using the expressions for the spherical harmonics (see e.g. P-H) this can be rewritten

$$\psi(r,\theta,\phi) = \frac{1}{2(2a)^{3/2}}\left(-Y_{21}+Y_{2-1}\right)e^{-r/2a} \ .$$

Then

$$N \equiv \int dV|\psi(r,\theta,\phi)|^2 = \frac{1}{2a^3}\int_0^\infty drr^2e^{-r/a}\int_0^{2\pi}d\phi\int_0^\pi d\theta\sin(\theta)\left(|Y_{21}|^2+|Y_{2-1}|^2\right)$$

where we used the orthogonality of the spherical harmonics. Using the hint

$$\int_0^\infty drr^2e^{-r/a} = 2a^3 \ .$$

Instead the normality of the spherical harmonics implies

$$\int_0^{2\pi}d\phi\int_0^\pi d\theta\sin\theta\left(|Y_{21}|^2+|Y_{2,-1}|^2\right) = 2 \ .$$

It follows that $N = 1/8$, hence the wave function is not normalized !

Note: Was not my intention to give a non-normalized w.f. I apologize for the misprint. The normalized wave function should be instead

$$\psi(x,y,z) = \sqrt{\frac{15}{8\pi}}\frac{1}{(a)^{3/2}}\frac{xz}{r^2}e^{-r/2a} \ .$$

b) Since the wave function is a linear combination of two spherical harmonic with the same index $l = 2$ it is evident that this is the only permitted value of the orbital quantum number. Anagously, since the two spherical harmonic have indeces $m = \pm 1$ these are the only possible values for the magnetic quantum number. Since the absolute values of the Y_{21} and Y_{2-1} coefficients are equal, the two values for L_z, $\hbar$ and $-\hbar$, will occour with the same probability 1/2.

c) The probability of finding $r > 2a$ is given by

$$P = \frac{1}{4a^3}\int_{2a}^\infty drr^2e^{-r/a}\int_0^{2\pi}d\phi\int_0^\pi d\theta\sin\theta\left(|Y_{21}|^2+|Y_{2-1}|^2\right) = \frac{1}{2a^3}\int_{2a}^\infty drr^2e^{-r/a} \ .$$

Integrating by parts we find

$$\int_{2a}^\infty drr^2e^{-r/a} = 10a^3e^{-2}$$

then

$$P = 5e^{-2} = 0.67$$

d) The Schrödinger equation in spherical coordinates is

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{\mathbf{L}^2}{2mr^2}+V(r)-E\right]e^{-r/2a}\left(-Y_{21}+Y_{2-1}\right) = 0 \ .$$

Since

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}e^{-r/2a}\right) = -\left(\frac{1}{ra}-\frac{1}{4a^2}\right)e^{-r/2a}$$

and

$$\mathbf{L}^2\left(-Y_{2\ 1}+Y_{2\ -1}\right) = 6\hbar^2\left(-Y_{2\ 1}+Y_{2\ -1}\right)$$

we have

$$\left[-\frac{\hbar^2}{8ma^2}+\frac{3\hbar^2}{mr^2}-E\right]e^{-r/2a}=0$$

hence

$$E=-\frac{\hbar^2}{8ma^2}+\frac{3\hbar^2}{mr^2}\ .$$

5. a) We can first note that the state χ is normalized. The general expansion of χ in the α, β basis is

$$\chi=a\alpha+b\beta$$

where α corresponds to the spin-up state and β to spin-down. The coefficients of such expansion are given by

$$a=\langle\alpha|\chi\rangle=(1\ 0)\begin{pmatrix}\frac{1}{2}\\ -i\sqrt{\frac{3}{4}}\end{pmatrix}=\frac{1}{2}$$

and

$$b=\langle\beta|\chi\rangle=(0\ 1)\begin{pmatrix}\frac{1}{2}\\ -i\sqrt{\frac{3}{4}}\end{pmatrix}=-i\sqrt{\frac{3}{4}}\ .$$

Then

$$P(L_z=+\frac{\hbar}{2})=|a|^2=\frac{1}{4}\qquad P(L_z=-\frac{\hbar}{2})=|b|^2=\frac{3}{4}\ .$$

b) Since (see P-H)

$$S_x^2|\alpha\rangle=S_x(S_x|\alpha\rangle)=\frac{\hbar^2}{4}|\alpha\rangle\qquad S_x^2|\beta\rangle=S_x(S_x|\beta\rangle)=\frac{\hbar^2}{4}|\beta\rangle$$

it follows

$$\langle\alpha|S_x^2|\alpha\rangle=\frac{\hbar^2}{4}\qquad\langle\beta|S_x^2|\beta\rangle=\frac{\hbar^2}{4}$$

and

$$\langle\alpha|S_x^2|\beta\rangle=\langle\beta|S_x^2|\alpha\rangle=0\ .$$

Then,

$$\langle\chi|S_x^2|\chi\rangle=|a|^2\langle\alpha|S_x^2|\alpha\rangle+|b|^2\langle\beta|S_x^2|\beta\rangle=\frac{\hbar^2}{4}\ .$$

c) If the spin of the particle is 1 the dimension of the matrices is 3×3.