LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS F0047T
Examination date: 2014-01-14
The solutions are just suggestions. They may contain several alternative routes.

1. A measurement of the spin component in the direction $\hat{n} = \hat{x}\sin(\varphi) + \hat{y}\cos(\varphi)$ gives the value $-\hbar/2$. The spin operator $S_{\hat{n}} = \hat{n} \cdot (S_x, S_y, S_z)$ is

$$S_{\hat{n}} = \frac{\hbar}{2}\begin{pmatrix} 0 & \sin\varphi - i\cos\varphi \\ \sin\varphi + i\cos\varphi & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & -ie^{i\varphi} \\ ie^{-i\varphi} & 0 \end{pmatrix} = \frac{-i\hbar}{2}\begin{pmatrix} 0 & e^{i\varphi} \\ -e^{-i\varphi} & 0 \end{pmatrix}$$

The eigenvalue equation is

$$S_{\hat{n}}\chi = \lambda\chi \Leftrightarrow \frac{i\hbar}{2}\begin{pmatrix} 0 & -e^{i\varphi} \\ e^{-i\varphi} & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix} \tag{1}$$

We find the eigenvalues from

$$\begin{vmatrix} -\lambda & \frac{-i\hbar}{2}e^{i\varphi} \\ \frac{i\hbar}{2}e^{-i\varphi} & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda^2 - (\frac{\hbar}{2})^2 = 0 \Rightarrow \lambda = \pm\frac{\hbar}{2}$$

(a) The spin state corresponding to $\lambda = -\hbar/2$ must satisfy the eigenvalue equation Eq. (1). This yields two equations that are liniearly dependent. Take any of these, say $iae^{-i\varphi} = -b$ and choose $a = 1$ and hence:

$$\chi_{\hat{n}-} = C\begin{pmatrix} 1 \\ -ie^{-i\varphi} \end{pmatrix} \Rightarrow \chi_{\hat{n}-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -ie^{-i\varphi} \end{pmatrix}, \text{ or differently } \frac{1}{\sqrt{2}}\begin{pmatrix} ie^{i\varphi} \\ 1 \end{pmatrix},$$

where the normalization condition $|a|^2 + |b|^2 = 1$ was used in the last step. Other correct solutions can be found by a multiplication with an arbitrary phase factor $e^{i\alpha}$.

N.B. this is for the other eigenvalue $\lambda = +\hbar/2$, not an answer to the question.
The spin state corresponding to $\lambda = \hbar/2$ must satisfy the eigenvalue equation Eq. (1). This yields two equations that are liniearly dependent. Take any of these, say $iae^{-i\varphi} = b$ and choose $a = 1$ and hence:

$$\chi_{\hat{n}+} = C\begin{pmatrix} 1 \\ ie^{-i\varphi} \end{pmatrix} \Rightarrow \chi_{\hat{n}+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ ie^{-i\varphi} \end{pmatrix}, \text{ or differently } \frac{1}{\sqrt{2}}\begin{pmatrix} -ie^{-i\varphi} \\ 1 \end{pmatrix},$$

where the normalization condition $|a|^2 + |b|^2 = 1$ was used in the last step. Other correct solutions can be found by a multiplication with an arbitrary phase factor $e^{i\alpha}$.

(b) A general spin state (for the z–direction) can be written as $\chi^z = a\chi_+^z + b\chi_-^z$, where $\chi_+^z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is the spin up and $\chi_-^z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is the spin down spinor in the z-direction. The outcomes of a measurement will be: For $\chi_{\hat{n}-}$ we find that the probability to measure spin up, *i.e.* $S_z = \hbar/2$ is $|a|^2 = |-e^{-i\varphi}/\sqrt{2}|^2 = 1/2$, and that the probability to measure spin down, *i.e.* $S_z = -\hbar/2$ is $|b|^2 = |1/\sqrt{2}|^2 = 1/2$.

(c) We would get 50% up and 50% down in the $\hat{n}$ direction. The reason is that the states (in b) we start from are eigenstates of S_z and this operator is not present in $S_{\hat{n}}$. Had S_z been part of $S_{\hat{n}}$ there would be a bias.

2. (a) The parity of a hydrogen eigenfunction $\psi_{nlm_l}(\mathbf{r})$ is given by $(-1)^l$. The given wave function $\Psi(\mathbf{r})$ consists of eigenfunctions with the same parity. Hence $\Psi(\mathbf{r})$ has a definite parity.

   (b) The probability is given by the absolute square of the coefficients.
   $(\Psi(\mathbf{r}, t = 0) = \frac{1}{\sqrt{15}}(3\psi_{100}(\mathbf{r}) - 2\psi_{200}(\mathbf{r}) + \psi_{320}(\mathbf{r}) - \psi_{322}(\mathbf{r})))$

   The probabilities are (in order) $\frac{9}{15}, \frac{4}{15}, \frac{1}{15}, \frac{1}{15}$. as a check they sum up to 1 as they should do.

   (c) The energy of a single eigenstate is given by: $E_n = -\frac{13.56}{n^2}$ eV. The expectation value is given by $<E> = \frac{9}{15}(-\frac{13.56}{1^2}) + \frac{4}{15}(-\frac{13.56}{2^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) = -13.56(\frac{9}{15} + \frac{4}{60} + \frac{1}{135} + \frac{1}{135}) = -9.240889 \approx -9.24$ eV

   The operator $\mathbf{L}^2$ has eigenvalues $\hbar^2 l(l+1)$. The expectation value is given by $<\mathbf{L}^2> = \frac{9}{15} \cdot 0 + \frac{4}{15} \cdot 0 + \frac{1}{15}(\hbar^2 2(2+1)) + \frac{1}{15}(\hbar^2 2(2+1)) = \frac{12}{15}\hbar^2 = \frac{4}{5}\hbar^2$

   The operator L_z has eigenvalues $\hbar m_l$. The expectation value is given by $<L_z> = \frac{9}{15} \cdot 0 + \frac{4}{15} \cdot 0 + \frac{1}{15} \cdot 0 + \frac{1}{15}(\hbar 2) = \frac{2}{15}\hbar$

3. (a) The mean position of the particle is

$$<x> = \int_{-\infty}^{\infty} \psi^*(x) x \psi^*(x) dx = \frac{\gamma}{\sqrt{\pi}} \int_{-\infty}^{\infty} x e^{-\gamma^2 x^2} dx = 0$$

   (b) The mean momentum of the particle is

$$<p> = \int_{-\infty}^{\infty} \psi^*(x) \frac{\hbar}{i} (\frac{d}{dx} \psi(x)) dx = \frac{\gamma \hbar}{\sqrt{i\pi}} \int_{-\infty}^{\infty} e^{-\gamma^2 x^2/2} \frac{d}{dx} e^{-\gamma^2 x^2/2} dx = 0$$

   (c) The Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x)$$

   can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = [E - V(x)]\psi(x).$$

   As

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}e^{-\gamma^2 x^2/2} = -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2)e^{-\gamma^2 x^2/2}$$

   we have

$$E - V(x) = -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2)$$

   or

$$V(x) = \frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2) + \frac{\hbar^2 \gamma^2}{2m} = \frac{\hbar^2 \gamma^4 x^2}{2m}$$

4. a) There are 4 states the system can have with the energys and (degeneracys) $\hbar\omega$ (1), $2\hbar\omega$ (2) and $3\hbar\omega$ (1). The partition sum is given by:

$$Z = \sum_{n_1=0,n_2=0}^{n_1=1,n_2=1} e^{-(n_1+n_2+1.0)\hbar\omega/k_B T} = e^{-1.0\hbar\omega/k_B T} + 2e^{-2.0\hbar\omega/k_B T} + e^{-3.0\hbar\omega/k_B T}$$

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b) There is one state of the lower energy and **two** states with the next higher energy. The probability to find the system in a state of energy is proportional to the Boltzmann factor, we arrive at the following equation.

$$\frac{1e^{-1,0\hbar\omega/k_BT}}{Z} = \frac{2e^{-2,0\hbar\omega/k_BT}}{Z} \tag{2}$$

and $e^{1\hbar\omega/k_BT} = 2$ which evaluates to $T = \frac{1\hbar\omega}{k_B\ln 2}$.

c) The partition sum at this specific temperature is given by: $(k_BT = \frac{1\hbar\omega}{\ln 2})$ $(\frac{1}{k_BT} = \frac{\ln 2}{1\hbar\omega})$ we arrive at the following

$$Z = e^{-1.0\hbar\omega/k_BT} + 2e^{-2.0\hbar\omega/k_BT} + e^{-3.0\hbar\omega/k_BT} = e^{-1.0\ln 2} + 2e^{-2.0\ln 2} + e^{-3.0\ln 2} =$$

$$\frac{1}{2} + 2\frac{1}{4} + \frac{1}{8} = \frac{1}{2} + \frac{1}{2} + \frac{1}{8} = 1 + \frac{1}{8} = \frac{9}{8}$$

The probability P will be (put Z into one of the terms in eq (2).

$$P = \frac{e^{-1,0\ln 2}}{\frac{9}{8}} = \frac{1}{2} \cdot \frac{8}{9} = \frac{4}{9} \approx 0.444...$$

As a check we can calculate for the state with the highest energy

$$P_3 = \frac{e^{-3,0\ln 2}}{\frac{9}{8}} = \frac{1}{8} \cdot \frac{8}{9} = \frac{1}{9} \approx 0.111...$$

and we can easily conclude the probabilities add up to one.

5. 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)

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

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 $\left(\Psi(-\frac{a}{2}) = \Psi(\frac{a}{2}) = 0\right)$ 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

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$A = 0$ and we get the following solution: The normalising constant $B = \sqrt{\frac{2}{a}}$ you get from the condition $\int_{-a/2}^{a/2} | \Psi |^2 \, dx = 1$. The condition $\sin(\frac{ka}{2}) = 0$ gives $\frac{ka}{2} = \frac{\pi}{2} * (even - integer)$. The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a}) \quad \text{with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 2, 4, 6, ... \quad (3)$$

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:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos(\frac{n\pi x}{a}) \quad \text{with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 3, 5, ... \quad (4)$$

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:

$$\Psi_{n,m}(x, y) = \psi_n(x) \cdot \psi_m(y) \text{ eigenenergys } E_{n,m} = E_n + E_m \text{where } n = 1, 2, , . \text{ and } m = 1, 2, , . \quad (5)$$

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:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a}) \quad \text{with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 2, 3, ... \quad (6)$$

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

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi}{a}(x + \frac{a}{2})) \quad \text{with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 2, 3, ... \quad (7)$$

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a} + \frac{n\pi}{2}) = \sqrt{\frac{2}{a}} \left(\sin(\frac{n\pi x}{a}) \cdot \cos(\frac{n\pi}{2}) + \cos(\frac{n\pi x}{a}) \cdot \sin(\frac{n\pi}{2}) \right)$. We see that we recover the solution in eq (3), (4) and (5) as we let n run from 1 to ∞.

b) The ground state eigenfunction is given by (using eq. (4))

$$\Psi_{n=1,m=1}(x, y) = \psi_1(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \cos(\frac{\pi x}{a}) \cdot \sqrt{\frac{2}{a}} \cos(\frac{\pi y}{a}) \quad (8)$$

The next lowest state eigenfunction is given by (using eq. (4) and (3)). Note there are two eigenfunctions with the same energy ($\Psi_{n=1,m=2}(x, y)$) you may use either one of them.

$$\Psi_{n=2,m=1}(x, y) = \psi_2(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \sin(2\frac{\pi x}{a}) \cdot \sqrt{\frac{2}{a}} \cos(\frac{\pi y}{a}) \quad (9)$$

Orthogonality is defined as

$$\int_x \int_y \Psi_{n_1,m_1}(x, y) \Psi_{n_2,m_2}(x, y) = \delta_{n_1,n_2} \, \delta_{m_1,m_2} \quad (10)$$

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by explicit calculation

$$\int_{x=-a/2}^{a/2} \int_{y=-a/2}^{a/2} \left(\frac{2}{a}\cos(\frac{\pi x}{a}) \cdot \cos(\frac{\pi y}{a})\right) \cdot \left(\frac{2}{a}\sin(2\frac{\pi x}{a}) \cdot \cos(\frac{\pi y}{a})\right) = \text{calculations} = 0 \qquad (11)$$

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.