HW #4

1. Hydrogen atom ground state

(a) We determine the normalization factor

```
Integrate[4 π r² (N E^(-r/a₀))², {r, 0, ∞}, Assumptions -> Re[a₀] > 0]
```

$N^2 \pi a_0^3$

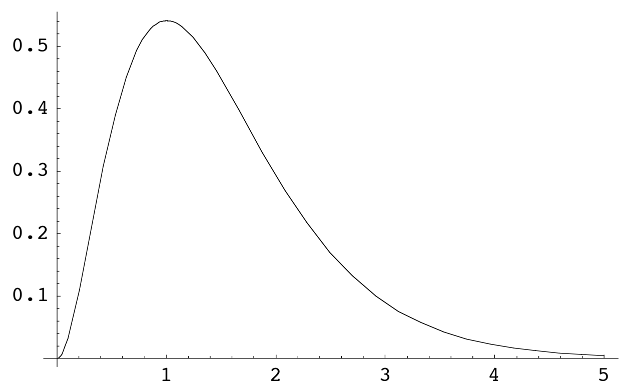
```
Solve[% == 1, N]
```

$\left\{\left\{N \to -\frac{1}{\sqrt{\pi}\, a_0^{3/2}}\right\}, \left\{N \to \frac{1}{\sqrt{\pi}\, a_0^{3/2}}\right\}\right\}$

Therefore, $N = 1 \big/ (\pi a_0{}^3)^{1/2}$.

(b) Probability distribution in the radius is

```
Plot[4 π r² (N E^(-r/a₀))² /. {N → 1/(√π a₀^(3/2))} /. {a₀ → 1}, {r, 0, 5}]
```



- Graphics -

The most likely value of r, namely the maximum of dP/dr, is obtained at

```
Solve[D[4 π r² (E^(-r/a₀))², r] == 0, r]
```

$\{\{r \to 0\}, \{r \to a_0\}\}$

Therefore the most likely value of r is $r_{\max} = a_0$, the Bohr radius.

(c) We calculate the wave function in the momentum space using the completeness relation $1 = \int \left| \vec{x} \right\rangle \left\langle \vec{x} \right| d\,\vec{x}$.

$\phi(\vec{p}) = \langle \vec{p} \mid 0 \rangle = \int \langle \vec{p} \mid \vec{x} \rangle \langle \vec{x} \mid 0 \rangle \, d\,\vec{x} = \int \frac{e^{-i\,\vec{p}\cdot\vec{x}/\hbar}}{(2\,\pi\,\hbar)^{3/2}}\,\psi(\vec{x})\,d\,\vec{x}$

$= \int \frac{e^{-i\,p\,r\cos\theta/\hbar}}{(2\,\pi\,\hbar)^{3/2}}\,N\,e^{-r/a_0}\,r^2\,d\,r\,d\cos\theta\,d\,\phi$

$= \int_0^\infty \frac{\hbar}{-i\,p\,r}\,\frac{e^{-i\,p\,r/\hbar} - e^{i\,p\,r/\hbar}}{(2\,\pi\,\hbar)^{3/2}}\,N\,e^{-r/a_0}\,r^2\,d\,r\,2\,\pi$

$= \frac{2\,\pi\,i\,\hbar}{p}\,\frac{N}{(2\,\pi\,\hbar)^{3/2}}\int_0^\infty (e^{-i\,p\,r/\hbar} - e^{i\,p\,r/\hbar})\,e^{-r/a_0}\,r\,d\,r$

For the last step I lazily use *Mathematica*,

```
Simplify[Integrate[E^(-I p r/ℏ) E^(-r/a0) r, {r, 0, Infinity},
   Assumptions -> Im[p] == 0 && Re[a0] > 0 && ℏ > 0 && Im[p/ℏ] == 0] - Integrate[E^(I p r/ℏ) E^(-r/a0) r,
   {r, 0, Infinity}, Assumptions -> Im[p] == 0 && Re[a0] > 0 && ℏ > 0 && Im[p/ℏ] == 0]]
```

$-\frac{2\,i\,\hbar^2\,\mathrm{Sin}[2\,\mathrm{ArcTan}[\frac{p\,a_0}{\hbar}]]\,a_0^2}{\hbar^2 + p^2\,a_0^2}$

```
FullSimplify[%]
```

$-\frac{4\,i\,p\,\hbar^3\,a_0^3}{(\hbar^2 + p^2\,a_0^2)^2}$

Therefore,

$\phi(\vec{p}) = \frac{2\,\pi\,i\,\hbar}{p}\,\frac{N}{(2\,\pi\,\hbar)^{3/2}}\,\frac{-4\,i\,p\,\hbar^3\,a_0^3}{(\hbar^2 + p^2\,a_0^2)^2}$

$= \frac{8\,\pi\,\hbar^4}{(2\,\pi\,\hbar)^{3/2}}\,\frac{1}{(\pi\,a_0{}^3)^{1/2}}\,\frac{a_0^3}{(\hbar^2 + p^2\,a_0^2)^2}$

$= \left(\frac{8\,\hbar^5\,a_0{}^3}{\pi^2}\right)^{1/2}\,\frac{1}{(\hbar^2 + p^2\,a_0^2)^2}$

(d) We calculate the normalization

$\int \phi(\vec{p})^*\,\phi(\vec{p})\,d\,\vec{p} = \int_0^\infty \frac{8\,\hbar^5\,a_0{}^3}{\pi^2}\,\frac{1}{(\hbar^2 + p^2\,a_0^2)^4}\,4\,\pi\,p^2\,\mathrm{dp}$

```
Integrate[1/(ℏ^2 + p^2 a0^2)^4 p^2, {p, 0, ∞}]
```

$\frac{i\,(\mathrm{Log}[-\frac{i\,a_0}{\hbar}] - \mathrm{Log}[\frac{i\,a_0}{\hbar}])}{32\,\hbar^5\,a_0^3}$

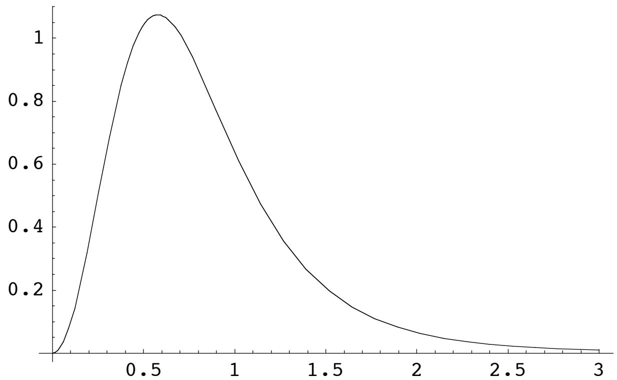
```
PowerExpand[%]
```

$\frac{\pi}{32\,\hbar^5\,a_0^3}$

Therefore, $\int \phi(\vec{p})^*\,\phi(\vec{p})\,d\,\vec{p} = \frac{8\,\hbar^5\,a_0{}^3}{\pi^2}\,\frac{\pi}{32\,\hbar^5\,a_0^3}\,4\,\pi = 1$

(e) Plot $4\,\pi\,p^2\,|\,\phi(p)\,|^2$

```
Plot[ (8 ℏ^5 a0^3)/π^2 1/(ℏ^2 + p^2 a0^2)^4 4 π p^2 /. {a0 → 1, ℏ → 1}, {p, 0, 3}]
```



- Graphics -

The maximum probability is obtained at

```
Solve[D[ 1/(ℏ^2 + p^2 a0^2)^4 4 π p^2, p] == 0, p]
```

$$\left\{\{p \to 0\},\ \left\{p \to -\frac{\hbar}{\sqrt{3}\, a_0}\right\},\ \left\{p \to \frac{\hbar}{\sqrt{3}\, a_0}\right\}\right\}$$

obviously the last solution is the one we are looking for: $p_{\max} = \hbar / \left(\sqrt{3}\, a_0\right)$.

The uncertainty relation can be seen to be satisfied crudely by approximating $\Delta p \approx p_{\max}$, $\Delta x \approx r_{\max}$, and hence $\Delta p \, \Delta x \approx \hbar$. (This is the level of answer I was looking for. But if you have done the rest, great!)

To see this more rigorously, we need to evaluate the uncertainties. Using the isotropy of the wave function, it is clearly that $\langle x \rangle = \langle y \rangle = \langle z \rangle = 0$, and $\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{1}{3} \langle r^2 \rangle$. It is easy to calculate $\langle r^2 \rangle = \int_0^\infty r^2 \left|\psi(r)\right|^2 4 \pi r^2 \, d r = 4 \pi N^2 \int_0^\infty r^4 e^{-2 r/a_0} \, d r = 4 \pi \frac{1}{\pi a_0{}^3} \frac{3 a_0{}^5}{4}$ and hence $(\Delta x)^2 = \frac{1}{3} \langle r^2 \rangle = a_0{}^2$. Similarly, $\langle p_x \rangle = \langle p_y \rangle = \langle p_z \rangle = 0$, and $\langle p_x{}^2 \rangle = \langle p_y{}^2 \rangle = \langle p_z{}^2 \rangle = \frac{1}{3} \langle p^2 \rangle$. We find $\langle p^2 \rangle = \int_0^\infty p^2 \left|\phi(p)\right|^2 4 \pi p^2 \, d p = \frac{8 \hbar^5 a_0{}^3}{\pi^2} \int_0^\infty p^2 \frac{1}{(\hbar^2 + p^2 a_0^2)^4} 4 \pi p^2 \, d p$

```
Integrate[ p^4/(ℏ^2 + p^2 a0^2)^4, {p, 0, ∞}]
```

$$\frac{i \left(\text{Log}\left[-\frac{i a_0}{\hbar}\right] - \text{Log}\left[\frac{i a_0}{\hbar}\right]\right)}{32 \hbar^3 a_0^5}$$

```
PowerExpand[%]
```

$$\frac{\pi}{32 \hbar^3 a_0^5}$$

Hence, $\langle p^2 \rangle = \frac{8 \hbar^5 a_0{}^3}{\pi^2} 4 \pi \frac{\pi}{32 \hbar^3 a_0^5} = \frac{\hbar^2}{a_0{}^2}$, and $(\Delta p_x)^2 = \frac{1}{3} \langle p^2 \rangle = \frac{\hbar^2}{3 a_0{}^2}$. Therefore $(\Delta x)^2 (\Delta p_x)^2 = \frac{\hbar^2}{3} \geqslant \frac{\hbar^2}{4}$ and hence the uncertainty relation is satisfied, but not saturated.

2. Spin Precession

```
Sx = ℏ/2 {{0, 1}, {1, 0}}; Sy = ℏ/2 {{0, -I}, {I, 0}}; Sz = ℏ/2 {{1, 0}, {0, -1}};
```

```
Sx // MatrixForm
```

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

```
Sy // MatrixForm
```

$$\begin{pmatrix} 0 & -\frac{i\hbar}{2} \\ \frac{i\hbar}{2} & 0 \end{pmatrix}$$

```
Sz // MatrixForm
```

$$\begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}$$

(a) $|S_z; +\rangle$ and $|S_z; -\rangle$ are eigenstates of S_z, and hence are eigenstates of the Hamiltonian with eigenvalues $E = \mp g \frac{e\hbar}{4mc} B$. The Schrödinger equation is $i\hbar \frac{\partial}{\partial t} |\alpha\rangle = H |\alpha\rangle$, and hence the time dependence of a Hamitonian eigenstate is $|\alpha, t\rangle = |\alpha, 0\rangle e^{-iEt/\hbar}$. Therefore,
$|S_z; +, t\rangle = |S_z; +\rangle e^{+ige\hbar Bt/(4mc)}$
$|S_z; -, t\rangle = |S_z; -\rangle e^{-ige\hbar Bt/(4mc)}$

(b) We start with the result in the class $|S_x; +\rangle = \frac{1}{\sqrt{2}} (|S_z; +\rangle + |S_z; -\rangle)$. In the S_z representation, therefore, $|S_x; +\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. (Sakurai would have put a "dot" on the equal sign.) Using the time-dependence obtained above, we find $|S_x; +\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{+ige\hbar Bt/(4mc)} \\ e^{-ige\hbar Bt/(4mc)} \end{pmatrix}$.

(c) We just calculate the product of the wave function daggered, matrix, and the wave function. To simplify the notation, I use the notation $\omega = g \frac{e\hbar}{2mc} B$. Then,

```
ket = 1/√2 {{E^(I ω t/2)}, {E^(-I ω t/2)}}
```

$$\left\{\left\{\frac{e^{\frac{i t \omega}{2}}}{\sqrt{2}}\right\}, \left\{\frac{e^{-\frac{1}{2} i t \omega}}{\sqrt{2}}\right\}\right\}$$

```
% // MatrixForm
```

$$\begin{pmatrix} \frac{e^{\frac{i t \omega}{2}}}{\sqrt{2}} \\ \frac{e^{-\frac{1}{2} i t \omega}}{\sqrt{2}} \end{pmatrix}$$

```
bra = 1/Sqrt[2] {{E^(-I ω t/2), E^(I ω t/2)}}
```

$$\left\{\left\{\frac{e^{-\frac{1}{2} i t \omega}}{\sqrt{2}}, \frac{e^{\frac{i t \omega}{2}}}{\sqrt{2}}\right\}\right\}$$

```
(bra.Sx.ket)[[1, 1]]
```

$$\frac{1}{4} e^{-i t \omega} \hbar + \frac{1}{4} e^{i t \omega} \hbar$$

```
ExpToTrig[%]
```

$$\frac{1}{2} \hbar \operatorname{Cos}[t \omega]$$

```
(bra.Sy.ket)[[1, 1]]
```

$$-\frac{1}{4} i e^{-i t \omega} \hbar + \frac{1}{4} i e^{i t \omega} \hbar$$

```
ExpToTrig[%]
```

$$-\frac{1}{2} \hbar \operatorname{Sin}[t \omega]$$

```
(bra.Sz.ket)[[1, 1]]
```

0

Therefore, there is no z-component of the spin at any time, while the x- and y-components precess with the spin precession frequency $\omega/2\pi$. Note that $\omega = \Delta E/\hbar$, not $E/\hbar$, as expected from the general discussion of the correlation amplitude in Sakurai.

(d) According to the Particle Data Group, the magnetic moment of the proton is $\mu = 2.79\,\mu_N$, where $\mu_N = \frac{e\hbar}{2 m_p c} = 3.15 \times 10^{-14}$ MeV/Tesla is the nuclear magneton. The energy eigenvalues are $\pm\mu B$ and hence the difference between two energy levels is $\Delta E = 2\mu B$. In order for the spin to be "frozen," namely that the excited state is not populated, we need the thermal energy to be much smaller than the energy difference, $k T \ll \Delta E$. For the room temperature, $k T \approx 0.03$ eV, and therefore $B \gg 1.7 \times 10^5$ Tesla. This is an enormous magnetic field even the most powerful superconducting magnet on the Earth cannot produce.

It is, however, possible to polarize nuclear spin. First of all, we can lower the temperature. If we go down to mK (milli Kelvin), the magnetic field needs to be $B \gg 0.57$ Tesla. In addition, there is a famous experiment by C.S. Wu that polarized the nuclear spin, and discovered that the parity is violated in nature. What she did was to first polarize the electron in Cobalt atom using a magnetic field and a low temperature. On the other hand, there is so-called hyperfine interaction between electron and nuclear spins. Once the electron spin is polarized, the hyperfine interaction prefers the nuclear spin to be anti-parallel. Namely that the elctron spin is an effective superstrong magnetic field on the nuclear spin. This way, she managed to polarize the nuclear pin at a much higher temperature. I suspect it was a few Kelvin, but the paper unfortunately doesn't say what it was.