Worksheet 3

(1) The wave function for the 1s state of an electron in the hydrogen atom is

$$\psi_{1s}(\rho) = \frac{1}{\sqrt{\pi a^3}} e^{-\rho/a}, \tag{1}$$

where a is the Bohr radius (a constant) and ρ is the distance from the center of the atom. The probability of finding the electron in a region $\mathcal{W}$ of $\mathbb{R}^3$ is equal to

$$\iiint_{\mathcal{W}} p(x, y, z)\, dV,$$

where, $p(x, y, z) = \psi_{1s}\left(\sqrt{x^2+y^2+z^2}\right)^2$. Show that the probability of finding the electron at a distance greater than the Bohr radius a is $5/e^2$ (this is roughly 67%).

Let $B(a)$ be the ball of radius a.

$$\iiint_{B(a)} p(x,y,z)\,dV = \int_0^{\pi}\int_0^{2\pi}\int_0^{a} \psi_{1s}(\rho)^2 \cdot \rho^2 \sin\phi \, d\rho\, d\theta\, d\phi$$

$$= \left(\int_0^{2\pi} d\theta\right)\left(\int_0^{a} \frac{e^{-2\rho/a}}{\pi a^3}\rho^2\, d\rho\right)\left(\int_0^{\pi}\sin\phi\, d\phi\right)$$

Now, $\displaystyle\int_0^{\pi} \sin\phi\, d\phi = -\cos\phi \Big|_0^{\pi} = 2$

$\displaystyle\int_0^{2\pi} d\theta = 2\pi$

and

$$\int_0^{a} \frac{e^{-2\rho/a}}{\pi a^3}\rho^2\, d\rho = \frac{-e^{-2\rho/a}\rho^2}{2\pi a^2}\Bigg|_0^{a} + \int_0^{a} \frac{e^{-2\rho/a}}{\pi a^2}\rho\, d\rho$$

$$= \frac{-e^{-2}a^2}{2\pi a^2} - \frac{e^{-2\rho/a}}{2\pi a}\rho \Bigg|_0^{a} + \int_0^{a} \frac{e^{-2\rho/a}}{2\pi a}\, d\rho$$

$$= -\frac{e^{-2}a^2}{2\pi a^2} - \frac{e^{-2}}{2\pi} - \frac{e^{-2\rho/a}}{4\pi}\Bigg|_0^a$$

$$= \frac{-e^{-2}}{\pi} - \frac{e^{-2}}{4\pi} + \frac{1}{4\pi} = \frac{1}{4\pi}\left(1 - 5e^{-2}\right)$$

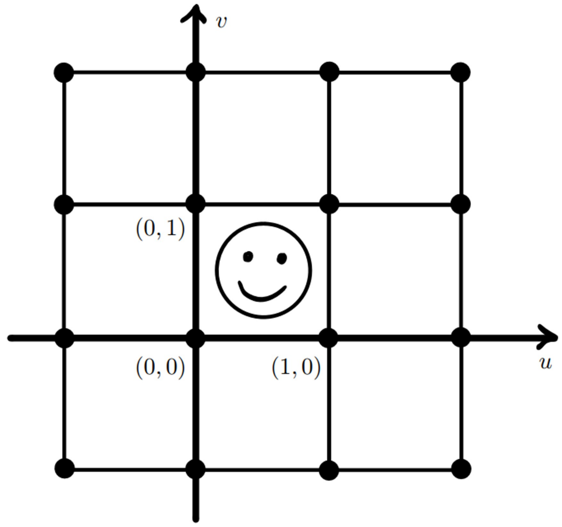
Hence, $\iiint_{B(a)} \rho(x,y,z)\, dV = 1 - 5e^{-2}$

This is the probability of finding the electron at most the bohr radius. Hence

$$\mathbb{P}(R > a) = 1 - P(R \leq a)$$
$$= 1 - (1 - 5e^{-2})$$
$$= 5e^{-2}.$$

(2) Consider the transformation $(x, y) = T(u, v) = (u - 2v, u + 2v)$.

(a) Compute the image under T of each vertex in the below grid and make a careful plot of them in the xy-plane on your paper; make it look nice, you will add to it later.
To speed this up, divide the task up among all members of your group.



(b) For each pair A and B of vertices of the grid joined by a line, add the line segment joining $T(A)$ to $T(B)$ to your plot. This gives a rough picture of what T is doing.

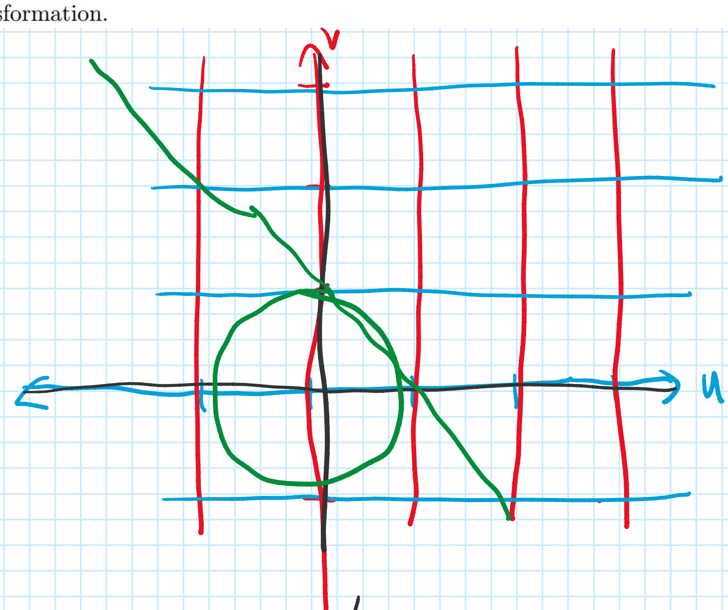
(c) What is the image of the u-axis under T? The v-axis?

(d) Consider the line L given by $u + v = 1$. What is the image of L under T? Is it a circle, an ellipse, a hyperbola, or something else?

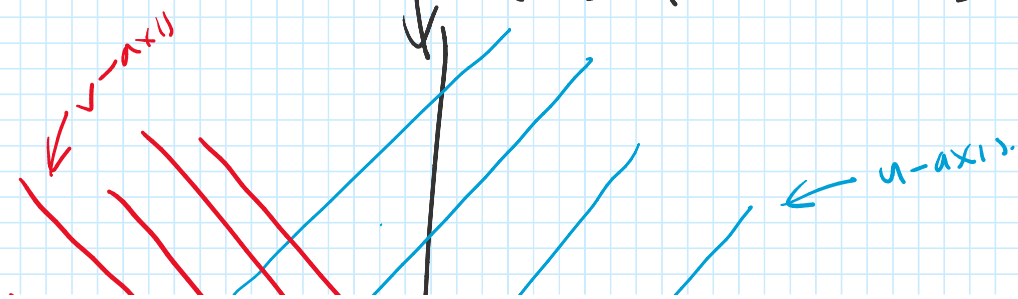
(e) Consider the circle C given by $u^2 + v^2 = 1$. What is the image of C under T?

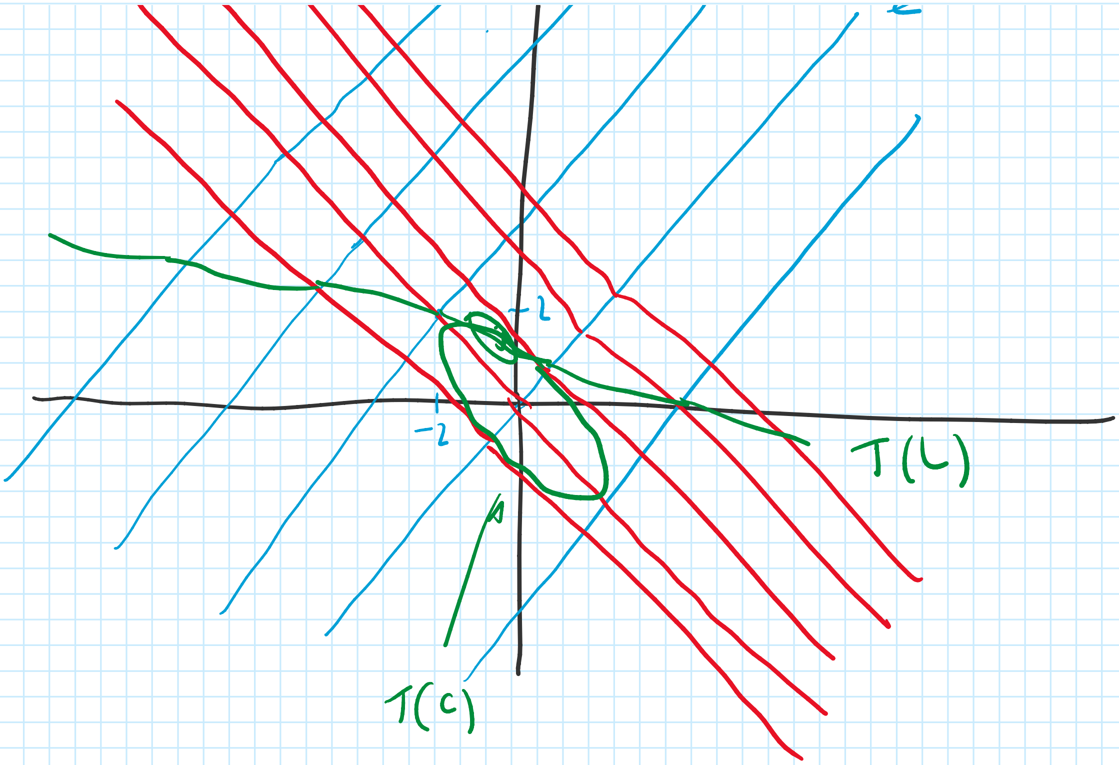
(f) Add $T(L)$, $T(C)$ and $T($☺$)$ to your picture.

(g) What does the transformation T do to the area of one of the unit boxes? Compute the Jacobian of this transformation.



$T(u,v) = (u-2v, u+2v)$





d) $u+v=1$, $\quad v=1-u \Rightarrow T(u,1-u) = (u-2(1-u),$
$u+2(1-u))$

$= (2u-2, -u-2)$ This is a line.

e) It is an ellipse. (The mapping squishes in one direction)

g) a unit box goes to one with dimensions $\sqrt{8} \times \sqrt{2}$ so has area $\sqrt{8}\cdot\sqrt{2} = 2\cdot\sqrt{2}\cdot\sqrt{2} = 4$.

$T_u(u,v) = (1,1)$

$T_v(u,v) = (-2,2)$.

Hence $|J(T)| = \left\| \begin{matrix} 1 & -2 \\ 1 & 2 \end{matrix} \right\| = 2+2 = 4.$

(3) Compute the Jacobian of the spherical coordinates transformation.

spherical coordinates are given by

$$G(\rho, \theta, \phi) = (\rho\cos\theta\sin\phi, \rho\sin\theta\sin\phi, \rho\cos\phi)$$

so

$$J(G) = \left\| \begin{matrix} \cos\theta\sin\phi & -\rho\sin\theta\sin\phi & \rho\cos\theta\cos\phi \\ \sin\theta\sin\phi & \rho\cos\theta\sin\phi & \rho\sin\theta\cos\phi \\ \cos\phi & 0 & -\rho\sin\phi \end{matrix} \right\|$$

$$= \left| \cos\phi \begin{vmatrix} -\rho\sin\theta\sin\phi & \rho\cos\theta\cos\phi \\ \rho\cos\theta\sin\phi & \rho\sin\theta\cos\phi \end{vmatrix} - \rho\sin\phi \begin{vmatrix} \cos\theta\sin\phi & -\rho\sin\theta\sin\phi \\ \sin\theta\sin\phi & \rho\cos\theta\sin\phi \end{vmatrix} \right|$$

$$= \left| \rho^2\cos^2\phi\sin\phi \begin{vmatrix} -\sin\theta & \cos\theta \\ \cos\theta & \sin\theta \end{vmatrix} - \rho^2\sin^3\phi \begin{vmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{vmatrix} \right|$$

$$= \left| \rho^2\cos^2\phi\sin\phi(-1) - \rho^2\sin^3\phi \right|$$

$$= \rho^2 \sin\phi .$$