Problem 1.5

The time-averaged potential of a neutral hydrogen atom is given by

$$\Phi = \frac{q}{4\pi\epsilon_0}\frac{e^{-\alpha r}}{r}\left(1+\frac{\alpha r}{2}\right)$$

where q is the magnitude of the electronic charge, and $\alpha^{-1} = a_0/2$, a_0 being the Bohr radius. Find the distribution of charge (both continuous and discrete) that will give this potential and interpret your result physically.

Solution

The governing equations of the electric field are Gauss's law and Faraday's law. In the context of electrostatics they are

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

$$\nabla \times \mathbf{E} = \mathbf{0}.$$

This second equation implies the existence of a potential function $-\Phi$ that satisfies

$$\mathbf{E} = \nabla(-\Phi) = -\nabla\Phi.$$

The minus sign is arbitrary mathematically, but physically it indicates that a charge in an electric field has more potential energy upstream than it does downstream. Substitute this formula into Gauss's law to obtain Poisson's equation.

$$\nabla \cdot (-\nabla\Phi) = \frac{\rho}{\epsilon_0}$$

$$-\nabla \cdot \nabla\Phi = \frac{\rho}{\epsilon_0}$$

$$\nabla^2\Phi = -\frac{\rho}{\epsilon_0}$$

Expand $\nabla^2\Phi$ in spherical coordinates (r, ϕ, θ), where θ is the angle from the polar axis, using the formula inside the back cover of the textbook.

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\Phi) + \underbrace{\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right)}_{=0} + \underbrace{\frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2}}_{=0} = -\frac{\rho}{\epsilon_0}$$

Since the given function for Φ is independent of ϕ and θ, these latter two terms disappear. Solve for ρ and simplify.

$$\begin{aligned}\rho(r) = -\frac{\epsilon_0}{r}\frac{d^2}{dr^2}(r\Phi) = -\frac{\epsilon_0}{r}\frac{d^2}{dr^2}\left[\frac{q}{4\pi\epsilon_0}e^{-\alpha r}\left(1+\frac{\alpha r}{2}\right)\right] &= -\frac{q}{4\pi r}\frac{d^2}{dr^2}\left[e^{-2r/a_0}\left(1+\frac{r}{a_0}\right)\right] \\ &= -\frac{q}{4\pi r}\left(\frac{4}{a_0^3}re^{-2r/a_0}\right) \\ &= -\frac{q}{\pi a_0^3}e^{-2r/a_0}\end{aligned}$$

Integrate this charge density over all of space.

$$\iiint_{\text{all space}} \rho\, dV = \int_0^\pi \int_0^{2\pi} \int_0^\infty \left(-\frac{q}{\pi a_0^3} e^{-2r/a_0}\right) r^2 \sin\theta\, dr\, d\phi\, d\theta$$

$$= -\frac{q}{\pi a_0^3} \left(\int_0^\pi \sin\theta\, d\theta\right) \left(\int_0^{2\pi} d\phi\right) \left(\int_0^\infty r^2 e^{-2r/a_0}\, dr\right)$$

$$= -\frac{q}{\pi a_0^3}(2)(2\pi)\left(\frac{a_0^3}{4}\right)$$

$$= -q$$

$\rho(r)$ is therefore the (continuous) charge density for the time-averaged electronic cloud around the nucleus. Because the given potential function Φ is not defined at $r = 0$, no information about the charge density at this point is known from the approach taken. We expect there to be a point charge $+q$ at $r = 0$ since the hydrogen atom is electrically neutral; this (discrete) charge density would be $+q\delta(r)$. In order to derive this, return to Poisson's equation.

$$\nabla^2 \Phi = -\frac{\rho}{\epsilon_0}$$

Integrate both sides over the volume of a sphere centered at the origin with radius ε, a really small positive number.

$$\iiint_{\substack{x^2+y^2\\+z^2\leq\varepsilon^2}} \nabla^2\Phi\, dV = \iiint_{\substack{x^2+y^2\\+z^2\leq\varepsilon^2}} \left(-\frac{\rho}{\epsilon_0}\right) dV$$

$$\iiint_{\substack{x^2+y^2\\+z^2\leq\varepsilon^2}} \nabla\cdot\nabla\Phi\, dV = -\frac{1}{\epsilon_0} \iiint_{\substack{x^2+y^2\\+z^2\leq\varepsilon^2}} \rho\, dV$$

Apply the divergence theorem on the left side and multiply both sides by $-\epsilon_0$.

$$\iiint_{\substack{x^2+y^2\\+z^2\leq\varepsilon^2}} \rho\, dV = -\epsilon_0 \oiint_{\substack{x^2+y^2\\+z^2=\varepsilon^2}} \nabla\Phi\cdot d\mathbf{S}$$

$$\iiint_{r\leq\varepsilon} \rho\, dV = -\epsilon_0 \oiint_{r=\varepsilon} \nabla\Phi\cdot\hat{\mathbf{r}}\, dS$$

$$= -\epsilon_0 \oiint_{r=\varepsilon} \frac{\partial\Phi}{\partial r}\, dS$$

$$= -\epsilon_0 \int_0^\pi \int_0^{2\pi} \left.\frac{\partial\Phi}{\partial r}\right|_{r=\varepsilon} (\varepsilon^2 \sin\theta\, d\phi\, d\theta)$$

Substitute the prescribed potential function and evaluate the derivative.

$$\begin{aligned}
\iiint\limits_{r\leq\varepsilon} \rho\, dV &= -\epsilon_0 \int_0^\pi \int_0^{2\pi} \left.\frac{d\Phi}{dr}\right|_{r=\varepsilon} (\varepsilon^2 \sin\theta\, d\phi\, d\theta) \\
&= -\epsilon_0 \int_0^\pi \int_0^{2\pi} \left.\frac{d}{dr}\left[\frac{q}{4\pi\epsilon_0}\frac{e^{-\alpha r}}{r}\left(1+\frac{\alpha r}{2}\right)\right]\right|_{r=\varepsilon} (\varepsilon^2 \sin\theta\, d\phi\, d\theta) \\
&= -\epsilon_0 \int_0^\pi \int_0^{2\pi} \left[-\frac{q}{4\pi\epsilon_0 a_0^2\varepsilon^2}(2\varepsilon^2 + 2a_0\varepsilon + a_0^2)e^{-2\varepsilon/a_0}\right] (\varepsilon^2 \sin\theta\, d\phi\, d\theta) \\
&= \frac{q}{4\pi a_0^2}(2\varepsilon^2 + 2a_0\varepsilon + a_0^2)e^{-2\varepsilon/a_0}\left(\int_0^\pi \sin\theta\, d\theta\right)\left(\int_0^{2\pi} d\phi\right) \\
&= \frac{q}{4\pi a_0^2}(2\varepsilon^2 + 2a_0\varepsilon + a_0^2)e^{-2\varepsilon/a_0}(2)(2\pi) \\
&= \frac{q}{a_0^2}(2\varepsilon^2 + 2a_0\varepsilon + a_0^2)e^{-2\varepsilon/a_0}
\end{aligned}$$

Take the limit of both sides as $\varepsilon \to 0$.

$$\lim_{\varepsilon\to 0} \iiint\limits_{r\leq\varepsilon} \rho\, dV = \lim_{\varepsilon\to 0} \frac{q}{a_0^2}(2\varepsilon^2 + 2a_0\varepsilon + a_0^2)e^{-2\varepsilon/a_0}$$

$$\lim_{\varepsilon\to 0} \iiint\limits_{r\leq\varepsilon} \rho\, dV = q$$

The only way an integral over an infinitesimal volume yields a nonzero result is if the integrand consists of a delta function. The sphere being integrated over is centered at the origin, so this delta function is $\delta(r)$. And because the right side is q, this is what the magnitude of the delta function has to be.

$$\rho(r) = q\delta(r)$$

Again, this (discrete) charge density represents the nucleus of the hydrogen atom. The final answer for the charge density is the sum of the discrete and continuous results.

$$\rho(r) = -\frac{q}{\pi a_0^3}e^{-2r/a_0} + q\delta(r)$$

This first term is valid everywhere except $r = 0$, and this second term is zero everywhere except $r = 0$. The integral of the final density over all of space is zero, indicating an electrically neutral hydrogen atom.