P] Obtenga y normalice la función de onda $\phi(r)$ del átomo de hidrógeno en su estado fundamental. Calcule su radio cuadrático medio $\sqrt{\langle r^2 \rangle}$.

indicación: Usar $\phi(r) = A e^{-\alpha r}$, con A y α por determinar.

Sol: ec. Schrödinger

$$-\frac{\hbar^2}{2m}\nabla^2 \phi(r) + V(r)\,\phi(r) = E\,\phi(r)$$

donde $\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)$ + derivadas angulares

$$V(r) = -\frac{e^2}{r} \quad \text{(átomo de hidrógeno)}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d\phi}{dr}\right) - \frac{e^2}{r}\phi = E\phi \quad ; \quad \phi = A e^{-\alpha r}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2 \cancel{A} e^{-\alpha r}(-\alpha)\right) - \frac{e^2}{r}\cancel{A} e^{-\alpha r} = E \cancel{A} e^{-\alpha r}$$

$$\Rightarrow \quad +\frac{\hbar^2}{2m}\frac{1}{r^2}\alpha\left(2r e^{-\alpha r} - r^2 e^{-\alpha r}\alpha\right) - \frac{e^2}{r}\cancel{e^{-\alpha r}} = E \cancel{e^{-\alpha r}}$$

$$\Rightarrow \quad \frac{\hbar^2}{m}\frac{\alpha}{r} - \frac{\hbar^2}{2m}\alpha^2 - \frac{e^2}{r} = E$$

$$\therefore \quad \alpha = \frac{m e^2}{\hbar^2} \quad \text{y} \quad E = -\frac{\hbar^2}{2m}\alpha^2 = -\frac{\hbar^2}{2m}\frac{m^2 e^4}{\hbar^4} = -\frac{m e^4}{2\hbar^2}$$

A se determina normalizando ϕ

$$1 = \int_0^\infty \phi^*(r)\,\phi(r)\,dr = \int_0^\infty A^2 e^{-2\alpha r}\,dr$$

$$= A^2 \left. e^{-2\alpha r}\right|_\infty^0 \frac{1}{2\alpha}$$

$$= \frac{A^2}{2\alpha}$$

$$\Rightarrow \quad A = \sqrt{2\alpha} = \sqrt{\frac{2 m e^2}{\hbar^2}}$$

Entonces la solución es

$$\boxed{\phi(r) = \frac{2me^2}{\hbar^2}\, e^{-\frac{me^2}{\hbar^2}r}}$$

Ahora calcular $\sqrt{\langle r^2 \rangle}$

Definiendo $a \equiv \frac{\hbar^2}{me^2} \Rightarrow \phi(r) = \sqrt{\frac{2}{a}}\, e^{-r/a}$

$$\langle r^2 \rangle = \int_0^\infty \phi(r)\, r^2\, \phi(r)\, dr$$

$$= \frac{2}{a} \int_0^\infty r^2 e^{-\frac{2r}{a}} dr$$

$$= \frac{2}{a} \left[\cancelto{0}{r^2 \left(\frac{-a}{2}\right) e^{-\frac{2r}{a}} \Big|_0^\infty} + \frac{a}{2} \int_0^\infty 2r\, e^{-2r/a} dr \right]$$

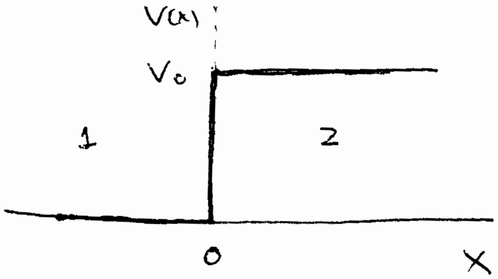
$$= \cancelto{0}{2r\left(-\frac{a}{2}\right) e^{-\frac{2r}{a}} \Big|_0^\infty} + \frac{a}{2} \int_0^\infty \cancel{2}\, e^{-2r/a} dr$$

$$= a\, \underbrace{e^{-2\frac{r}{a}} \Big|_\infty^0}_{1}\, \frac{a}{2}$$

$$= \frac{a^2}{2}$$

$$\therefore \quad \boxed{\sqrt{\langle r^2 \rangle} = \frac{a}{\sqrt{2}}}$$

P1



Considere una partícula moviéndose desde $-\infty$ a $+\infty$ con energía $E > V_0$. Encuentre los coeficientes de reflexión R y de transmisión T.

Sol: $R \equiv \left|\frac{J_R}{J_i}\right|$ y $T \equiv \left|\frac{J_T}{J_i}\right|$; donde $J(x) = -\frac{i\hbar}{2m}\left[\phi^*(x)\frac{\partial\phi}{\partial x}(x) - \phi(x)\frac{\partial\phi^*}{\partial x}(x)\right]$

Hay que resolver la ec de Schrödinger en cada región y luego ocupar las condiciones de borde

ec. Sch: $-\frac{\hbar^2}{2m}\phi''(x) + V(x)\phi(x) = E\phi(x)$; $V(x) = \begin{cases} 0 & x<0 \\ V_0 & x>0 \end{cases}$

En la región 1 $(x<0)$

$$-\frac{\hbar^2}{2m}\phi_1''(x) = E\phi_1(x)$$

$$\Rightarrow \quad \phi_1''(x) = -K_1^2\phi_1(x) \quad , \quad K_1^2 = \frac{2mE}{\hbar^2}$$

$$\Rightarrow \quad \phi_1(x) = \underbrace{A_1 e^{iK_1x}}_{\text{onda incidente}} + \underbrace{B_1 e^{-iK_1x}}_{\text{onda reflejada}}$$

En la región 2 $(x>0)$

$$-\frac{\hbar^2}{2m}\phi_2''(x) + V_0\phi_2(x) = E\phi_2(x)$$

$$\Rightarrow \quad \phi_2''(x) = -K_2^2\phi_2(x) \quad ; \quad K_2^2 = \frac{2m(E-V_0)}{\hbar^2}$$

$$\Rightarrow \quad \phi_2(x) = \underbrace{A_2 e^{iK_2x}}_{\text{onda transmitida}} + B_2 e^{-iK_2x}$$

$= 0$, pues no hay onda desde $+\infty$ a $-\infty$

Para la onda incidente $A_1 e^{ik_1 x}$:

$$J_i = \frac{-i\hbar}{2m}\left[A_1^* e^{-ik_1 x} \cdot A_1 e^{ik_1 x} \cdot ik_1 - A_1 e^{ik_1 x} \cdot A_1^* e^{-ik_1 x}(-ik_1)\right]$$

$$= \frac{-i\hbar}{2m}\left[|A_1|^2 ik_1 + |A_1|^2 ik_1\right]$$

$$= \frac{\hbar k_1 |A_1|^2}{m}$$

Para las ondas reflejadas y transmitidas es análogo:

$$J_R = -\frac{\hbar k_1}{m}|B_1|^2$$

$$J_T = \frac{\hbar k_2}{m}|A_2|^2$$

Entonces, $R = \left|\frac{J_R}{J_i}\right| = \left|\frac{B_1}{A_1}\right|^2$ y $T = \left|\frac{J_T}{J_i}\right| = \frac{k_2}{k_1}\left|\frac{A_2}{A_1}\right|^2$

$|B_1/A_1|^2$ y $|A_2/A_1|^2$ se determinan aplicando las condiciones de borde

$\phi_1(0) = \phi_2(0) \Rightarrow A_1 + B_1 = A_2$

$\phi_1'(0) = \phi_2'(0) \Rightarrow ik_1 A_1 - ik_1 B_1 = ik_2 A_2$

En forma matricial $\begin{bmatrix} -1 & 1 \\ k_1 & k_2 \end{bmatrix}\begin{bmatrix} B_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} A_1 \\ k_1 A_1 \end{bmatrix}$

$$\Rightarrow B_1 = \frac{A_1 k_2 - k_1 A_1}{-k_2 - k_1} = \frac{k_1 - k_2}{k_1 + k_2} A_1$$

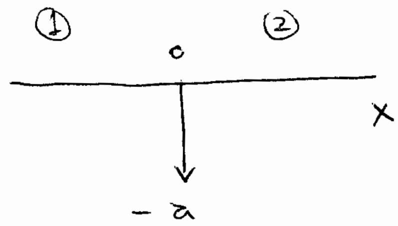
$$\text{y} \quad A_2 = \frac{-k_1 A_1 - k_1 A_1}{-k_2 - k_1} = \frac{2k_1}{k_1 + k_2} A_1$$

Luego, $R = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2 = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \boxed{1 - \frac{4k_1 k_2}{(k_1 + k_2)^2}}$

y $T = \frac{k_2}{k_1}\left|\frac{2k_1}{k_1 + k_2}\right|^2 = \frac{k_2}{k_1}\frac{(2k_1)^2}{(k_1 + k_2)^2} = \boxed{\frac{4k_1 k_2}{(k_1 + k_2)^2}}$

Notar que $R + T = 1$

P] Encuentre la función de onda y la energía $E<0$ de una partícula en un potencial $V(x) = -a\,\delta(x)$. $(a>0)$



Sol: $-\dfrac{\hbar^2}{2m}\phi''(x) + V(x)\,\phi(x) = E\,\phi(x)$

• Si $x<a$: $-\dfrac{\hbar^2}{2m}\phi_1''(x) = E\,\phi_1(x)$

$$\Rightarrow \quad \phi_1''(x) = \underbrace{-\frac{2mE}{\hbar^2}}_{\equiv k^2}\phi_1(x)$$

$$\Rightarrow \quad \phi_1(x) = A_1 e^{kx} + \underbrace{B_1}_{=0} e^{-kx}$$

$\uparrow = 0$, porque e^{-kx} diverge en $-\infty$

• Si $x>a$: es análogo

$$\Rightarrow \quad \phi_2(x) = \underbrace{A_2}_{=0} e^{kx} + B_2 e^{-kx}$$

$= 0$, porque e^{kx} diverge en $+\infty$

Entonces,

$$\phi(x) = \begin{cases} \phi_1 = A_1 e^{kx} & x<0 \\ \phi_2 = B_2 e^{-kx} & x>0 \end{cases} \qquad k^2 = -\frac{2mE}{\hbar^2}$$

CB_1 : $\phi_1(0) = \phi_2(0) \Rightarrow A_1 = B_2 \equiv C$

$$\Rightarrow \quad \phi(x) = C\,e^{-k|x|} \qquad x \in \mathbb{R}$$

CB_2 : $-\dfrac{\hbar^2}{2m}\phi''(x) - a\,\delta(x)\,\phi(x) = E\,\phi(x) \Big/ \displaystyle\int_{-\varepsilon}^{\varepsilon}$

$$-\frac{\hbar^2}{2m}\underbrace{\int_{-\varepsilon}^{\varepsilon}\phi''(x)\,dx}_{\phi'(\varepsilon)-\phi'(-\varepsilon)} - a\underbrace{\int_{-\varepsilon}^{\varepsilon}\delta(x)\,\phi(x)\,dx}_{\phi(0)} = E\underbrace{\int_{-\varepsilon}^{\varepsilon}\phi(x)\,dx}_{\approx 2\varepsilon\,\phi(0)}$$

tomando $\lim \varepsilon \to 0$ $\Rightarrow$ $-\frac{\hbar^2}{2m}\left[\phi'(0^+) - \phi'(0^-)\right] = a\,\phi(0)$

$$\Rightarrow \quad \underbrace{\phi'(0^+)}_{-CK} - \underbrace{\phi'(0^-)}_{CK} = -\frac{2ma}{\hbar^2}\underbrace{\phi(0)}_{C}$$

$$\Rightarrow \quad K = \frac{ma}{\hbar^2}$$

Y como $E = -\frac{\hbar^2}{2m}K^2$ $\Rightarrow$ $\boxed{E = -\frac{ma^2}{2\hbar^2}}$

Además, $\phi(x) = C\,e^{-K|x|} = C\,e^{-\frac{ma}{\hbar^2}|x|}$

C se obtiene normalizando

$$1 = \int_{-\infty}^{\infty} \phi^*(x)\,\phi(x)\,dx = C^2 \int_{-\infty}^{\infty} e^{-\frac{2ma}{\hbar^2}|x|}\,dx$$

$$= 2C^2 \int_0^{\infty} e^{-\frac{2max}{\hbar^2}}\,dx$$

$$= \cancel{2}C^2 \cdot \underbrace{e^{-\frac{2max}{\hbar^2}}\Big|_{\infty}^{0}}_{1} \frac{\hbar^2}{\cancel{2}ma}$$

$$= C^2 \cdot \frac{\hbar^2}{ma}$$

$$\Rightarrow \quad C = \frac{\sqrt{ma}}{\hbar}$$

$$\therefore \quad \boxed{\phi(x) = \frac{\sqrt{ma}}{\hbar}\, e^{-\frac{ma|x|}{\hbar^2}}}$$