Electron Hydrogen scattering

Abstract

We use the Born approximation to compute the differential cross section for the elastic scattering of a fast electron by a hydrogen atom in the ground state. We will treat the hydrogen atom as a fixed target with a time-independent charge distribution.

Index Terms

Born aproximation, scattering, cross-section

In Born approximation the differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \left| \frac{m}{2\pi} \int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} V_I(r) \right|^2, \tag{1}$$

where $V_I(r) = eV(r)$ is the interaction energy of the incoming electron with the hydrogen atom. It will be better to do the calculation in two parts since $V(r)$ is contributed by two charge constituents, the proton and the electron. The contribution from the proton is straightforward to compute since we know $V_p(r)$ right away: $V_p(r) = \frac{e}{r}$. The corresponding integral to be calculated as

$$I_1 \equiv \frac{m}{2\pi} \int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} \frac{e^2}{r}. \tag{2}$$

Unfortunately this integral is divergent, but we can regularize it by introducing an exponentially decaying function $e^{-\epsilon r}$, with $\epsilon > 0$. What we do is to evaluate the integral with $V_p(r) = \frac{e^2 e^{-\epsilon r}}{r}$ and let $\epsilon \to 0$ in the final answer (unlike physicists, mathematicians would strongly object: "You cannot change the order of integration and the limit $\epsilon \to 0$". We can think of it as assigning a finite number to a divergent integral by the renormalization procedure. Physically $e^{-\epsilon r}/r$ terms represents the potential due a massive particle of mass ϵ.) In this case we have

$$\begin{aligned} I_1 &\equiv \frac{me^2}{2\pi} \int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} \frac{e^{-\epsilon r}}{r} = 2me^2 \int dr \frac{\sin(qr)}{q} e^{-\epsilon r} = \frac{2me^2}{q} \Im \left\{ \int_0^\infty dr e^{-r(\epsilon - iq)} \right\} \\ &= \frac{2me^2}{q} \Im \left\{ \frac{1}{\epsilon - iq} = \frac{2me^2}{\epsilon^2 + q^2} \right\} = \frac{2me^2}{q^2}, \end{aligned} \tag{3}$$

where we finally set $\epsilon = 0$.

The second contribution comes from the electron cloud. The potential due to electron in the ground state is given as

$$V_e(r) = e\left(\frac{e^{-r/a_0}}{r} - \frac{1}{r} + \frac{1}{a_0} e^{-r/a_0}\right). \tag{4}$$

The first idea would be to plug this into the integral, and have fun... It can be done, but let's try something else,

$$I_2 \equiv \frac{me}{2\pi} \int d^3 r e^{-i\mathbf{q}\cdot\mathbf{r}} V_e(r) = \frac{2me}{q} \int_0^\infty r V_e(r) \sin(qr) dr \tag{5}$$

Now the idea is the integration by parts twice with the definitions $\mathcal{U} = rV(r)$ an $d\mathcal{V} = \sin(qr)$ for the first one and $\mathcal{U} = \frac{d}{dr}(rV(r))$ an $d\mathcal{V} = \cos(qr)$ for the second one. Note that we can drop $\mathcal{U}\mathcal{V}|_0^\infty$ since $\mathcal{U}$ vanishes at the boundaries. After two integration by parts we get

$$I_2 = -\frac{2m}{q^3} \int_0^\infty \frac{d^2}{dr^2}(rV_e(r)) \sin(qr) dr. \tag{6}$$

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What we have achieved is $\frac{d^2}{dr^2}(rV_e(r))$ term, which is r $\nabla^2 V_e$. By Poisson's equation it can be replaced by $r(-4\pi\rho_e(r))$ where

$$\rho_e(r) = -e|\psi(r)|^2 = -\frac{e}{\pi a_0^3} e^{-2r/a_0} \tag{7}$$

So the integral we need to deal with is

$$\begin{aligned} I_2 &= -\frac{8me^2}{a_0^3 q^3}\int_0^\infty re^{-2r/a_0}\sin(qr)dr = -\frac{8me^2}{a_0^3 q^3}\Im\left\{\int_0^\infty re^{-(2/a_0-iq)r}dr\right\} \\ &= -\frac{8me^2}{a_0^3 q^3}\Im\left\{\left(\frac{-d}{d\alpha}\right)_{\alpha=(2/a_0-iq)}\int_0^\infty e^{-\alpha r}dr\right\} \\ &= -\frac{8me^2}{a_0^3 q^3}\Im\left\{\frac{qa_0}{(2-iqa_0)^2}\right\} = -\frac{32me^2}{[4+(qa_0)^2]^2 q^2}. \end{aligned} \tag{8}$$

Combining both terms we have

$$\frac{d\sigma}{d\Omega} = \frac{4m^2e^4}{q^4}\left(1-\frac{16}{[4+(qa_0)^2]^2}\right)^2. \tag{9}$$

Before we discuss the limiting cases, let's solve the problem one more time using a shortcut. The object we are dealing with is,

$$I = \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} V(r), \tag{10}$$

which is nothing but the Fourier transform of the potential energy. Instead of jumping onto the problem head on, let's follow a detour. Consider the Poisson's equation,

$$\nabla^2 V(r) = -4\pi\rho(r) = -4\pi e(\delta(\overrightarrow{r}) - \rho_e(r)). \tag{11}$$

Instead of Fourier transforming the potential itself, we can Fourier transform Eq. (11) which gives

$$-q^2\tilde{V}(q) = -4\pi e(1-\mathcal{F}\{\rho_e(r)\}) \rightarrow \tilde{V}(q) = \frac{4\pi e(1-\mathcal{F}\{\rho_e(r)\})}{q^2}. \tag{12}$$

$\mathcal{F}\{\rho_e(r)\}$ term is to be calculated by usual means, and in reproduces the second term in Eq (9).

For large qa_0 the second term in Eq. (9), which accounts for the electron cloud, can be neglected. So the incoming electrons are deflected only by the proton. For small qa_0 the cross section becomes zero which is a manifestation of the fact that the hydrogen atom is neutral. This means that only highly deflected electrons can probe into the electron cloud, and "see" the proton.