CALCULATION OF PHASE SHIFTS FOR A CENTRAL POTENTIAL

The Schrödinger equation in the presence of a potential is

$$u'' + \left[k^2 - \frac{\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2} U(r) \right] u = 0 \qquad \text{--- (1)}$$

where $u = rR$ is the "radial" part of the wavefunction.

The equation in the absence of $U(r)$ is satisfied by $u^{(0)}$:

$$u^{(0)\,''} + \left[k^2 - \frac{\ell(\ell+1)}{r^2} \right] u^{(0)} = 0 \qquad \text{--- (2)}$$

We wish to determine the phase shift between $u^{(0)}$ and u as $r \to \infty$.

We multiply (1) by $u^{(0)}$ and (2) by u and subtract to get

$$u^{(0)} u'' - u\, u^{(0)\,''} = \frac{2m U(r)}{\hbar^2} u^{(0)} u$$

If we integrate this eqn (LHS integrated by parts) we obtain

$$u^{(0)} u' - u\, u^{(0)\,'} = \frac{2m}{\hbar^2} \int U(r)\, u^{(0)} u \, dr$$

In the limit $r \to \infty$, $u^{(0)} = 2 \sin(kr - \ell\pi/2)$ and $u = 2\sin(kr - \ell\pi/2 + \delta_\ell)$

If $U(r)$ can be treated as a perturbation then the RHS integrand can be approximated as $U(r)\, u^{(0)} u^{(0)}$, since $u \approx u^{(0)}$

THUS

$$u^{(0)} u' - u\, u^{(0)\,'} = \frac{2m}{\hbar^2} \int U(r) \left[u^{(0)} \right]^2 dr$$

Putting in the expressions for $u^{(0)}$ and u we get the LHS:

$$4k \sin(kr - \ell\pi/2) \cos(kr - \ell\pi/2 + \delta_\ell) - 4k \sin(kr - \ell\pi/2 + \delta) \cos(kr - \ell\pi/2)$$

i.e. $\quad 4k\,(-\sin \delta_\ell)$

$$\therefore \quad \sin \delta_\ell = \frac{-m}{2\hbar^2 k} \int U(r) \left[u^{(0)}_\ell \right]^2 dr$$

$\because \quad u^{(0)}_\ell = (2\pi kr)^{1/2} J_{\ell+\frac{1}{2}}(kr)$,

$$\sin \delta_\ell = \frac{-\pi m}{\cancel{2k}\,\hbar^2} \int U(r) \left[J_{\ell+\frac{1}{2}}(kr) \right]^2 dr$$

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ELASTIC SCATTERING OF FAST ELECTRONS

The differential cross-section for this case can't be written in terms of the first Born approximation:

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2\hbar^2}\left|\int U(r)\, e^{-i\vec{q}\cdot\vec{r}}\, d\tau\right|^2.$$

where $\vec{q} = \vec{k} - \vec{k}'$
and $|q| = 2k\sin(\chi/2)$

By choosing the $\vec{q}$ to be along the $\hat{z}$ axis, the exponent can be written as $iqr\cos\theta$ where θ is the polar angle (w.r.t. $\vec{q}$)

Then $$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi\hbar^2}\left|\int U(r)\,\frac{\sin qr}{q}\, r\, dr\right|^2$$ [only for a central potential.]

The potential energy operator for the electron-atom system is

$$U = \frac{Ze^2}{r} - \sum_{j=1}^{Z}\frac{e^2}{|\vec{r}-\vec{r}_j|}$$

Z ≡ atomic number
$\vec{r}_j$ ≡ position of j^{th} electron

We can write this operator in a form that does not involve $\vec{r}$

To do this we recognise first that $U = e\Phi$ where Φ is the electrostatic potential of the atomic constituents, and satisfies the Poisson equation $\nabla^2\Phi = -4\pi\rho$, in which

$$\rho(\vec{r}) = Ze\,\delta(\vec{r}) - e\,n(\vec{r})$$

$n(\vec{r})$: position distrib. of electrons

We can define the fourier components of ρ and Φ:

$$\Phi_q = \int \Phi(r)\, e^{-i\vec{q}\cdot\vec{r}}\, d\tau \quad \text{and} \quad \rho_q = \int \rho(r)\, e^{-i\vec{q}\cdot\vec{r}}\, d\tau$$

Since Φ_q and ρ_q are both independent of r, we have

$$\nabla^2\left[\Phi_q e^{-i\vec{q}\cdot\vec{r}}\right] = -q^2\Phi_q e^{-i\vec{q}\cdot\vec{r}} \quad \text{and} \quad \nabla^2\left[\rho_q e^{-i\vec{q}\cdot\vec{r}}\right] = -q^2\rho_q e^{-i\vec{q}\cdot\vec{r}}$$

For each fourier component $\nabla^2\Phi_q e^{i\vec{q}\cdot\vec{r}} = -4\pi\rho_q e^{i\vec{q}\cdot\vec{r}}$

i.e $-q^2\Phi_q e^{i\vec{q}\cdot\vec{r}} = -4\pi\rho_q e^{i\vec{q}\cdot\vec{r}}$

$$\Rightarrow \Phi_q = \frac{4\pi}{q^2}\rho_q$$

Since $\Phi_q = \int \Phi(r)\, e^{-i\vec{q}\cdot\vec{r}}\, d\tau$, etc

$$\int \Phi(r)\, e^{-i\vec{q}\cdot\vec{r}}\, d\tau = \frac{4\pi}{q^2}\int \rho(r)\, e^{-i\vec{q}\cdot\vec{r}}\, d\tau$$

$$\Rightarrow \int U(r)\, e^{-i\vec{q}\cdot\vec{r}}\, d\tau = \frac{4\pi e}{q^2}\int \left[Ze\,\delta(r) - e\,n(\vec{r})\right] e^{-i\vec{q}\cdot\vec{r}}\, d\tau$$

DEFINE $F(q) = \int n(r)\, e^{-i\vec{q}\cdot\vec{r}}\, d\tau$ "FORM FACTOR"

THEN $\int U(r)\, e^{-iqr}\, d\tau = \frac{4\pi e^2}{q^2}\left[Z - F(q)\right]$

$$\Rightarrow \quad \frac{d\sigma}{d\Omega} = \frac{4m^2e^4}{\hbar^4 q^4}\left[Z - F(q)\right]^2 \qquad q = 2K\sin(\chi/2) = \frac{2mv}{\hbar}\sin\chi/2$$

CASE I : $qa_0 \ll 1$, where $a_0 \sim$ atomic size

Since q is small we can write $q \simeq \frac{mv}{\hbar}\chi$

If we define $v_0 \sim \hbar/ma_0$, this implies $\chi \ll v_0/v$ and $\vec{q}\cdot\vec{r} \equiv qr$

In this case we can ~~expand~~ get $F(q)$ by expanding the exponential

$$F(q) = \int n(r)\left[1 - i\vec{q}\cdot\vec{r} - \frac{q^2r^2}{2!} \cdots\right] d\tau$$

the first term integrates out to Z, the total charge, the second term integrates to zero due to odd parity. The third term is significant, and $F(q) = Z - \int n(r)\, r^2 d\tau$

$$Z - F(q) = \frac{1}{6}q^2 \int n(r)\, r^2\, d\tau$$

$$\text{so} \quad \frac{d\sigma}{d\Omega} = \left(\frac{me^2}{3\hbar^2}\right)^2 \left|\int n(r)\, r^2\, dV\right|^2$$

applies to fwd. scatt. and is independent of the angle of scattering

CASE II

$qa_0 \gg 1$ or $\chi \gg v_0/v$ then the $F(q)$ integrand oscillates very rapidly and the integral is nearly zero. So only the term in Z survives and

$$\frac{d\sigma}{d\Omega} = \left(\frac{Ze^2}{2mv^2}\right)^2 \frac{1}{\sin^4(\chi/2)}$$

which is the Rutherford formula.

This corresponds to large angle scatt.