37

POTENTIAL FUNCTION OF HELIUM-LIKE ATOMS AND ELECTRON SCATTERING BY THE BORN APPROXIMATION

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ABSTRACT. In this paper the potential function of helium-like atoms has been derived by using the wave function of Hartree and Ingman (1933) and the scattering cross section of electron by the helium like atoms has been calculated by the method of Born approximation. The theoretical results at low angular range are found to be in excellent agreement with the experimental findings of Hughes, McMillen and Webb (1932).

INTRODUCTION

In calculating the energy eigen values of helium-like atoms by the variational methods the trial wave function has often been chosen as a product of two functions i.e. $f(r_1)\cdot f(r_2)$, where r_1 and r_2 are the position vectors of the two electrons with respect to the nucleus as origin (c.f. Huzinaga, 1960). This type of wave function makes the calculation simple, however, from physical grounds we would expect some dependence of the wave function on r_{12} the mutual distance between the two electrons. Therefore the simple wave function $f(r_1)f(r_2)$ may be modified by a multiplication of a function $\chi(r_{12})$ which depends on the distance between the electrons. This function $\chi(r_{12})$ is called the correlation function. Several authors like Hylleraas (1929), Hartree and Ingman (1933), and Roothan (1960) have suggested this type of improved approximation of analytical wave function for helium like atoms.

In the present paper we propose to evaluate the nature of the potential functional function and to calculate the cross section of elastic scattering of electron by helium-like atom in the ground state by taking a wave function as suggested by Hartree and Ingman (1933). They have taken both the electrons in the K shell and they argue that the correlation function should approach a constant value for $r_{12}\rightarrow\infty$, expressing the separability of the wave function when the electrons are far apart and the decrease to a finite though smaller value for $r_{12}\rightarrow 0$. The success of such a wave function can also be judged by the improvement in the value of the eigen-energy. The upper limit for the ground state energy of the helium atom obtained by Hartree and Ingman using the above wave function is $-2.89e^2/a_0$, a_0 being the Bohr radius, the experimental value being $-2.904e^2/a_0$, whereas Hylleraas, using a wave function without $\chi(r_{12})$, has obtained $-2.847e^2/a_0$ as the value for the same.

In the first part of this paper the function due to Hartree and Ingman has been normalized and the potential function has been evaluated by using the above mentioned wave function. In the second part the differential scattering cross section of electron has been calculated by the Born approximation method neglecting the exchange effect. At 500 eV (the range of energy where the Born approximation method is fairly valid) the differential cross section of scattering of electron by helium atom agrees very well at small angles with the experimental findings of Hughes, McMillen and Webb (1932), but for large angles our theoretical results deviate slightly from the experimental ones. By comparing our results at 700 eV with those of Sachl (1958) who has calculated the same problem in higher Born approximation we find that in the angular range 60° to 135°, our expression gives better agreement with experimental findings than that of Sachl (1958). No data below 60° angle has been given by Sachl.

METHODS OF CALCULATION

The wave function ψ due to Hartree and Ingman is

$$\psi \sim e^{-\xi(r_1+r_2)}(1-Ce^{-\eta r_{12}})$$

where $\xi = 1.8395, \quad C = 0.88784, \quad \eta = 0.047827,$

and the distances are represented in Bohr unit.

The wave function is normalized as shown in Appendix 1.

The potential function is calculated by the formula (vide Mott and Massey, 1949).

$$V(r) = -e^2\int\left(\frac{Z}{r}-\sum_{n=1,2}\frac{1}{|\boldsymbol{r}-\boldsymbol{r}_n|}\right)|\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)|^2\, d\boldsymbol{r}_1\, d\boldsymbol{r}_2, \qquad \dots (1)$$

where Z is the atomic number and ψ is the wave function.

Thus

$$V(r) = -\frac{Ze^2}{r}+\frac{2e^2}{N^2}\{I(2\xi, 0)-2CI(2\xi, \eta)+C^2I(2\xi, 2\eta)\} \qquad \dots (2)$$

where N is the normalization factor (vide Appendix 1) and

$$I(\mu, \eta) = \int \frac{e^{-\mu(r_1+r_2)-\eta r_{12}}}{|\boldsymbol{r}-\boldsymbol{r}_1|}\, d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2.$$

From the identity

$$\frac{e^{-\lambda r}}{r} = \frac{1}{2\pi^2}\int\frac{e^{\pm i\boldsymbol{p}\cdot\boldsymbol{r}}}{p^2+\lambda^2}\, d^3\boldsymbol{p}$$

we get

$$I(\mu, \eta) = \frac{\mu^2\eta}{2\pi^8} \int \frac{e^{-i\mathbf{p}.\mathbf{r}_1 + i\mathbf{q}.\mathbf{r}_2 + i\mathbf{s}.(\mathbf{r}_1 - \mathbf{r}_2) - i\mathbf{k}.(\mathbf{r} - \mathbf{r}_1)}}{(p^2+\mu^2)^2(q^2+\mu^2)^2(s^2+k^2)} d^3\boldsymbol{r}_1 \cdot d^3\boldsymbol{r}_2 \cdot d^3\mathbf{p}\, d^3\boldsymbol{q} \cdot d^3\boldsymbol{s} \cdot d^3\boldsymbol{k}$$

Applying the properties of δ-function

$$\int_{-\infty}^{\infty} e^{i(\mathbf{p}-\mathbf{k}).\mathbf{x}}\, d^3\boldsymbol{x} = (2\pi)^3\, \delta(\boldsymbol{p}-\boldsymbol{k})$$

we get

$$\therefore \qquad I(\mu, \eta) = \frac{\mu^2\eta\, 2^5}{\pi^2} \int e^{-i\mathbf{k}.\mathbf{r}}\, d^3\boldsymbol{k} \,.\, f(k^2)$$

where
$$f(k^2) = \int \frac{d^3\mathbf{s}}{\{(s+k)^2+\mu^2\}^2(s^2+\mu^2)^2(s^2+\eta^2)^2 \,.\, k^2}$$

i.e.
$$I(\mu, \eta) = \frac{\mu\,\eta\, 2^6\pi}{r} \int \frac{1}{ik}\, e^{ikr} \left[\frac{1}{(\mu^2-\eta^2)^2} \left\{ \frac{\mu+\eta}{\eta(k^2+\delta^2)(k^2+\lambda^2)} - \frac{4\mu(\mu+\eta)}{(k^2+\delta^2)^2(k^2+\lambda^2)} \right.\right.$$

$$\left.\left. + \frac{2}{(k^2+4\mu^2)^2} \right\} - \frac{2}{(\mu^2-\eta^2)^3} \left\{ \frac{1}{(k^2+\delta^2)} - \frac{1}{(k^2+4\mu^2)} \right\} \right] dk$$

where
$$\mu+\eta = \delta; \quad \mu-\eta = \lambda$$

After evaluation of the integral we have

$$I(\mu, \eta) = \frac{2^6\mu\eta\pi^2}{r(\mu^2-\eta^2)^2} \left\{ \frac{\mu+\eta}{\eta(\delta^2-\lambda^2)} \left[\frac{1}{\lambda^2} - \frac{e^{-\lambda r}}{\lambda^2} - \frac{1}{\delta^2} + \frac{e^{-\delta r}}{\delta^2} \right] \right.$$

$$-4\mu(\mu+\eta) \left[\frac{1}{\delta^4\lambda^2} - \frac{e^{-\lambda r}}{\lambda^2(\delta^2-\lambda^2)^2} + \frac{e^{-\delta r}}{\delta^2(\delta^2-\lambda^2)^2} + \frac{e^{-\delta r}}{\delta^4(\delta^2-\lambda^2)} + \frac{e^{-\delta r}r}{2\delta^3(\delta^2-\lambda^2)} \right]$$

$$\left. + \frac{1}{8\mu^3} \left[\frac{1}{\mu} - \frac{e^{-2\mu r}}{\mu} - e^{-2\mu r}r \right] - \frac{2}{\delta^2(\mu^2-\eta^2)} [1-e^{-\delta r}] + \frac{[1-e^{-2\mu r}]}{2\mu^2(\mu^2-\eta^2)} \right\}$$

The scattering amplitude, by the Born approximation method is given by

$$f(\theta) = \frac{1}{4\pi} \frac{2m}{\hbar^2} \int V(r) e^{i\mathbf{k}.\mathbf{r}}\, d^3\boldsymbol{r} \qquad \ldots \quad (3)$$

where $V(r)$ is the potential and $\boldsymbol{k} = \frac{2mv}{\hbar} (\boldsymbol{n}_0 - \boldsymbol{n})$, $\boldsymbol{n}_0$ and $\boldsymbol{n}$ are the unit vectors along the incident and scattered directions respectively. Substituting in Eq. (3) the value of $V(r)$ from Eq. (1) we have,

$$f(\theta) = \frac{e^2}{4\pi}\frac{2m}{\hbar^2}\left[-\int\frac{Z}{r}e^{\mathbf{ik.r}}d^3\boldsymbol{r}+\frac{2}{N^2}\{I'(2\xi,0)-2CI'(2\xi,\eta)+C^2I'(2\xi,2\eta)\}\right] \tag{4}$$

where $$I'(\mu,\nu) = \int^{\infty}\frac{e^{-\mu(\mathbf{r}_1+\mathbf{r}_2)-\nu\mathbf{r}_{12}+\mathbf{ik.r}}}{|\boldsymbol{r}-\boldsymbol{r}_n|}d^3\boldsymbol{r}_1\,d^3\boldsymbol{r}_2d^3\boldsymbol{r}$$

with $$n = 1, 2$$

After integration (vide Appendix 2), we obtain

$$I'(\mu,\nu) = \frac{2^8\pi^3\mu\nu}{\boldsymbol{k}^2}\left[\frac{1}{(\mu^2-\nu^2)^2}\left\{\frac{\lambda/\nu+2}{(\boldsymbol{k}^2+\delta^2)(\boldsymbol{k}^2+\lambda^2)}-\frac{4\mu\delta}{(\boldsymbol{k}^2+\delta^2)^2(\boldsymbol{k}^2+\lambda^2)}-\frac{2}{(\boldsymbol{k}^2+4\mu^2)^2}\right\}-\frac{2}{(\mu^2-\nu^2)^3}\left\{\frac{1}{\boldsymbol{k}^2+\delta^2}-\frac{1}{\boldsymbol{k}^2+4\mu^2}\right\}\right]$$

where $$\mu+\nu = \delta, \quad \mu-\nu = \lambda$$

TABLE I

Comparison of the differential scattering cross section of electron of energy 500 eV scattered by helium atom

Angle in degrees	Experimental value	Theoretical results (present author)
	Differential cross section in units of 10^{-20}cm2	
9.5	1195.0	1190.4
12.0	1047.0	1037.16
22.0	467.0	475.64
27.0	284.5	287 01
47.0	60.8	69.8
67.0	15.88	20.04
87.0	6.14	9.23

TABLE II

Comparison of the differential scattering cross section of electron of energy 700eV scattered by helium atom

Angle in degrees	Differential cross section in units of 10^{-20} cm2		
	Experimental value	Theoretical results Sachl	Theoretical results (present author)
60	15	24	15.75
90	5	8.6	4.04
120	3.5	5.2	1.864
135	3.4	1.8	1.405

DISCUSSION

From the calculation it is observed that the screening effect is more prominent far small angles of scattering whereas for large angles it becomes negligible. This is because when the scattering angle is large the particle moves very near the nucleus, where the screening effect due to the surrounding electrons is negligible.

The better agreement of our theoretical calculations with experiment for small angles of scattering is due to the fact that in these cases the particle passes far from the nucleus, where the potential is very weak on account of the screening effect and as such, the perturbation calculations are quite valid.

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APPENDIX I

In the present case the wave function is

$$\psi = \frac{1}{N} e^{-\xi(r_1+r_2)} (1 - Ce^{-\eta r_{12}}),$$

the normalization factor N is evaluated from the requirement

$$\int \psi \psi^* d\tau = 1.$$

Thus, $$N^2 = I''(2\xi, 0) - 2CI''(2\xi, \eta) + C^2 I''(2\xi, 2\eta)$$

where $$I''(\mu,\lambda)=\int e^{-\mu(r_1+r_2)}\quad e^{-\lambda r_{12}}\quad d^3r_1\, d^3r_2$$

$$=2\pi^2\int_0^\infty ds\int_0^s du\int_0^u dt\, e^{-\mu s}\ e^{-\lambda u}\ u(s^2-t^2)$$

where $s=r_1+r_2,\quad t=-r_1+r_2,\ u=r_{12}$ (vide Hylleraas, 1929)

$$=2\pi^2\int_0^\infty ds\int_0^s du\ e^{-\mu s}e^{-\lambda u}\left(s^2u^2-\frac{u^4}{3}\right)$$

$$=2\pi^2\int_0^\infty ds\ e^{-\mu s}\,(s^2I_2-\tfrac{1}{3}I_4)$$

where $I_n=\int_0^s e^{-\lambda u}\ u^n du=\left(-\frac{\partial}{\partial\lambda}\right)^n I_0\ ;\ I_0=\int_0^s e^{-\lambda u}\,du=\left[\frac{e^{-\lambda u}}{-\lambda}\right]_0^s$

$$\therefore\ I''(\mu,\lambda)=\Bigg[\int_0^\infty e^{-\mu s}\, s^2\frac{2}{\lambda^3}ds-\int_0^\infty \tfrac{1}{3}e^{-\mu s}\,\frac{24}{\lambda^5}ds$$

$$-\int_0^\infty e^{-(\lambda+\mu)s}\left\{\frac{2}{\lambda^3}\,s^2+\frac{2}{\lambda^2}\,s^3+\frac{1}{\lambda}\ \ s^4\right\}ds$$

$$+\tfrac{1}{3}\int_0^\infty e^{-(\lambda+\mu)s}\left\{\frac{24}{\lambda^5}+\frac{24}{\lambda^4}s+\frac{12}{\lambda^3}s^2+\frac{4}{\lambda^2}\,s^3+\frac{1}{\lambda}\,s^5\right\}ds\ \Bigg]$$

i.e., $$I''(\mu,\lambda)=\frac{8\pi^2}{\mu^3(\lambda+\mu)^5}\ \{\lambda^2+5\lambda\mu+8\mu^2\}$$

Since $$\int_0^\infty e^{-\nu s}\ s^n\, ds=\frac{n!}{\nu^{n+1}}$$

APPENDIX 2

The value of $I'(\mu,\nu)$ we get as

$$I'(\mu,\nu)=\int\int\int\frac{e^{-\mu(r_1+r_2)-\nu r_{12}+i\mathbf{k}\cdot\mathbf{r}}\quad d^3\mathbf{r}_1\, d^3\mathbf{r}_2\, d^3\mathbf{r}_3}{|\mathbf{r}-\mathbf{r}_1|}$$

$$= \frac{\mu^2\nu}{(\pi^2)^3 2\pi^2} \int\int\int \frac{e^{-i\mathbf{p}.\mathbf{q}(\mathbf{r}-\mathbf{r}_1)}}{p^2} d^3\boldsymbol{p} \int \frac{e^{i\mathbf{q}.\mathbf{r}}}{(q^2+\mu^2)^2} d^3\boldsymbol{q} \int \frac{e^{i\mathbf{t}.\mathbf{r}_2}}{(t^2+\mu^2)^2} d^3\boldsymbol{t}$$

$$\int \frac{e^{i\mathbf{s}.(\mathbf{r}_1-\mathbf{r}_2)}}{(s^2+\nu^2)^2} d^3\boldsymbol{s} \int e^{i\mathbf{k}.\mathbf{r}} d^3\boldsymbol{r}\, d^3\boldsymbol{r}_1\, d^3\boldsymbol{r}_2$$

Since
$$\frac{e^{-\lambda r}}{r} = \frac{1}{2\pi^2} \int_{-\infty}^{\infty} \frac{e^{i\mathbf{p}.\mathbf{r}}}{p^2+\lambda^2} d^3\boldsymbol{p}$$

and
$$e^{-\lambda r} = \int_{-\infty}^{\infty} \frac{e^{i\mathbf{p}.\mathbf{r}} d^3\boldsymbol{p}}{(p^2+\lambda^2)^2}$$

$$\therefore \quad I'(\mu,\nu) = \frac{\mu^2\nu(2\pi)^9}{2\pi^8} \int \frac{\delta(\boldsymbol{k}-\boldsymbol{p})\delta(\boldsymbol{p}+\boldsymbol{q}+\boldsymbol{s})\delta(\boldsymbol{t}-\boldsymbol{s}) d^3\boldsymbol{p}\, d^3\boldsymbol{q}\, d^3\boldsymbol{t}\, d^3\boldsymbol{s}}{p^2(q^2+\mu^2)^2(t^2+\mu^2)^2(s^2+\nu^2)^2}$$

$$= \frac{2^8\mu^2\nu\pi}{\boldsymbol{k}^2} \int \frac{d^3\boldsymbol{s}}{(|\boldsymbol{k}+\boldsymbol{s}|^2+\mu^2)^2(s^2+\mu^2)^2(s^2+\nu^2)^2}$$

$$= \frac{2^8\pi^2\mu^2\nu}{\boldsymbol{k}^3} \int \frac{\boldsymbol{s}\, d\boldsymbol{s}}{(s^2+\mu^2)^2(s^2+\nu^2)^2\{(s-k)^2+\mu^2\}}$$

Applying the following identity,

$$\left[(p^2+\mu^2)(p^2+\nu^2)\right]^{-2} = \frac{1}{(\mu^2-\nu^2)^2}\left[\frac{1}{(p^2+\nu^2)^2}+\frac{1}{(p^2+\mu^2)^2}\right]$$

$$-\frac{2}{(\mu^2-\nu^2)^3}\left[\frac{1}{(p^2+\nu^2)}-\frac{1}{(p^2+\mu^2)}\right]$$

$$\therefore\ I'(\mu,\nu) = \frac{2^8\pi^3\mu\nu}{\boldsymbol{k}^2}\left[\frac{1}{(\mu^2-\nu^2)^2}\left\{\frac{1}{(\boldsymbol{k}^2+\delta^2)(\boldsymbol{k}^2+\lambda^2)}\left\{\frac{\mu-\nu}{\nu}+2\right] - \frac{4\mu(\mu+\nu)}{(\boldsymbol{k}^2+\delta^2)^2(\boldsymbol{k}^2+\lambda^2)}\right.\right.$$

$$\left.\left.+\frac{2}{(\boldsymbol{k}^2+4\mu^2)^2}\right\} - \frac{2}{(\mu^2-\nu^2)^3}\left\{\frac{1}{\boldsymbol{k}^2+\delta^2}-\frac{1}{\boldsymbol{k}^2+4\mu^2}\right\}\right]$$

where
$$\mu+\nu = \delta \quad \text{and} \quad \mu-\nu = \lambda$$

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