Potential for a Fermi Charge Distribution

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Abstract

The generalization of the nuclear Coulomb potential is derived for the case where the nuclear charge is described by a Fermi distribution. The purpose of this note is to check the validity of the formulas for the potential on pages 153-154 of *Atomic Structure Theory*. Errors are discovered and pointed out in the formulas for S_k and P_k on the bottom of page 153.

Normalization

Basic assumption: The nuclear charge density is given by

$$\rho(r) = \frac{\rho_0}{1 + \exp[(r-c)/a]} \tag{1}$$

The constant c is the 50% falloff radius of the charge distribution and a is related to the 90% - 10$ falloff distance t by $t = 4\ln(3)a$. The constant ρ_0 is chosen by requiring that the total charge of the nucleus is Z:

$$Z = 4\pi\rho_0 \int_0^\infty \frac{r^2}{1 + \exp[(r-c)/a]} dr \tag{2}$$

It is convenient to introduce the dimensionless positive constant $\mu = c/a$ and rewrite Eq.(2) as

$$Z = 4\pi\rho_0 a^3 \int_0^\infty \frac{x^2}{1 + \exp(x-\mu)} dx, \tag{3}$$

where $x = r/a$ The integral above can be conveniently separated into two parts:

$$K_1 = \int_0^\mu \frac{x^2}{1 + \exp(x-\mu)} dx \tag{4}$$

$$K_2 = \int_\mu^\infty \frac{x^2}{1 + \exp(x-\mu)} dx \tag{5}$$

The two parts above are expanded as

$$K_1 = \frac{\mu^3}{3} + \sum_{n=1}^{\infty}(-1)^n e^{-n\mu}\int_0^{\mu} x^2 e^{nx} dx \tag{6}$$

$$K_2 = -\sum_{n=1}^{\infty}(-1)^n e^{n\mu}\int_{\mu}^{\infty} x^2 e^{-nx} dx \tag{7}$$

These integrals have the following values:

$$e^{-n\mu}\int_0^{\mu} x^2 e^{nx} dx = \frac{2}{n^3} - \frac{2\mu}{n^2} + \frac{\mu^2}{n} - \frac{2e^{-n\mu}}{n^3} \tag{8}$$

$$e^{n\mu}\int_{\mu}^{\infty} x^2 e^{-nx} dx = \frac{2}{n^3} + \frac{2\mu}{n^2} + \frac{\mu^2}{n} \tag{9}$$

It follows that

$$K_1 + K_2 = \frac{\mu^3}{3} + 4\mu\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n^2} + 2\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n^3}e^{-n\mu} \tag{10}$$

Noting that

$$\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n^2} = \frac{\pi^2}{12}, \tag{11}$$

Eq.(2) can be reexpressed as

$$\rho_0 = \frac{3}{4\pi c^3}\frac{Z}{\mathcal{N}}, \tag{12}$$

where the normalization constant $\mathcal{N}$ is

$$\mathcal{N} = 1 + \frac{a^2}{c^2}\pi^2 + 6\frac{a^3}{c^3}S_3. \tag{13}$$

Here, the function S_k is defined by

$$S_k = \sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n^k}e^{-n\mu} \tag{14}$$

Nuclear potential: $c < r$

Assuming $\mu < x$, the nuclear potential is divided into three parts:

$$V_{c<r}(r) = 4\pi\rho_0 a^2\left[I_1 + I_2 + I_3\right], \tag{15}$$

with

$$I_1 = \frac{1}{x}\int_0^{\mu} \frac{x^2}{1+\exp(x-\mu)}dx \tag{16}$$

$$I_2 = \frac{1}{x}\int_{\mu}^{x} \frac{x^2}{1+\exp[(x-\mu)}dx \tag{17}$$

$$I_3 = \int_x^{\infty} \frac{x}{1+\exp(x-\mu)}dx, \tag{18}$$

where, as before, $x = r/a$. These three terms are as follows:

$$I_1 = \frac{1}{x}\left(\frac{\mu^3}{3} + \sum_{n=1}^{\infty}(-1)^n e^{-n\mu}\int_0^{\mu} y^2 e^{ny}dy\right) \tag{19}$$

$$I_2 = \frac{1}{x}\left(-\sum_{n=1}^{\infty}(-1)^n e^{n\mu}\int_{\mu}^{x} y^2 e^{-ny}dy\right) \tag{20}$$

$$I_3 = -\sum_{n=1}^{\infty}(-1)^n e^{n\mu}\int_x^{\infty} y e^{-ny}dy. \tag{21}$$

Evaluating the three integrals above, we find

$$e^{-n\mu}\int_0^{\mu} y^2 e^{ny}dy = \frac{2}{n^3} - \frac{2e^{-n\mu}}{n^3} - \frac{2\mu}{n^2} + \frac{\mu^2}{n} \tag{22}$$

$$\begin{aligned} e^{n\mu}\int_{\mu}^{x} y^2 e^{-ny}dy &= \frac{2}{n^3} + \frac{2\mu}{n^2} + \frac{\mu^2}{n} - \frac{2e^{-n(x-\mu)}}{n^3} \\ &\quad - \frac{2xe^{-n(x-\mu)}}{n^2} - \frac{2x^2 e^{-n(x-\mu)}}{n} \end{aligned} \tag{23}$$

$$e^{n\mu}\int_x^{\infty} y e^{-ny}dy = \frac{e^{-n(x-\mu)}}{n^2} + \frac{xe^{-n(x-\mu)}}{n} \tag{24}$$

Combining, we have

$$\begin{aligned} I_1 + I_2 + I_3 &= \frac{1}{x}\left\{\frac{\mu^3}{3}\right. \\ &\quad \left. + \sum_{n=1}^{\infty}(-1)^{n-1}\left[\frac{2e^{-n\mu}}{n^3} - \frac{2e^{-n(x-\mu)}}{n^3} - \frac{xe^{-n(x-\mu)}}{n^2} + \frac{4\mu}{n^2}\right]\right\} \\ &= \frac{c^3}{3a^2 r}\left\{1 + 6\frac{a^3}{c^3}[S_3 - P_3] - 3\frac{a^2 r}{c^3}P_2 + \frac{a^2\pi^2}{c^2}\right\}, \end{aligned} \tag{25}$$

where

$$P_k = \sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n^k}e^{-n|x-\mu|} \tag{26}$$

With the aid of Eqs. (12 & 15), we find

$$V_{c<r}(r) = \frac{Z}{\mathcal{N}r}\left\{1 + 6\frac{a^3}{c^3}\left[S_3 - P_3\right] \; -3\frac{a^2 r}{c^3}P_2 + \frac{a^2\pi^2}{c^2}\right\}. \tag{27}$$

Nuclear potential: $c > r$

Assuming $\mu > x$, the nuclear potential is divided into three parts:

$$V_{c>r}(r) = 4\pi\rho_0 a^2 \left[J_1 + J_2 + J_3\right], \tag{28}$$

with

$$J_1 = \frac{1}{x}\int_0^x \frac{x^2}{1+\exp(x-\mu)}dx \tag{29}$$

$$J_2 = \int_x^\mu \frac{x}{1+\exp[(x-\mu)}dx \tag{30}$$

$$J_3 = \int_\mu^\infty \frac{x}{1+\exp(x-\mu)}dx. \tag{31}$$

These three terms are expanded as

$$J_1 = \frac{1}{x}\left(\frac{x^3}{3} + \sum_{n=1}^{\infty}(-1)^n e^{-n\mu}\int_0^x y^2 e^{ny}dy\right) \tag{32}$$

$$J_2 = \frac{1}{2}(\mu^2 - x^2) + \sum_{n=1}^{\infty}(-1)^n e^{-n\mu}\int_x^\mu y e^{ny}dy \tag{33}$$

$$J_3 = -\sum_{n=1}^{\infty}(-1)^n e^{n\mu}\int_\mu^\infty y e^{-ny}dy. \tag{34}$$

$$\begin{aligned} J_1 + J_2 + J_3 = &\left\{\frac{\mu^2}{2} - \frac{x^2}{6}\right. \\ &\left. + \sum_{n=1}^{\infty}(-1)^{n-1}\left[\frac{2}{n^2} + \frac{e^{-n(\mu-x)}}{n^2} + \frac{1}{x}\left(\frac{2e^{-n\mu}}{n^3} - \frac{2e^{-n(\mu-x)}}{n^3}\right)\right]\right\} \\ = &\frac{c^2}{3a^2}\left\{\frac{3}{2} - \frac{r^2}{2c^2} + \frac{a^2\pi^2}{2c^2} + \frac{3a^2}{c^2}P_2 + \frac{6a^3}{c^2 r}[S_3 - P_3]\right\}. \end{aligned} \tag{35}$$

It follows that

$$V_{c>r} = \frac{Z}{c\mathcal{N}}\left\{\frac{3}{2} - \frac{r^2}{2c^2} + \frac{a^2\pi^2}{2c^2} + \frac{3a^2}{c^2}P_2 + \frac{6a^3}{c^2 r}[S_3 - P_3]\right\}. \tag{36}$$

Summary

$$V_{r<c}(r) = \frac{Z}{c\mathcal{N}}\left\{\frac{3}{2} - \frac{r^2}{2c^2} + \frac{a^2\pi^2}{2c^2} + \frac{3a^2}{c^2}P_2 + \frac{6a^3}{c^2 r}[S_3 - P_3]\right\} \tag{37}$$

$$V_{r>c}(r) = \frac{Z}{\mathcal{N}r}\left\{1 + \frac{a^2\pi^2}{c^2} - 3\frac{a^2 r}{c^3}P_2 + 6\frac{a^3}{c^3}\left[S_3 - P_3\right]\right\} \tag{38}$$

In the above,

$$S_k = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^k} \exp[-nc/a] \tag{39}$$

$$P_k = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^k} \exp[-n|r-c|/a], \tag{40}$$

correcting errors in the formulas at the bottom of page 153 of the book. In the limiting case $r \to c$,

$$V_{r<c} \to \frac{Z}{c\mathcal{N}} \left\{ 1 + \frac{3\pi^2 a^2}{4c^2} \right\} \tag{41}$$

$$V_{r>c} \to \frac{Z}{c\mathcal{N}} \left\{ 1 + \frac{3\pi^2 a^2}{4c^2} \right\}, \tag{42}$$

confirming the continuity of the expressions for V(r) in the at $r = c$. In the limit $a \to 0$,

$$V_{c>r} \to \frac{Z}{c} \left(\frac{3}{2} - \frac{r^2}{2c^2} \right) \tag{43}$$

$$V_{c<r} \to \frac{Z}{r}. \tag{44}$$

The figure below compares a Coulomb potential with $Z = 1$, shown in the dot-dashed black curve, with the potential from a uniform distribution with $Z = 1$ and $c = 1$, shown in orange, and the potential from a Fermi distribution with $Z = 1$, $c = 1$ and $a = 1/4$, shown in blue.