

MOMENTS OF THE TWO-PARAMETER FERMI CHARGE DISTRIBUTION

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Abstract

Moments $\langle r^m \rangle$ and isotopic differences $\delta\langle r^m \rangle$ of the spherical two-parameter Fermi charge distribution are presented for $m = 1$ to 10 as a function of the half-density radius c and diffusity a ; the introduction of the parameter $\beta \equiv \pi a/c$ proved to be useful. First, the Fermi integrals $F_n(k)$ are derived. Then, even and odd orders are treated separately for $F_n(k)$ as well as for $\langle r^m \rangle$ and $\delta\langle r^m \rangle$; in calculating $\delta\langle r^m \rangle$ the diffusity a is assumed to be constant. The differences $\delta\langle r^m \rangle$ for even m are also given in terms of $\delta\langle r^2 \rangle$.

I. Introduction. The Fermi integral $F_n(k)$

Moments of model charge distributions are often used in atomic and nuclear physics. Isotope shifts $\delta\nu$ in optical and characteristic X-ray frequencies can be expressed with differences in even moments $\delta\langle r^m \rangle_{A2,A1}$ for two isotopes [1]. Another example: the energy of transitions in muonic atoms determine the *Barrett moment* $\langle r^k e^{-\alpha r} \rangle$ [2], which can be approximated by a series of moments $\langle r^m \rangle$ ($m = 2, 3, \dots$) [3]. A frequently used charge distribution is the spherically symmetric *two-parameter Fermi distribution* ($2pF$):

$$\rho_F(r; c, a) = \frac{\rho_0}{1 + e^{\frac{r-c}{a}}} \equiv \frac{\rho_0}{1 + e^{x-k}} \quad (r \geq 0) \quad (1)$$

where c is the half-density radius, a is the surface diffusity, $x \equiv r/a$, $k \equiv c/a$; the dimensionless quantity $\beta \equiv \pi/k = \pi a/c$ is also used where practical. The m -th absolute moment of the $2pF$ charge distribution is

$$\langle r^m \rangle = \frac{\int r^m \rho_F(r; c, a) dv}{\int \rho_F(r; c, a) dv} = \frac{\int r^{m+2} \rho_F(r; c, a) dr}{\int r^2 \rho_F(r; c, a) dr} = a^m \frac{F_{m+2}(k)}{F_m(k)} \quad (2)$$

where the *Fermi-integral*

$$F_n(k) = \int \frac{x^n}{1 + e^{x-k}} dx \quad (3)$$

is introduced; the limits of integration in r and x are from zero to infinity. The Fermi integral can be expressed by the sums [4, Appendix C; note the misprint in the exponent of the last term!]:

$$\begin{aligned} F_n(k) &= \frac{k^{n+1}}{n+1} + \sum_{r=0}^n [1 - (-1)^r] \frac{n!}{(n-r)!} k^{n-r} \left(1 - \frac{1}{2^r}\right) \zeta(r+1) \\ &\quad - \sum_{v=1}^{\infty} (-1)^{v+n} \frac{n!}{v^{n+1}} e^{-vk} \end{aligned} \quad (4)$$

where ζ is the *Riemann function* (see later).

In the present paper, formulae for the Fermi integrals $F_n(k)$, for moments $\langle r^m \rangle$ and for isotopic differences $\delta \langle r^m \rangle$ are given using the parameters c, a and β . In order to meet practical requirements (evaluation of optical isotope shift measurements) isotopic differences $\delta \langle r^m \rangle$ with even m are expressed by $\delta \langle r^2 \rangle$, too. Parts of this work have been published in [5, 3]. However, the present full version contains several completions.

II. Estimation of the exponential terms

It is worth estimating the value of the last sum of exponential terms

$$E_n(k) = - \sum_{v=1}^{\infty} (-1)^{v+n} \frac{n!}{v^{n+1}} e^{-vk} = (-1)^n n! e^{-k} \left(1 + \frac{e^{-k}}{2^{n+1}} + \dots\right) \quad (5)$$

Even for the very light nucleus 4He [6, p.489] $k = 1.0/0.32 = 3.12$, i.e. $e^{-k} \approx 0.045$, the second and any further terms in the parentheses can be neglected; i.e.:

$$|E_n(k)| \approx n!e^{-k} \quad (6)$$

Compare the $|E_n(k)|$ values with the sum of the leading terms:

$$\begin{aligned} F_2(k) &\approx \frac{k^3}{3}(1+1) = \frac{30}{3} \times 2 = 20 \\ |E_2(k)| &\approx 2 \times 0.045 \approx 0.09 \\ \\ F_6(k) &\approx \frac{k^7}{7}(1+7+16.3+10.3) = \frac{2873}{7} \times 34.6 = 14200 \\ |E_6(k)| &\approx 32 \\ \\ F_{10}(k) &\approx \frac{k^{11}}{11}(1+18+154+682+1397+852) = 7.7 \times 10^8 \\ |E_{10}(k)| &\approx 1.6 \times 10^5 \end{aligned} \quad (7)$$

It can be seen that for 4He the values $|E_n(k)|$ are three orders of magnitudes less than $F_n(k)$; consequently, $E_n(k)$ can be neglected. For heavier nuclei the difference between $E_n(k)$ and $F_n(k)$ is even more significant.

III. $F_n(k)$ for $m = 2, 4, \dots, 10$ and $m = 1, 3, \dots, 9$

In the first sum, for even r the value of the bracket vanishes: $[1 - (-1)^r] = 0$; therefore, only terms with odd r remain. For odd r i.e. for even arguments $(r+1)$ the value of the *Riemann ζ function* is [7, p.807]:

$$\zeta(r+1) = \frac{(2\pi)^{r+1}}{2(r+1)!} |B_{r+1}| \quad (8)$$

with the *Bernoulli numbers* B_{r+1} [7, pp.804, 810]:

$$\begin{aligned} B_2 &= \frac{1}{6}, & B_4 &= -\frac{1}{30}, & B_6 &= \frac{1}{42}, \\ B_8 &= -\frac{1}{30}, & B_{10} &= \frac{5}{66}, & B_{12} &= -\frac{691}{2730} \end{aligned} \quad (9)$$

$$\begin{aligned}
\zeta(2) &= \frac{(2\pi)^2}{2 \times 2!} \frac{1}{6} = \frac{\pi^2}{6}, & \zeta(4) &= \frac{(2\pi)^4}{2 \times 4!} \frac{1}{30} = \frac{\pi^4}{90}, \\
\zeta(6) &= \frac{(2\pi)^6}{2 \times 6!} \frac{1}{42} = \frac{\pi^6}{945}, & \zeta(8) &= \frac{(2\pi)^8}{2 \times 8!} \frac{1}{30} = \frac{\pi^8}{9450}, \\
\zeta(10) &= \frac{(2\pi)^{10}}{2 \times 10!} \frac{5}{66} = \frac{\pi^{10}}{93555}, & \zeta(12) &= \frac{(2\pi)^{12}}{2 \times 12!} \frac{691}{2730} \quad (10)
\end{aligned}$$

(The value of $\zeta(12)$ will be necessary for the closed expression of the 9th moment $\langle r^9 \rangle$.)

For even n

$$\begin{aligned}
F_n(k) &= \frac{k^{n+1}}{n+1} + \sum_{r=0}^n [1 - (-1)^r] \frac{n!}{(n-r)!} k^{n-r} \frac{2^r - 1}{2^r} \frac{(2\pi)^{r+1}}{2(r+1)!} |B_{r+1}| \\
&= \frac{k^{n+1}}{n+1} \left[1 + \sum_{r=1,3,\dots}^{n-1} 2(2^r - 1) |B_{r+1}| \frac{(n+1)!}{(n-r)!(r+1)!} \left(\frac{\pi}{k}\right)^{r+1} \right] \quad (11)
\end{aligned}$$

With $\beta \equiv \pi/k = \pi a/c$ and using numerical values of the *Bernoulli numbers* B_{r+1} , we have

$$\begin{aligned}
F_n(k) &\approx \frac{k^{n+1}}{n+1} \left[1 + \frac{(n+1)!}{(n-1)!3!} \beta^2 + \frac{7}{3} \frac{(n+1)!}{(n-3)!5!} \beta^4 + \frac{31}{3} \frac{(n+1)!}{(n-5)!7!} \beta^6 \right. \\
&\quad + \frac{381}{5} \frac{(n+1)!}{(n-7)!9!} \beta^8 + \frac{2555}{3} \frac{(n+1)!}{(n-9)!11!} \beta^{10} \\
&\quad \left. + \frac{1414477}{105} \frac{(n+1)!}{(n-11)!13!} \beta^{12} + \dots + (\dots) \beta^n \right] \quad (12)
\end{aligned}$$

the sum in the brackets terminates with β^n . For $n = 2, 4, 6, 8$ and 10 we

have:

$$\begin{aligned}
F_2(k) &= \frac{k^3}{3} (1 + \beta^2) \\
F_4(k) &= \frac{k^5}{5} \left(1 + \frac{10}{3}\beta^2 + \frac{7}{3}\beta^4 \right) \\
F_6(k) &= \frac{k^7}{7} \left(1 + 7\beta^2 + \frac{49}{3}\beta^4 + \frac{31}{3}\beta^6 \right) \\
F_8(k) &= \frac{k^9}{9} \left(1 + 12\beta^2 + \frac{294}{5}\beta^4 + 124\beta^6 + \frac{381}{5}\beta^8 \right) \\
F_{10}(k) &= \frac{k^{11}}{11} \left(1 + \frac{55}{3}\beta^2 + 154\beta^4 + 682\beta^6 + 1397\beta^8 + \frac{2555}{3}\beta^{10} \right) \quad (13)
\end{aligned}$$

For odd n the sum over r ends on n , the terms in the brackets contain even powers of β the last term is $\sim \beta^{n+1}$:

$$\begin{aligned}
F_1(k) &= \frac{k^2}{2} \left(1 + \frac{1}{3}\beta^2 \right) \\
F_3(k) &= \frac{k^4}{4} \left(1 + 2\beta^2 + \frac{7}{15}\beta^4 \right) \\
F_5(k) &= \frac{k^6}{6} \left(1 + 5\beta^2 + 7\beta^4 + \frac{31}{21}\beta^6 \right) \\
F_7(k) &= \frac{k^8}{8} \left(1 + \frac{28}{3}\beta^2 + \frac{98}{3}\beta^4 + \frac{124}{3}\beta^6 + \frac{127}{15}\beta^8 \right) \\
F_9(k) &= \frac{k^{10}}{10} \left(1 + 15\beta^2 + 98\beta^4 + 310\beta^6 + 381\beta^8 + \frac{2555}{33}\beta^{10} \right) \quad (14)
\end{aligned}$$

IV. $\langle r^m \rangle$ for $m = 2, 4, \dots, 10$ and $m = 1, 3, \dots, 9$

Using $F_2(k)$ the ratio $F_{m+2}(k)/F_2(k)$ can be formed.

For even m :

$$\begin{aligned} \frac{F_{m+2}(k)}{F_2(k)} = & \frac{3}{m+3} k^m \frac{1}{1+\beta^2} \left[1 + \frac{(m+3)!}{(m+1)!3!} \beta^2 + \frac{7}{3} \frac{(m+3)!}{(m-1)!5!} \beta^4 \right. \\ & + \frac{31}{3} \frac{(m+3)!}{(m-3)!7!} \beta^6 + \frac{381}{5} \frac{(m+3)!}{(m-5)!9!} \beta^8 \\ & + \frac{2555}{3} \frac{(m+3)!}{(m-7)!11!} \beta^{10} + \frac{1414477}{105} \frac{(m+3)!}{(m-9)!13!} \beta^{12} \\ & \left. + \dots + (\dots) \beta^{m+2} \right] \end{aligned} \quad (15)$$

For odd m the last term contains $\sim \beta^{m+3}$.

In the case of 4He , $\beta \approx 1$, while for ${}^{12}C$: $k = 2.36/0.52 = 4.54$ [6, p.489]
 $\beta \approx 0.69$ i.e. $\beta^2 \approx 0.48$. Therefore, the series expansion

$$\frac{1}{1+\beta^2} = 1 - \beta^2 + \beta^4 - \beta^6 + \beta^8 - \beta^{10} + \beta^{12} - + \dots \quad (16)$$

is valid –except for the lightest elements (as perhaps Li, Be and B)–. Using Eq. (16) we have the general formula for the m -th moment:

$$\begin{aligned} \langle r^m \rangle = a^m \frac{F_{m+2}(k)}{F_2(k)} = & \frac{3}{m+3} c^m \times \\ & \left\{ 1 + \left[\frac{(m+3)(m+2)}{3!} - 1 \right] \beta^2 + \left[\frac{7}{3} \frac{(m+3)(m+2)(m+1)m}{5!} - \right. \right. \\ & \left. \left. \frac{(m+3)(m+2)}{3!} + 1 \right] \beta^4 + \left[\frac{31}{3} \frac{(m+3)(m+2)\dots(m-1)(m-2)}{7!} \right. \right. \\ & \left. \left. - \frac{7}{3} \frac{(m+3)(m+2)(m+1)m}{5!} + \frac{(m+3)(m+2)}{3!} - 1 \right] \beta^6 \right. \\ & \left. + \left[\frac{381}{5} \frac{(m+3)\dots(m-3)(m-4)}{9!} - \frac{31}{3} \frac{(m+3)\dots(m-2)}{7!} \right. \right. \end{aligned}$$

$$\begin{aligned}
& + \left[\frac{7}{3} \frac{(m+3)\dots m}{5!} - \frac{(m+3)(m+2)}{3!} + 1 \right] \beta^8 \\
& + \left[\frac{2555}{3} \frac{(m+3)\dots(m-5)(m-6)}{11!} \right. \\
& - \left(\frac{381}{5} \frac{(m+3)\dots(m-3)(m-4)}{9!} - \dots - 1 \right) \left. \right] \beta^{10} \\
& + \left[\frac{1414477}{105} \frac{(m+3)\dots(m-7)(m-8)}{13!} \right. \\
& - \left(\frac{2555}{3} \frac{(m+3)\dots(m-5)(m-6)}{11!} + \dots + 1 \right) \left. \right] \beta^{12} + \dots \} \quad (17)
\end{aligned}$$

It can be seen that for $\langle r^m \rangle$ the coefficients of $\beta^{m+2}, \beta^{m+4}, \dots$ vanish exactly. Applying the above general formula to *even* m values and substituting $\beta = \pi a/c$ we have:

$$\begin{aligned}
\langle r^2 \rangle &= \frac{3}{5} c^2 \left(1 + \frac{7}{3} \beta^2 \right) = \frac{3}{5} c^2 + \frac{7}{5} (\pi a)^2 \\
\langle r^4 \rangle &= \frac{3}{7} c^4 \left(1 + 6\beta^2 + \frac{31}{3} \beta^4 \right) \\
\langle r^6 \rangle &= \frac{1}{3} c^6 \left(1 + 11\beta^2 + \frac{239}{5} \beta^4 + \frac{381}{5} \beta^6 \right) \quad (18)
\end{aligned}$$

$$\begin{aligned}
\langle r^8 \rangle &= \frac{3}{11} c^8 \left(1 + \frac{52}{3} \beta^2 + \frac{410}{3} \beta^4 + \frac{1636}{3} \beta^6 + \frac{2555}{3} \beta^8 \right) \\
\langle r^{10} \rangle &= \frac{3}{13} c^{10} \left(1 + 25\beta^2 + \frac{926}{3} \beta^4 + \frac{46714}{21} \beta^6 + \frac{910573}{210} \beta^8 \right. \\
&\quad \left. + \frac{19447}{210} \beta^{10} \right) \quad (19)
\end{aligned}$$

For *odd* m , from β^{m+2} the signs alternate, with the same non-zero absolute

values. This alternating series can be written in the closed form $1/(1+\beta^2)$

$$\begin{aligned}
\langle r \rangle &= \frac{3}{4}c \left[1 + \beta^2 - \frac{8}{15}\beta^4(1 - \beta^2 + \beta^4 - \beta^6 + \beta^8 - \dots) \right] \\
&= \frac{3}{4}c \left[1 + \beta^2 - \frac{8}{15} \frac{\beta^4}{1 + \beta^2} \right] \\
\langle r^3 \rangle &= \frac{1}{2}c^3 \left[1 + 4\beta^2 + 3\beta^4 - \frac{32}{21} \frac{\beta^6}{1 + \beta^2} \right] \\
\langle r^5 \rangle &= \frac{3}{8}c^5 \left[1 + \frac{25}{3}\beta^2 + \frac{73}{3}\beta^4 + 17\beta^6 - \frac{128}{15} \frac{\beta^8}{1 + \beta^2} \right] \\
\langle r^7 \rangle &= \frac{3}{10}c^7 \left[1 + 14\beta^2 + 84\beta^4 + 226\beta^6 + 155\beta^8 - \frac{2560}{33} \frac{\beta^{10}}{1 + \beta^2} \right] \\
\langle r^9 \rangle &= \frac{1}{4}c^9 \left[1 + 21\beta^2 + 210\beta^4 + 1154\beta^6 + 3037\beta^8 + 2073\beta^{10} \right. \\
&\quad \left. - \frac{1415168}{1365} \frac{\beta^{12}}{1 + \beta^2} \right]
\end{aligned} \tag{20}$$

V. $\delta\langle r^m \rangle$ for $m = 2, 4, \dots, 10$

Assuming a constant *surface diffusity* $a = const.$, and a mass number dependence $c = r_0 A^{1/3}$ for the *half-density radius* c , we have

$$\delta c = \frac{1}{3}c \frac{\delta A}{A}. \tag{21}$$

The change in the second moment corresponding to a change $\delta A \equiv A_2 - A_1$ in the mass number is

$$\delta\langle r^2 \rangle = \frac{3}{5}2c \frac{1}{3} \frac{r_0}{A^{2/3}} \delta A = \frac{2}{5}c^2 \frac{\delta A}{A} \tag{22}$$

and the shifts in the higher even moments:

$$\begin{aligned}
\delta\langle r^4 \rangle &= \frac{4}{7}c^4 [1 + 3\beta^2] \frac{\delta A}{A} \\
\delta\langle r^6 \rangle &= \frac{2}{3}c^6 \left[1 + \frac{22}{3}\beta^2 + \frac{239}{15}\beta^4 \right] \frac{\delta A}{A} \\
\delta\langle r^8 \rangle &= \frac{8}{11}c^8 \left[1 + 13\beta^2 + \frac{205}{3}\beta^4 + \frac{409}{3}\beta^6 \right] \frac{\delta A}{A} \\
\delta\langle r^{10} \rangle &= \frac{10}{13}c^{10} \left[1 + 20\beta^2 + \frac{1852}{10}\beta^4 + \frac{186856}{210}\beta^6 \right. \\
&\quad \left. + \frac{1821146}{2100}\beta^8 \right] \frac{\delta A}{A}
\end{aligned} \tag{23}$$

VI. $\delta\langle r^m \rangle$ in terms of for $\langle r^m \rangle$ for $m = 4, 6, \dots, 10$

For some applications e.g. for the evaluation of isotope shifts in optical and characteristic X -ray spectra the isotopic differences in higher moments $\delta\langle r^4 \rangle, \delta\langle r^6 \rangle, \dots$, should be expressed in terms of $\delta\langle r^2 \rangle$ [5]. This can be done easily because the formula of the previous section allows to express c^2 by $\delta\langle r^2 \rangle$:

$$c^2 = \frac{5}{2} \frac{A}{\delta A} \delta\langle r^2 \rangle = \frac{5}{4} \frac{A_1 + A_2}{A_2 - A_1} \delta\langle r^2 \rangle \tag{24}$$

where A is now replaced by $(A_1 + A_2)/2$ and δA by $A_2 - A_1$. Using Eq. (24), the isotope shifts of higher order are:

$$\begin{aligned}
\delta\langle r^4 \rangle &= \frac{25}{14} \frac{A_1 + A_2}{A_2 - A_1} (\delta\langle r^2 \rangle)^2 + \frac{30}{7}(\pi a)^2 \delta\langle r^2 \rangle \\
\delta\langle r^6 \rangle &= \frac{125}{48} \left(\frac{A_1 + A_2}{A_2 - A_1} \right)^2 (\delta\langle r^2 \rangle)^3 + \frac{275}{18}(\pi a)^2 \frac{A_1 + A_2}{A_2 - A_1} (\delta\langle r^2 \rangle)^2 \\
&\quad + \frac{239}{9}(\pi a)^4 \delta\langle r^2 \rangle \\
\delta\langle r^8 \rangle &= \frac{625}{176} \left(\frac{A_1 + A_2}{A_2 - A_1} \right)^3 (\delta\langle r^2 \rangle)^4 + \frac{1625}{44}(\pi a)^2 \left(\frac{A_1 + A_2}{A_2 - A_1} \right)^2 (\delta\langle r^2 \rangle)^3 \\
&\quad + \frac{5125}{33}(\pi a)^4 \frac{A_1 + A_2}{A_2 - A_1} (\delta\langle r^2 \rangle)^2 + \frac{8180}{33}(\pi a)^6 \delta\langle r^2 \rangle
\end{aligned}$$

$$\begin{aligned}
\delta\langle r^{10} \rangle &= \frac{15625}{3328} \left(\frac{A_1 + A_2}{A_2 - A_1} \right)^4 (\delta\langle r^2 \rangle)^5 \\
&\quad + \frac{15625}{208} (\pi a)^2 \left(\frac{A_1 + A_2}{A_2 - A_1} \right)^3 (\delta\langle r^2 \rangle)^4 \\
&\quad + \frac{57875}{104} (\pi a)^4 \left(\frac{A_1 + A_2}{A_2 - A_1} \right)^2 (\delta\langle r^2 \rangle)^3 \\
&\quad + \frac{583925}{273} (\pi a)^6 \frac{A_1 + A_2}{A_2 - A_1} (\delta\langle r^2 \rangle)^2 + \frac{910573}{546} (\pi a)^8 \delta\langle r^2 \rangle
\end{aligned} \tag{25}$$

VII. $\delta\langle r^m \rangle$ for $m = 1, 3, \dots, 9$

Here the derivative and the series sum

$$\begin{aligned}
\delta \left(\frac{\beta^3}{1 + \beta^2} \right) &= -\beta^3 \frac{1 + \frac{1}{3}\beta^2}{(1 + \beta^2)^2} \frac{\delta A}{A}, \\
1 - \frac{5}{3}\beta^2 + \frac{7}{3}\beta^4 - 3\beta^6 + \frac{11}{3}\beta^8 - \dots &= \frac{1 + \frac{1}{3}\beta^2}{(1 + \beta^2)^2}
\end{aligned} \tag{26}$$

are used in the expressions for $\delta\langle r^m \rangle$:

$$\begin{aligned}
\delta\langle r \rangle &= \frac{1}{4}c \left[1 - \beta^2 + \frac{8}{5}\beta^4 \frac{1 + \frac{1}{3}\beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A} \\
\delta\langle r^3 \rangle &= \frac{1}{2}c^3 \left[1 + \frac{4}{3}\beta^2 - \beta^4 + \frac{32}{21}\beta^6 \frac{1 + \frac{1}{3}\beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A} \\
\delta\langle r^5 \rangle &= \frac{5}{8}c^5 \left[1 + 5\beta^2 + \frac{73}{15}\beta^4 - \frac{17}{5}\beta^6 + \frac{128}{25}\beta^8 \frac{1 + \frac{1}{3}\beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A} \\
\delta\langle r^7 \rangle &= \frac{7}{10}c^7 \left[1 + 10\beta^2 + \frac{18}{5}\beta^4 + \frac{226}{7}\beta^6 - \frac{155}{7}\beta^8 \right. \\
&\quad \left. + \frac{2560}{77}\beta^{10} \frac{1 + \frac{1}{3}\beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A} \\
\delta\langle r^9 \rangle &= \frac{3}{4}c^9 \left[1 + \frac{49}{3}\beta^2 + \frac{350}{3}\beta^4 + \frac{1154}{3}\beta^6 + \frac{3037}{9}\beta^8 - \frac{691}{3}\beta^{10} \right. \\
&\quad \left. + \frac{1415168}{4095}\beta^{12} \frac{1 + \frac{1}{3}\beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A}
\end{aligned} \tag{27}$$

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