

## Barrett Moments and *rms* Charge Radii

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**Abstract.** An empirical relation is established between Barrett equivalent radii  $R_{k,\alpha}$  and *rms* charge radii  $\langle r^2 \rangle^{1/2}$  based on the results of model-independent and *Fermi model* analyses of  $2p \rightarrow 1s$  transitions in muonic atoms. This relation follows simple  $Z$  dependence, and can be usefully applied to derive *rms* radii  $\langle r^2 \rangle^{1/2}$  or differences  $\delta^{AA'} \langle r^2 \rangle^{1/2}$  in cases where only  $R_{k,\alpha}$  data or isotope shifts  $\delta^{AA'} R_{k,\alpha}$  are published. The atomic number dependence of the Barrett parameters  $k(Z)$  and  $\alpha(Z)$  is also given by empirical formulae. It is shown that the Barrett moment can be expanded in a sum of integer moments  $\langle r^m \rangle$  ( $m \geq 2$ ) using an effective exponential parameter  $\alpha_{\text{eff}}(Z)$ . The moments  $\langle r^m \rangle$  and isotopic differences  $\delta \langle r^m \rangle$  of the two-parameter Fermi distribution expressed in terms of the parameters  $c$  and  $a$  are given in the Appendix for  $m = 1 - 10$ .

*Keywords:* nuclear *rms* charge radii, Barrett moments

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### 1. Introduction

Energy levels of muonic atoms are strongly influenced by the nuclear charge distribution  $\rho(r)$ . Consequently, the energies of gamma rays arising from transitions between energy levels contain valuable information on the electric charge distribution. However, this information is “coded” in a form that cannot be unambiguously translated into the usual characteristics of the charge distribution, e.g. half-density radius, surface thickness, etc. Barrett [1] has shown that the energy of a transition in a muonic atom is determined — to a very good approximation — by the quantity

$$B_{k,\alpha} \equiv \langle r^k e^{-\alpha r} \rangle = \int \rho(r) r^k e^{-\alpha r} \cdot dv \quad (1)$$

independently of the form of  $\rho(r)$ . This quantity is called now *Barrett moment*, and is determined with high accuracy ( $\leq 0.1\%$ ). The parameters  $k$  and  $\alpha$  depend on the atomic number  $Z$  and on the specific transition  $nl_j \rightarrow n'l'_j$ .

To comply with our need for illustrative models, the *Barrett equivalent radius*  $R_{k,\alpha}$  is also introduced [2]. This is the radius of the uniform charge distribution  $\rho(r)_{\text{unif}}$  having the same total charge  $Ze$  and the same Barrett moment as the actual nuclear charge distribution  $\rho(r)$ . Formally, it is defined by the implicit equation:

$$\frac{3}{R_{k,\alpha}^3} \int_0^{R_{k,\alpha}} r^k e^{-\alpha r} r^2 \cdot dr = B_{k,\alpha}. \quad (2)$$

Quite often, only  $R_{k,\alpha}$  or the isotopic differences  $\delta^{AA'} R_{k,\alpha}$  are given as the result of a muonic X-ray measurement. Although this quantity is more illustrative than the Barrett moment, the comparison of radii  $R_{k,\alpha}$  of nuclei with different atomic number is still difficult owing to the  $Z$  dependence of the parameters  $k$  and  $\alpha$ .

Other types of experiments, e.g. electron scattering,  $K_\alpha$  X-ray isotope shift (KIS) and optical isotope shift (OIS) measurements yield the second moment  $\langle r^2 \rangle$  or the isotopic difference  $\delta \langle r^2 \rangle$  of the charge distribution. Therefore, it is of importance to express the results of muonic atom experiments also in terms of  $\langle r^2 \rangle$ . Sometimes, it is determined simultaneously with  $R_{k,\alpha}$  using some model charge distribution e.g. the *two-parameter Fermi distribution* (2pF) or some model-independent procedure.

For the most important muonic transition  $2p \rightarrow 1s$  the value of  $k$  is slightly higher than 2 ( $k \approx 2.0 - 2.3$ ), while  $\alpha$  takes on small positive values  $\alpha \approx 0.02 - 0.16$ . Consequently, the integrand of the Barrett moment is fairly close to that of the second moment  $\langle r^2 \rangle$ , see Fig. 6 in Ref. [3], p. 187. Therefore, it is expected that — for  $2p \rightarrow 1s$  transitions — the ratio

$$v = \frac{\langle r^2 \rangle^{1/2}}{\sqrt{3/5} R_{k,\alpha}} \quad (3)$$

is close to unity:  $v \approx 1$ . (The symbol  $v$  is chosen to remind of the similar quantity  $V^e$  used in the evaluation of electron scattering measurements [4,5].) It will be seen that  $v(Z)$  shows a fairly regular dependence on the atomic number. This can be exploited to determine  $\langle r^2 \rangle$  or  $\delta \langle r^2 \rangle$  in cases when only  $R_{k,\alpha}$  or  $\delta R_{k,\alpha}$  data are known.

In Section 2 the derivation of  $v(Z)$  from  $R_{k,\alpha}$  and  $\langle r^2 \rangle$  data is presented together with the resulting curve and formulae. In addition, formulae for the  $Z$  dependence of the parameters  $\alpha(Z)$  and  $k(Z)$  will also be given for  $2p \rightarrow 1s$  transitions. In Section 3 a momentum expansion method is developed, which renders possible the approximation of the Barrett moment by a sum of integral moments  $\langle r^m \rangle$ . This can be applied to express the second moment  $\langle r^2 \rangle$  in terms of  $B_{k,\alpha}$  using an iteration procedure. In the expansion method and also in other

applications (e.g. evaluation of KIS and OIS results) integer moments and their isotopic differences are used. Therefore, in the Appendix a summary of expressions for  $\langle r^m \rangle$  and  $\delta \langle r^m \rangle$  ( $m = 1 - 10$ ) in terms of the parameters  $c$  and  $a$  of the 2pF charge distribution is presented.

## 2. Interpolation Formulae for $v(Z)$ , $\alpha(Z)$ and $k(Z)$

In the literature, root-mean-square (*rms*) charge radii  $\langle r^2 \rangle^{1/2}$  are derived from the high accuracy  $R_{k,\alpha}$  values in two ways: model-independently or using a model function for  $\rho(r)$ . In the model-independent procedure results from electron scattering experiments are also applied: elastic scattering cross sections are used to construct the charge distribution in a model-independent way, e.g. by determining the coefficients of a Fourier-Bessel series [6]. Having the form of the charge density distribution from electron scattering and the Barrett moments from muonic X rays,  $\langle r^2 \rangle^{1/2}$  values are calculated, e.g. [7]. In the recent compilation of *rms* charge radii [3] Table IX contains both  $R_{k,\alpha}$  and  $\langle r^2 \rangle$  data for 20 isotopes of 9 elements evaluated by model-independent method. The  $Z$  dependence of the ratio (3) formed by these data shows simple, monotonic trend.

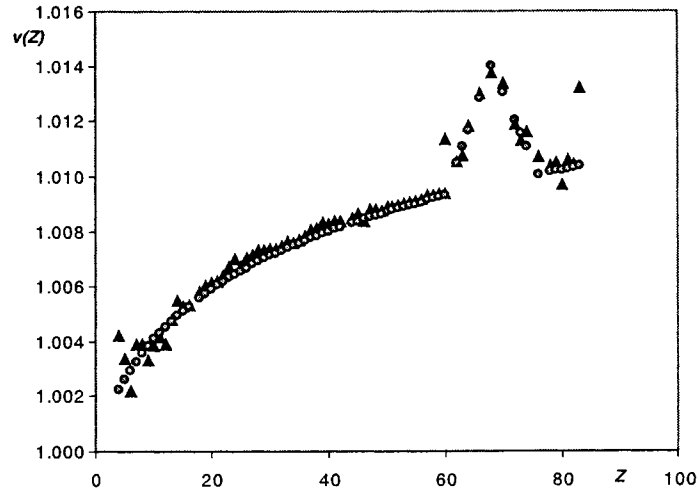


Fig. 1.  $Z$  dependence of the ratio  $v$ , Eq. (3). Triangles:  $v$  values derived from  $R_{k,\alpha}$  and  $\langle r^2 \rangle^{1/2}$  data; circles: calculated by the empirical formula (5).

There are much more  $R_{k,\alpha}$  and  $\langle r^2 \rangle$  data based on evaluations using 2pF and 3pF (deformed) charge distributions: Tables III.A and III.C of [3] contain altogether 231 isotopes of 73 elements. Triangles in Fig. 1 show the  $v$  values calculated from both the model-independent and from the Fermi model procedures. For elements

where both model-independent and Fermi model results are available, the simple average is plotted. For atomic numbers  $Z < 60$  and  $Z > 77$  the two data sets follow the *same* smooth, slowly increasing trend, and they both can be described by the empirical formula:

$$v(Z) = 1 + 0.0035 \times \ln(0.22 \times Z + 1). \quad (4)$$

This is the result of a simple least-squares fit assuming equal weights and imposing the constraint  $v(0) = 1$ .

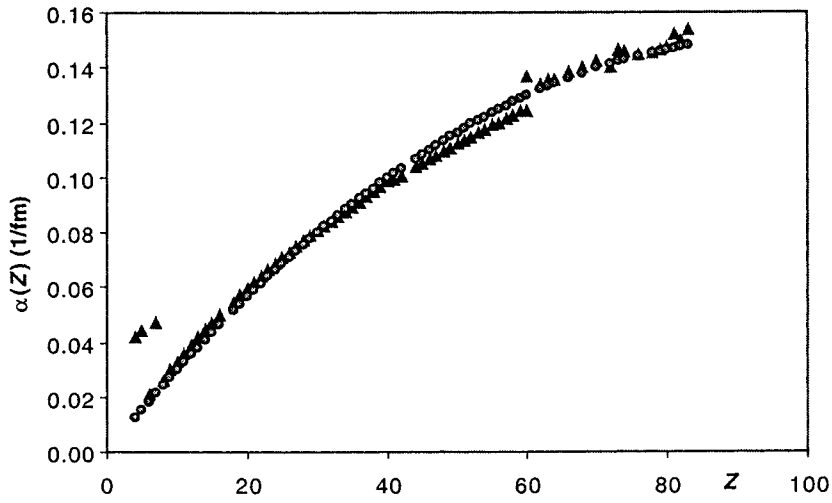


Fig. 2.  $Z$  dependence of the parameter  $\alpha$ , Eq. (1). Triangles: experimental  $\alpha$  values; circles: calculated by the empirical formula (8).

There are, however, significant deviations from the smooth behaviour for three light elements ( $Z = 4, 5$  and  $7$ ) and also in the region of deformed nuclei. In the former case, the deviations are probably caused by the limited accuracy of the experiment for very light elements. This is supported by the observation that the strongly correlated  $\alpha$  and  $k$  values have both strikingly high values for these same nuclei, see Figs 2 and 3.

In the *deformed* region ( $60 \leq Z \leq 77$ ) the experimental  $v$  values follow a triangular peak superimposed on the smooth, monotone trend. This can be well described by:

$$v(Z)_{\text{def}} = v(Z) + 0.00054 \times \min(Z - 60; 77 - Z). \quad (5)$$

The deformation term reminds to that found for the description of the mass number dependence of *rms* charge radii in terms of the *P-factor* (*nucleonic promiscuity*) [8]. Filled circles in Fig. 1 show  $v$  values calculated by Eq. (5).

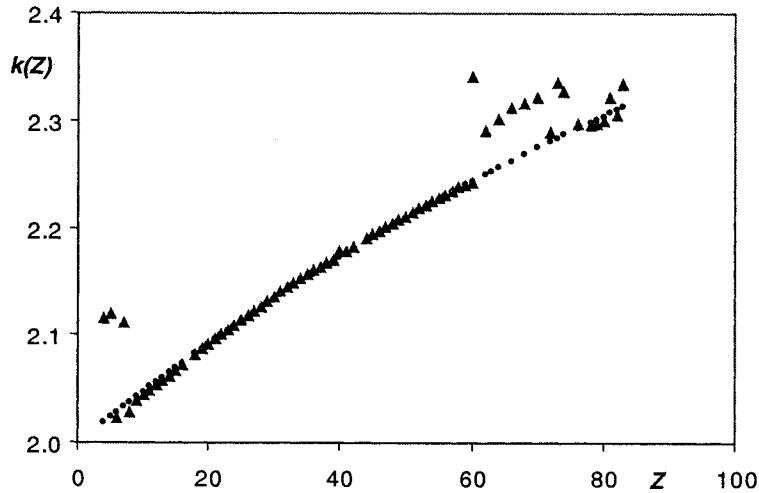


Fig. 3.  $Z$  dependence of the parameter  $k$ , Eq. (1). Triangles: experimental  $k$  values; circles: calculated by the empirical formula (9).

### 2.1. Application and uncertainties

The main motivation for the present work was the need for accurate isotopic differences  $\delta \langle r^2 \rangle^{1/2}$  [9]. In Table V of [3] the  $\delta R_{k,\alpha}$  values are listed. Now, having the empirical formulae (4,5) at hand,  $\delta \langle r^2 \rangle^{1/2}$  values can be derived from  $\delta R_{k,\alpha}$  simply by

$$\delta \langle r^2 \rangle^{1/2} = v(Z) \sqrt{3/5} \delta R_{k,\alpha}. \quad (6)$$

Otherwise, one would have no other choice but to put  $\delta \langle r^2 \rangle^{1/2} = \sqrt{3/5} \delta R_{k,\alpha}$  and to add a systematic error of about 1.0% to all isotopic differences.

Regarding the uncertainty of  $v(Z)$ , the following observations should be taken into account. The individual  $v_i$  values from the Fermi models (Tables III.A and III.C of [3]) follow the smooth trend within  $\pm 0.0002$ , while those from the model-independent evaluation (Table IX) have a spread of  $\pm 0.0003-8$  around the common  $v(Z)$  dependence. As the calculation error is about  $\pm 0.0001$  [7], these latter deviations must be of physical origin; they probably reflect the effect of the individual  $\rho(r)_i$  charge distributions, which differ from each other as well as from the ‘‘average’’ Fermi distribution.

### 2.2. $Z$ dependence of the parameters $\alpha$ and $k$

The large body of data in [3] allows to derive empirical formulae for the atomic number dependence of the parameters  $\alpha$  and  $k$  plotted in Figs 2 and 3. Most of

the individual  $\alpha$  and  $k$  values follow the smooth behaviour. There are significant — and probably correlated — deviations from the general trend for  $Z = 4, 5$  and  $7$ , and — for  $k$  — also in the region of deformed nuclei. These elements are not included in the fit. In fitting empirical formulae to the data, the constraints

$$\alpha(0) = 0, \quad k(0) = 2, \quad v(0) = 1 \quad (7)$$

may be imposed. Imposing these constraints we have

$$\alpha(Z) = 0.00316 \times Z - 0.0000166 \times Z^2 \quad (8)$$

and

$$k(Z) = 0.00484 \times Z - 0.0000128 \times Z^2. \quad (9)$$

### 3. Expansion of the Barrett Moment in Integer Moments

In some papers [10, 11], the value of  $B_{k,\alpha}$  is given as the result of the experiment. The Barrett moment

$$B_{k,\alpha} \equiv \langle r^2 r^\kappa e^{-\alpha \cdot r} \rangle = 4\pi \int \rho(r) y(r) r^4 dr, \quad \kappa \equiv k - 2 \quad (10)$$

can be simplified in two ways: the function

$$y(r) = r^\kappa e^{-\alpha \cdot r} \quad (11)$$

is replaced either by

$$\hat{y}(r) = r^{\kappa_{\text{eff}}} \quad (12)$$

or by

$$\tilde{y}(r) = e^{-\alpha_{\text{eff}} \cdot r}. \quad (13)$$

The first choice results in the moment  $\langle r^{\kappa_{\text{eff}}} \rangle$  introduced by Ford and Wills [12], and will not be discussed here. The second choice — not exploited until now — has the advantage that the function (13) can be expanded into the power series

$$\tilde{y}(r) = 1 - \frac{1}{1!} (\alpha_{\text{eff}} \cdot r) + \frac{1}{2!} (\alpha_{\text{eff}} \cdot r)^2 - + \dots, \quad (14)$$

i.e. the Barrett moment can be written in a series of *integer* moments:

$$\tilde{B}_{\alpha_{\text{eff}}} = \langle r^2 e^{-\alpha_{\text{eff}} \cdot r} \rangle = \langle r^2 \rangle - \frac{1}{1!} \alpha_{\text{eff}} \langle r^3 \rangle + \frac{1}{2!} \alpha_{\text{eff}}^2 \langle r^4 \rangle - + \dots \quad (15)$$

Based on this expression, and provided  $\alpha_{\text{eff}}$  is chosen in a way that  $\tilde{B}_{\alpha_{\text{eff}}} = B_{k,\alpha}$ , an iteration procedure can be developed for the determination of the mean-squared radius from the experimental  $B_{k,\alpha}$  value:

$$\langle r^2 \rangle_{i+1} = B_{k,\alpha} + \frac{1}{1!} \alpha_{\text{eff}} \langle r^3 \rangle_i - \frac{1}{2!} \alpha_{\text{eff}}^2 \langle r^4 \rangle_i + \dots \quad (16)$$

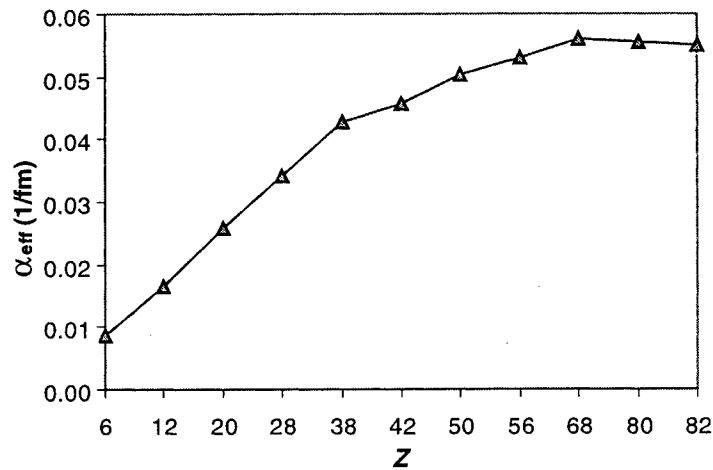
In order to carry out this program, two tasks are to be solved. First, the value of the parameter  $\alpha_{\text{eff}}$  should be determined for all atomic numbers  $Z$ . Second, the integer moments  $\langle r^m \rangle_i$  ( $m \geq 3$ ) should be expressed by  $\langle r^2 \rangle_i$ .

### 3.1. Determination of the parameter $\alpha_{\text{eff}}$

The exponential function  $\tilde{y}(r)$  is *empirically equivalent* to  $y(r)$  if

$$\tilde{B}_{\alpha_{\text{eff}}} \equiv \langle e^{-\alpha_{\text{eff}} r} \rangle = B_{k,\alpha} \quad (17)$$

for the same  $\rho(r)$ . The exact form of the charge distribution is not crucial, because the energies of muonic X rays depend — to a good approximation — on the integral quantity  $B_{k,\alpha}$  but not on the form of  $\rho(r)$ . Therefore, the simple two-parameter Fermi charge distribution (2pF) was assumed with half-value radius  $c = 1.1 \times A^{1/3}$  fm and with constant surface diffusivity  $a = 0.523$  fm. The value of  $B_{k,\alpha}$  was calculated using Eqs (8) and (9) for  $\alpha(Z)$  and  $k(Z)$ , respectively. The resulting “direct”  $\alpha_{\text{eff}}$  values (Fig. 4) can be well approximated by



**Fig. 4.**  $Z$  dependence of the effective exponential parameter  $\alpha_{\text{eff}}$ . Triangles:  $\alpha_{\text{eff}}$  values derived from equating the moments  $B_{k,\alpha}$  and  $\tilde{B}_{\alpha_{\text{eff}}}$ , Eq. (17); full curve: empirical formula (18).

$$\alpha_{\text{eff}}(Z) = 0.001521 \times Z - 0.00001031 \times Z^2, \quad (18)$$

where the constraint  $\alpha_{\text{eff}}(0) = 0$  has been taken into account. These  $\alpha_{\text{eff}}$  values can be used in the iteration Eq. (16).

In addition to determining the values of  $\alpha_{\text{eff}}$  directly, it may be of interest how it can be composed from the strongly correlated primary parameters  $\alpha$  and  $\kappa$ . Therefore, the equality of the integrals  $\tilde{B}_{\alpha_{\text{eff}}}$  and  $B_{k,\alpha}$  was also searched using the expression

$$\alpha_{\text{eff}}(Z) = \alpha(Z) - f \times \kappa(Z) \quad (19)$$

with  $f$  as a free parameter; i.e. this is an indirect way of determining  $\alpha_{\text{eff}}$ . Performing the fit for a wide range of elements ( $Z = 6, 12, 20, 28, 38, 42, 50, 56, 68, 80$  and  $82$ ) the value of  $f$  varied only within the narrow interval from 0.30 to 0.35. More exactly, the fairly smooth behaviour can be well described by the empirical formula

$$f = 0.3499 - 0.000826 \times Z + 0.00000225 \times Z^2. \quad (20)$$

In calculating the effective exponential moment  $\tilde{B}_{\alpha_{\text{eff}}}$ , the direct  $\alpha_{\text{eff}}(Z)$  values from Eq. (18) are used. Application of the indirect  $\alpha_{\text{eff}}(Z)$  values from Eqs (19) and (20) would contain hardly traceable, correlated systematic deviations  $\delta\alpha$  and  $\delta k$  from Eqs (8) and (9). It is worth noting that the downward bending of  $\alpha_{\text{eff}}(Z)$  at the highest  $Z$  values occurs both in the case of the direct and in the indirect approach.

### 3.2. Expression of higher moments $\langle r^m \rangle$ ( $m \geq 3$ ) in terms of $\langle r^2 \rangle$

Integer moments  $\langle r^m \rangle$  ( $1 \leq m \leq 10$ ) of 2pF charge distributions as the function of the parameters  $c$  and  $a$  are listed in the Appendix. Starting the iteration procedure of Eq. (16) with

$$\langle r^2 \rangle_1 = B_{k,\alpha} \quad (21)$$

and applying Eq. (37) from the Appendix, we have

$$c_1 = \sqrt{\frac{5}{3} \langle r^2 \rangle_1 - \frac{7}{3} (\pi a)^2}. \quad (22)$$

This is inserted to Eqs (43, 38, ...) to get  $\langle r^m \rangle_1$  for  $m = 3, 4, \dots$  and with these the second step of iteration yields

$$\langle r^2 \rangle_2 = B_{k,\alpha} + \frac{1}{1!} \alpha_{\text{eff}} \langle r^3 \rangle_1 - \frac{1}{2!} \alpha_{\text{eff}}^2 \langle r^4 \rangle_1 - + \dots \quad (23)$$

Now,  $c_2$  can be calculated by Eq. (37), and so forth.



### 3.3. Uncertainties in the momentum expansion method

The relative difference of the effective exponential moment  $\tilde{B}_{\alpha_{\text{eff}}}$  and the Barrett moment  $B_{k,\alpha}$  is a few times  $10^{-4}$  for light nuclei and less than  $6 \times 10^{-5}$  for medium weight and heavy nuclei. (It should be reminded here that the experimental accuracy of muonic X-ray energies is also less for light nuclei.) The error from the approximation of the exponential function (13) by a finite sum of powers  $(\alpha_{\text{eff}} \cdot r)^m$  in Eqs (14) and (15) can be made as small as required simply by including more terms to the sum. That is why — to be on the safe side — the Appendix contains moments up to  $m = 10$ .

## 4. Summary

The wealth of data in recent compilations allowed to develop some tools for the further improvement in the evaluation of muonic X-ray results. In Section 2 a quantitative relationship was found between the Barrett equivalent radius  $R_{k,\alpha}$  and the *rms* radius  $\langle r^2 \rangle^{1/2}$ , see Eqs (3), (4) and (5). This relationship facilitates the calculation of  $\delta \langle r^2 \rangle^{1/2}$  values from the published  $\delta R_{k,\alpha}$  data, Eq. (6). At the same time, a possible source of systematic error is avoided. In the same section simple interpolation formulae are given for the atomic number dependence of the Barrett parameters  $\alpha(Z)$  and  $k(Z)$ , see Eqs (8) and (9).

In Section 3 an iteration procedure is developed, defined by Eq. (16), which connects the value of  $\langle r^2 \rangle$  with the measured quantity, the Barrett moment  $B_{k,\alpha}$ . In this procedure several integer moments ( $m \geq 2$ ) of the two-parameter Fermi distribution (2pF) are used. Therefore, a list of explicit expressions of 2pF moments  $\langle r^m \rangle$  and isotopic differences of moments  $\delta \langle r^m \rangle$  is presented in the Appendix for  $m = 1 - 10$  making use of the parameters  $c$ ,  $a$  (and also  $\beta \equiv \pi a/c$ ) of the Fermi distribution function.

## Appendix: Moments of the Two-Parameter Fermi Distribution

### *The Fermi integral*

Moments of model charge distributions are often used in atomic and nuclear physics both in theoretical work and in the evaluation of experimental results. For example, the energy of transitions in muonic atoms determine the *Barrett moment*  $\langle r^k \cdot e^{-\alpha r} \rangle$  [1]. In Section 3 Eq. (14) it is shown that this Barrett moment can be approximated by a sum of integer moments  $\langle r^m \rangle$  ( $m = 2, 3, \dots$ ). An other example: isotope shifts  $\delta\nu$  in optical and characteristic X-ray frequencies can be expressed as linear combinations of differences in even moments  $\delta \langle r^m \rangle$  ( $m = 2, 4, \dots$ ) [13]. A broad, systematic review of model functions for nuclear charge distributions can be found in [14]. The simplest models are the one-parameter equivalent uniform, and the two-parameter trapezoidal distributions. A more realistic and fre-

quently used charge distribution is the spherically symmetric *two-parameter Fermi distribution* (2pF):

$$\rho_F(r; c, a) = \frac{\rho_0}{1 + e^{(r-c)/a}} \equiv \frac{\rho_0}{1 + e^{x-k}} \quad (r \geq 0), \quad (24)$$

where  $c$  is the half-density radius and  $a$  the surface diffusivity. The introduction of the dimensionless parameters  $x \equiv r/a$ ,  $k \equiv c/a$  and  $\beta \equiv \pi/k = \pi a/c$  proved also to be useful during this work.

The  $m$ th moment of the 2pF charge distribution is

$$\langle r^m \rangle \equiv \frac{\int r^m \rho_F(r; c, a) \cdot dv}{\int \rho_F(r; c, a) \cdot dv} = \frac{\int r^{m+2} \rho_F(r; c, a) \cdot dr}{\int r^2 \rho_F(r; c, a) \cdot dr} = a^m \frac{F_{m+2}(k)}{F_2(k)}, \quad (25)$$

where the *Fermi integral*

$$F_n(k) = \int \frac{x^n}{1 + e^{x-k}} dx \quad (26)$$

is introduced. The limits of integration in  $r$  and  $x$  are taken from zero to infinity. The Fermi integral can be expressed by the sums [15] Appendix C (note the misprint in the exponent of the last term):

$$\begin{aligned} F_n(k) &= \frac{k^{n+1}}{n+1} + \sum_{r=0}^n [1 - (-1)^r] \frac{n!}{(n-r)!} k^{n-r} \left(1 - \frac{1}{2^r}\right) \zeta(r+1) \\ &\quad - \sum_{v=1}^{\infty} (-1)^{v+n} \frac{n!}{v^{n+1}} e^{-vk}, \end{aligned} \quad (27)$$

where  $\zeta$  is the *Riemann function* (see later).

In this Appendix formulae for the moments  $\langle r^m \rangle$  and for isotopic differences  $\delta \langle r^m \rangle$  are presented from  $m = 1$  to 10 using the parameters  $c$ ,  $a$  and  $\beta$ . First, the Fermi integrals  $F_n(k)$  are derived from the general formula given by Elton; it is shown that the sum of the exponential terms can be neglected. Then, even and odd orders are treated separately for  $\langle r^m \rangle$  as well as for  $\delta \langle r^m \rangle$ ; in calculating  $\delta \langle r^m \rangle$  the diffusivity  $a$  was assumed to be constant. Finally, the formulae for 2pF moments are compared to those based on simpler distributions: uniform and trapezoidal.

It is worth while to estimate the value of the last sum of exponential terms

$$E_n(k) = - \sum_{v=1}^{\infty} (-1)^{v+n} \frac{n!}{v^{n+1}} e^{-vk} = (-1)^n n! e^{-k} \left(1 - \frac{e^{-k}}{2^{n+1}} + \dots\right). \quad (28)$$

Even for the very light nucleus  ${}^4\text{He}$  [16]  $k = 1.0/0.32 = 3.12$ , i.e.  $e^{-k} \approx 0.045$ , it can be seen that  $|E_n(k)|$  is less than  $F_n(k)$  by two or three orders of magnitude

depending on  $n$ . In the case of medium and heavy nuclei the difference between  $|E_n(k)|$  and  $F_n(k)$  is even higher. Consequently, the sum  $E_n(k)$  can be neglected.

Returning to the first sum, one can see that 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  $\zeta$  function is [17]

$$\zeta(r + 1) = \frac{(2\pi)^{r+1}}{2(r + 1)!} |B_{r+1}| \quad (29)$$

with the Bernoulli numbers  $B_{r+1}$  [17]:

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

$$\begin{aligned} \zeta(2) &= \pi^2/6, & \zeta(4) &= \pi^4/90, & \zeta(6) &= \pi^6/945, \\ \zeta(8) &= \pi^8/9450, & \zeta(10) &= \pi^{10}/93555, & \zeta(12) &= 691\pi^{12}/638512875. \end{aligned} \quad (31)$$

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

For even  $n$

$$F_n(k) = \frac{k^{n+1}}{n+1} \left[ 1 + \sum_{r=1,3,\dots}^{n-1} 2(2^r - 1) |B_{r+1}| \frac{(n+1)!}{(n-r)!(r+1)!} \left(\frac{\pi}{k}\right)^{r+1} \right]. \quad (32)$$

Substituting numerical values for the Bernoulli numbers  $B_{r+1}$ , we have

$$\begin{aligned} F_n(k) &\approx \frac{k^{n+1}}{n+1} \left[ 1 + \frac{(n+1)!}{(n-1)!3!} \beta^2 + \frac{7}{3} \frac{(n+1)!}{(n-3)!5!} \beta^4 + \frac{31}{3} \frac{(n+1)!}{(n-5)!7!} \beta^6 \right. \\ &+ \frac{381}{5} \frac{(n+1)!}{(n-7)!9!} \beta^8 + \frac{2555}{3} \frac{(n+1)!}{(n-9)!11!} \beta^{10} \\ &\left. + \frac{1414477}{105} \frac{(n+1)!}{(n-11)!13!} \beta^{12} + \dots + (\dots) \beta^n \right] \quad (33) \end{aligned}$$

the sum in the brackets terminates with  $\beta^n$ . For  $n = 2$  we have

$$F_2(k) = \frac{k^3}{3} (1 + \beta^2). \quad (34)$$

For odd  $n$  the sum over  $r$  ends with  $n$ , the terms in the brackets contain even powers of  $\beta$ , here, too; the last term contains  $\beta^{n+1}$ .

### Moments of 2pF charge distributions

With  $F_2(k)$  the ratio  $F_{m+2}(k)/F_2(k)$  can be formed. For  ${}^4\text{He}$   $\beta \approx 1$ , while for  ${}^{12}\text{C}$ ,  $k = 2.36/0.52 = 4.54$  [16]  $\beta \approx 0.69$ , i.e.  $\beta^2 \approx 0.48$ . Therefore, except for the lightest

elements, as perhaps Li, Be and B, the series expansion

$$\frac{1}{1+\beta^2} = 1 - \beta^2 + \beta^4 - \beta^6 + \beta^8 - \beta^{10} + \beta^{12} - + \dots \quad (35)$$

is valid (we will need it up to  $\beta^{12}$ ). Using this in Eq. (25) we have the general formula for the  $m$ th moment

$$\begin{aligned} \langle r^m \rangle = & a^m \frac{F_{m+2}(k)}{F_2(k)} = \frac{3}{m+3} c^m \left\{ 1 + \left[ \frac{(m+3)(m+2)}{3!} - 1 \right] \beta^2 \right. \\ & + \left[ \frac{7(m+3)(m+2)(m+1)m}{3 \cdot 5!} - \frac{(m+3)(m+2)}{3!} + 1 \right] \beta^4 \\ & + \left[ \frac{31(m+3)(m+2)\dots(m-1)(m-2)}{3 \cdot 7!} - \frac{7(m+3)(m+2)(m+1)m}{3 \cdot 5!} \right. \\ & + \left. \frac{(m+3)(m+2)}{3!} - 1 \right] \beta^6 + \left[ \frac{381(m+3)\dots(m-3)(m-4)}{5 \cdot 9!} \right. \\ & - \left. \frac{31(m+3)\dots(m-2)}{3 \cdot 7!} + \frac{7(m+3)\dots m}{3 \cdot 5!} - \frac{(m+3)(m+2)}{3!} + 1 \right] \beta^8 \quad (36) \\ & + \left[ \frac{2555(m+3)\dots(m-5)(m-6)}{3 \cdot 11!} - \left( \frac{381(m+3)\dots(m-3)(m-4)}{5 \cdot 9!} \right. \right. \\ & - \dots + 1) \left. \right] \beta^{10} + \left[ \frac{1414477(m+3)\dots(m-7)(m-8)}{105 \cdot 13!} \right. \\ & \left. - \left( \frac{2555(m+3)\dots(m-5)(m-6)}{3 \cdot 11!} + \dots - 1 \right) \right] \beta^{12} + \dots \left. \right\}. \end{aligned}$$

As it can be seen from this form the first (and second, ...) terms in the bracket multiplying  $\beta^{m+4}$  ( $\beta^{m+6}$ , ...) are equal to zero, i.e. the number of non-zero terms in the brackets multiplying  $\beta^{m+2}$  ( $\beta^{m+4}$ , ...) remains the same; moreover, these terms cancel each other.

Applying the above general formula to *even*  $m$  values we have:

$$\langle r^2 \rangle = \frac{3}{5} c^2 \left( 1 + \frac{7}{3} \beta^2 \right) = \frac{3}{5} c^2 + \frac{7}{5} (\pi a)^2, \quad (37)$$

$$\langle r^4 \rangle = \frac{3}{7} c^4 \left( 1 + 6\beta^2 + \frac{31}{3} \beta^4 \right), \quad (38)$$

$$\langle r^6 \rangle = \frac{1}{3} c^6 \left( 1 + 11\beta^2 + \frac{239}{5} \beta^4 + \frac{381}{5} \beta^6 \right), \quad (39)$$

$$\langle r^8 \rangle = \frac{3}{11} c^8 \left( 1 + \frac{52}{3} \beta^2 + \frac{410}{3} \beta^4 + \frac{1636}{3} \beta^6 + \frac{2555}{3} \beta^8 \right), \quad (40)$$

$$\langle r^{10} \rangle = \frac{3}{13} c^{10} \left( 1 + 25\beta^2 + \frac{926}{3} \beta^4 + \frac{46714}{21} \beta^6 + \frac{910573}{210} \beta^8 + \frac{19447}{210} \beta^{10} \right). \quad (41)$$

Note that in the expression for the moment  $\langle r^m \rangle$  the coefficients of  $\beta^{m+2}$ ,  $\beta^{m+4}$ , ... vanish exactly; the non-zero coefficients are all positive.

For odd  $m$  moments, the coefficients up to  $\beta^{m+1}$  are also positive; but from  $\beta^{m+2}$  the signs alternate, with the same non-zero absolute value. This alternating series can be written in the closed form  $1/(1 + \beta^2)$ .

$$\begin{aligned} \langle r \rangle &= \frac{3}{4}c \left[ 1 + \beta^2 - \frac{8}{15}\beta^4 (1 - \beta^2 + \beta^4 - \beta^6 + \beta^8 + \dots) \right] \\ &= \frac{3}{4}c \left( 1 + \beta^2 - \frac{8}{15} \frac{\beta^4}{1 + \beta^2} \right) \end{aligned} \quad (42)$$

and similarly:

$$\langle r^3 \rangle = \frac{1}{2}c^3 \left( 1 + 4\beta^2 + 3\beta^4 - \frac{32}{21} \frac{\beta^6}{1 + \beta^2} \right), \quad (43)$$

$$\langle r^5 \rangle = \frac{3}{8}c^5 \left( 1 + \frac{25}{3}\beta^2 + \frac{73}{3}\beta^4 + 17\beta^6 - \frac{128}{15} \frac{\beta^8}{1 + \beta^2} \right), \quad (44)$$

$$\langle r^7 \rangle = \frac{3}{10}c^7 \left( 1 + 14\beta^2 + 84\beta^4 + 226\beta^6 + 155\beta^8 - \frac{2560}{33} \frac{\beta^{10}}{1 + \beta^2} \right), \quad (45)$$

$$\begin{aligned} \langle r^9 \rangle &= \frac{1}{4}c^9 \left( 1 + 21\beta^2 + 210\beta^4 + 1154\beta^6 + 3037\beta^8 + 2073\beta^{10} \right. \\ &\quad \left. - \frac{1415168}{1365} \frac{\beta^{12}}{1 + \beta^2} \right). \end{aligned} \quad (46)$$

*Isotopic differences  $\delta \langle r^m \rangle$*

Assuming a constant surface diffusivity  $a$  and a mass number dependence  $c = r_0 A^{1/3}$  for the half-density radius, the change in the second moment corresponding to a change  $\delta A \equiv A_2 - A_1$  in the mass number is

$$\delta \langle r^2 \rangle = \frac{2}{5}c^2 \frac{\delta A}{A} \quad (47)$$

and the shifts in the higher even moments:

$$\delta \langle r^4 \rangle = \frac{4}{7}c^4 (1 + 3\beta^2) \frac{\delta A}{A}, \quad (48)$$

$$\delta \langle r^6 \rangle = \frac{2}{3}c^6 \left( 1 + \frac{22}{3}\beta^2 + \frac{239}{15}\beta^4 \right) \frac{\delta A}{A}, \quad (49)$$

$$\delta \langle r^8 \rangle = \frac{8}{11}c^8 \left( 1 + 13\beta^2 + \frac{205}{3}\beta^4 + \frac{409}{3}\beta^6 \right) \frac{\delta A}{A}, \quad (50)$$

$$\delta \langle r^{10} \rangle = \frac{10}{13}c^{10} \left( 1 + 20\beta^2 + \frac{926}{5}\beta^4 + \frac{93428}{105}\beta^6 + \frac{910573}{1050}\beta^8 \right) \frac{\delta A}{A}. \quad (51)$$

*Expression of  $\delta \langle r^m \rangle$  ( $m > 2$ ) in terms of  $\delta \langle r^2 \rangle$ .* For some applications, e.g. for the evaluation of isotope shifts in optical and characteristic X-ray spectra

the isotopic differences in  $\delta \langle r^4 \rangle$ ,  $\delta \langle r^6 \rangle$  are expressed in terms of  $\delta \langle r^2 \rangle$  [9]. This can be done easily because Eq. (47) allows to express  $c^2$  by  $\delta \langle r^2 \rangle$ :

$$c^2 = \frac{5}{2} \frac{A}{\delta A} \delta \langle r^2 \rangle = \frac{5}{4} \frac{A_1 + A_2}{A_2 - A_1} \delta \langle r^2 \rangle, \quad (52)$$

where  $A$  is replaced by  $(A_1 + A_2)/2$ . This  $c^2$  value is inserted in Eqs (48)–(51) and the differences  $\delta \langle r^m \rangle$  of higher order result.

For the *differences of odd moments* the closed forms in  $\beta$  are used:

$$\delta \langle r \rangle = \frac{1}{4} c \left[ 1 - \beta^2 + \frac{8}{5} \beta^4 \frac{1 + \frac{1}{3} \beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A}, \quad (53)$$

$$\delta \langle r^3 \rangle = \frac{1}{2} c^3 \left[ 1 + \frac{4}{3} \beta^2 - \beta^4 + \frac{32}{21} \beta^6 \frac{1 + \frac{1}{3} \beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A}, \quad (54)$$

$$\delta \langle r^5 \rangle = \frac{5}{8} c^5 \left[ 1 + 5\beta^2 + \frac{73}{15} \beta^4 - \frac{17}{5} \beta^6 + \frac{128}{25} \beta^8 \frac{1 + \frac{1}{3} \beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A}, \quad (55)$$

$$\delta \langle r^7 \rangle = \frac{7}{10} c^7 \left[ 1 + 10\beta^2 + \frac{252}{7} \beta^4 + \frac{226}{7} \beta^6 - \frac{155}{7} \beta^8 + \frac{2560}{77} \beta^{10} \frac{1 + \frac{1}{3} \beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A}, \quad (56)$$

$$\delta \langle r^9 \rangle = \frac{3}{4} c^9 \left[ 1 + \frac{49}{3} \beta^2 + \frac{350}{3} \beta^4 + \frac{1154}{3} \beta^6 + \frac{3037}{9} \beta^8 - \frac{691}{3} \beta^{10} + \frac{1415168}{4095} \beta^{12} \frac{1 + \frac{1}{3} \beta^2}{(1 + \beta^2)^2} \right] \frac{\delta A}{A}. \quad (57)$$

### Comparison to simpler distributions

The case of the *uniform* distribution is very simple: it can be regarded as a limiting 2pF distribution of Eq. (36) with  $c = R$  and  $a = 0$ , i.e.  $\beta = 0$ . In this case the formula for the moments reduces to the first term:

$$\langle r^m \rangle = \frac{3}{m+3} R^m. \quad (58)$$

The sum of the subsequent terms in the 2pF moments is always positive. Therefore, the use of the equivalent uniform distribution instead of 2pF results in a *systematic underestimation of all moments*. The thicker the surface relative to the radius, i.e. the higher  $\beta^2$  (light nuclei!) the stronger the deviation.

For a *trapezoidal* charge distribution with half-density radius  $c_T$  and surface thickness  $t_T$  the  $m$ th moment is [18]:

$$\begin{aligned} \langle r^m \rangle_T &= \frac{3}{m+3} c_T^m \left\{ 1 + \left[ \frac{(m+3)(m+2)}{3!} - 1 \right] \beta_T^2 \right. \\ &\quad \left. + \left[ \frac{(m+3)(m+2)(m+1)m}{5!} - \frac{(m+3)(m+2)}{3!} + 1 \right] \beta_T^4 + \dots \right\}, \end{aligned} \quad (59)$$

where  $\beta_T \equiv t_T/2c_T$ . It can be seen that for the trapezoidal distribution both the first term and the bracket before the quadratic term are equal to those of the 2pF distribution. That means that the moments of the equivalent trapezoidal distribution are much closer to those of the 2pF distribution than the moments of the uniform distribution.

The quantity of series expansion  $\beta_T \equiv t_T/2c_T$  corresponds to  $\beta \equiv \pi a/c$  of the 2pF distribution. One may look for the parameters of the trapezoidal distribution *equivalent* to a 2pF distribution, in the sense that all moments should be equal up to terms  $\beta^2$  ( $\beta_T^2$ ). To meet this demand  $c_T = c$  and  $\beta_T = \beta$  should be chosen, and from the latter

$$t_T = 2\pi a \quad (60)$$

follows. This *equivalent surface thickness* corresponds to a density decrease from 96% to 4% in the 2pF distribution — instead of the conventional  $s = 2 \ln(9) \times a \approx 4.4 \times a$  thickness defined by a density drop from 90% to 10%. This is an example for defining a surface thickness based on physical requirements (equivalence of moments) rather than on the biological accident that we happen to have ten fingers.

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*Dedicated to Valentine Telegdi on the occasion of his 80th birthday*

## Note

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