# Bound on Screening Corrections in Beta Decay

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A determinantal method is employed to provide a rigorous bound on the screening corrections in beta decay in the nonrelativistic approximation. Our results suffice to demonstrate that a previous numerical calculation of these corrections is inaccurate.

we have

### 1. INTRODUCTION

I N the preceding paper,<sup>1</sup> L. Durand, III, has discussed some discrepancies which exist among the published values of the atomic screening correction to beta-decay spectra, and has derived the value of this correction for an exactly soluble model of the screened Coulomb potential. Here we shall provide a rigorous upper bound on the screening correction in the nonrelativistic approximation. We shall employ in our discussion a Fredholm determinant method which has been used recently to analyze analyticity properties in potential scattering theory. It is hoped that some of the techniques and intermediate results of our work may prove useful in contexts other than that considered here.

We shall assume that the screened Coulomb potential in which the emitted beta-decay electron moves may be represented by a superposition of Yukawa potentials,

$$V(r) = (1/r) \int_{\mu_0}^{\infty} d\mu \sigma(\mu) e^{-\mu r}.$$
 (1)

At great distances this potential must closely approximate the pure Coulomb potential of the residual singly charged ion. We shall make the not unphysical requirement that this part of the potential has a large, but finite, range characterized by  $\mu_0^{-1}$ . This affects only the intermediate steps of our calculation, and the limit  $\mu_0 \rightarrow 0$  may be taken without difficulty in our result. At small distances the potential must approach the Coulomb potential of the residual nucleus,

$$V(r) = Z\alpha/r + \text{const} + O(r^2)$$
,

with  $Z\alpha$  a positive or negative quantity according to whether we consider positron or electron decay. This condition requires that

$$\int_{\mu_0}^{\infty} d\mu \sigma(\mu) = Z\alpha.$$
 (2)

It should be observed that the potential cannot contain a term linear in r; for such a term implies that the charge density of the screening atomic electrons diverges as  $r^{-1}$  at the nucleus, which is not true. Accordingly, the spectral weight  $\sigma(\mu)$  must change sign at least once.

<sup>1</sup>L. Durand, III, preceding paper, Phys. Rev. 135, B310 (1964).

The nonrelativistic screened Fermi function,  $\mathfrak{F}_s$ , is the absolute square of the electron wave function evaluated at the origin divided by the correspondingly normalized quantity for a free electron. In terms of the radial *S*-state wave function, normalized by the asymptotic boundary condition

$$u_0(r) \to e^{i\delta_0} \sin(kr + \delta_0), \ r \to \infty,$$
  
$$\mathfrak{F}_s = \lim_{r \to 0} |u_0(r)/kr|^2. \tag{3}$$

It is the ratio of the screened to the pure Coulomb value of this function which we shall bound.

In Ref. 2 it is shown that the limit which we need is related to the Jost function  $f_l(k)$  by

$$f_l(k)^{-1} = \lim_{r \to 0} \left[ \frac{u_l(r)}{(kr)^{l+1}} \right], \tag{4}$$

and that the Jost function may be written as a Fredholm determinant,

$$f_l(k) = \operatorname{Det}[1 - \mathcal{G}_l(k)V].$$
(5)

Here  $g_l(k)$  is the radial Green's function which satisfies

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right] \mathcal{G}_l(k; r, r') = 2m\delta(r - r'), \quad (6)$$

and has outgoing wave boundary conditions at infinity, or equivalently, is analytic in the upper half k plane. We shall initially work with an arbitrary value of the angular momentum since it entails no complication and gives general results which may prove useful in other contexts.

#### 2. THE COULOMB "JOST FUNCTION"

We begin our development by obtaining a "Jost function" for a pure Coulomb potential. This task will illustrate well the techniques we employ and will provide us with some results that will be needed later. Since the determinant is invariant under similarity transformations, we may replace the kernel  $G_l(k)(Z\alpha/r)$ 

<sup>&</sup>lt;sup>2</sup> L. Brown, D. I. Fivel, B. W. Lee, and R. F. Sawyer, Ann. Phys. (N. Y.) **23**, 187 (1963). There are, unfortunately, a large number of misprints in this paper. The Jost and Green's functions,  $f_i(k)$  and  $G_i(k)$ , used in the present paper are denoted by  $f_i^{(+)}(k)$  and  $G_i^{(+)}(k)$  in this reference.

occurring in it by the symmetrical form

$$Z \alpha r^{-1/2} \mathfrak{G}_l(k) r^{-1/2} = r^{-1/2} [\mathfrak{G}_l(k) (Z \alpha/r)] r^{1/2}.$$

It is advantageous to make use of a further similarity transformation

$$[r^{-1/2}\mathcal{G}_l(k)r^{-1/2}] \longrightarrow e^{-\varphi rp}[r^{-1/2}\mathcal{G}_l(k)r^{-1/2}]e^{\varphi rp},$$

where p is the momentum operator with the configuration-space representation p((1/i)(d/dr)) when acting to the right or  $p = -(1/i)(d^T/dr)$  when acting to the left. On referring to the differential equation (6) satisfied by the configuration-space representation of the Green's function, we easily conclude on dimensional grounds that it is of the form m/k multiplying a function of the dimensionless variables kr and kr'. Accordingly, by varying  $\varphi$  one may readily verify that

$$e^{-\varphi r p} \mathcal{G}_l(k; \mathbf{r}, \mathbf{r}') e^{\varphi r p} = e^{i\varphi} \mathcal{G}_l(k; e^{i\varphi} \mathbf{r}, e^{i\varphi} \mathbf{r}')$$
  
=  $e^{2i\varphi} \mathcal{G}_l(e^{i\varphi} k; \mathbf{r}, \mathbf{r}'),$ 

and

$$e^{-\varphi r p} [r^{-1/2} \mathfrak{g}_{l}(k) r^{-1/2}] e^{\varphi r p} = e^{i\varphi} [r^{-1/2} \mathfrak{g}_{l}(e^{i\varphi}k) r^{-1/2}].$$

We shall take  $\varphi = \pi/2$ , for in this case we have

$$Z\alpha[r^{-1/2}\mathcal{G}_l(k)r^{-1/2}] \to -iZ\alpha K_l(ik), \qquad (7)$$

where the Coulomb kernel

$$K_l(ik) = -r^{-1/2} \mathcal{G}_l(ik) r^{-1/2} \tag{8}$$

is a symmetrical, and in fact, a real, positive-definite operator.

The positive imaginary argument *ik* corresponds to negative energy and the bound-state region of the Coulomb problem. At certain critical values of the potential strength,  $(Z\alpha)' < 0$ , bound states will occur for any given negative energy  $-k^2/2m$ . This implies that the integral form of the radial Schrödinger equation possesses homogeneous solutions for these critical potential strengths, or that its associated Fredholm determinant vanishes,

$$\operatorname{Det}[1+(Z\alpha)'K_l(ik)]=0.$$

Thus, the eigenvalues of  $K_l(ik)$  are the reciprocals of the set  $-(Z\alpha)'$ , and we may immediately conclude from the Balmer formula that they are given by

$$K_l(ik)' = (m/k)(n+l+1),^{-1} \quad n=0, 1, \cdots$$
 (9)

The corresponding eigenvectors satisfy

$$K_{l}(ik)\phi_{n,l}(k) = (m/k)(n+l+1)^{-1}\phi_{n,l}(k), \quad (10a)$$

or

$$\begin{split} \tilde{r}(n+l+1)(k/mr)[r^{1/2}\phi_{n,l}(k;r)] \\ &= -G_l(ik)^{-1}[r^{1/2}\phi_{n,l}(k;r)] \\ &= -(1/2m)\{d^2/dr^2 - l(l+1)/r^2 - k^2\} \\ &\times [r^{1/2}\phi_{n,l}(k;r)]. \quad (10b) \end{split}$$

The regular solution of this differential equation is simply related to the familiar bound-state solution of the Coulomb problem, and we have

$$r^{1/2}\phi_{n,l}(k;r) = \left[\frac{n!}{(2l+1+n)!}\right]^{1/2} (2kr)^{l+1} \\ \times e^{-kr}L_n^{2l+1}(2kr), \quad (11)$$

where  $L_n^{2l+1}(2kr)$  is a Laguerre polynomial. These functions form a complete orthonormal set with the inner product

$$(n(lk)|n'(lk)) = \int_0^\infty dr \phi_{n,l}(k;r) \phi_{n';l}(k;r) = \delta_{n,n'}. \quad (12)$$

A general Fredholm determinant may be written in the form

$$Det[1 - \lambda A] = exp\{Tr ln[1 - \lambda A]\}$$
$$= exp\{-\sum_{s=1}^{\infty} (\lambda^{s}/s) TrA^{s}\}, \quad (13)$$

for sufficiently small values of the parameter  $\lambda$ . Thus the determinantal definition (5) of the Jost function cannot be used for the case of a pure Coulomb potential, for here the first trace occurring in the expansion diverges. We shall remedy this situation by working with a modified determinant in which this trace is removed,

$$\operatorname{Det}'[1 - \lambda A] = e^{\lambda \operatorname{Tr} A} \operatorname{Det}[1 - \lambda A].$$
(14)

The evaluation of this modified determinant for the Coulomb case is easily accomplished by using the sequence of similarity transformations which brought the original kernel into the form  $-iZ\alpha K_l(ik)$  and then computing the sum of traces which occurs in exponential of the modified version of (13). This sum converges only for small values of  $Z\alpha$ , but we shall obtain a result which clearly expresses its analytic continuation for arbitrary values of this parameter. According to the eigenvalue spectrum (9), the required traces are simply

$$\operatorname{Tr}[K_{l}(ik)]^{s} = (m/k)^{s} \sum_{n=0}^{\infty} (n+l+1)^{-s}$$
$$= \left(\frac{m}{k}\right)^{s} \frac{(-1)^{s}}{(s-1)!} \left(\frac{\partial}{\partial l}\right)^{s} \ln\Gamma(l+1)$$

The identification of the sum with the *s*th derivative of the logarithm of the gamma function follows from the observation that both possess the same singularities and both vanish as  $l \rightarrow \infty$ . We thus find

Det'[1-
$$G_l(k)(Z\alpha/r)$$
]  

$$= \exp\left\{-\sum_{s=2}^{\infty} \left(\frac{iZ\alpha m}{k}\right)^s \frac{1}{s!} \left(\frac{\partial}{\partial l}\right)^s \ln\Gamma(l+1)\right\}$$

$$= \exp\left\{-\ln\Gamma\left(l+1+i\frac{Z\alpha m}{k}\right) + \ln\Gamma(l+1) + \frac{iZ\alpha m}{k}\psi(l+1)\right\}$$
where

where

$$\psi(z) = (d/dz) \ln\Gamma(z). \tag{15}$$

This leads us to define a Coulomb Jost function by

$$f_{l}^{(C)}(k) = \exp\{-i\eta\psi(l+1)\} \operatorname{Det}'[1-\mathfrak{g}_{l}(k)Z\alpha/r] = \frac{\Gamma(l+1)}{\Gamma(l+1+i\eta)},$$
(16)

where  $\eta = (Z\alpha m/k)$  is the usual Coulomb parameter.

#### 3. FACTORIZATION OF THE JOST FUNCTION

We turn now to a discussion of the ratio of the screened Jost function to the Coulomb Jost function which we have just defined

$$\frac{f_{l}(k)}{f_{l}^{(C)}(k)} = \frac{\operatorname{Det}[1 - \mathfrak{g}_{l}(k)V]}{\exp\{-i\eta\psi(l+1)\}\operatorname{Det}'[1 - \mathfrak{g}_{l}(k)(Z\alpha/r)]}.$$

After rewriting the modified determinant in terms of a normal determinant and making use of the fact that the ratio of determinants is a determinant of the ratio of the operators that they contain, we find

$$f_{l}(k) = f_{l}^{(C)}(k) \exp\{-\mathrm{Tr}[1 - \mathcal{G}_{l}(k)(Z\alpha/r)]^{-1}\mathcal{G}_{l}(k)V\} \\ \times \exp\{\mathrm{Tr}[1 - \mathcal{G}_{l}(k)(Z\alpha/r)]^{-1}[\mathcal{G}_{l}(k)(Z\alpha/r)]^{2} \\ + i\eta\psi(l+1)\}R_{l}(k), \quad (17)$$

where

$$R_{l}(k) = \operatorname{Det}'\{1 - [1 - \mathcal{G}_{l}(k)(Z\alpha/r)]^{-1} \\ \times \mathcal{G}_{l}(k)[V - (Z\alpha/r)]\}.$$
(18)

Although the formal procedure outlined to obtain this relation is not justified since the first trace of the Coulomb kernel diverges, the relation itself is true; for it merely expresses a combinatorial relationship among well-defined traces.

We may express the trace which occurs first in Eq. (17) as

$$\Gamma r [1 - \mathfrak{G}_{l}(k)(Z\alpha/r)]^{-1} \mathfrak{G}_{l}(k) V$$

$$= \operatorname{Tr} [\mathfrak{G}_{l}(k)^{-1} - (Z\alpha/r)]^{-1} V$$

$$= \operatorname{Tr} \mathfrak{G}_{l}^{\eta}(k) V, \qquad (19)$$

where  $G_{l^{\eta}}(k)$  is a Green's function which includes the effect of the Coulomb potential. It satisfies the differential equation

$$\frac{1}{2m}\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right] - \frac{Z\alpha}{r} \\ \times G_{l^{\eta}}(k; r, r') = \delta(r - r')$$

with an outgoing wave boundary condition. It proves useful to write

$$\operatorname{Tr} G_{l}^{\eta}(k) V = \int_{\mu_{0}}^{\infty} d\mu \sigma(\mu) \mathfrak{A}_{l}(\mu, k) , \qquad (21)$$

(20)

where, on using the previous sequence of similarity transformations, we have

$$\alpha_{l}(\mu,k) = -i \operatorname{Tr} \frac{K_{l}(ik)}{1 + iZ\alpha K_{l}(ik)} e^{-i\mu r}.$$
 (22)

On making further use of this sequence of similarity transformation we obtain

$$R_l(k) = \operatorname{Det}'[1 - B_l(k)], \qquad (23)$$

with

$$B_{l}(k) = \frac{-iK_{l}(ik)}{1 + iZ\alpha K_{l}(ik)} (irV(ir) - Z\alpha), \qquad (24)$$

and also, recalling the eigenvalue spectrum (9),

$$\operatorname{Tr}[1-\mathfrak{g}_{l}(k)(Z\alpha/r)]^{-1}[\mathfrak{g}_{l}(k)(Z\alpha/r)]^{2}+i\eta\psi(l+1)$$
$$=-\eta^{2}\sum_{n=0}^{\infty}\frac{1}{n+l+1+i\eta}\frac{1}{n+l+1}+i\eta\psi(l+1)$$

$$=i\eta\psi(l+1+i\eta). \tag{25}$$

The last equality follows from a consideration of the singularities and asymptotic behaviour in the variable l of the structure which precedes it.

It is perhaps well to pause here and collect our results by writing

$$f_{l}(k) = f_{l}^{(C)}(k)$$

$$\times \exp\{-\operatorname{Tr}G_{l}^{\eta}(k)V + i\eta\psi(l+1+i\eta)\}R_{l}(k). \quad (26)$$

# 4. BOUNDS ON $R_l(k)$

The upper bound on the modified determinant

 $|\operatorname{Det}'[1-B]| \le e^{\frac{1}{2}||B||^2},$  in which

$$||B||^2 = \mathrm{Tr}BB^{\dagger}, \qquad (27)$$

is fairly well known,<sup>2–4</sup> A lower bound on this quantity can be obtained with the aid of the inequalities

$$|\operatorname{Tr} AB| \leq ||A|| ||B||,$$
$$||AB|| \leq ||A|| ||B||,$$

which follow from the Schwartz inequality. For the

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<sup>&</sup>lt;sup>3</sup> J. Schwinger, Phys. Rev. 93, 615 (1954).

<sup>&</sup>lt;sup>4</sup> F. Smithies, Integral Equations (Cambridge University Press, Cambridge, 1958).

first inequality implies that for  $s \ge 2$ 

 $|\operatorname{Tr} B^{s}| \leq ||B|| ||B^{s-1}||,$ 

and the repeated use of the second yields

$$|\operatorname{Tr} B^s| \leq ||B||^s.$$

Hence it follows from the expansion (13) that

$$Det'[1-B]| \ge \exp\{-\sum_{s=2}^{\infty} (1/s) |\operatorname{Tr} B^s|\} \\ \ge \exp\{-\sum_{s=2}^{\infty} (1/s) ||B||^s\} \\ \ge \exp\{\ln(1-||B||) + ||B||\},$$

so long as ||B|| < 1. We may thus bound the remainder function occurring in the decomposition of the Jost function given in the preceding section by

$$[1 - ||B_l(k)||]e^{||B_l(k)||} \le |R_l(k)| \le e^{\frac{1}{2}||B_l(k)||^2}.$$
 (28)

We note that when the norm  $||B_l(k)||$  is small we have the more detailed statement

$$R_{l}(k) = 1 + O(||B_{l}(k)||^{2}).$$
<sup>(29)</sup>

The bounding of the remainder function is now reduced to the evaluation of

$$||B_{l}(k)||^{2} = \operatorname{Tr} \frac{K_{l}(ik)^{2}}{1 + (Z\alpha K_{l}(ik))^{2}} \times [irV(ir) - Z\alpha][-irV(-ir) - Z\alpha]. \quad (30)$$

Since the factor involving the potential is positive semidefinite, this norm is at most increased if we neglect the positive definite operator  $(Z\alpha K_l(ik))^2$  occurring in the denominator<sup>5</sup>

$$||B_{l}(k)||^{2} \leq \int_{\mu_{0}}^{\infty} d\mu_{1} d\mu_{2} \sigma(\mu_{1}) \sigma(\mu_{2}) \\ \times \operatorname{Tr} K_{l}(ik)^{2} (e^{-i\mu_{1}r} - 1) (e^{i\mu_{2}r} - 1).$$

We may exploit the symmetry of this double integral and write

$$||B_{l}(k)||^{2} \leq \int_{\mu_{0}}^{\infty} d\mu_{1} d\mu_{2} \sigma(\mu_{1}) \sigma(\mu_{2}) \\ \times \{b_{l}(\mu_{1},k) + b_{l}(\mu_{2},k) - b_{l}(\mu_{1}-\mu_{2},k)\}, \quad (31)$$

where

$$b_l(\mu,k) = \operatorname{Tr} K_l(ik)^2 (1 - \cos \mu r).$$
 (32)

Recalling the definition (22), we see that we may write this function as

$$b_{l}(\mu,k) = \operatorname{Re} \frac{\partial}{\partial (Z\alpha)} \{ \alpha_{l}(\mu,k) - \alpha_{l}(0,k) \}_{Z\alpha=0}.$$
(33)

The evaluation of the function  $\alpha_l(\mu,k)$  therefore yields both the Born term  $TrG_i^{\eta}(k)V$  and bounds on the remainder function  $R_l(k)$ .

#### 5. CALCULATION OF THE COULOMB-BORN APPROXIMATION

We employ the Coulomb basis discussed in Sec. 2. to secure

$$\mathfrak{A}_{l}(\mu,k) = -i(m/k) \sum_{n=0}^{\infty} \frac{1}{n+l+1+i\eta}$$

in which

$$(n(lk)|e^{-i\mu r}|n(lk)) = \int_0^\infty dr \phi_{nl}(k;r)e^{-i\mu r} \phi_{nl}(k;r).$$

 $\times (n(lk) | e^{-i\mu r} | n(lk)),$  (34)

Integrals of this general type may be evaluated in terms of hypergeometric functions.<sup>6</sup> In our particular case the hypergeometric function reduces to a Jacobi polynomial  $P_n^{(\alpha,\beta)}(z)$ , and one finds

$$(n(lk) | e^{-i\mu r} | n(lk)) = \left(\frac{\zeta^2}{\zeta^2 + 1}\right)^{l+1} e^{-2i\varphi(n+l+1)} P_n^{(0,2l+1)}(\cos 2\varphi), \quad (35)$$
where

where

$$\zeta = (2k/\mu), \quad \varphi = \arg(\zeta + i) > 0. \tag{36}$$

Since the Jacobi polynomials possess a simple generating function,<sup>7</sup> we may convert the infinite sum into a more manageable integral,

$$\begin{aligned} \alpha_{l}(\mu,k) &= -i(m/k) \sum_{n=0}^{\infty} \int_{0}^{\infty} dl e^{-(n+l+1+i\eta)t} \\ &\times (n(lk) | e^{-i\mu r} | n(lk)) \\ &= i(m/k) (\frac{1}{2})^{2l+1} (1+i/\zeta)^{2l} \\ &\times \int_{0}^{\infty} dl e^{(l-i\eta)t} R^{-1} (R - e^{-2i\varphi} e^{-t} - 1)^{2l+1}, \end{aligned}$$
(37) with

$$R = [(1 - e^{-t})(1 - e^{-4i\varphi}e^{-t})]^{1/2}.$$
 (38)

This integral representation has the virtue of having its dependence on the Coulomb parameter  $\eta$  isolated in the simple factor  $e^{-i\eta t}$ . Other methods of calculation generally lead to integrals with a complicated de-

<sup>&</sup>lt;sup>5</sup> The convergence of this bound requires that  $|V(ir)| \leq r^{-1}$  as  $r \to \infty$ , which is tantamount to the condition that weight  $\sigma(\mu)$ contain no derivatives of the  $\delta$  function. This is a somewhat stringent condition on the behaviour of the potential in an unphysical region. It arises from the use of the similarity transformation to rotate k into ik so that the denominator in Eq. (30) becomes positive-definite and the kernel K occuring in it may be neglected. This procedure appears to be necessary if a simple form of the bound is to be obtained.

<sup>&</sup>lt;sup>6</sup> See, for example, L. D. Landau and E. M. Lifshitz Quantum Mechanics (Pergamon Press Ltd., London, 1958), p. 505. <sup>7</sup> The generating function used here is equivalent to that given

in the Bateman Project Staff, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 172.

pendence on this parameter, and these integrals are  $b_0(\mu_1 - \mu_2, k)$ , and we secure the simple result correspondingly difficult to evaluate.

It is at this point that we specialize our discussion to the case l=0. In this case the integral can be evaluated without great algebraic difficulty, for it is related to a standard representation<sup>8</sup> of the Legendre function of the second kind, and one finds

$$\begin{aligned} 
\alpha_0(\mu,k) &= -\left(im/2k\right)\left\{i/\eta + e^{-2\varphi\eta} \\ \times \left[Q_{i\eta-1}(\cos 2\varphi + i\epsilon) + Q_{i\eta}(\cos 2\varphi + i\epsilon)\right]\right\}. \quad (39)
\end{aligned}$$

The argument of the Legendre function is in the region of its cut. The  $i\epsilon$  indicates that this cut is to be approached from above. It is the real part of  $\alpha_0$  that enters into the Fermi function and also into the bound which was developed previously. This real part may be computed with the aid of various relations among Legendre functions<sup>9</sup> with the result:

$$\operatorname{Re}\alpha_{0}(\mu,k) = -\frac{m}{2k} \{1/\eta + e^{-2\varphi\eta}\pi(\operatorname{coth}\pi\eta + 1) \\ \times \frac{1}{2} [P_{i\eta}(\cos 2\varphi) + P_{-i\eta}(\cos 2\varphi)]\}.$$
(40)

The derivative of this function with respect to  $Z\alpha$ , evaluated at  $Z\alpha = 0$ , is related to the bounding function  $b_0$ . This derivative may be obtained by expressing the Legendre function  $P_{i\eta}(z)$  in terms of a hypergeometric function.9 The resulting terms contain logarithms and an Euler dilogarithm. They can be expressed succinctly by the integral

$$b_{0}(\mu,k) = (m^{2}/2k^{2})$$

$$\times \int_{0}^{|\mu/2k|} dx(x^{2}+1)^{-1} [2\pi - 4 \arctan x], \quad (41)$$

$$0 \le b_{0}(\mu,k) \le (m^{2}/2k^{2}) |\mu/k| \pi.$$

We may bound the double integral (31) by

$$||B_{0}(k)||^{2} \leq 2 \int_{\mu_{0}}^{\infty} d\mu_{1} |\sigma(\mu_{1})| \int_{\mu_{0}}^{\mu_{1}} d\mu_{2} |\sigma(\mu_{2})| |b_{0}(\mu_{1},k) + b_{0}(\mu_{2},k) - b_{0}(\mu_{1}-\mu_{2},k)|.$$

Since

$$(\partial/\partial\mu)b_0(\mu,k) \ge 0,$$

within the integration range  $b_0(\mu_1 - \mu_2, k)$  decreases with  $\mu_2$  and is thus always smaller than  $b_0(\mu_1,k)$ . Accordingly, the bound increases with the neglect of

$$||B_{0}(k)||^{2} \leq 2 \int_{\mu_{0}}^{\infty} d\mu_{1} |\sigma(\mu_{1})| \int_{\mu_{0}}^{\infty} d\mu_{2} |\sigma(\mu_{2})| b_{0}(\mu_{2},k)$$

$$\leq \pi m^{2} k^{-3} \int_{\mu_{0}}^{\infty} d\mu_{1} |\sigma(\mu_{1})| \int_{\mu_{0}}^{\infty} d\mu_{2} \mu_{2} |\sigma(\mu_{2})|. \quad (42)$$

If the weight  $\sigma(\mu)$  does not change sign we may write this bound as

$$||B_0(k)||^2 \leq \eta \langle \mu \rangle / k , \qquad (43)$$

in which

$$\langle \mu \rangle = (Z\alpha)^{-1} \int_{\mu_0}^{\infty} d\mu \mu \sigma(\mu) = \lim_{r \to 0} \left[ r^{-1} - (Z\alpha)^{-1} V(r) \right].$$
(44)

The remarkably simple structure of this bound, which depends only on the behaviour of the potential at the origin, is a consequence of the analyticity of the potential which we have assumed.

#### 6. DISCUSSION

The bound  $||B_0(k)||^2$  is quite small for light to medium weight nuclei and for moderate energies of the emitted beta particle, energies of the order of a few hundred kilovolts. Although such energies exceed the range in which the nonrelativistic approximation is accurate, relativistic corrections will not alter very greatly the magnitude of the screening corrections themselves. A quantitative estimate of the bound may be obtained by fitting the Hartree potential function of various atoms by a discrete sum of Yukawa potentials. Such a fit has been performed by Byatt.<sup>10</sup> His results give various averaged inverse-range parameters that all lie close to the value

$$\langle \mu \rangle = 1.5 Z^{1/3} \alpha m \,, \tag{45}$$

in agreement with the estimate of Durand.<sup>1</sup> In many cases he obtained an accurate fit with a sum of terms of the same sign, and in these cases the very simple formula (43) can be applied. For the other cases in which terms of differing sign occur, one finds from Byatt's work that (43) differs at most by 30% from the correct value given by (42). As a specific example, we note that for an energy of 200 keV and with Z=16, Eqs. (43) and (45) give

$$||B_0(k)||^2 < 2 \times 10^{-3}$$

<sup>&</sup>lt;sup>8</sup> Bateman Project Staff, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. I, p. 160, Eq. (32). There are two misprints in this formula. The curly brackets should be raised to the power  $-\mu - 1/2$ , and the term  $(z^2-1)$  occurring inside these brackets should be replaced by  $(z^2-1)^{1/2}$ . <sup>9</sup> Such formulas may be found in Ref. 8, Chap. III. There is

another misprint in this reference. A minus sign should appear on the right of Eq. (8), p. 144.

<sup>&</sup>lt;sup>10</sup> W. J. Byatt, Phys. Rev. 104, 1298 (1956). Our discussion is simplified by the neglect of the long-range Coulomb potential of the residual ion. The inclusion of this potential modifies our results by at most 10%. We should also note that Byatt's potentials contain a term proportional to r and hence violate the general considerations given in the Introduction on the behaviour of the correct potential near the origin. Moreover, they do not possess the correct behaviour at infinity. However, the difference between the true atomic screening potential and that given by a model such as Byatt's can be made very small, the major relative error occurring in a region where the potential is itself quite small. These very small differences will have little effect on the value of the wave function at the origin, and we may employ the model potential in our calculations even though it violates some general requirements.

Thus, for the conditions considered here, the remainder function  $R_0(k)$  can differ from unity by at most a few tenths of a percent, and within this accuracy we may use

$$f_0(k) = f_0^{(C)}(k) \exp\{-\mathrm{Tr}G_0^{\eta}(k)V + i\eta\psi(l+1+i\eta)\},\$$

or

$$= \mathfrak{F}_{o} \exp\{(\pi \eta^{2} \langle \mu \rangle / k) [\operatorname{cotanh} \pi \eta + 1]\}. \quad (46)$$

Here  $\mathcal{F}_{c}$  is the Fermi function of a pure Coulomb potential,

$$\mathfrak{F}_c = |\Gamma(1+i\eta)|^2 e^{-\pi\eta}, \qquad (47)$$

and we have retained only terms to order  $\mu$  in an expansion of the function  $\operatorname{Re} \mathfrak{A}_0(\mu, k)$  which determines ReTr $G_0^{\eta}V$ . As an illustration of the order of the screening corrections, and to compare our results with the numerical calculation of Reitz,<sup>11</sup> we consider again the example of E = 200 keV, Z = 16. In this case<sup>12</sup>

$$\mathfrak{F}_{s}/\mathfrak{F}_{c} = \begin{cases} 1+7\times10^{-3}(1+38\times10^{-3}), \text{ positron decay} \\ 1-3\times10^{-3}(1+0\times10^{-3}), \text{ electron decay.} \end{cases}$$

<sup>11</sup> J. R. Reitz, Phys. Rev. 77, 10 (1950).

 $\mathfrak{F}_{n} = |f_{n}(k)|^{-2}$ 

<sup>12</sup> It must be noted that these values are of the same order as that of the error bound  $||B_0(k)||^2$ . Indeed, the correction terms

The parenthesis enclose the corresponding values found by Reitz. His value for the positron-decay correction disagrees quite strongly with ours. We also note that, to within terms of order  $(\langle \mu \rangle / k)^2$ , we may write our result (46) for the Fermi function as

$$\mathfrak{F}_s = (k'/k)\mathfrak{F}_c', \qquad (48)$$

where  $\mathfrak{F}_{c}'$  is the pure Coulomb Fermi function evaluated at the shifted energy  $E' = E + Z\alpha \langle \mu \rangle$ , and k' is the wave number corresponding to this shifted energy. This form agrees with the WKB result of Rose.<sup>13</sup>

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<sup>13</sup> M. E. Rose, Phys. Rev. 49, 727 (1936).

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## Empirical Screening Correction for *M*-Subshell Internal Conversion Coefficients\*

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The only theoretical values which are available for coefficients of internal conversion in the M shell have been calculated without the inclusion of screening, and they are in disagreement with experimental values by factors as large as 3. From the comparison of these theoretical values with new accurate measurements on the M-subshell electron lines of the M4 transitions occuring in the decay of Te<sup>121m</sup> and of Te<sup>123m</sup>, it was possible to effect a tentative semiempirical screening correction. Essentially, this is the replacement of the nuclear charge Z for the evaluation of the coefficient by  $Z_{effM} = Z - \sigma_i$ , where  $\sigma_i = 7.0, 7.9, \text{ and } 10.0 \text{ for } M_I (3s), M_{II, III}$ (3p), and  $M_{IV,V}$  (3d) electrons, respectively. This correction to the theoretical values is found to produce agreement with other experimental M conversion results, both measured in this work and taken from the literature, over a wide range of multipolarities and of Z and energy values. The nonspecific characteristic of the correction is interpreted to mean that the screening is chiefly an effect on the electron wave functions of the initial bound states of the atom.

#### I. INTRODUCTION

T has been recognized that experimentally determined values of internal conversion coefficients in the M levels are considerably smaller than the theoretical values now available.<sup>1</sup> For simplicity, two effects included in the later theoretical work on K and L shell

conversion coefficients<sup>1,2</sup> were neglected in the M-shell calculations. The first of these, the effect of finite nuclear size, was thought to be of little importance in most cases; it was recognized that the second effect, the screening of the M electrons from the nuclear charge by the other electrons in the atom could produce

in (46) and  $||B_0(k)||^2$  are both of order  $\langle \mu \rangle / k$ . However, an inspection of the determinantal representation of the remainder function  $R_0(k)$  of Eq. (23) shows that its absolute value is *not* of order  $\langle \mu \rangle / k$  as indicated by the bound  $||B_0(k)||^2$ , but rather of the smaller order  $(\langle \mu \rangle / k)^2$ . The reason for this discrepancy is that  $||B_0(k)||^2$  gives essentially a bound on the logarithm of  $R_0(k)$ , and  $R_0(k)$  has a large phase of order  $\langle \mu \rangle / k$ .

<sup>\*</sup> Research performed under the auspices of the U.S. Atomic Energy Commission.

<sup>&</sup>lt;sup>1</sup> M. E. Rose, Internal Conversion Coefficients (North-Holland Publishing Company, Amsterdam, 1958).

<sup>&</sup>lt;sup>2</sup>L. A. Sliv and A. M. Band, Academy of Sciences of the U.S.S.R., *Coefficients of Internal Conversion of Gamma Radiation* (English transl.: Physics Department, University of Illinois, Urbana, Reports 57 ICC K1 and 58 ICC L1, 1957 and 1958).