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ADDENDUM

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Abstract. The finite-radius Fourier transform of the first-order vacuum-polarization correction to the Coulomb potential of a point charge, required for a Fourier–Bessel evaluation of vacuum-polarization potentials of extended charges, is calculated by an efficient analytical method.

The need for an accurate and efficient method for the calculation of vacuum-polarization potentials of extended charges has recently received new emphasis in connection with the problem of muon-catalysed fusion, as vacuum polarization leads to the single most important correction to the non-relativistic energies of the ddμ and dtμ molecular states [1] and the effects of finite nuclear size in the vacuum-polarization potential are significant at the distances relevant to μ-mesic molecular physics [2]. The first-order vacuum-polarization potentials of extended charge distributions have been calculated in [3] by using an efficient Fourier–Bessel method for the evaluation of folding integrals. The application of the Fourier–Bessel method requires here the calculation of the finite-radius Fourier transform of the vacuum-polarization potential of a point charge, the so-called Uehling potential, and this addendum describes a rapidly converging expansion method for such a calculation. This completes the analytical treatment of the vacuum-polarization effects of extended charges described in [3].

The Uehling potential [4] is a first-order vacuum-polarization correction of quantum electrodynamics to the Coulomb potential of a point charge e. It can be written as

$$U(r) = \frac{2\alpha e}{3\pi r}\chi_1(2r/\lambda\!\!\!^{-}_{\mathrm{e}}) \qquad (1)$$

where $\alpha = e^2/\hbar c = 1/137.036$ is the fine-structure constant, $\lambda\!\!\!^{-}_{\mathrm{e}} = \hbar/m_{\mathrm{e}}c = 386.159$ fm is the reduced Compton wavelength of the electron and the function $\chi_1(x)$ belongs to a class of functions defined by the integrals

$$\chi_k(x) = \int_1^\infty \frac{\mathrm{e}^{-xt}}{t^k}\left(1+\frac{1}{2t^2}\right)\sqrt{1-\frac{1}{t^2}}\,\mathrm{d}t. \qquad (2)$$

These functions can be expressed in closed form [5] in terms of the modified Bessel functions $K_0(x)$ and $K_1(x)$ and the modified Bessel function integral $\mathrm{Ki}_1(x)$ [6] (accurate and efficient Chebyshev polynomial approximations of these special functions are given, for example, in

[7]). Use will be made here of the functions $\chi_k(x)$ with k in the range $-4 \leqslant k \leqslant 1$ the closed-form expressions of which are as follows

$$\begin{aligned}
\chi_{-4}(x) &= \frac{1}{2x^3}(24+3x^2)K_0(x) + \frac{6}{x^4}(4+x^2)K_1(x) \\
\chi_{-3}(x) &= \frac{3}{x^2}K_0(x) + \frac{3}{2x^3}(4+x^2)K_1(x) \\
\chi_{-2}(x) &= \frac{1}{x}K_0(x) + \frac{1}{2x^2}(4+x^2)K_1(x) - \frac{1}{2}\mathrm{Ki}_1(x) \\
\chi_{-1}(x) &= \frac{1}{2}K_0(x) + \frac{1}{2x}(2-x^2)K_1(x) + \frac{x}{2}\mathrm{Ki}_1(x) \\
\chi_0(x) &= -\frac{x}{4}K_0(x) + \frac{1}{4}(4+x^2)K_1(x) - \frac{1}{4}(3+x^2)\mathrm{Ki}_1(x) \\
\chi_1(x) &= \frac{1}{12}(12+x^2)K_0(x) - \frac{x}{12}(10+x^2)K_1(x) + \frac{x}{12}(9+x^2)\mathrm{Ki}_1(x).
\end{aligned} \tag{3}$$

A recursive scheme has been given in [8] for the calculation of the functions $\chi_k(x)$ with $k \leqslant -3$.

The infinite-radius Fourier transform of the Uehling potential can be expressed in terms of elementary functions [3]

$$\begin{aligned}
\tilde{U}^{(\infty)}(q) &= 4\pi \int_0^\infty U(r) j_0(qr) r^2 \, \mathrm{d}r \\
&= \frac{4\alpha e}{3q^2}\left[\left(1-\frac{2}{\lambda_e^2 q^2}\right)\left(s \ln\frac{s+1}{s-1} - 2\right) + \frac{1}{3}\right] \qquad s = \sqrt{1+\left(\frac{2}{\lambda_e q}\right)^2}.
\end{aligned} \tag{4}$$

Unfortunately, it does not seem possible to evaluate the finite-radius Fourier transform of the Uehling potential

$$\tilde{U}^{(R)}(q) = 4\pi \int_0^R U(r) j_0(qr) r^2 \, \mathrm{d}r \tag{5}$$

in closed form; in [3] it has been expressed for a set of discrete arguments q_n as

$$\begin{aligned}
\tilde{U}^{(R)}(q_n) &= \tilde{U}^{(\infty)}(q_n) + (-1)^n \frac{4\alpha e \lambda_e}{3q_n} I\left(\frac{2R}{\lambda_e}, \frac{\lambda_e q_n}{2}\right) \\
q_n &= \left(n - \frac{1}{2}\right)\frac{\pi}{R} \qquad n = 1, 2, 3, \ldots
\end{aligned} \tag{6}$$

where the finite-radius correction to the Fourier transform $\tilde{U}^{(\infty)}(q_n)$ is given in terms of the integral

$$I(\mu, \nu) = \int_1^\infty \frac{\mathrm{e}^{-\mu t}}{\nu^2 + t^2}\left(1 + \frac{1}{2t^2}\right)\sqrt{1 - \frac{1}{t^2}} \, \mathrm{d}t. \tag{7}$$

While the integral $I(\mu, \nu)$, for all the values of μ and ν of physical interest, is not difficult to evaluate with good accuracy by a numerical quadrature, taking appropriate care of the square-root 'singularity' at $t = 1$, it would be preferable to be able to evaluate this integral by an analytical method.

It is convenient to define a class of integrals

$$\phi_k(\mu, \nu) = \int_1^\infty \frac{e^{-\mu t}}{\nu^2 + t^2} \frac{1}{t^k} \left(1 + \frac{1}{2t^2}\right) \sqrt{1 - \frac{1}{t^2}}\, dt. \tag{8}$$

The integral $I(\mu, \nu)$ is thus

$$I(\mu, \nu) = \phi_0(\mu, \nu). \tag{9}$$

The functions $\phi_k(\mu, \nu)$ are related to the functions $\chi_k(\mu)$ in the recurrence relation, valid for any integer k,

$$\phi_k(\mu, \nu) = \frac{1}{\nu^2}[\chi_k(\mu) - \phi_{k-2}(\mu, \nu)] \tag{10}$$

which follows from the relation between the integrands in the integral definitions (2) and (8) of these functions. The finite-radius Fourier transform of the Uehling potential at an arbitrary point q is now expressed as

$$\tilde{U}^{(R)}(q) = \tilde{U}^{(\infty)}(q) - \frac{4\alpha e \lambda\!\!\!^{-}_e}{3q} \sin(qR)\phi_0\left(\frac{2R}{\lambda\!\!\!^{-}_e}, \frac{\lambda\!\!\!^{-}_e q}{2}\right) - \frac{2\alpha e \lambda\!\!\!^{-2}_e}{3} \cos(qR)\phi_1\left(\frac{2R}{\lambda\!\!\!^{-}_e}, \frac{\lambda\!\!\!^{-}_e q}{2}\right). \tag{11}$$

The problem of the evaluation of $\tilde{U}^{(R)}(q)$ is thus equivalent to the problem of the evaluation of the functions $\phi_0(\mu, \nu)$ and $\phi_1(\mu, \nu)$. Expanding $(1+1/2t^2)(1-1/t^2)^{1/2}$ in the integrand of the integral definition (8) of $\phi_k(\mu, \nu)$ in powers of $1/t^2$, the following series representation of these functions is obtained:

$$\begin{gathered} \phi_k(\mu, \nu) = \sum_{n=0}^{\infty} a_n \int_1^\infty \frac{e^{-\mu t}}{\nu^2 + t^2} \frac{dt}{t^{2n+k}} = \sum_{n=0}^{\infty} a_n F_{2n+k}(\mu, \nu) \\ a_0 = 1 \qquad a_1 = 0 \qquad a_2 = -\frac{3}{8} \qquad a_n = \frac{(n-1)(2n-5)}{2n(n-2)} a_{n-1}. \end{gathered} \tag{12}$$

Using tabulated integrals (5.1.43 of [6] and 5.221,1 of [9]), the expansion functions $F_m(\mu, \nu)$ in this series can be evaluated in closed form in terms of the exponential integral $E_1(z)$ of a complex argument and the exponential integrals $E_k(\mu)$ as

$$F_m(\mu, \nu) = \int_1^\infty \frac{e^{-\mu t}}{\nu^2 + t^2} \frac{dt}{t^m} = -\frac{1}{\nu} \operatorname{Im}\left[\left(\frac{i}{\nu}\right)^m e^{i\mu\nu} E_1(\mu + i\mu\nu) - \sum_{k=0}^{m-1} \left(\frac{i}{\nu}\right)^{m-k} E_{k+1}(\mu)\right] \tag{13}$$

for non-negative integers m. This supplies starting functions $F_0(\mu, \nu)$ and $F_1(\mu, \nu)$ that can be used in a recurrence evaluation of $F_m(\mu, \nu)$ for any integer m

$$\begin{aligned} F_0(\mu, \nu) &= -\frac{1}{\nu} \operatorname{Im}[e^{i\mu\nu} E_1(\mu + i\mu\nu)] \\ F_1(\mu, \nu) &= -\frac{1}{\nu^2} \{\operatorname{Re}[e^{i\mu\nu} E_1(\mu + i\mu\nu)] - E_1(\mu)\} \\ F_m(\mu, \nu) &= \frac{1}{\nu^2}[E_m(\mu) - F_{m-2}(\mu, \nu)]. \end{aligned} \tag{14}$$

The above recurrence relation is analogous to that of equation (10); it is numerically stable for values $\nu > 1$. The exponential integral $E_1(z)$ with a complex argument can be evaluated by a continued fraction [10]

$$E_1(z) = \mathrm{e}^{-z}\left(\frac{1}{1+z-}\frac{1^2}{3+z-}\frac{2^2}{5+z-}\cdots\right) \tag{15}$$

which converges rapidly for arguments with absolute values $|z| > 1$, which is satisfied amply at points $q_n = (n-\frac{1}{2})\pi/R$ or $n\pi/R$ required in a Fourier–Bessel expansion where $|\mu + \mathrm{i}\mu\nu| > \mu\nu = (n-\frac{1}{2})\pi$ or $n\pi$. The exponential integrals $E_m(\mu), m > 1$ are calculated easily from the standard special function $E_1(\mu)$ using the recurrence relations

$$\begin{aligned} E_m(\mu) &= \frac{\mathrm{e}^{-\mu} - \mu E_{m-1}(\mu)}{m-1} \qquad m \neq 1 \\ E_m(\mu) &= \frac{(m-2-\mu)\mathrm{e}^{-\mu} + \mu^2 E_{m-2}(\mu)}{(m-1)(m-2)} \qquad m \neq 1, 2. \end{aligned} \tag{16}$$

Functions $E_m(\mu)$ with $m \leqslant 0$ are expressible in terms of the exponential function and can be obtained from $E_0(\mu) = \mathrm{e}^{-\mu}/\mu$ with the above recurrence relations.

The terms of the series (12) for the functions $\phi_k(\mu, \nu)$ can be thus calculated accurately and efficiently but the series itself converges very slowly (approximately as the series $\sum_n n^{-5/2}$) and as such is impractical for an accurate evaluation of the functions $\phi_k(\mu, \nu)$ with arguments of physical interest. This problem is solved by expressing the series (12) in terms of a series whose coefficients are the differences $a_n - a_{n+1}$ of the coefficients of (12) and which converges much more rapidly. To this effect the recurrence relation (14) is used for the $n \geqslant 1$ terms in (12):

$$\begin{aligned} \nu^2\phi_k(\mu, \nu) &= \nu^2 a_0 F_k(\mu, \nu) + \sum_{n=1}^{\infty} a_n[E_{2n+k}(\mu) - F_{2n+k-2}(\mu, \nu)] \\ &= \nu^2 a_0 F_k(\mu, \nu) + \chi_k(\mu) - a_0 E_k(\mu) - \sum_{n=0}^{\infty} a_{n+1} F_{2n+k}(\mu, \nu). \end{aligned} \tag{17}$$

Here, the series representation of the functions $\chi_k(\mu)$ in terms of the exponential integrals

$$\chi_k(\mu) = \sum_{n=0}^{\infty} a_n \int_1^{\infty} \frac{\mathrm{e}^{-\mu t}}{t^{2n+k}}\,\mathrm{d}t = \sum_{n=0}^{\infty} a_n E_{2n+k}(\mu) \tag{18}$$

is employed. Adding equations (12) and (17) and using the recurrence relation (14) to write $a_0[\nu^2 F_k(\mu, \nu) - E_k(\mu)]$ as $-a_0 F_{k-2}(\mu, \nu)$, the functions $\phi_k(\mu, \nu)$ are now expressed as

$$\phi_k(\mu, \nu) = \frac{1}{\nu^2+1}[\chi_k(\mu) - a_0 F_{k-2}(\mu, \nu) + \phi_k^{(1)}(\mu, \nu)] \tag{19}$$

where $\phi_k^{(1)}(\mu, \nu)$ represents a series whose coefficients are the differences of the original coefficients. More generally,

$$\phi_k^{(l)}(\mu, \nu) = \sum_{n=0}^{\infty} a_n^{(l)} F_{2n+k}(\mu, \nu) \qquad a_n^{(l)} = a_n^{(l-1)} - a_{n+1}^{(l-1)} \qquad a_n^{(0)} = a_n. \tag{20}$$

The coefficents $a_n^{(l)}$ have the values

$$a_0^{(l)} = \frac{(l-3)(2l+1)}{2l(l-4)} a_0^{(l-1)} \qquad a_n^{(l)} = \frac{(3n+l-3)(2n-5)}{2(n+l)(3n+l-6)} a_{n-1}^{(l)}$$
$$(a_0^{(4)} = -\tfrac{105}{128}) \qquad\qquad (a_1^{(3)} = \tfrac{105}{128}). \tag{21}$$

The series for $\phi_k^{(1)}(\mu, \nu)$ converges sufficiently rapidly so that the expression (19) can be already used for an accurate evaluation of the functions $\phi_k(\mu, \nu)$.

It is useful to repeat the above procedure several times, thus obtaining successive series (20) with higher-order-difference coefficients that converge progressively more rapidly (the rate of convergence of the series $\phi_k^{(l)}(\mu, \nu)$ is approximately that of the series $\sum_n n^{-(l+5/2)}$). In analogy with equation (19), the lth-order series (20) is then expressed in terms of $\phi_k^{(l+1)}(\mu, \nu)$ as

$$\phi_k^{(l)}(\mu, \nu) = \frac{1}{\nu^2+1}[\chi_k^{(l)}(\mu) - a_0^{(l)} F_{k-2}(\mu, \nu) + \phi_k^{(l+1)}(\mu, \nu)] \tag{22}$$

where $\chi_k^{(l)}(\mu)$ are functions defined by series representations in terms of the exponential integrals

$$\chi_k^{(l)}(\mu) = \sum_{n=0}^{\infty} a_n^{(l)} E_{2n+k}(\mu). \tag{23}$$

As $a_n^{(l)} = a_n^{(l-1)} - a_{n+1}^{(l-1)}$, the lth-order functions $\chi_k^{(l)}(\mu)$ are related to functions of order $l-1$ by the relation

$$\chi_k^{(l)}(\mu) = \chi_k^{(l-1)}(\mu) - \chi_{k-2}^{(l-1)}(\mu) + a_0^{(l-1)} E_{k-2}(\mu) \qquad \chi_k^{(0)}(\mu) = \chi_k(\mu). \tag{24}$$

By a repeated use of (24), the lth-order functions can be expressed in terms of the functions $\chi_m(\mu)$ and $E_m(\mu)$ with m decreasing from $m = k$ and $k-2$, respectively, to $m = k-2l$. More explicitly,

$$\chi_k^{(l)}(\mu) = \Delta_{-2}^l \chi_k(\mu) + \sum_{m=0}^{l-1} a_0^{(m)} \Delta_{-2}^{l-1-m} E_{k-2}(\mu) \tag{25}$$

where Δ_{-2}^l is the operator of the backward two-step difference $\Delta_{-2} f_k = f_k - f_{k-2}$ to be applied l-times. It is now seen from equation (22) that $\phi_k^{(l)}(\mu, \nu)/(\nu^2+1)^l$ is the lth-order remainder term in an expansion of $\phi_k(\mu, \nu)$ in powers of $1/(\nu^2+1)$

$$\phi_k(\mu, \nu) = \sum_{n=0}^{l-1} \frac{\chi_k^{(n)}(\mu) - a_0^{(n)} F_{k-2}(\mu, \nu)}{(\nu^2+1)^{n+1}} + \frac{\phi_k^{(l)}(\mu, \nu)}{(\nu^2+1)^l}. \tag{26}$$

The use of equation (25) for the evaluation of the functions $\chi_k^{(n)}(\mu)$, which are needed for the coefficients of the expansion (26), involves the calculation of the differences of numbers that become increasingly large as the expansion order l increases, and so, in principle, this procedure is unstable numerically. The functions $\chi_k^{(n)}(\mu)$ with $n \geqslant 1$ can be calculated accurately, however, by summing directly the series (23). In any case, the lth-order remainder term in the expansion (26) can be evaluated accurately by summing the series (20) for $\phi_k^{(l)}(\mu, \nu)$, which converges rapidly when $l > 1$, and, moreover, the remainder term is a small correction when $l \geqslant 2$ and $\nu \gg 1$. This means that the use of the expansion (26) in Fourier–Bessel calculations of the vacuum-polarization potentials of nuclear charge distributions does not require the expansion order l to be higher than the value $l = 3$, say, and thus, the only functions $\chi_k^{(n)}(\mu)$, $k = 0, 1$ that are then, in fact, needed are of order not greater than $n = 2$ and, therefore, still calculable sufficiently accurately using equation (25) with the functions $\chi_m(\mu)$ with m from $m = 1$ to $m = -4$ (see equation (3)).

Numerical tests were performed with the values of μ and ν employed in the calculations of [3]. They showed that, using equation (26) with $l = 3$ and equation (25), the evaluation of $\phi_k(\mu, \nu)$, $k = 0, 1$ to an accuracy within two digits of the double floating-point precision (i.e. 16 digits) requires a calculation of $\phi_k^{(3)}(\mu, \nu)$, $k = 0, 1$ that included only for the lowest values of ν more than a few terms in the series (20). A computer program VACPOL [11], which can calculate the first-order vacuum-polarization potentials of extended nuclear charge distributions to more than ten-digit accuracy, has been written as an implementation of the analytical methods presented here and those of [3].

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