Accurate and efficient methods for the evaluation of vacuum-polarization potentials of order $Z\alpha$ and $Z\alpha^2$ *

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Rational approximations are presented for the second-order (Uehling) and fourth-order (Källén-Sabry) vacuum-polarization potentials in configuration space. These approximations may be applied to point-charge or finite-inducing-charge distributions. For the second-order potential, two approximations are given, with nominal accuracies of nine and four figures for the range $0 \leq r \leq \infty$. For the fourth-order potential, one approximation of about three-figure accuracy is given for the range $0 \leq r \leq \lambda\!\!\!^{-}_e$.

Although the solution for the lowest-order electron-positron vacuum-polarization potential (second-order correction to the photon propagator) around a point charge was reduced to quadrature[1] in 1935, no entirely satisfactory means of evaluating this result in routine problems has yet been given. This potential is needed for several applications, including the calculation of exotic (and electronic) atom energy levels, and the calculation of some charged-particle scattering cross sections. The best methods of evaluation available to date are two expansions about $r=0$ (r is the distance from the point charge). One is a series due to McKinley.[2] The other is a different expansion[3] based on the so-called Glauber technique,[4] a technique which is apparently due to Rarita and Sommerfield[4] and which involves exponential integrals. Both of these methods fail at large r, and they suffer from unnecessary computational effort for the level of accuracy that they yield. In the present note we report two rational approximations to this function. These approximations are valid over the entire range $0 \leq r \leq \infty$, and they represent considerably improved levels of accuracy and/or efficiency. In addition, we report a somewhat less accurate polynomial fit to the fourth-order vacuum-polarization function.

The second-order vacuum-polarization potential around a static point charge $Z\alpha$, acting on a particle of charge $-e$, is

$$V_2(r) = -\frac{2}{3}\frac{Z\alpha e^2}{\pi r} K_1\left(\frac{2r}{\lambda\!\!\!^{-}_e}\right), \tag{1}$$

where

$$K_1(x) = \int_1^\infty dt\, e^{-xt}\left(\frac{1}{t^2}+\frac{1}{2t^4}\right)(t^2-1)^{1/2} \tag{2}$$

and where $e^2 \approx 1.44$ MeV fm is the square of the electron charge and $\lambda\!\!\!^{-}_e \approx 386.159$ fm is the reduced electron Compton wavelength. For a charge distribution $\rho(\vec{r})$ of finite extent, the corresponding potential is

$$V_2(\vec{r}) = -\frac{2}{3}\frac{\alpha e^2}{\pi}\int d^3r' \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} K_1\left(\frac{2}{\lambda\!\!\!^{-}_e}|\vec{r}-\vec{r}\,'|\right), \tag{3}$$

where $\int d^3r' \rho(\vec{r}\,') = Z$. If $\rho(\vec{r})$ is spherically symmetric, the angular integrations may be performed to obtain

$$V_2(r) = -\frac{2}{3}\frac{\alpha e^2 \lambda\!\!\!^{-}_e}{r}\int_0^\infty dr'\, r'\rho(r')\left[K_0\left(\frac{2}{\lambda\!\!\!^{-}_e}|r-r'|\right) - K_0\left(\frac{2}{\lambda\!\!\!^{-}_e}|r+r'|\right)\right], \tag{4}$$

where

$$K_0(x) = -\int^x dx\, K_1(x) = \int_1^\infty dt\, e^{-xt}\left(\frac{1}{t^3}+\frac{1}{2t^5}\right)(t^2-1)^{1/2}. \tag{5}$$

If the charge distribution $\rho(r')$ is confined to some finite radius, then for relatively large values of r we may expand $K_0(r\pm r')$ in a Taylor series about r, yielding

$$V_2(r) \approx -\frac{2}{3}\frac{Z\alpha e^2}{\pi r}\left[K_1\left(\frac{2r}{\lambda\!\!\!^{-}_e}\right)+\frac{1}{6}\left\langle\left(\frac{2r}{\lambda\!\!\!^{-}_e}\right)^2\right\rangle K_3\left(\frac{2r}{\lambda\!\!\!^{-}_e}\right) + \frac{1}{120}\left\langle\left(\frac{2r}{\lambda\!\!\!^{-}_e}\right)^4\right\rangle K_5\left(\frac{2r}{\lambda\!\!\!^{-}_e}\right)\right], \tag{6}$$

where

$$\left\langle\left(\frac{2r}{\lambda\!\!\!^{-}_e}\right)^n\right\rangle = \frac{1}{Z}\int d^3r' \rho(\vec{r})\left(\frac{2r}{\lambda\!\!\!^{-}_e}\right)^n \tag{7}$$

and where

$$K_n(x) = (-1)^n \frac{d^n}{dx^n} K_0(x). \tag{8}$$

With this definition, all K_n are positive for all x. The fourth-order vacuum-polarization potential is[5]

$$V_4(\vec{r}) = -\frac{e^2\alpha^2}{\pi^2} \int d^3r' \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} L_1\left(\frac{2}{\lambda_e}|\vec{r}-\vec{r}'|\right), \tag{9}$$

where

$$L_1(x) = \int_1^\infty dt\, e^{-xt}\Bigg[\left(-\frac{13}{54t^2}-\frac{7}{108t^4}-\frac{2}{9t^6}\right)(t^2-1)^{1/2}+\left(\frac{44}{9t}-\frac{2}{3t^3}-\frac{5}{4t^5}-\frac{2}{9t^7}\right)\ln[t+(t^2-1)^{1/2}]$$
$$+\left(-\frac{4}{3t^2}-\frac{2}{3t^4}\right)(t^2-1)^{1/2}\ln[8t(t^2-1)]$$
$$+\left(\frac{8}{3t}-\frac{2}{3t^5}\right)\int_t^\infty dy\left(\frac{3y^2-1}{y(y^2-1)}\ln[y+(y^2-1)^{1/2}]-\frac{1}{(y^2-1)^{1/2}}\ln[8y(y^2-1)]\right)\Bigg]. \tag{10}$$

If $L_0(x) = -\int^x dx\, L_1(x)$, then for spherically symmetric $\rho(r)$,

$$V_4(r) = -\frac{e^2\alpha^2}{\pi}\frac{\lambda_e}{r}\int_0^\infty dr'\, r'\rho(r')\left[L_0\left(\frac{2}{\lambda_e}|r-r'|\right) - L_0\left(\frac{2}{\lambda_e}|r+r'|\right)\right]. \tag{11}$$

For large r, we recover

$$V_4(r) \approx -\frac{Ze^2\alpha^2}{\pi^2 r} L_1\left(\frac{2r}{\lambda_e}\right). \tag{12}$$

The approximations of K_n are best in the sense of Chebyshev; that is, the maximum error is minimized with respect to an appropriate weight. The approximations were calculated by using the Remes iteration.[6] The accurate values needed to produce the approximations were obtained from high-order ascending series and asymptotic expansions. If we let $y = xt$ in the expression for $K_n(x)$, we find

$$K_n(x) = \frac{1}{2x^{n-1}}\int_x^\infty dy\,\frac{(2y^2+x^2)(y^2-x^2)^{1/2}y^n e^{-y}}{y^5}. \tag{13}$$

The ascending series is derived by substituting the Taylor-series expansion for e^{-y} and integrating only to a finite upper limit U. The integral is therefore reduced to a sum of elementary forms:

$$\int_x^U dy\, y^m(y^2-x^2)^{1/2} = (U^2-x^2)^{3/2}\sum_{i=0}^{N}\frac{(m-1)!!(m-2i)!!}{(m-2i-1)!!(m+2)!!} \times U^{m-2i-1}x^{2i} + T, \tag{14}$$

where $m \geqslant 0$, $N=[m/2]$, the greatest integer $\leqslant m/2$, and where $T=0$ for m odd and

$$T = \frac{(m-1)!!x^{2N+2}}{(m+2)!!}\left[\frac{(U^2-x^2)^{1/2}}{U} - \ln\left(\frac{U+(U^2-x^2)^{1/2}}{x}\right)\right]$$

for m even. Similar expressions for negative m can be derived. This ascending series is extremely unstable against round-off error. For $U \approx 56$ and $x \approx 35$, a 100-term series evaluated with 57-decimal-digit arithmetic yields K_0 accurate to six significant figures.

The asymptotic series may be derived by substituting $t = 1+\epsilon$ in the expression for $K_n(x)$:

$$K_n(x) = \frac{e^{-x}}{\sqrt{2}}\int_0^\infty d\epsilon\,(3+4\epsilon+2\epsilon^2) \times \epsilon^{1/2}(1+\epsilon/2)^{1/2}(1+\epsilon)^{n-5}e^{-x\epsilon}. \tag{15}$$

Binomial expansions reduce the integral to the elementary form

$$K_n(x) \sim \frac{e^{-x}}{\sqrt{2}}\int_0^\infty d\epsilon \sum_{i=0}^{L}\beta_{n,i}\epsilon^{i+1/2}e^{-x\epsilon} \tag{16}$$

$$= \frac{e^{-x}}{x^{3/2}}\left(\frac{\pi}{2}\right)^{1/2}\sum_{i=0}^{L}\frac{\beta_{n,i}(2i+1)!!}{2^{i+1}x^i}. \tag{17}$$

The coefficients $\beta_{n,i}$ were determined with an algebraic computer language ALTRAN.[7] For K_0,

TABLE I. Coefficients of nine-figure approximations to the second-order functions for $0 \le x \le 1$.

	i	K_0	K_1	K_3	K_5
			Function		
a_i	0	0.883 572 933 75	−0.717 401 817 54	0.999 999 999 87	6.000 000 0002
	1	−0.282 598 173 81	1.178 097 2274	0.000 000 019 7702	−0.000 000 064 3052
	2	−0.589 048 795 78	−0.374 999 630 87	−0.750 000 501 90	0.000 002 104 9413
	3	0.125 001 334 34	0.130 896 755 30	0.785 403 063 16	−0.000 026 711 2715
	4	−0.032 729 913 852	−0.038 258 286 439	−0.349 886 016 55	−0.137 052 361 52
	5	0.008 288 857 4511	−0.000 024 297 2873	0.000 064 596 3330	−0.000 634 761 0409
	6	−0.000 010 327 7658	−0.000 359 201 4867	−0.009 818 908 0747	−0.078 739 801 501
	7	0.000 063 643 6689	−0.000 017 170 0907	0.000 086 513 1458	−0.001 964 174 0173
	8			−0.000 239 692 3662	−0.003 475 236 9349
	9				−0.000 731 453 1622
b_i	0	−319.999 594 323	−64.051 484 3293	5190.101 3646	318.150 793 824
	1	2.539 009 959 81	0.711 722 714 285	82.849 549 620	43.389 886 7347
	2	1.0	1.0	1.0	1.0
c_i	0	−319.999 594 333	64.051 484 3287	27 680.540 606	848.402 116 837
	1	2.539 010 206 62	−0.711 722 686 403	−327.039 477 79	−25.693 986 7765
	2		0.000 804 220 7748		0.320 844 906 346

TABLE II. Coefficients of four-figure approximations to the second-order functions for $0 \le x \le 1$.

	i	K_0	K_1	K_3	K_5
			Function		
a_i	0	0.883 67	−0.717 4042	0.999 93	5.9994
	1	−0.286 08	1.178 207	0.003 2027	0.026 197
	2	−0.568 54	−0.375 8012	−0.772 54	−0.189 39
	3	0.083 589	0.132 8592	0.838 76	0.455 86
	4		−0.039 9244	−0.393 69	−0.514 16
b_i	0	1.0003	−63.999	0.187 49	8.226 53
	1	−0.002 5452	0.709 536	0.005 3068	1.0
	2		1.0		
c_i	0	1.0	63.999	1.0	21.9375
	1		−0.709 539		−0.991 862

TABLE III. Coefficients of nine-figure approximations to the second-order functions for $1 \le x \le \infty$.

	i	K_0	K_1	K_3	K_5
			Function		
d_i	0	5.018 065 179	217.238 6409	8.540 770 444	0.592 430 158 65
	1	71.518 912 62	1643.364 528	60.762 427 66	2.059 631 2871
	2	211.620 9929	2122.244 512	97.146 305 84	3.778 519 0424
	3	31.403 274 78	−45.120 040 44	31.549 735 93	3.561 485 3214
	4	−1.0	1.0	1.0	1.0
e_i	0	2.669 207 401	115.558 9983	4.543 392 478	0.315 118 678 16
	1	51.725 496 69	1292.191 441	35.149 201 69	0.347 324 522 20
	2	296.980 9720	3831.198 012	60.196 686 56	0.038 791 936 870
	3	536.432 4164	2904.410 075	8.468 839 579	−0.001 305 974 1497
	4	153.533 5924			

TABLE IV. Coefficients of four-figure approximations to the second-order functions for $1 \le x \le \infty$.

	i	K_0	K_1	K_3	K_5
d_i	0	10.494	47.946	1.550 30	0.245 685
	1	−1.0	1.0	6.088 30	0.414 457
	2			1.0	1.0
e_i	0	5.7308	27.797	0.806 556	0.122 176
	1	25.305	73.389	3.897 28	−0.016 4658

a 30-term asymptotic series is accurate to more than six significant figures for $x \approx 35$. For K_1, K_3, and K_5 the asymptotic series are accurate to six significant figures for smaller $x \approx 20$.

The approximations themselves are split into two intervals. The form of the approximations for $0 \le x \le 1$ is

$$\begin{aligned} K_0(x) &\approx P_k^{(0)}(x) + xR_{mn}^{(0)}(x^2)\ln x,\\ K_1(x) &\approx P_k^{(1)}(x) + R_{mn}^{(1)}(x^2)\ln x,\\ K_3(x) &\approx x^{-2}P_k^{(3)}(x) + x^2R_{mn}^{(3)}(x^2)\ln x,\\ K_5(x) &\approx x^{-4}P_k^{(5)}(x) + R_{mn}^{(5)}(x^2)\ln x. \end{aligned} \tag{18}$$

TABLE V. Coefficients of three-figure approximations to the fourth-order functions for $0 \le x \le 2$.

	i	L_0	L_1
f_i	0	1.990 159	1.646 407
	1	−2.397 605	−2.092 942
	2	1.046 471	0.962 310
	3	−0.367 066	−0.254 960
	4	0.063 740	0.164 404
	5	−0.037 058	
g_i	0	0.751 198	0.137 691
	1	0.138 889	−0.416 667
	2	0.020 886	−0.097 486
h_i	0	−0.444 444	0.444 444
	1	−0.003 472	0.017 361

$P_k(z)$ denotes a polynomial in z of order k such that

$$P_k(z) = \sum_{i=0}^{k} a_i z^i ,$$

and $R_{mn}(z)$ denotes a rational polynomial such that

TABLE VI. Values of approximate second-order functions. For $x = 1$, the first and second listed values are computed using the small- and large-x approximations, respectively.

x	K_0	K_1	K_3	K_5
		Nine-figure approximations		
0.0	0.883 572 9338	∞	∞	∞
0.25	0.431 371 8736	0.941 790 4049	15.408 171 2707	1535.332 454 0159
0.50	0.262 344 7922	0.484 329 7280	3.521 904 9469	95.571 525 9677
0.75	0.169 089 7271	0.284 529 6070	1.386 096 4849	18.660 744 9367
1.00	0.112 539 5580	0.177 933 5790	0.675 609 0734	5.777 377 5414
1.0	0.112 539 5580	0.177 933 5785	0.675 609 0725	5.777 377 5414
2.0	0.026 012 7364	0.035 932 7228	0.084 134 5872	0.295 219 2271
4.0	0.001 942 7993	0.002 405 2217	0.004 027 2268	0.007 944 0791
8.0	0.000 017 2849	0.000 019 7200	0.000 026 5456	0.000 037 8183
16.0	$2.522\,48 \times 10^{-9}$	$2.722\,43 \times 10^{-9}$	$3.206\,95 \times 10^{-9}$	$3.844\,66 \times 10^{-9}$
		Four-figure approximations		
0.0	0.883 67	∞	∞	∞
0.25	0.431 30	0.941 79	15.407 96	1535.277
0.50	0.262 49	0.484 33	3.521 82	95.5691
0.75	0.169 05	0.284 53	1.386 18	18.6619
1.00	0.112 64	0.177 94	0.675 66	5.777 91
1.0	0.112 54	0.177 95	0.675 61	5.777 42
2.0	0.026 012	0.035 944	0.084 131	0.295 18
4.0	0.001 9452	0.002 3913	0.004 0301	0.007 9858
8.0	0.000 017 284	0.000 019 277	0.000 026 666	0.000 038 646
16.0	2.508×10^{-9}	2.607×10^{-9}	3.240×10^{-9}	3.999×10^{-9}

$$R_{mn}(z)=\frac{\sum_{i=0}^{m} b_i z^i}{\sum_{j=0}^{n} c_i z^i}.$$

The coefficients a_i, b_i, and c_i of the approximations of K_n are given in Table I, and these approximations have an absolute error less than 10^{-9}. The coefficients for four-figure approximations are given in Table II.

On the interval $1 \leqslant x \leqslant \infty$, all the approximations are of the form

$$K_n(x) \approx \frac{e^{-x}}{x^{3/2}} \frac{\sum_{i=0}^{m} d_i x^{-i}}{\sum_{i=0}^{s} e_i x^{-i}}, \tag{19}$$

and Table III contains coefficients for approximations with a maximum absolute error of 10^{-9} and maximum relative error of 10^{-4}. Table IV contains coefficients of approximations with maximum absolute error of 10^{-4} and maximum relative error about 10.

The fourth-order vacuum-polarization integrals $L_0(x)$ and $L_1(x)$ [Eq. (10)] are somewhat more tedious to evaluate, and we have not applied the above methods in this case. Instead, we have used the series due to Blomqvist[5] and the tabulated results of Vogel[8] to produce the Chebyshev approximation

$$L_1(x) \approx \sum_{i=0}^{4} f_i^{(1)} x^i + \sum_{i=0}^{2} g_i^{(1)} x^{2i} \ln x + \sum_{i=0}^{1} h_i^{(1)} x^{4i} \ln^2 x, \tag{20}$$

where the coefficients f_i, g_i, and h_i are given in Table V. Here, the maximum absolute and relative errors over the range $0 < x \leqslant 2$ are less than 10^{-3} and 10^{-2}, respectively. Integration of this expression with respect to x gives

$$L_0(x) \approx \sum_{i=0}^{5} f_i^{(0)} x^i + x \sum_{i=0}^{2} g_i^{(0)} x^{2i} \ln x + x \sum_{i=0}^{1} h_i^{(0)} x^{4i} \ln^2 x, \tag{21}$$

TABLE VII. Values of the approximate fourth-order functions. For $x > 2$, order-of-magnitude estimates are given on the basis of Eq. (22).

	Three-figure approximations	
x	L_0	L_1
0.0	1.990 16	∞
0.25	0.973 72	1.8800
0.50	0.630 27	1.0140
0.75	0.429 10	0.636 38
1.00	0.298 64	0.425 22
1.50	0.148 05	0.207 11
2.00	0.072 65	0.106 58
4.0	4×10^{-3}	6×10^{-3}
8.0	2×10^{-5}	3×10^{-5}
16.0	2×10^{-9}	3×10^{-9}

where the coefficients are also given in Table V. The constant of integration $f_0^{(0)}$ [which drops out in Eq. (11)] has been chosen through a simple assumption about the asymptotic form of $L_0(x)$. We assume that

$$L_0(x) \underset{x\to\infty}{\longrightarrow} \frac{e^{-x}}{x^2}(A + Bx^{-1/2}) \tag{22}$$

and choose A and B to fit $L_1(x)$ near $x=2$. This provides the value of $f_0^{(0)}$ in Table V, along with $A=6.720$ and $B=-6.647$. Clearly, this ansatz is only slightly better than setting the functions to zero for $x > 2$. We note finally that the formulas for L_0 and L_1 are somewhat unstable numerically; presumably a rational approximation would provide a more satisfying fit.

Tables VI and VII contain numerical values of each of these functions K_n and L_n for selected values of x, computed with each approximation.

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