

Tables for Use in Quadrature Formulas Involving Derivatives of the Integrand

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1. Introduction. Tables of the a_j and x_j in the approximate quadrature formulas developed by Hammer and Wicke [1]

$$(1) \int_{-1}^1 f(x) dx = 2 \sum_{i=0}^{(k-1)/2} \frac{f^{(2i)}(0)}{(2i+1)!} + \sum_{j=1}^m a_j [f^{(k)}(x_j) - f^{(k)}(-x_j)], k \text{ odd}$$

$$(2) \int_{-1}^1 f(x) dx = 2 \sum_{i=0}^{(k-2)/2} \frac{f^{(2i)}(0)}{(2i+1)!} + \sum_{j=1}^m a_j [f^{(k)}(x_j) + f^{(k)}(-x_j)], k \text{ even}$$

are given in table 2 for $k = 1, 2, m = 1(1)10$. Coefficients of related orthogonal polynomials are given in table 1 for $k = 1, 2, m = 0(1)11$. The remainder terms for formulas (1) and (2) are

$$(3) R_{k,m} = \begin{cases} \frac{f^{(4m+k+1)}(\eta)}{(4m+1)!} C_{k,m}, k \text{ odd} \\ \frac{f^{(4m+k)}(\eta)}{(4m)!} C_{k,m}, k \text{ even.} \end{cases}$$

The $C_{k,m}$ are listed in table 3, for the same k and m as in table 2.

2. Calculations. The polynomials $P_{m,k}(x)$ were generated by orthonormalization of the sequence $1, x, \dots, x^m$ with weight functions

$$(4) W_k(x) = \begin{cases} \frac{(1-\sqrt{x})^k}{k!}, k \text{ odd} \\ \frac{(1-\sqrt{x})^k}{k! \sqrt{x}}, k \text{ even} \end{cases}$$

on the interval $(0, 1)$. Their coefficients were obtained as solutions to systems of linear equations. The x_j are the square roots of the zeros r_j of $P_{m,k}(x)$. The numbers a_j are determined by

$$(5) a_j = \begin{cases} \frac{A_{m+1,k}}{2x_j P'_{m,k}(r_j) P_{m+1,k}(r_j)}, k \text{ odd} \\ \frac{A_{m+1,k}}{2P'_{m,k}(r_j) P_{m+1,k}(r_j)}, k \text{ even} \end{cases}$$

where $A_{m,k}$ is the quotient of leading coefficients of $P_{m,k}$ and $P_{m-1,k}$. The values of $C_{k,m}$ for use in the remainder terms were derived from

$$(6) C_{k,m} = \begin{cases} 2 \left[\frac{(4m+1)!}{(4m+k+2)!} - \sum_{j=1}^m a_j x_j^{4m+1} \right], k \text{ odd} \\ 2 \left[\frac{(4m)!}{(4m+k+1)!} - \sum_{j=1}^m a_j x_j^{4m} \right], k \text{ even,} \end{cases}$$

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TABLE 1

$k = 1$

$P_0 = 1.73205\ 08075\ 6888$
 $P_1 = 7.53370\ 80350\ 0884x - 2.26011\ 24105\ 0265$
 $P_2 = 30.89988\ 23741\ 862x^2 - 23.66207\ 20883\ 408x + 2.68435\ 27159\ 0420$
 $P_3 = 125.09567\ 55614\ 90x^3 - 156.54342\ 49462\ 16x^2 + 49.95110\ 87256\ 310x - 3.04662\ 58269\ 2541$
 $P_4 = 503.92224\ 31999\ 51x^4 - 878.56845\ 42019\ 08x^3 + 480.77283\ 44538\ 39x^2 - 87.74164\ 92632\ 052x + 3.36803\ 13248\ 0860$
 $P_5 = 2025.03058\ 73957\ 9x^5 - 4532.89143\ 04158\ 0x^4 + 3554.73528\ 18164\ 0x^3 - 1152.71421\ 91499\ 2x^2 + 138.22772\ 15120\ 70x - 3.65996\ 50721\ 1686$
 $P_6 = 8126.60217\ 35502\ x^6 - 22225.89230\ 7314x^5 + 22794.37521\ 9445x^4 - 10831.68147\ 2854x^3 + 2371.48444\ 08556\ x^2 - 202.49633\ 19667\ 4x + 3.92935\ 16425\ 271$
 $P_7 = 32585.34917\ 364x^7 - 1\ 05329.15543\ 67x^6 + 1\ 33708.35590\ 97x^5 - 84369.53936\ 860x^4 + 27562.57790\ 493x^3 - 4390.47486\ 2558x^2 + 281.55199\ 51626x - 4.18076\ 36516\ 86$
 $P_8 = 1\ 30585.72574\ x^8 - 4\ 87145.05832\ x^7 + 7\ 37945.40041\ x^6 - 5\ 82772.09740\ x^5 + 2\ 56072.42057\ x^4 - 61782.59435\ 9x^3 + 7521.30300\ 46x^2 - 376.33313\ 306x + 4.41740\ 68709$
 $P_9 = 5\ 23121.399x^9 - 22\ 12241.35x^8 + 38\ 96351.95x^7 - 37\ 02822.37x^6 + 20\ 55853.62x^5 - 6\ 74493.559x^4 + 1\ 25947.128x^3 - 12137.5185x^2 + 487.72367\ 9x - 4.63163\ 193$
 $P_{10} = 20\ 95022.5x^{10} - 99\ 04599.4x^9 + 198\ 92582.x^8 - 221\ 24981.x^7 + 148\ 91824.x^6 - 62\ 25087.3x^5 + 15\ 95661.1x^4 - 2\ 38415.82x^3 + 18678.058x^2 - 616.56109x + 4.85521\ 90$
 $P_{11} = 83\ 88194.x^{11} - 438\ 42170.x^{10} + 989\ 11790.x^9 - 1261\ 15400.x^8 + 999\ 31000.x^7 - 509\ 73540.x^6 + 167\ 70010.x^5 - 34\ 68084.x^4 + 4\ 25177.7x^3 - 27649.29x^2 + 763.6075x - 5.05931\ 2$

$k = 2$

$P_0 = 1.73205\ 08075\ 6888$
 $P_1 = 12.70977\ 81860\ 449x - 1.27097\ 78186\ 0449$
 $P_2 = 59.88757\ 23920\ 599x^2 - 29.17599\ 68063\ 882x + 1.20652\ 61837\ 2282$
 $P_3 = 259.32961\ 55268\ 10x^3 - 242.98324\ 64964\ 47x^2 + 50.37043\ 53148\ 982x - 1.18192\ 23907\ 2002$
 $P_4 = 1087.36971\ 21542\ 1x^4 - 1531.67966\ 14027\ 7\ x^3 + 633.73798\ 31134\ 97x^2 - 76.31728\ 62592\ 196x + 1.16909\ 13241\ 5856$
 $P_5 = 4487.70266\ 55197\ 8x^5 - 8483.52105\ 08986\ 2x^4 + 5405.81028\ 77031\ 0x^3 - 1335.91407\ 05265\ 8x^2 + 106.99341\ 52181\ 20x - 1.16124\ 14205\ 1600$
 $P_6 = 18355.66707\ 8423x^6 - 43644.30820\ 7345x^5 + 37942.62659\ 3113x^4 - 14721.14915\ 1884x^3 + 2472.29781\ 31355\ x^2 - 142.37405\ 03369\ 3x + 1.15594\ 79227\ 687$
 $P_7 = 74659.95872\ 219x^7 - 2\ 14151.18872\ 09x^6 + 2\ 36965.50353\ 31x^5 - 1\ 27161.63787\ 63x^4 + 34058.68565\ 987x^3 - 4184.54516\ 3429x^2 + 182.43804\ 37977x - 1.15213\ 67777\ 11$
 $P_8 = 3\ 02544.85398\ 6x^8 - 10\ 16908.12494\ x^7 + 13\ 69647.20094\ x^6 - 9\ 45055.96574\ 0x^5 + 3\ 54167.19148\ 2x^4 - 70308.79999\ 50\ x^3 + 6633.07482\ 984x^2 - 227.16794\ 4900x + 1.14926\ 09079\ 5$
 $P_9 = 12\ 22819.3856x^9 - 47\ 14584.9219x^8 + 74\ 930684.8783x^7 - 63\ 42588.4460x^6 + 30\ 83282.8184x^5 - 8\ 64946.91266x^4 + 1\ 33312.13054x^3 - 9996.98758\ 11x^2 + 276.54933\ 828x - 1.14701\ 28163$
 $P_{10} = 49\ 33033.914x^{10} - 214\ 63128.26x^9 + 393\ 48240.15\ x^8 - 395\ 46800.17x^7 + 237\ 46979.27x^6 - 87\ 07972.887x^5 + 19\ 12893.189x^4 - 2\ 36576.7122x^3 + 14474.00552\ x^2 - 330.57026\ 87x + 1.14520\ 6765$
 $P_{11} = 198\ 72572.1x^{11} - 963\ 24095.7x^{10} + 2001\ 94335.x^9 - 2332\ 57625.x^8 + 1672\ 30868.x^7 - 762\ 13570.1x^6 + 220\ 33307.3x^5 - 39\ 12962.35x^4 + 3\ 98072.797x^3 - 20280.6219\ x^2 + 389.22470\ 8x - 1.14373\ 626$

TABLE 2

m	j	k = 1	
		x_j	e_j
1	1	.5477225575 05166	.3042903097 25092
2	1	.3721456511 38755	.2998694151 77678
	2	.7920059217 60865	.0695342880 47154
3	1	.2820900214 17742	.2625168155 42158
	2	.6268601608 87658	.1158516504 33743
	3	.8825310979 63249	.0226513358 72470
4	1	.2273288824 80793	.2283023164 62706
	2	.5140806061 43694	.1313690234 71769
	3	.7563681074 02448	.0510204966 76312
	4	.9248839673 29570	.0093443207 77566
5	1	.1904841804 26525	.2005148719 02275
	2	.4344049427 27343	.1330163257 25257
	3	.6535558761 15115	.0693217404 15712
	4	.8292980447 85322	.0254519669 74067
	5	.9479286287 01912	.0045107921 65497
6	1	.1639811690 9936	.1782134815 8969
	2	.3756528865 1806	.1290409387 9439
	3	.5724366400 9800	.0790426562 2466
	4	.7417866536 8859	.0393058004 7950
	5	.8740336979 4142	.0139874045 8116
	6	.9618129567 5531	.0024324030 3689
7	1	.1439912886 45	.1601387035 18
	2	.3307098113 32	.1229802576 16
	3	.5079816905 42	.0833391819 77
	4	.6669327097 06	.0490821180 75
	5	.8006064071 09	.0237352491 28
	6	.9033361608 21	.0082842932 84
	7	.9708112198 58	.0014235185 93
8	1	.1283703842	.1452769503
	2	.2952852684	.1163542537
	3	.4559661731	.0844453524
	4	.6038699343	.0553533943
	5	.7338622714	.0318100298
	6	.8415994425	.0151045544
	7	.9235314840	.0052043396
	8	.9769705854	.0008871299
9	1	.115823631	.132878407
	2	.266673730	.109816541
	3	.413291816	.083725810
	4	.550684038	.059056710
	5	.674964515	.037887335
	6	.782771237	.021412447
	7	.871235919	.010039513
	8	.938022434	.003428033
	9	.981369607	.000581047
10	1	.10552258	.12239571
	2	.24309589	.10363706
	3	.37773918	.08198747
	4	.50552941	.06098113
	5	.62345737	.04220687
	6	.72888457	.02667176
	7	.81949694	.01489473
	8	.89332330	.00691990
	9	.94876470	.00234732
	10	.98461980	.00039623

TABLE 2—Continued

m	j	k = 2	
		x_j	a_j
1	1	.3162277660 16838	.1666666666 66667
2	1	.2136036212 56443	.1437779500 85321
	2	.6644945298 23701	.0228887165 81346
3	1	.1638297723 39671	.1224797344 91539
	2	.5118494949 80572	.0395183540 10279
	3	.8050693913 12212	.0046685781 64849
4	1	.1336140770 13473	.1060360979 05865
	2	.4169305407 03968	.0469644870 94641
	3	.6739890075 18818	.0123633215 15102
	4	.8733068456 92833	.0013027601 51060
5	1	.1131072568 64736	.0933196598 68176
	2	.3520392516 58368	.0494739624 16079
	3	.5769763210 36054	.0188805340 81087
	4	.7683849647 09291	.0045407258 01483
	5	.9112358854 64930	.0004517844 99852
6	1	.0982014632 7176	.0832757144 1884
	2	.3048169927 4399	.0495578221 5891
	3	.5034255107 0724	.0234294328 9172
	4	.6810857911 4211	.0083180426 8343
	5	.8274681084 1897	.0019025149 7640
	6	.9344124389 0913	.0001831395 3766
7	1	.0868450485 199	.0751675980 885
	2	.2688827298 199	.0484760818 692
	3	.4461187708 020	.0263277958 602
	4	.6095094010 734	.0117357442 186
	5	.7517394338 839	.0039910960 716
	6	.8666985675 800	.0008849203 899
	7	.9495850305 493	.0000834301 748
8	1	.0778891768 89	.0684940996 00
	2	.2406041327 18	.0468585232 40
	3	.4003534653 41	.0280343978 67
	4	.5505429051 14	.0145005204 06
	5	.6858231067 44	.0062300015 19
	6	.8015939596 43	.0020600871 63
	7	.8940032842 24	.0004474372 29
	8	.9600499057 83	.0000415997 26
9	1	.0706369010 2	.0629090570 4
	2	.2177597386 8	.0450255142 4
	3	.3630238378 6	.0289225611 3
	4	.5014536828 7	.0166061935 8
	5	.6290237349 3	.0083212591 4
	6	.7422126043 9	.0034868683 1
	7	.8379675527 1	.0011308362 0
	8	.9137418873 3	.0002420894 9
	9	.9675684295 0	.0000222879 4
10	1	.0646394150	.0581677528
	2	.1989137370	.0431420181
	3	.3320234405	.0292595373
	4	.4601078372	.0181452843
	5	.5800614933	.0101353888
	6	.6891397684	.0049671598
	7	.7849102517	.0020445253
	8	.8652666620	.0006538257
	9	.9284600004	.0001385086
	10	.9731500562	.0000126607

TABLE 3*

$k = 1$		$k = 2$	
m	$C_{1,m}$	m	$C_{2,m}$
1	1.7619×10^{-2}	1	6.1905×10^{-3}
2	1.0473×10^{-3}	2	2.7882×10^{-4}
3	6.3902×10^{-5}	3	1.4869×10^{-5}
4	3.9380×10^{-6}	4	8.4576×10^{-7}
5	2.4386×10^{-7}	5	4.9654×10^{-8}
6	1.5142×10^{-8}	6	2.9680×10^{-9}
7	9.4185×10^{-10}	7	1.7940×10^{-10}
8	6.3112×10^{-11}	8	1.0922×10^{-11}
9	7.7×10^{-11}	9	6.8464×10^{-12}
10	-3.3×10^{-10}	10	-2.8×10^{-13}

* These figures include round-off errors.

and thus show effects of round-off errors in a_j and x_j as well as the theoretical remainder. Since the matrix of the linear system solved to find the coefficients of $P_{m,k}(x)$ is ill-conditioned, the accuracy of the figures decreases rapidly with increasing m . Figures are kept to the upper limit of accuracy. If results are rounded to one or two fewer significant figures than are carried in the table of x_j , there is no doubt of the accuracy of the digits kept.

The formulas were derived in [1]. The calculations were carried out in the Numerical Analysis Laboratory of the University of Wisconsin on the IBM 650. An 18-digit floating-decimal interpretive routine by Eugene Albright and a linear systems solver by Gerald Thorne were used. I am indebted to William Kammerer for several helpful suggestions.

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1. P. C. HAMMER & H. H. WICKE, "Quadrature formulas involving derivatives of the integrand," *Math. Comp. (MTAC)*, v. 14, 1960, p. 3-7.