

RATIONAL APPROXIMATIONS FOR THE HOLTSMARK DISTRIBUTION, ITS CUMULATIVE AND DERIVATIVE

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Abstract—The convergent series expansions of the Holtsmark distribution $P(\beta)$, its cumulative $Q(\beta)$, its derivative $R(\beta)$ and the semiconvergent asymptotic series for these functions are used to calculate rational approximations for P , Q , and R , which are valid for all positive β and have maximum errors of approximately 10^{-8} , 10^{-9} and 10^{-7} , respectively.

1. INTRODUCTION

Despite the great advances over the past three decades in the theory of plasma microfield distribution functions, which has been conveniently summarized by Iglesias, Hooper and DeWitt,¹ the distribution function derived by Holtsmark² is still of considerable value in dealing with certain properties of low-density, high-temperature plasmas in which particle correlations are unimportant. Recently, the need for the evaluation of the Holtsmark distribution, its cumulative and derivative has arisen in the calculation of atomic partition functions.³ The technique of Padé approximants is used to calculate rational approximations for these three functions which are valid for all values of the reduced field strength β .

2. ANALYSIS

We consider the Holtsmark distribution function

$$P(\beta) = (2\beta/\pi) \int_0^\infty dt t \sin \beta t e^{-t^{3/2}} = (2/\beta\pi) \int_0^\infty dt t \sin t e^{-(t/\beta)^{3/2}}, \quad (1)$$

its cumulative

$$Q(\beta) = \int_0^\beta d\beta' P(\beta') \quad (2)$$

and its derivative, which we here call $R(\beta)$. Expanding $\sin \beta t$ in the first integral in Eq. (1) and integrating term by term, we obtain

$$P(\beta) = (4/3\pi) \beta^2 \sum_{n=0}^{\infty} a_n \beta^{2n}, \quad a_n \equiv (-1)^n \Gamma\left(\frac{4}{3}n + 2\right) / \Gamma(2n + 2). \quad (3)$$

Integrating and differentiating this expression yields

$$Q(\beta) = (4/9\pi) \beta^3 \sum_{n=0}^{\infty} b_n \beta^{2n}, \quad b_n \equiv 3 a_n / (2n + 3), \quad (4)$$

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and

$$R(\beta) = (8/3\pi) \beta \sum_n c_n \beta^{2n}, \quad c_n \equiv (n+1) a_n. \quad (5)$$

The coefficients in Eqs. (3), (4) and (5) are normalized so that $a_n = b_n = c_n = 1$; values for larger values of n are readily generated by recursion.

To obtain asymptotic expressions, we follow Holtmark² by expanding $[\exp - (t/\beta)^{3/2}]$ in the second form of Eq. (1), then replacing $\sin t$ by $\text{Im } e^{it}$. Defining a new variable of integration $u = -it$, we obtain

$$P(\beta) \sim (2/\pi\beta) \sum_{n=0}^{\infty} (-1)^{n+1} \sin(3n\pi/4) \Gamma\left(\frac{3n}{2} + 2\right) \beta^{-3n/2}/n!. \quad (6)$$

Terms with $n = 0, 4, 8, \dots$ vanish. It is convenient to shift the index of summation by one so that the first term is nonzero:

$$P(\beta) \sim (15/8) \sqrt{2/\pi} \beta^{-5/2} \sum_{m=0}^{\infty} \tilde{a}_m \beta^{-3m/2}, \quad (7)$$

where

$$\tilde{a}_m \equiv (8/15) \sqrt{2/\pi} \sin(3(m+1)\pi/4) \Gamma\left(\frac{3m+7}{2}\right) / \Gamma(m+2); \quad (8)$$

we have chosen the normalization so that $\tilde{a}_0 = 1$. Recursion relations for \tilde{a}_m are easily derived from those for $\Gamma(n)$. Integrating and recalling that $P(\beta)$ is normalized to unity, we have

$$Q(\beta) = 1 - \int_{\beta}^{\infty} d\beta' P(\beta') \sim 1 - (5/4) \sqrt{2/\pi} \beta^{-3/2} \sum_{m=0}^{\infty} \tilde{b}_m \beta^{-3m/2},$$

$$\tilde{b}_m = \tilde{a}_m / (m+1). \quad (9)$$

Differentiating Eq. (7) leads immediately to

$$R(\beta) \sim (-75/16) \sqrt{2/\pi} \beta^{-7/2} \sum_{m=0}^{\infty} \tilde{c}_m \beta^{-3m/2}, \quad \tilde{c}_m = (1 + 3m/5) \tilde{a}_m. \quad (10)$$

3. RATIONAL APPROXIMATIONS

We now calculate rational approximations to $P(\beta)$, $Q(\beta)$ and $R(\beta)$ in the following form:

$$0 \leq \beta \leq \beta^*: \quad P(\beta) = (4/3\pi) \beta^2 u_1(x)/v_1(x), \quad (11)$$

$$Q(\beta) = (4/9\pi) \beta^3 u_2(x)/v_2(x), \quad (12)$$

$$R(\beta) = (8/3\pi) \beta u_3(x)/v_3(x); \quad (13)$$

$$\beta^* \leq \beta < \infty: \quad P(\beta) = (15/8) \sqrt{2/\pi} \beta^{-5/2} u_4(y)/v_4(y), \quad (14)$$

Table 1. Coefficients for $P(\beta)$.

n	c_{1n}			d_{1n}			c_{4n}			d_{4n}		
$\beta^* = 5.35, \quad L_1 = 12, \quad M_1 = 13, \quad L_4 = M_4 = 12$												
1	5.3213	58196	9315-2	5.1623	99953	7559-1	-5.8279	10992	3206+1	-6.3385	57111	2344+1
2	9.6792	05787	7047-3	1.2611	69195	1988-1	1.5802	12612	3226+3	1.8894	51071	1591+3
3	4.0835	19154	2469-4	1.9324	87786	9202-2	-2.5497	91301	9232+4	-3.4231	19239	9947+4
4	3.1725	79323	7450-5	2.0744	70827	3751-3	2.6383	10629	3289+5	4.1165	14954	9442+5
5	9.3347	92974	9771-7	1.6494	11125	0278-4	-1.7461	32102	3968+6	-3.3708	17266	3750+6
6	4.0297	73892	3818-8	1.0006	54492	1671-5	6.6626	75117	1900+6	1.8369	81594	1601+7
7	7.2634	59051	1209-10	4.6967	04829	4008-7	-7.3155	45947	2329+6	-5.9159	11859	7522+7
8	1.8177	22697	7773-11	1.7082	31490	7411-8	-5.2626	44361	9572+7	4.9132	01859	9912+7
9	1.5079	59904	3503-13	4.7633	89532	2910-10	2.4110	43181	9602+8	4.5437	54584	6985+8
10	2.0246	46471	2406-15	9.9179	96748	2997-12	-3.1988	13057	5441+8	-2.1012	34228	3505+9
11	1.4246	57599	3322-19	1.4634	21335	3989-13	-2.6036	18538	7058+7	3.8908	91660	4974+9
12	1.5130	90778	2746-20	1.3749	76403	5118-15	-3.7993	38432	7787+6	-2.7548	75377	6661+9
13				6.2306	99595	2226-18						

$$Q(\beta) = 1 - (5/4) \sqrt{2/\pi} \beta^{-3/2} u_5(y)/v_5(y), \quad (15)$$

$$R(\beta) = (-75/16) \sqrt{2/\pi} \beta^{-7/2} u_6(y)/v_6(y), \quad (16)$$

where

$$x \equiv \beta^2, \quad y \equiv \beta^{-3/2}, \quad (17)$$

and

$$u_i(t) \equiv \sum_{n=0}^{L_i} c_{in} t^n, \quad v_i(t) \equiv \sum_{n=0}^{M_i} d_{in} t^n, \quad i = 1, 2, \dots, 6. \quad (18)$$

The coefficients c_{in} and d_{in} are independent of β^* and are equal to unity for $n = 0$. The value of β^* may be different for each of the three functions, and is chosen after the coefficients are evaluated so as to minimize the error.

The coefficients c_{in} and d_{in} are determined by equating in turn each rational expression (11)–(16) to the appropriate series from Sec. 2, cross multiplying and formally equating like powers of x or y , as described, for example, by Baker;⁴ this is the simplest form of the Padé approximation procedure. The resulting linear systems are described by matrices with elements that depend only on the *difference* of row and column indices, i.e. so-called Toeplitz matrices. We exploit this feature of the system matrix, using a subroutine written by G. B. Rybicki, in order to reduce computing time and to increase accuracy. The calculations have been carried out with 30 sf arithmetic for a number of choices of the polynomial orders L_i and M_i .

To select the optimum values of L_i , M_i and β^* , accurate values of $P(\beta)$ and $R(\beta)$ were evaluated by direct numerical integration using the form

$$P(\beta) = (2/\beta\pi) \int_0^{2\pi} dt \sin t \sum_{n=0}^{\infty} (2n\pi + t) \exp\{-[(2n\pi + t)/\beta]^{3/2}\}, \quad (19)$$

Table 2. Coefficients for $Q(\beta)$.

n	c_{1n}	d_{1n}	c_{5n}	d_{5n}
$\beta^* = 5.40$, $L_2 = M_2 = L_4 = M_4 = 12$				
1	1.8966 -2013	8780-1	4.6768 -6494	3157-1
2	2.5317 91426	7416+2	1.0267 05493	0802+1
3	2.1210 29801	3271+3	1.4014 74346	7985+2
4	1.3479 85005	8071+4	1.3281 43573	8511+3
5	6.2081 05054	2043+6	9.1250 02904	7627+5
6	2.1963 85329	1836+7	4.2617 42187	3130+6
7	5.6533 16102	3147+9	1.8740 12759	8294+7
8	1.0682 77496	3144+10	5.5486 91202	7141+9
9	1.3129 60298	0283+12	1.2082 08502	7751+10
10	9.5647 53100	6326+15	1.8199 90125	8672+12
11	1.8572 76100	1340+17	1.7633 87494	2625+14
12	-1.4989 85216	0908+20	8.0671 51538	7642+17

together with a similar expression for $R(\beta)$. Error curves were computed for each rational approximation for the interval $4.0 \leq \beta \leq 6.0$, in which the small- β and large- β forms were expected to have comparable errors. By choosing the small- β and large- β form with the smallest errors, plotting the error curves and locating the intersection point, we determined for $P(\beta)$ the optimum value $\beta^* = 5.35$, which corresponds to a maximum relative error $\epsilon_{\max} = 8.9 \times 10^{-9}$ for the approximations with $L_1 = 12$, $M_1 = 13$, $L_4 = M_4 = 12$. For $R(\beta)$, we find $\beta^* = 5.15$, $\epsilon_{\max} = 1.6 \times 10^{-7}$ for $L_3 = 13$, $M_3 = 14$, $L_6 = 14$, $M_6 = 13$. No check values were computed for $Q(\beta)$, but by comparing the small- β and large- β forms for $L_2 = M_2 = L_5 = M_5 = 12$ in the neighborhood of $\beta = 5.0$, we find $\beta^* = 5.40$ and $\epsilon_{\max} \simeq 1 \times 10^{-9}$. The coefficients of the rational approximations

Table 3. Coefficients for $R(\beta)$.

n	c_{1n}	d_{1n}	c_{5n}	d_{5n}
$\beta^* = 5.15$, $L_3 = 13$, $M_3 = 14$, $L_6 = 14$, $M_6 = 13$				
1	-3.7714 53756	2388-1	5.4890 74511	8867-1
2	2.8658 82706	1726-3	1.4339 80601	8754-1
3	-2.4970 47597	8578-3	2.3655 23418	8604-2
4	-1.0908 00305	5922-5	2.7557 98165	8846-3
5	-5.9411 20278	1125-6	2.4012 66306	8210-4
6	-3.0835 58842	5598-8	1.6159 55789	5932-5
7	-6.0080 85045	0585-9	8.5441 37592	2706-7
8	-1.3513 40679	4647-11	3.5723 07268	9829-8
9	-2.4485 98156	7752-12	1.1773 49943	0426-9
10	4.5538 91752	5173-15	3.0167 15665	4715-11
11	-3.2230 60591	6261-16	5.8399 29379	7887-13
12	1.5088 21629	8286-18	8.0938 93466	2632-15
13	-7.4026 17976	4104-21	7.2087 55477	9050-17
14			3.1227 32286	7957-19

Table 4. Values of Functions.

β	$P(\beta)$	$Q(\beta)$	$R(\beta)$
1.0	2.7122 08070-1	1.0860 77296-1	3.0773 83690-1
2.0	3.3693 87827-1	4.5176 18482-1	-1.3340 16902-1
3.0	1.7606 29272-1	7.0774 78512-1	-1.3848 70538-1
4.0	8.0673 54136-2	8.2946 55532-1	-5.9639 21261-2
5.0	4.1180 23725-2	8.8754 44652-1	-2.4943 81058-2
6.0	2.3822 08458-2	9.1896 59950-1	-1.1778 55295-2
7.0	1.5164 57557-2	9.3800 57335-1	-6.2662 27225-3
8.0	1.0349 76409-2	9.5054 78667-1	-3.6610 34529-3
9.0	7.4383 07487-3	9.5932 91180-1	-2.2977 05335-3
10.0	5.5613 46283-3	9.6576 48611-1	-1.5242 96364-3

defined by Eqs. (11)–(16) are given in Tables 1, 2 and 3 for $P(\beta)$, $Q(\beta)$ and $R(\beta)$, respectively. To enable users to check that these coefficients are correctly entered into their programs, we give in Table 4 ten-digit values of the functions for $\beta = 1(1)10$ generated by the approximations given here; not all of the digits are necessarily significant.

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REFERENCES

1. C. A. Iglesias, C. F. Hooper, Jr. and H. E. DeWitt, *DeWitt, Phys. Rev. A* **28**, 361 (1983).
2. J. Holtzmark, *Ann. Phys.* **58**, 577 (1919).
3. D. G. Hummer and D. Mihalas, *Astrophys. J.* In press.
4. G. A. Baker, Jr., *Essentials of Padé Approximants*, p. 5. Academic Press, New York (1975).