

Numerical Evaluation of Debye Function

$$D(x) = \frac{3}{x^3} \int_0^x \frac{t^3 dt}{e^t - 1}$$

Algorithm:

A. Given x , determine D according to:

- $x = 0; D = 1;$
- $0 < x \leq 0.1; D = 1 - 0.375 * x + x^2 * (0.05 - 5.952380953 \times 10^{-4} * x^2);$
- $0.1 < x \leq 7.25; D = \frac{((0.0946173*x-4.432582)*x+85.07724)*x-800.6087}{((x+15.121491)*x+143.155337)*x+682.0012} * x + 3953.632;$
- $x > 7.25; D$ is determined as follows:

Obtain the integer N from:

$$N = 25.0/x;$$

Determine $D(x)$ from the following loop:

$$D = 0;$$

$$D2 = 1;$$

if $x \leq 25$, do the loop from 1 to truncated integer value of N

for $I = 1:N$

$$\text{DS} = I; D2 = D2 * x^2; x3 = DS * x;$$

$$D = D + D2 * \frac{6.0 + x3 * (6.0 + x3 * (3.0 + x3))}{DS^4};$$

end;

if $x > 25$, skip the loop, and obtain D as follows:

$$D = 3 * \frac{6.493939402 - D}{x^3};$$

The figure below compares the calculated values with reference values. Differences are $< 10^{-6}$. See below for FORTRAN subroutine

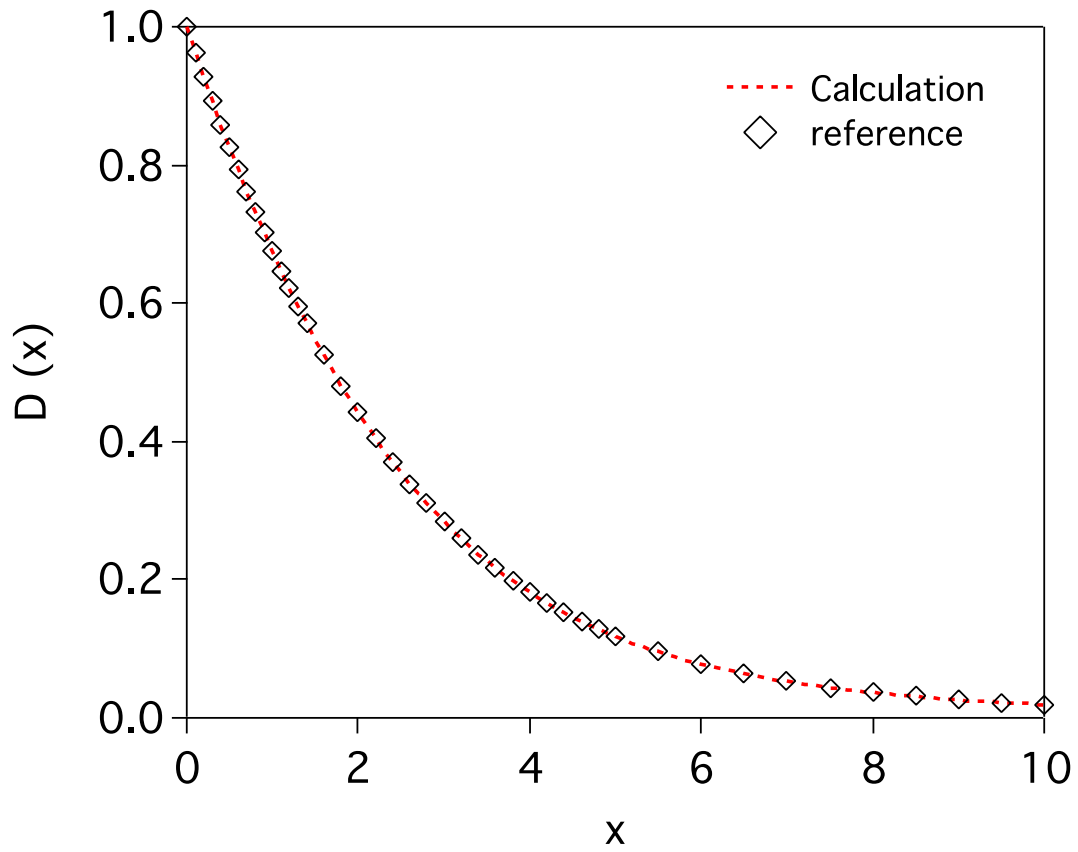


Fig. 1 $D(x)$ versus x up to 10. Dash line is the calculation and diamond symbols are from reference table.

Reference: J. W. Swegle, Sandia report, SAN89-1443 UC-404, 1989.

(Jue Wang, Apr. 2012)

Table 1.

x	D(x) Calculated	D(x) Table
0.0	1.000000	1.000000
0.1	0.963000	0.963000
0.2	0.926999	0.926999
0.3	0.891995	0.891995
0.4	0.857985	0.857985
0.5	0.824963	0.824963
0.6	0.792924	0.792924
0.7	0.761859	0.761859
0.8	0.731759	0.731759
0.9	0.702615	0.702615
1.0	0.674416	0.674416
1.1	0.647148	0.647148
1.2	0.620798	0.620798
1.3	0.595351	0.595351
1.4	0.570793	0.570793
1.5	0.547106	
1.6	0.524274	0.524275
1.7	0.502279	
1.8	0.481102	0.481103
1.9	0.460725	
2.0	0.441128	0.441129
2.1	0.422290	
2.2	0.404193	0.404194
2.3	0.386815	
2.4	0.370136	0.370137
2.5	0.354135	
2.6	0.338792	0.338793
2.7	0.324085	
2.8	0.309994	0.309995
2.9	0.296499	
3.0	0.283579	0.283580
3.1	0.271214	
3.2	0.259384	0.259385
3.3	0.248070	
3.4	0.237252	0.237252
3.5	0.226911	
3.6	0.217029	0.217030
3.7	0.207588	
3.8	0.198571	0.198571

3.9	0.189959	
4.0	0.181737	0.181737
4.1	0.173888	
4.2	0.166396	0.166396
4.3	0.159246	
4.4	0.152424	0.152424
4.5	0.145914	
4.6	0.139704	0.139704
4.7	0.133780	
4.8	0.128129	0.128129
4.9	0.122738	
5.0	0.117597	0.117597
5.1	0.112693	
5.2	0.108015	
5.3	0.103554	
5.4	0.099299	
5.5	0.095240	0.095241
5.6	0.091368	
5.7	0.087675	
5.8	0.084151	
5.9	0.080789	
6.0	0.077581	0.077581
6.1	0.074519	
6.2	0.071597	
6.3	0.068808	
6.4	0.066146	
6.5	0.063604	0.063604
6.6	0.061177	
6.7	0.058858	
6.8	0.056644	
6.9	0.054528	
7.0	0.052506	0.052506
7.1	0.050573	
7.2	0.048726	
7.3	0.046960	
7.4	0.045271	
7.5	0.043655	0.043655
7.6	0.042109	
7.7	0.040630	
7.8	0.039214	
7.9	0.037858	

8.0	0.036560	0.036560
8.1	0.035317	
8.2	0.034126	
8.3	0.032984	
8.4	0.031890	
8.5	0.030840	0.030840
8.6	0.029834	
8.7	0.028869	
8.8	0.027942	
8.9	0.027053	
9.0	0.026200	0.026200
9.1	0.025380	
9.2	0.024593	
9.3	0.023837	
9.4	0.023110	
9.5	0.022411	0.022411
9.6	0.021739	
9.7	0.021092	
9.8	0.020470	
9.9	0.019872	
10.0	0.019296	0.019296

27. Miscellaneous Functions

27.1. Debye Functions

Series Representations

27.1.1

$$\int_0^x \frac{t^n dt}{e^t - 1} = x^n \left[\frac{1}{n} - \frac{x}{2(n+1)} + \sum_{k=1}^{\infty} \frac{B_{2k} x^{2k}}{(2k+n)(2k)!} \right]$$

($|x| < 2\pi, n \geq 1$)

(For Bernoulli numbers B_{2k} , see chapter 23.)

27.1.2

$$\int_x^{\infty} \frac{t^n dt}{e^t - 1} = \sum_{k=1}^{\infty} e^{-kx} \left[\frac{x^n}{k} + \frac{nx^{n-1}}{k^2} + \frac{(n)(n-1)x^{n-2}}{k^3} + \dots + \frac{n!}{k^{n+1}} \right] (x > 0, n \geq 1)$$

Relation to Riemann Zeta Function (see chapter 23)

27.1.3

$$\int_0^{\infty} \frac{t^n dt}{e^t - 1} = n! \zeta(n+1).$$

[27.1] J. A. Beattie, Six-place tables of the Debye energy and specific heat functions, *J. Math. Phys.* **6**, 1-32 (1926).

$$\frac{3}{x^3} \int_0^x \frac{y^3 dy}{e^y - 1}, \frac{12}{x^5} \left[\int_0^x \frac{y^3 dy}{e^y - 1} - \frac{3x}{e^x - 1} \right], x=0(.01)24, \quad 6S.$$

[27.2] E. Grüneisen, Die Abhängigkeit des elektrischen Widerstandes reiner Metalle von der Temperatur, *Ann. Physik.* (5) **16**, 530-540 (1933).

$$\frac{20}{x^5} \int_0^x \frac{t^4 dt}{e^t - 1} - \frac{4x}{e^x - 1}, \quad x=0(.1)13(.2)18(1)20(2)52(4)80, \quad 4S.$$

Table 27.1

Debye Functions

x	$\frac{1}{x} \int_0^x \frac{t dt}{e^t - 1}$	$\frac{2}{x^2} \int_0^x \frac{t^2 dt}{e^t - 1}$	$\frac{3}{x^3} \int_0^x \frac{t^3 dt}{e^t - 1}$	$\frac{4}{x^4} \int_0^x \frac{t^4 dt}{e^t - 1}$
0.0	1.000000	1.000000	1.000000	1.000000
0.1	0.975278	0.967083	0.963000	0.960555
0.2	0.951111	0.934999	0.926999	0.922221
0.3	0.927498	0.903746	0.891995	0.884994
0.4	0.904437	0.873322	0.857985	0.848871
0.5	0.881927	0.843721	0.824963	0.813846
0.6	0.859964	0.814940	0.792924	0.779911
0.7	0.838545	0.786973	0.761859	0.747057
0.8	0.817665	0.759813	0.731759	0.715275
0.9	0.797320	0.733451	0.702615	0.684551
1.0	0.777505	0.707878	0.674416	0.654874
1.1	0.758213	0.683086	0.647148	0.626228
1.2	0.739438	0.659064	0.620798	0.598599
1.3	0.721173	0.635800	0.595351	0.571967
1.4	0.703412	0.613281	0.570793	0.546317
1.6	0.669366	0.570431	0.524275	0.497882
1.8	0.637235	0.530404	0.481103	0.453131
2.0	0.606947	0.493083	0.441129	0.411893
2.2	0.578427	0.458343	0.404194	0.373984
2.4	0.551596	0.426057	0.370137	0.339218
2.6	0.526375	0.396095	0.338793	0.307405
2.8	0.502682	0.368324	0.309095	0.278355
3.0	0.480435	0.342614	0.283580	0.251879
3.2	0.459555	0.318834	0.259385	0.227792
3.4	0.439962	0.296859	0.237252	0.205915
3.6	0.421580	0.276565	0.217030	0.186075
3.8	0.404332	0.257835	0.198571	0.168107
4.0	0.388148	0.240554	0.181737	0.151855
4.2	0.372958	0.224615	0.166396	0.137169
4.4	0.358696	0.209916	0.152424	0.123913
4.6	0.345301	0.196361	0.139704	0.111957
4.8	0.332713	0.183860	0.128129	0.101180
5.0	0.320876	0.172329	0.117597	0.091471
5.5	0.294240	0.147243	0.095241	0.071228
6.0	0.271260	0.126669	0.077581	0.055677
6.5	0.251331	0.109727	0.063604	0.043730
7.0	0.233948	0.095707	0.052506	0.034541
7.5	0.218698	0.084039	0.043655	0.027453
8.0	0.205239	0.074269	0.036560	0.021968
8.5	0.193294	0.066036	0.030840	0.017702
9.0	0.182633	0.059053	0.026200	0.014368
9.5	0.173068	0.053092	0.022411	0.011747
10.0	0.164443	0.047971	0.019296	0.009674

$$\left[\begin{matrix} (-4)5 \\ 5 \end{matrix} \right]$$

$$\left[\begin{matrix} (-4)6 \\ 5 \end{matrix} \right]$$

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IF (TAU3(K3) .GT. 0. .AND. P .GT. TAU3(K3)) THEN
  X=XFROZN
  RETURN
ENDIF
X=XFROZN-TAU1(K3)*(XFROZN-XRVSBL)**TAU2(K3)*DV/
1 (VOA(K3,1)-VOA(K3,2))
X=MIN(X,XFROZN)
X=MAX(X,XRVSBL)
ENDIF
RETURN
END
SUBROUTINE DEBYEF(X,D)
SAVE
C EVALUATE DEBYE FUNCTIONS. TAKEN FROM ANEOS PACKAGE
C PARAMETERS:
C X = ARGUMENT (THETA/T) (INPUT)
C D = DEBYE FUNCTION (OUTPUT)
C D(X)=(3/X**3)*INTEGRAL( (Y=0,X) OF Y**3/(EXP(Y)-1) )
  IF(X.EQ.0.)THEN
    D=1.
    RETURN
  ENDIF
  EXX=EXP(-X)
  IF(X.GT.0.1) GO TO 5
  X2=X*X
  D=1.-.375*X+X2*(.05-5.952380953E-4*X2)
  RETURN
5 IF(X-7.25) 10,10,13
10 D=(((.0946173*X-4.432582)*X+85.07724)*X-800.6087)*X+3953.632)
  1 /(((X+15.121491)*X+143.155337)*X+682.0012)*X+3953.632)
  RETURN
13 N=25./X
  D=0.
  IF (N.LE.0) GO TO 20
  D2=1.
  DO 15 I=1,N
    DS=I
    D2=D2*EXX
    X3=DS*X
  15 D=D+D2*(6.+X3*(6.+X3*(3.+X3)))/(DS**4)
  20 D=3.*(6.493939402-D)/(X**3)
  RETURN
  END
SUBROUTINE PHMP(L,TOM,V01)

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