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;
- $0 < x \leq 0.1$; $D = 1 - 0.375 * x + x^2 * (0.05 - 5.952380953 \times 10^{-4} * x^2)$;
- $0.1 < x \leq 7.25$; $D = \frac{\left(((0.0946173*x-4.432582)*x+85.07724)*x-800.6087\right)*x+3953.632}{\left(((x+15.121491)*x+143.155337)*x+682.0012\right)*x+3953.632}$;
- $x > 7.25$; 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 the truncated integer value of N

For i=1:N   where i is a counter in all formulae below
$D2 = D2 * e^{-x}$;
$x3 = i * x$;

$$D = D + D2 * \frac{6 + x3 * \left(6 + x3 * \left(6 + x3 * (3 + x3)\right)\right)}{i^4}$$

end loop

After the loop, calculate the final D value by:

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

If $x > 25$, skip the loop and obtain D by the final equation given directly above.

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

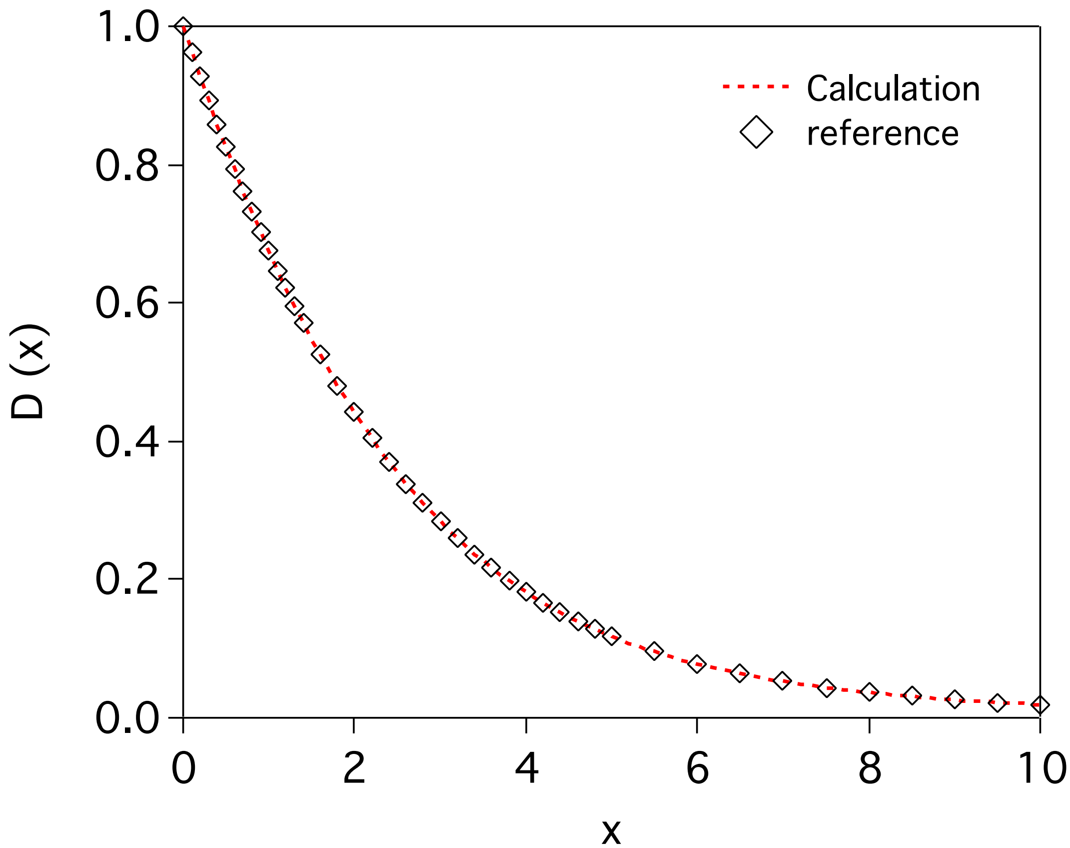

Fig. 1 D (x) versus x up to 10. Dash line is the calculation and diamond symbols are from reference table.

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

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

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

27.1.2

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

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).

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

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

$\frac{20}{x^4}\int_0^x \frac{t^4dt}{e^t-1} - \frac{4x}{e^x-1}$,

$x=0(.1)13(.2)18(1)20(2)52(4)80$, 4S.

Table 27.1 **Debye Functions**

x	$\frac{1}{x}\int_0^x \frac{t\,dt}{e^t-1}$	$\frac{2}{x^2}\int_0^x \frac{t^2dt}{e^t-1}$	$\frac{3}{x^3}\int_0^x \frac{t^3dt}{e^t-1}$	$\frac{4}{x^4}\int_0^x \frac{t^4dt}{e^t-1}$
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	0.598598
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	0.309995	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
	$\left[{(-4)5 \atop 5}\right]$	$\left[{(-4)6 \atop 5}\right]$	$\left[{(-4)6 \atop 5}\right]$	$\left[{(-4)6 \atop 5}\right]$

```
      IF(TAU3(K3).GT.O..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=O,X) OF Y**3/(EXP(Y)-1) )
      IF(X.EQ.O.)THEN
       D=1.
       RETURN
      ENDIF
      EXX=EXP(-X)
      IF(X.GT.O.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=O.
      IF (N.LE.O) 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,VO1)
```

```
function D = Debye( x )
%Numerical evaluation of Debye Function
format long
if x==0
    D=1;
elseif x>0 && x<=0.1
        D=1-0.375*x+x^2*(0.05-5.952380953e-4*x^2);

elseif x>0.1 && x<=7.25
    D=((((0.0946173*x-4.432582)*x+85.07724)*x-800.6087)*x+3953.632)/((((x+15.121491)↙
*x+143.155337)*x+682.0012)*x+3953.632);

elseif x>7.25
                N=25/x;
                D=0;
                D2=1;

                if x<=25
                    for i=1:floor(N)
                        D2=D2*exp(-x);
                        x3=i*x;
                        D=D+D2*(6+x3*(6.0+x3*(3+x3)))/i^4;
                    end
                D=3*(6.493939402-D)/x^3;
                elseif x>25
                        D=3*(6.493939402-D)/x^3;
                    end

else disp('something is wrong')
end


end
```