TABLES OF FUNCTIONS WHICH OCCUR
IN THE THEORY OF THERMAL VIBRATIONS

by

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ABSTRACT

Tables of the population function, the average energy function, the Einstein and Debye specific heat functions, and the Debye diffraction function are given. These functions are of value in elementary calculations of the specific heat and diffraction effects of crystals.
1. **INTRODUCTION**

Most of these functions are tabulated in various places. However, for convenience they have been re-calculated with short FORTRAN programmes and presented together.

2. **THE FUNCTIONS**

(i) The Bose-Einstein population function, defined by:

\[ P(x) = (e^x - 1)^{-1} \]

(ii) The average energy function of a harmonic quantum oscillator, defined by:

\[ \gamma(x) = x/2 + x/(e^x - 1) = x/2 \coth x/2 \]

The average energy is \( \langle (w,T) = kT \gamma(\hbar w/kT) \)

(iii) The specific heat function for a quantum oscillator, defined by:

\[ E(x) = x^2 e^x (e^x - 1)^{-2} \]

(iv) The specific heat of a Debye continuum, defined by:

\[ C_{v/3R} = D(x) = \frac{3}{x^3} \int_0^x y^4 e^y (e^y - 1)^{-2} dy \]

(v) The diffraction function of a Debye continuum defined by:

\[ \varphi(x) = x^4 + 1/x \int_0^x y (e^y - 1)^{-1} dy \]

In all these functions \( x \) is to be interpreted as \( \hbar w/kT \) or as \( \theta_D/T \) where \( \theta_D \) is the Debye Temperature.

3. **METHOD OF CALCULATION**

3.1 **Large \( x \) (greater than 1.7)**

The functions were calculated using the EXP routine and expanding the two integrals in power series of exponentials.

This Table is presented in intervals of 1/x from 1/x = .01 to 1/x = .6 in steps of .01.
3.2 Small x (less than 2.5)

The following power series were used:

(i) \( P(x) = \frac{1}{x} - \frac{1}{2} + \frac{x}{12} - \frac{x^3}{6!} + \frac{x^5}{5!} - \frac{x^7}{30} \).

(ii) \( \gamma(x) = 1 + \frac{x^2}{12} - \frac{x^4}{6!} + \frac{x^6}{6.7!} - \frac{x^8}{30} \).

(iii) \( E(x) = 1 - \frac{x^2}{12} + \frac{x^4}{240} - \frac{x^6}{6048} + \frac{x^8}{518400} \).

(iv) \( D(x) = 1 - \frac{x^2}{20} + \frac{x^4}{560} - \frac{x^6}{18144} + \frac{x^8}{1900800} \).

(v) \( \psi(x) = 1 + \frac{x^2}{36} - \frac{x^4}{30.5!} + \frac{x^6}{42.7!} - \frac{x^8}{30.9!} \).

NOTE that for \( E(x) \) this series does not converge fast enough and is 4% in error at \( x = 2.5 \) and 0.5% in error at \( x = 20 \). For the other series the error is less; the worst is \( D(x) \) for which the error is 0.15% at \( x = 2.5 \).

4. ACKNOWLEDGEMENTS

The FORTRAN programmes were written by Mr. A. Hewat (vacation student from Melbourne University).
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