On the Determination of the Elastic Spectra of Solids from Specific Heat Data

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A new method is proposed which allows to express the frequency-distribution-function of solids by real functions. The result can be written in such a way that it contains the experimental data in terms of a modified Debye-temperature.

§ 1. Introduction

The problem to find the elastic spectra of solids from the specific heat has recently received much interest. Montroll\(^{1}\) has solved the problem by the method of Fourier-transforms. This solution involves complex functions which make a direct application to actual problems impossible. Grayson-Smith and Stanley\(^{2}\) have solved the integral equation in question by expanding the frequency-distribution into a Fourier-series. This method is appropriate only when low-temperature data of the specific heat are used.

We intend to find an expression for the frequency-distribution in terms of real functions and we propose the following way.

§ 2. Method

We write the number of eigen-vibrations of the solid in the frequency-interval between \(\nu\) and \(\nu+d\nu\) as \(f(\nu/\nu_0)\ d\nu/\nu_0\), where \(\nu_0\) is a frequency in unit of which we express the frequencies. Its value we choose in a way explained later. The specific heat per mode \(C(T)\) at the temperature \(T\) is then written as

\[
C(T) = \frac{k}{\nu_0} \int_0^\nu d\nu \frac{(\hbar \nu / kT)^2 f(\nu/\nu_0)}{(e^{\hbar \nu / kT} - 1) (1 - e^{-\hbar \nu / kT})}.
\]

Introducing \(x = kT/\hbar \nu_0\) and \(s = \hbar \nu / kT\), we obtain with \(f(s) \equiv s^2 g(s)\) and \(C(x) \equiv k x^2 F(x)\)

\[
F(x) = \int_0^\infty ds \frac{s^2 g(xs)}{(e^s - 1) (1 - e^{-s})}.
\]

Our problem to determine the frequency-distribution \(g(s)\) by means of the specific heat \(F(x)\) is now to solve this integral equation (1) of \(g(s)\). Using the Fourier-integral of \(F(x)\)
\[ F(x) = \frac{2}{\pi} \int_0^\infty dt \varphi(t) \cos xt, \quad \varphi(t) = \int_0^\infty du F(u) \cos tu, \quad (2, 2a) \]

we express \( g(x) \) by the integral

\[ g(x) = \frac{2}{\pi} \int_0^\infty dt \varphi(t) \gamma(xt), \quad (3) \]

\[ = \frac{2}{\pi} \int_0^\infty dt \gamma(xt) \int_0^\infty du F(u) \cos tu, \quad (3a) \]

where \( \gamma(x) \) has to satisfy the following equation obtained by insertion of eqs. (2) and (3) into eq. (1)

\[ \cos x = \int_0^\infty ds \frac{s^\gamma(xs)}{(e^s - 1) (1 - e^{-s})}. \quad (4) \]

If we could find the solution of this integral equation (4) in real functions then eq. (3a) would be a form satisfying our intention.

In order to solve eq. (4) we observe that the homogeneous equation:

\[ \frac{d^n}{dz^n} \varphi(z) = \frac{\varphi(z)}{z} \]

\[ \frac{dz}{dz^2} = \frac{1}{z} \]

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has the solutions \( \varphi(z) = z^a \) where \( a \) can take any value for which the integral has a meaning. Since \( \cos x \) can be expanded into a power series, we are allowed to assume that \( \gamma(x) \) can also be expanded into a power series and find then easily

\[ \gamma(x) = \sum_{\nu=0}^\infty (-1)^\nu \frac{x^{2\nu}}{(2\nu)! (2\nu+4)! \zeta(2\nu+2)}, \quad (6) \]

\[ \zeta(x) \]

being the Riemann \( \zeta \)-function. With the relations

\[ \sum_{\nu=0}^\infty (-1)^\nu \frac{x^{2\nu}}{(2\nu)! (2\nu+4)!} = \Re \left[ \frac{J_4(2\sqrt{ix})}{ix^2} \right] \quad (7) \]

and

\[ \frac{1}{\zeta(x)} = \sum_{n=1}^\infty \frac{\mu(n)}{n^x}, \quad (8) \]

\( \mu(n) \) being the Moebius function, eq. (6) takes the form aimed by us as follows.

\[ \gamma(x) = \sum_{n=1}^\infty \frac{\mu(n)}{n^x} \Re \left[ \frac{J_4(2\sqrt{i\zeta(x)}/n)}{i(\zeta(x)/n)^2} \right], \quad (9) \]

To get further, we express the temperature dependence of the specific heat, \( F(x) \), in terms of a modified Debye-temperature \( \vartheta(x) \) as

\[ F(x) = 3 \int_0^\infty ds \frac{s^4}{(e^s - 1) (1 - e^{-s})}. \quad (10) \]
Now we come to a definition of the frequency \( \nu_0 \). It seems convenient to choose \( \nu_0 \) in such a way that \( \hbar \nu_0 / k \) is the minimum Debye-temperature of the solid in question. With this expression eq. (10) for \( F(x) \), we rewrite eq. (2a)

\[
\varphi(t) = 3 \int_0^\infty du \cos tu \int_0^\infty dz \frac{e^z}{(e^z-1)(1-e^{-z})}. \tag{11}
\]

By a partial integration and a change of the integration variable \( u \) into \( v \)

\[
\vartheta(v)/u = \varTheta(v) \quad \text{or} \quad u = \varTheta(v), \tag{12}
\]

\( \varTheta \) being the inversion of the definition of \( v \), we obtain

\[
\varphi(t) = 3 \int_0^\infty dv \sin(t\varTheta(v)) \frac{v^4}{(e^v-1)(1-e^{-v})}, \tag{13}
\]

the insertion of which into eq. (3) gives our final result

\[
g(z) = 3 \int_0^\infty \frac{dt}{t} \sin t \int_0^\infty dv \frac{v^4 \vargamma(zt/\varTheta(v))}{(e^v-1)(1-e^{-v})}. \tag{14}
\]

Especially, in the Debye case, \( \vartheta(x) \) has the constant value unity and \( \varTheta(v) = 1/v \). Then with eq. (4) we find

\[
g(z) = 3 \int_0^\infty \frac{dt}{t} \sin t \cos zt = \begin{cases} 3 : 0 \leq z \leq 1, \\ 0 : z > 1, \end{cases} \tag{15}
\]

which leads to the well known Debye frequency-distribution

\[
\frac{1}{\nu_0} f\left(\frac{\nu}{\nu_0}\right) = \begin{cases} \frac{3}{\nu^4} : 0 \leq \nu \leq \nu_0, \\ 0 : \nu > \nu_0, \end{cases} \tag{16}
\]
as it must be.

A discussion of our results we reserve for another publication.

**Appendix**

It may be of interest here to see that the integral-expression of \( g(z) \), eq. (3), is allowable. We observe that \( g(z) \) can obviously be expressed as a Fourier-integral

\[
g(z) = \frac{2}{\pi} \int_0^\infty dt \cos zt \int_0^\infty du \cos tu \cdot g(u). \]

Applying for \( \cos zt \) eq. (4)

\[
g(z) = \frac{2}{\pi} \int_0^\infty dt \int_0^\infty dv \frac{v^4 \vargamma(ztv)}{(e^v-1)(1-e^{-v})} \int_0^\infty du \cos tu \cdot g(u),
\]

\[
= \frac{2}{\pi} \int_0^\infty dt \vargamma(zt) \int_0^\infty du \cos tu \int_0^\infty dv \frac{v^4 g(uv)}{(e^v-1)(1-e^{-v})},
\]
\[ \frac{2}{\pi} \int_{0}^{\infty} dt \varphi(t) \int_{0}^{\infty} du F(u) \cos tu, \]

\[ = \frac{2}{\pi} \int_{0}^{\infty} dt \varphi(t) \gamma(st). \]

References