ANALYSIS OF THE PHONON SURFACE SPECIFIC HEAT USING GREEN FUNCTION TECHNIQUES

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Abstract

Green functions are derived for the displacement associated with acoustic vibrations in isotropic elastic media and used to evaluate the surface specific heat in the harmonic approximation. ~~We consider~~ only the low-temperature limit case since, provided K_B $1/\hbar$ is very small, ~~we can replace~~ the dispersion relation for the three acoustic branches by ~~its~~ long-wavelenghts form. The contributions of surface elastic waves of the Rayleigh and Love types are pointed out and their features discussed. The nature of the result and their relations to previous work in this field is also presented and discussed.

1. Introduction

In this paper we present a Green function calculation of the surface contribution to the specific heat of a crystal at low temperatures.

The majority of the previous calculations in this subject were carried out by the use of a lattice-dynamical calculation [1 - 4] togheter with Born cyclic boundary conditions, justified by the relation between the vibrational spectrum and the propagation of disturbances through the crystal lattice [5]. On the other hand if one consider $G(\vec{r}, t)$ as the evolution matrix or propagator for the system, a great deal of the surface system dynamics is very neatly contained in it. Burt [6] used this technique to set up a very useful method to calculate the surface specific heat, since the density in frequency of the normal modes of a crystal is equal to the trace of the Fourier transform $G(\vec{r}, \omega)$. It is the aim of this paper the use of linear response theory, to calculate the contributions to the surface specific heat, at low temperatures, from surface waves of the Rayleigh and Love types.

2. Results and Discussions

We start showing briefly how to obtain the specific heat from displacement Green functions. Later we apply this result to some physical situations. (Rayleigh and Love range of frequencies)

2.1 - The Method

In the harmonic approximation, the thermodynamical functions are aditive, so the specific heat is given by

$$C(T) = \int d\omega \quad F(\omega) \quad D(\omega) \tag{1}$$

Where $F(\omega)$ is the specific heat of an harmonic oscilator of frequency ω, and $D(\omega)$ is the density of modes. The density of modes can be obtained from Green functions, already derived in the linear response approximation [7, 8], according to

$$D(\omega) = -\frac{1}{\pi} \operatorname{Im} \; 2\omega \int \sum_{\alpha} \rho d^3r \; \langle\langle u^{\alpha}(\vec{r}); u^{\alpha}(r) \rangle\rangle_{\omega} \tag{2}$$

To obtain the specific heat due to surface acoustic phonons, we consider in (2) only the contributions from localized modes. The use of elasticity theory is justified once only long-wave phonons are considered [9]

2.2 - Rayleigh Wave Contribution

Consider an isotropic material occupying the half-space $z < 0$ with a flat surface, with area $\bar{A}$, in the $z=0$ plane and vacuum in the half-space $z > 0$. Due to translational invariance, $\langle\langle u^{\alpha}(r); u^{\alpha}(r) \rangle\rangle_{\omega}$ is independent of the components of $\vec{r}$ parallel to the surface. Therefore

(2) is reduced to

$$D(\omega) = -\frac{1}{\pi} \text{ Im } 2\omega \bar{A}\rho \sum_{\alpha} \int dz \ll u^{\alpha}(z); u^{\alpha}(z) \gg_{\omega} \quad (3)$$

For modes polarized in the plane of propagation there is a frequency region where ω is below the treshold for transverse waves, i.e. $\omega < \omega_t$ ($\vec{K}$, 0). Only surface wave of the Rayleigh type can propagate in this region obeying the following dispersion relation

$$4v_T^3 (v_L^2 - v_R^2)^{1/2} (v_T^2 - v_R^2)^{1/2} = v_L(2v_T^2 - v_R^2)^2 \quad (4)$$

Here v_T and v_L are respectivelly the transverse and longitudinal velocity of the acoustic wave in the semi-infinite crystal; v_R is the velocity of the surface Rayleigh wave.

Now, using (1) with the Green functions as calculated by Loudon [7] we get

$$\Delta C = 12 \hbar K_B \zeta(3) \left[\frac{K_B T}{h v_R} \right]^2 \quad (5)$$

in agreement with Burt [6]. Here $\zeta(x)$ is the Riemann zeta function; K_B and h are the Boltzmann and PlancK constant respectively.

2.3 - Love Wave Contribution

Consider a film of thickness H deposited on a substrate whose thickness H' is effectively infinite. The film and substrate are made from different materials, both optically and elastically isotropic. For modes with polarization perpendicular to the plane of propagation there is a frequency region given by

$$vq^x < \omega < v'q^x \quad (6)$$

Where the system supports the propagation of another kind of surface wave, namely the Love waves. In (6) v (v') are the transversal velocities of the acoustic wave of wave vector q (q') in the film (substrate). The dispersion relation of this wave is [8]

$$C^{44} q^z \tan q^z H = C'^{44} \alpha'^z \quad (7)$$

where C^{44} and C'^{44} are components of the elastic tensor in the film and substrate respectivelly, and

$$q'^z = i\,\alpha'^z = \sqrt{(\omega/v')^2 - (q^x)^2} \qquad (8)$$

with similar expression for q^z

The Love -wave contribution for the surface specific heat can now be calculated using [10]

$$\Delta C = -\frac{1}{\pi}\,\mathrm{Im}\int_0^\infty d\omega\, F(\omega)\, 2\omega\bar{A}\left[\int_{-\infty}^{-H} dz \ll u^y(z); \overset{*}{u}^y(z) \gg_\omega + \int_{-H}^{0} dz \ll u^y(z); u^y(z) \gg_\omega\right] \qquad (9)$$

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