characteristics: They all have a rather broad band overlapped by a narrow $3d$ band. The numbers electrons which can be accommodated are two per for the $4s$ band and ten per atom for the $3d$ band, that the density of allowed energy states is much higher in the $3d$ than in the $4s$ band. For these metals, Fermi level lies somewhere within the $3d$ band. Thus, owing to the large difference in the density of states between the two bands, a small movement of the band with respect to the $4s$ band caused by high pressure could result in a substantial redistribution of the electronic population. Therefore, the conclusion from the results is that in the bcc structure, for first-row transition metals, the relative positions and relative widths of the bands arising from the $s$ and $d$ atomic levels are independent of density, at least for modest density changes. For the closer packed metals apparently there is a relative lowering of the $d$ band with increasing density so that there is some transfer of electrons from the $s$ band to the $d$ band, which slows the rate of increase of $s$-electron density at the nucleus.

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# Anharmonic Lattice in One Dimension: Energy Shift and Lifetime of an Excitation

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The self-energy and lifetime of a long-wavelength one-dimensional phonon are calculated by Van Hove's resolvent operator formalism using the first anharmonic term. The results are valid for zero temperature.

THE problem considered here is that of a one-dimensional anharmonic lattice. The dependences of the lifetime and energy shift of a phonon on the wave vector (at long wavelength) have been obtained by the resolvent operator method. The results are valid at zero temperature. The corresponding results for high temperatures have been obtained by Maradudin.[1] Thus, the results of this note supplement the results of Maradudin. His results indicate that at high temperatures the lifetime of all phonons is the same. But here we find that at zero temperature the lifetime of a phonon is a function of the wave vector. The notation used is the same as that of Van Hove[2] and Hugenholtz.[3]

The Hamiltonian for the harmonic lattice without zero-point energy is

$$H_0=\int_{-\pi/a}^{\pi/a} dk A_k^{\dagger} A_k \omega_k ,$$

where $A_k^{\dagger}$ and $A_k$ are the usual creation and annihilation operators for phonons, and

$$\omega_k=(4\alpha/m)^{1/2}|\sin\tfrac{1}{2}ka| .$$

We assume that $a$, the interatomic distance, is small and that we can take

$$\omega_k=A|k| ,$$

where

$$A=(\alpha a^2/m)^{1/2}.$$

The first anharmonic term is

$$V^{(3)}=\int_{-\pi/a}^{\pi/a} dk_1 \int_{-\pi/a}^{\pi/a} dk_2 \int_{-\pi/a}^{\pi/a} dk_3 C_{k_1,k_2,k_3}(A_{k_1}+A^{\dagger}_{-k_1}) \times(A_{k_2}+A^{\dagger}_{-k_2})(A_{k_3}+A^{\dagger}_{-k_3})\delta(k_1+k_2+k_3) ,$$

where

$$C_{k_1k_2k_3}=\frac{\beta a^3}{i3!}\left(\frac{1}{8m^3\omega_{k_1}\omega_{k_2}\omega_{k_3}}\right)^{1/2} k_1k_2k_3$$

and $\alpha$, $\beta$ are force constants. The diagonal part of the resolvent is given by

$$D_k(z)=\frac{1}{\omega_k-G_k(z)-z} .$$

The definition of these has been given by Van Hove and Hugenholtz. Here we evaluate the function approximately by considering the simplest diagram which contributes to it, i.e., the diagram of Fig. 1. We have left out a large number of diagrams and we work in

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[1] A. A. Maradudin, Phys. Letters 2, 298 (1962).
[2] L. Van Hove, Physica 21, 901 (1955); L. Van Hove, in *Lectures in Physics* (W. A. Benjamin, Inc., New York, 1961).
[3] N. M. Hugenholtz, Physica 23, 481 (1957).