...ing characteristics: They all have a rather broad ...band overlapped by a narrow 3*d* band. The numbers ...electrons which can be accommodated are two per ...for the 4*s* band and ten per atom for the 3*d* band, ...that the density of allowed energy states is much ...er in the 3*d* than in the 4*s* band. For these metals, ...Fermi level lies somewhere within the 3*d* band. ...s, owing to the large difference in the density of ...es between the two bands, a small movement of the ...band with respect to the 4*s* band caused by high ...ure could result in a substantial redistribution of ...electronic population. Therefore, the conclusion ...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.

ACKNOWLEDGMENT

The authors acknowledge the assistance of P. Baron in preparing the samples.

...YSICAL REVIEW VOLUME 138, NUMBER 3A 3 MAY 1965

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

C. MANOHAR

Chemistry Division, Atomic Energy Establishment Trombay, Bombay, India

(Received 2 November 1964; revised manuscript received 21 December 1964)

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 ...wave vector (at long wavelength) have been obtained by the resolvent operator method. The results ...valid at zero temperature. The corresponding results for high temperatures have been obtained by ...adudin.[1] Thus, the results of this note supplement ...results of Maradudin. His results indicate that at ...temperatures the lifetime of all phonons is the ...e. But here we find that at zero temperature the ...time of a phonon is a function of the wave vector. The notation used is the same as that of Van Hove[2] ...Hugenholtz.[3]

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

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

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

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

...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 α, β 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

---

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