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# KOHN EFFECT AND THE LATTICE VIBRATION FREQUENCY DISTRIBUTION IN METALS

by

W. KLEY, I. PELAH and J. PERETTI

**1963**

**Joint Nuclear Research Centre**
**Ispra Establishment - Italy**
**Department of Reactor Physics**

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# KOHN EFFECT AND THE LATTICE VIBRATION FREQUENCY DISTRIBUTION IN METALS

J. PERETTI, I. PELAH * and W. KLEY
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Kohn [1] has shown how the screening of the lattice vibrations in a metal by the conduction electrons results in a singular behaviour of the frequency $\omega(\boldsymbol{q})$ on a certain surface $S$. We intend to show here that, in certain circumstances, this Kohn effect produces some additional peaks in the frequency distribution $g(\omega)$ of the lattice, which can be clearly distinguished from those due to the usual dispersion of the lattice waves.

The Kohn effect is such that on one side (I) of $S$ the value of $\omega$ is larger by an amount $\Delta\omega$ than on the other side (II). Let us call the side (I) the interior and the side (II) the exterior of the surface $S$ (fig. 1). Let us call $\Sigma(\omega)$ the surface drawn in $q$ space on which the frequency is constant and equal to $\omega$, in the absence of the Kohn effect. The surface $\Sigma'(\omega)$ of constant frequency obtained by taking into account the Kohn effect coincides with $\Sigma$ except in the vicinity of $S$, where it is displaced from $\Sigma$ by an amount of the order of $\Delta\omega/2c$, in opposite direction on each side of $S$, as shown for example in fig. 2 ($c$ is the sound velocity). Two cases can occur: either

a) $\Sigma(\omega)$ cuts $S$ making a certain angle different from zero (fig. 2), or
b) $\Sigma(\omega)$ is tangent to $S$ on the interior (or exterior) side as in fig. 3.

The value $g(\omega)\,\mathrm{d}\omega$ is proportional to the volume

* On leave from Israel Atomic Energy Commission.

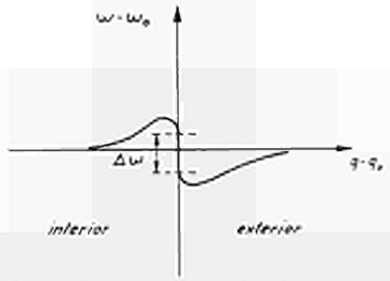


Fig. 1. Behaviour of $\omega$ near the point $(\omega_0, q_0)$ on the Kohn surface $S$. There is almost a discontinuity $\Delta\omega$.

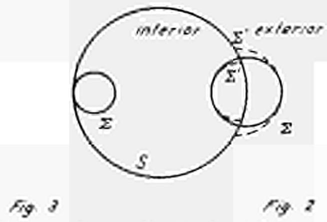


Fig. 2-3. $\Sigma$ is the surface of constant frequency without Kohn effect (solid line) which is changed to $\Sigma'$ (dotted line) when Kohn effect is taken into account.

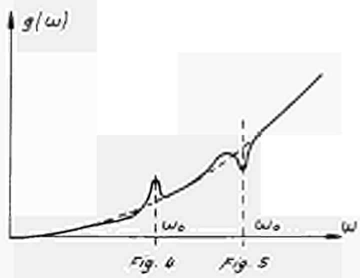


Fig. 4-5. Expected peaks in the $g(\omega)$ curve near the value $\omega_0$ such that $\Sigma(\omega_0)$ touches $S$.

in $q$ space enclosed between surfaces $\Sigma(\omega)$ and $\Sigma(\omega + d\omega)$. The displacement from $\Sigma$ to $\Sigma'$ gives a second-order, that is to say a negligible, contribution to $g(\omega)$ in the case a). But in case b) there is a finite contribution to $g(\omega)$, which is "positive" when the contact is on the interior side as in fig. 4, and "negative" when on the exterior side as in fig. 5. We therefore expect a positive or negative peak superimposed on the regular $g(\omega)$ curve at every frequency $\omega_i$ such that $\Sigma(\omega_i)$ touches the surface $S$ at point $\boldsymbol{q}_i$ in $q$ space.

The area under $g(\omega)$ being fixed, a positive contribution at frequency $\omega_0$ is accompanied by a lowering of $g(\omega)$ at frequencies less than $\omega_0$, and a negative contribution by an increase of $g(\omega)$ at frequencies less than $\omega_0$ *.

The exact position of the peaks depends on the crystal structure and on the shape and filling of the conduction band, but we can evaluate an order of magnitude if we assume that: a) the conduction electrons are free and the conduction band is half filled, b) the lattice is a b.c.c. lattice with parameter $a$ and the lattice vibrations follow a Debye model. Under those assumptions $S$ is a set of spheres of radius $2k_F = 2(6\pi^2)^{1/3}/a = 2 \times 3.897\ a^{-1}$, centred at the reciprocal lattice points. The surfaces $\Sigma$ are spheres centred at the origin, with the maximum possible radius $q_{max} = (12\pi^2)^{1/3}/a = 4.904\ a^{-1}$, and the reciprocal vectors $\boldsymbol{K}_\nu$ belong to a f.c.c. lattice with an edge whose length is $K = 2\pi/a = 6.283\ a^{-1}$. There are two interesting surfaces $\Sigma$ which touch $S$. One is $\Sigma_1$ of radius $q_1 = K/2 - 2k_F = 1.090\ a^{-1}$, which touches the sphere centred at the point 110; the other $\Sigma_2$ of radius $q_2 = 2k_F - K = 1.511\ a^{-1}$ which touches the sphere centred at the point 100. They are on opposite sides of $S$ and thus correspond to two peaks of opposite sign, occurring at frequencies $\omega_1 = 0.222\ \omega_{max}$ and $\omega_2 = 0.308\ \omega_{max}$. These peaks are in the region where the frequency distribution is usually well represented by a quadratic law $g(\omega) = d\omega^2$, and if experimentally observed, will be difficult to explain by any reasonable Born-Von Karman model **.

Finally, we would like to remark that, if the filling of the conduction band changes gradually from the value that we have assumed, one of the two peaks will move to lower and lower frequencies, and could give finally an anomalous contribution to the low temperature specific heat of the lattice.

*Reference*


1) W. Kohn, Phys. Rev. Letters 2 (1959) 393.


* The area under each bump is of the order of $(\Delta\omega/\omega)^2$.

** Recent measurements of vanadium, at the slow chopper facility at the Ispra reactor, have shown the existence of a small peak in this energy region. The experimental results have been presented at the Chalk River Symposium on Inelastic Scattering of Neutrons in Solids and Liquids (10 - 14 September 1962).