# CONNECTION BETWEEN TRUE EFFECTIVE MASS AND OPTICAL ABSORPTION IN INSULATORS

Vinay Ambegaokar and Walter Kohn
Carnegie Institute of Technology, Pittsburgh, Pennsylvania
(Received April 10, 1959)

In the independent-electron model of an insulator with cubic symmetry, the effective mass $m^*$ associated with a simple band $n=0$ is given by the well-known sum rule[1]

$$\frac{m}{m^*} = 1 - \sum_{n\neq 0} f_{0n}, \tag{1}$$

where the oscillator strength $f_{0n}$ is defined by

$$f_{0n} = \frac{2}{m}\frac{|p_{0n}|^2}{E_n - E_0}. \tag{2}$$

Consider, in the same model, a small number, $n_0$, of electrons per unit volume in the band 0. Their contribution to the real part of the complex conductivity is

$$\sigma(\omega) = \frac{\omega_p^2}{8}\sum_{n\neq 0} f_{0n}\,\hbar[\delta(E_n - E_0 - \hbar\omega) + \delta(E_n - E_0 + \hbar\omega)], \tag{3}$$

where

$$\omega_p^2 = 4\pi n_0 e^2/m. \tag{4}$$

Thus one has the following connection:

$$\frac{m}{m^*} = 1 - \frac{8}{\omega_p^2}\int_0^\infty \sigma(\omega)\,d\omega. \tag{5}$$

We have studied a more realistic model of an insulator in which the Coulomb interactions between all electrons are included to all orders of perturbation theory,[2] and have found that a relation very similar to (5) still holds.

In this model the effective mass of a free carrier is defined as follows. The many-electron wave functions of the insulator with one free carrier can be characterized by a wave vector $\vec{k}$ and other quantum numbers $n$. The energy spectrum of this system will be denoted by $E_n(\vec{k})$. Let $E_0(0)$ be the lowest energy. Then the many-particle effective mass $m^*$ is defined by the expansion

$$E_0(\vec{k}) = E_0(0) + (\hbar^2/2m^*)k^2 + \ldots. \tag{6}$$

Now let $\sigma_0(\omega)$ and $\sigma(\omega)$ be the real parts of the conductivity of the perfect insulator, without any free carriers, and of the insulator, with $n_0$ carriers per unit volume in the lowest "conduction band," respectively. Then one finds the following exact[3] relationship:

$$\frac{m}{m^*} = 1 - \frac{8}{\omega_p^2}\int_0^\infty [\sigma(\omega) - \sigma_0(\omega)]\,d\omega. \tag{7}$$

Under favorable circumstances, when $m^*$ is very small, this relation may enable one to determine the effective mass by optical measurements. The main effect of the presence of carriers in such a case is to reduce the optical absorption of the perfect insulator near the absorption threshold. The amount of this reduction gives an estimate of $m^*$ by means of Eq. (7).[4]

We should like to take this opportunity to thank Dr. M. Suffczynski for many stimulating discussions.

---

[1]See, e.g., N. F. Mott and H. Jones, Theory of the Properties of Metals and Alloys (Oxford University Press, Oxford, 1936), Chap. III.

[2]W. Kohn, Phys. Rev. 105, 509 (1957); 110, 857 (1958); Vinay Ambegaokar and Walter Kohn, Bull. Am. Phys. Soc. Ser. II, 4, 276 (1959). It should be remarked that in all this work the lattice is taken to be rigid.

[3]In particular, all exchange effects are completely contained in this relation. This may be contrasted with the analyses of E. O. Kane, J. Phys. Chem. Solids 6, 236 (1958), and J. C. Phillips, J. Phys. Chem. Solids 7, 52 (1958).

[4]Compare H. Y. Fan and G. W. Gobeli, Bull. Am. Phys. Soc. Ser. II, 3, 111 (1956); W. G. Spitzer and H. Y. Fan, Phys. Rev. 106, 882 (1957).