Electromagnetic Properties of Insulators. I*

VINAY AMBEGAOKAR AND WALTER KOHN
Department of Physics, Carnegie Institute of Technology, Pittsburgh, Pennsylvania

(Received August 3, 1959)

We discuss the response of a perfect insulator to weak external electromagnetic fields of long wavelength from a many-particle point of view. Our method is to treat the Coulomb interaction between all electrons to all orders of perturbation theory and analyze the structure of the corresponding Feynman graphs. As a result of this graphical analysis we are able to show that the response of the many-particle system to long-wavelength external fields of arbitrary polarization is completely described by a single frequency-dependent dielectric constant. In the limit of long wavelengths as well as low frequencies, we also include, in terms of a magnetic permeability, the magnetic effects of an external field on our system.

1. INTRODUCTION

IT has been customary for a long time to describe the response of an insulator to a weak electromagnetic field by means of a complex dielectric constant κ and permeability μ. However, the only models for which such a description has been rigorously justified treat the charge carriers either as localized[1] or as distributed throughout the insulator but not interacting with each other.[2]

In the present paper we verify the correctness of this conventional description for a more realistic model of an insulator.[3,4] We take the insulator to be a perfectly periodic cubic crystal with fixed nuclei and electrons which interact with these nuclei as well as with each other. Magnetic effects are very small in such a system, as evidenced by the small magnitude of the diamagnetic susceptibility ($\chi \approx 10^{-6}$); they will be neglected in the main body of this paper. What will be done is to derive explicitly and rigorously the usual constitutive equations of Maxwell's theory in terms of the frequency dependent dielectric constant $\kappa(\omega)$, with the single restriction that the wavelengths of the electromagnetic field be long compared to a lattice parameter. Similar results have been recently obtained by Nozières and Pines[5] who however treat the electron-electron interaction in the "random phase approximation."

The parameter $\kappa(\omega)$ can be defined either by means of a formal expression involving the exact wave functions of the insulator, or by a perturbation series in the Coulomb interaction between the electrons. The terms of this series can be represented by Feynman graphs.[6] To establish our results, it is not necessary to evaluate quantitatively the contribution of any of these graphs, but only to recognize some general characteristics. One crucial point is this. In describing the response of the electrons to a longitudinal electric field (i.e., to a time-dependent embedded charge distribution) one encounters so-called "improper" polarization graphs (see Fig. 1), while the response

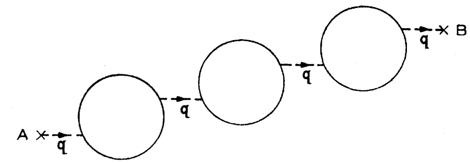
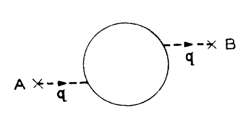


FIG. 1. An improper polarization graph that occurs in the response to a longitudinal field.

to a transverse electric field involves only "proper" polarization graphs (see Fig. 2). These graphs, which were introduced by Hubbard[7] in a somewhat different connection, will be more fully discussed in subsequent sections. At this point the following qualitative remarks may suffice. In Fig. 1 the dotted line originating at A describes the direct interaction of the longitudinal electric field due to the embedded charge with the system of electrons, while the line terminating at B represents the current set up by the response of the electrons. Each circle stands for a proper polarization part, i.e., an arbitrary graph of interacting electrons with the restriction that it cannot be split by cutting a single interaction line carrying momentum $\mathbf{q}$. On the other hand in Fig. 2 the line originating at A represents the interaction of the *total* transverse electric field with the electrons. The circle and the line terminating at B have the same significance as in Fig. 1. In spite of the different structure of the graphs of Figs. 1 and 2, one finds the same connection between the induced

FIG. 2. A proper polarization graph that occurs for both transverse and longitudinal fields.



* A preliminary report of this work was made at the 1959 Spring meeting of the American Physical Society in Washington, D. C. [V. Ambegaokar and W. Kohn, Bull. Am. Phys. Soc. 4, 276 (1959)]. It is based on a thesis submitted by one of us (V.A.) to the Carnegie Institute of Technology in partial fulfillment of the requirements for the Ph.D., and was supported in part by the Office of Naval Research.

[1] H. A. Lorentz, *Theory of Electrons* (B. Teubner and Sons, Leipzig, 1909), Chap. IV.

[2] A. H. Wilson, *Theory of Metals* (Cambridge University Press, Cambridge, 1936), first edition, Chap. IV.

[3] Some aspects of this model have been discussed in W. Kohn, Phys. Rev. **105**, 509 (1957); V. Ambegaokar and W. Kohn, Phys. Rev. Letters **2**, 385 (1959), and in reference 4.

[4] W. Kohn, Phys. Rev. **110**, 857 (1958).

[5] P. Nozières and D. Pines, Phys. Rev. **113**, 1254 (1959). This article gives references to earlier work by these authors.

[6] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).

[7] J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957).

polarization current and the total electric field

$$\mathbf{j}(\omega)=-i\omega\frac{\kappa(\omega)-1}{4\pi}\mathbf{E}_{\mathrm{tot}}(\omega), \tag{1.1}$$

in both the transverse and longitudinal cases.

Since the electron-electron interactions are taken into account completely in this theory, all internal field effects are included in the spectrum of energy levels of the insulator, and, thus, the dielectric constant defined here includes the Lorentz-Lorenz correction.

In the limit of long wavelengths *and* low frequencies (compared with a characteristic electronic frequency) it is possible also to include simply the magnetic effects on our system in terms of a magnetic permeability μ. This is done in Sec. 5, where both the electric and magnetic constitutive equations of Maxwell's theory are derived.

In this paper, then, we derive no new physical results but merely elucidate the graphical representation of an electromagnetic field interacting with an insulating crystal. This analysis will also serve as a preparation for the discussion in a following paper of the interaction of an electromagnetic field with charge carriers in an insulator.

2. RESPONSE TO A LONGITUDINAL FIELD

In this section, we shall calculate the polarization induced in the insulator by an external longitudinal electric field of long wavelength. We shall see that the magnitude of the induced polarization is critically dependent on the long range nature of the Coulomb interaction between electrons. To bring out this point, we shall compare the insulator with a hypothetical medium in which the extreme tail of the Coulomb interaction has been cut off. We shall exhibit a simple relation between the responses of these two media which will prove useful for our later discussion of the response of the real insulator to a transverse field since, in that case, long range Coulomb effects play no role.

At first, we shall treat the Coulomb interaction between the electrons as a perturbation, to all orders of perturbation theory, and examine the structure of the corresponding graphs. The results obtained by this formal device will then be directly expressed in terms of the many-particle wave functions of the insulator.

The Hamiltonian which describes the insulator may be written as

$$H=H_0+H_C+H_L. \tag{2.1}$$

Here

$$H_0=\textstyle\sum_i (T_i+V_i), \tag{2.2}$$

where T_i is the kinetic energy of the ith electron and V_i its interaction with the lattice of nuclei; H_C describes the Coulomb interaction between the electrons and H_L the electrostatic energy of the lattice of nuclei. When account is taken of the over-all charge-neutrality of the system, H_C may be written as

$$H_C=\frac{4\pi e^2}{\Omega}\sum_{i<j}\sum_{\mathbf{k}}{}'\frac{e^{i\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{x}_j)}}{k^2}, \tag{2.3}$$

where the prime on the sum over $\mathbf{k}$ indicates that the term with $\mathbf{k}=0$ is to be omitted. (Ω is the volume of the normalization box.)

Into the system described by (2.1) we introduce a time-dependent distribution of charge density, $\rho_{\mathrm{ext}}(\mathbf{x},t)$, which we Fourier analyze as follows:

$$\rho_{\mathrm{ext}}(\mathbf{x},t)=\int\rho_{\mathrm{ext}}(\mathbf{q},\omega)e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}d\mathbf{q}d\omega. \tag{2.4}$$

The reality of $\rho_{\mathrm{ext}}(\mathbf{x},t)$ implies

$$\rho_{\mathrm{ext}}^*(\mathbf{q},\omega)=\rho_{\mathrm{ext}}(-\mathbf{q},-\omega). \tag{2.5}$$

We restrict ourselves to charge distributions whose characteristic wavelengths are long compared to a lattice spacing. Further, we assume that $\omega/q\ll c^2/v_e$ (where c is the velocity of light and v_e a typical electronic velocity), so that we can neglect the magnetic effects of the charge density (2.4). Let us describe its electric field by a scalar potential. Then the Hamiltonian which describes its interaction with the system is, apart from an irrelevant interaction with the nuclei,

$$V(t)=\int\frac{4\pi e}{q^2}\rho_{\mathrm{ext}}(\mathbf{q},\omega)\rho(\mathbf{q})e^{-i\omega t}d\mathbf{q}d\omega, \tag{2.6}$$

where the operator $\rho(\mathbf{q})$ is defined as

$$\rho(\mathbf{q})=\textstyle\sum_i e^{i\mathbf{q}\cdot\mathbf{x}_i}. \tag{2.7}$$

We imagine that the Coulomb interactions (2.3) and the external perturbation (2.6) have been turned on gradually in the past with exponential time factors. The total perturbation to the one particle Hamiltonian H_0 may then be written as

$$H'(t)=H_Ce^{\eta t}+V(t)e^{st}, \tag{2.8}$$

where η and s are small quantities which will later be allowed to approach zero.

Let Φ_0 be the time-independent wave function corresponding to the ground state of H_0. In our case of an insulator this is a state in which a number of Brillouin zones are completely filled. The time development operator, which operating on Φ_0 in the infinite past transforms it into the perturbed wave function of the real insulator, is

$$U(t,-\infty)=1+\sum_{n=1}^{\infty}(-i)^n\int_{-\infty}^{t}dt_1\int_{-\infty}^{t_1}dt_2\cdots\int_{-\infty}^{t_{n-1}}\times dt_nH_I'(t_1)H_I'(t_2)\cdots H_I(t_n), \tag{2.9}$$

where

$$H_I'(t)=e^{iH_0t}H'(t)e^{-iH_0t}.$$

(Here and in all that follows we use units such that $\hbar=1$.) The Schrödinger representation wave function

generated by (2.9) is

$$\Psi(t)=e^{-iH_0t}U(t,-\infty)\Phi_0. \tag{2.10}$$

The electron charge density induced in the insulator is given by the expectation value of the charge density operator in the state $\Psi(t)$. In calculating this quantity we work to first order in $\rho_{\text{ext}}(\mathbf{q},\omega)$ and, furthermore, neglect the charge fluctuations with wave vector $\mathbf{q}+\mathbf{K}_\nu$ which are excited by the external perturbation. ($\mathbf{K}_\nu$ is a nonvanishing vector of the reciprocal lattice.) These induced short wavelength charge fluctuations, while themselves comparable to those of wave vector $\mathbf{q}$, make a negligible contribution to the total field within the insulator in our long wavelength limit ($q\ll K_\nu$).

The charge density operator is

$$\rho(\mathbf{x})=e\sum_i \delta(\mathbf{x}-\mathbf{x}_i)=\frac{e}{\Omega}\sum_{\mathbf{k}}\rho(-\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{2.11}$$

and the induced charge density, $\rho_{\text{ind}}(\mathbf{x},t)$, is

$$\rho_{\text{ind}}(\mathbf{x},t)=(\Psi(t),\rho(\mathbf{x})\Psi(t))'. \tag{2.12}$$

The prime on the right of (2.12) indicates the restrictions discussed in the previous paragraph. Let us Fourier analyze $\rho_{\text{ind}}(\mathbf{x},t)$ as in Eq. (2.4).[8] We then obtain a linear relation between the Fourier coefficients of the induced and external charge densities of the form

$$\rho_{\text{ind}}(\mathbf{q},\omega)=\alpha(\mathbf{q},\omega)\rho_{\text{ext}}(\mathbf{q},\omega), \tag{2.13}$$

where, when the time integrations indicated in Eq. (2.9) are carried out, $\alpha(\mathbf{q},\omega)$ becomes

$$\begin{aligned}
\alpha(\mathbf{q},\omega)
&=\frac{4\pi e^2}{q^2\Omega}\sum_{l,m,n}\Bigg\{\Bigg(\Phi_0,H_C\frac{1}{E_0-H_0-i\eta}H_C\frac{1}{E_0-H_0-2i\eta}\cdots\\
&\times\frac{1}{E_0-H_0-il\eta}\rho(-\mathbf{q})\frac{1}{E_0-H_0+\omega+im\eta+is}H_C\cdots\\
&\times\frac{1}{E_0-H_0+\omega+in\eta+is}\rho(\mathbf{q})\cdots\frac{1}{E_0-H_0+i\eta}H_C\Phi_0\Bigg)\\
&+\Bigg(\Phi_0,H_C\frac{1}{E_0-H_0-i\eta}\cdots\\
&\times\rho(\mathbf{q})\frac{1}{E_0-H_0-\omega-in\eta-is}H_C\cdots\\
&\times\frac{1}{E_0-H_0-\omega-im\eta-is}\rho(-\mathbf{q})\frac{1}{E_0-H_0+il\eta}\cdots\\
&\qquad\times\frac{1}{E_0-H_0+i\eta}H_C\Phi_0\Bigg)\Bigg\}.
\end{aligned} \tag{2.14}$$

[8] The quantity $\rho_{\text{ind}}(\mathbf{x},t)$ contains time factors of the form $e^{(n\eta+s)t}$ where n is an integer. Before making the Fourier analysis we take the limit $\eta,s\to 0$ in these factors.

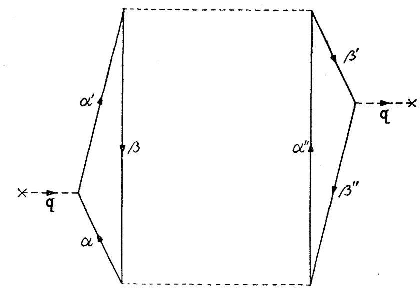


FIG. 3. A simple polarization graph. The directed solid lines running upward represent electrons in normally unoccupied Bloch states; the solid lines running downward represent holes in normally occupied states. The dashed horizontal internal lines represent Coulomb interactions.

Here E_0 is the energy of the independent particle state Φ_0, l,m,n are integers, and the dots indicate the successive occurrence of the Coulomb interaction Hamiltonian, H_C, and the appropriate energy denominators. In Eq. (2.14) the operator $\rho(\mathbf{q})$ comes from the interaction with the external perturbation (2.6), and the operator $\rho(-\mathbf{q})$ from the expectation value of the charge density operator.[9] In writing (2.14) we have made use of the reality condition (2.5).

The terms of the perturbation expansion (2.14) may, following Goldstone,[6] be represented by Feynman graphs. The graphs that occur here are almost exactly the $\mathfrak{D}$ graphs of reference 4 which described the interaction of two fixed charges in the perfect insulator. A simple but typical graph which occurs in (2.14) is Fig. 3. The two ρ operators act at the external interaction lines starting or ending at crosses. In the typical polarization graph Fig. 3, no unlinked or vacuum part has been shown because, although the linked cluster theorem as proved by Goldstone does not apply to our problem of a time-dependent perturbation, vacuum parts may be omitted for the following well-known reason.[10] In (2.14) all possible vacuum graphs occur with each polarization graph of the form of Fig. 3. The contribution of the sum of all vacuum graphs may be separated as a multiplicative factor. However, this factor may be omitted since it is the normalization sum for the clothed ground state wave function of the insulator and thus equal to one.

When the vacuum parts have been eliminated, the limit $\eta\to 0$ can be taken without any formal difficulties. Finally we let q approach zero and define the long wavelength complex polarizability $\alpha(\omega)$ by

$$\alpha(\omega)\equiv\lim_{q\to 0}\alpha(\mathbf{q},\omega). \tag{2.15}$$

[9] It is clear from the conservation of crystal momentum that the only Fourier coefficients of the charge density operator that can contribute are $\rho(-\mathbf{q}+\mathbf{K}_\nu)$. As pointed out earlier, we only retain the long wavelength response.

[10] J. M. Jauch and F. Rohrlich, *Theory of Photons and Electrons* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1955), p. 176 ff.

Then (2.14) results in

$$\alpha(\omega)=\lim_{q\to 0}\frac{4\pi e^2}{q^2\Omega}\sum_L\bigg(\Phi_0,H_C\frac{1}{E_0-H_0}\cdots\times\rho(-\mathbf{q})\frac{1}{E_0-H_0+\omega+is}H_C\cdots\times H_C\frac{1}{E_0-H_0+\omega+is}\rho(\mathbf{q})\frac{1}{E_0-H_0}\cdots H_C\Phi_0\bigg)+(\mathbf{q}\to-\mathbf{q},\quad\omega\to-\omega,\quad s\to -s).\quad(2.16)$$

Here $\sum_L$ means the sum over all linked graphs.

Let us now examine the graphs corresponding to the expansion (2.16) of $\alpha(\omega)$ in greater detail. Such graphs fall into two classes.[7] Graphs of the first class cannot be separated into two disconnected parts by cutting one Coulomb interaction line carrying momentum $\mathbf{q}$. We shall call such graphs *proper* polarization graphs. Graphs of the second class, which we call *improper* polarization graphs, can be so separated. Note that we include among the proper graphs those in which two otherwise disconnected parts are connected by a Coulomb interaction line carrying momentum $\mathbf{q}+\mathbf{K}_\nu$.

To clarify the physical meaning of the distinction between proper and improper graphs, let us for the moment consider a model of an insulator in which the interactions between charged particles are described by a cutoff Coulomb potential. Then, the part of the Hamiltonian describing the electron-electron interactions will be

$$H_C'=\frac{4\pi e^2}{\Omega}\sum_{k>\delta}\sum_{i<j}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{x}_j)}}{k^2},\qquad(2.17)$$

where δ is a small limiting wave number. The response of this system to a longitudinal electric field of long wavelength may also be described by polarization graphs. However, if $q<\delta$ ($\mathbf{q}$ being as usual, the wave vector of the external field) the Hamiltonian (2.17) contains no Fourier coefficient of the form q^{-2}. In the language of graphs, there are no electron-electron interaction lines carrying momentum $\mathbf{q}$ and, in particular, no improper polarization graphs. The long range effects of the Coulomb interactions are, thus, contained in the improper graphs.

We turn now to the connection between the sum of all polarization graphs, $\alpha(\omega)$, and that of the proper graphs alone which we call $\alpha_P(\omega)$. The connection arises from the fact that an arbitrary improper polarization graph (see Fig. 1) can be factored into the product of the two graphs obtained from it by removing a Coulomb interaction line carrying momentum $\mathbf{q}$ and in its place attaching two external interaction lines that preserve the sense of the momentum transfer. It follows from this theorem, which is discussed in Appendix A, that the sum of all improper graphs is $\alpha_P(\omega)\alpha(\omega)$, the $\alpha_P(\omega)$ coming from the proper parts which can be factored out of the improper graphs and the $\alpha(\omega)$ from the remaining parts, these parts themselves being either proper or improper. Thus one has the relation

$$\alpha(\omega)=\alpha_P(\omega)+\alpha(\omega)\alpha_P(\omega)\qquad(2.18)$$

(cf. reference 7). We shall show later that Eq. (2.18) implies that the dielectric constants which describe the response of the insulator to longitudinal and transverse fields are exactly equal.

We end this section by writing $\alpha(\omega)$ and $\alpha_P(\omega)$ in terms of the many-particle oscillator strengths of the insulator.[5] The sum rule these oscillator strengths satisfy arises from the following operator identities:

$$[H,\rho(\mathbf{q})]=\mathbf{q}\cdot\mathbf{j}(\mathbf{q}),\qquad(2.19)$$

$$[[H,\rho(\mathbf{q})],\rho(-\mathbf{q})]=-Nq^2/m,\qquad(2.20)$$

where

$$\mathbf{j}(\mathbf{q})\equiv(1/2m)\textstyle\sum_i(\mathbf{p}_ie^{i\mathbf{q}\cdot\mathbf{x}_i}+e^{i\mathbf{q}\cdot\mathbf{x}_i}\mathbf{p}_i),\qquad(2.21)$$

N is the total number of electrons in the insulator, and $\mathbf{p}_i$ the momentum operator for the ith electron. The longitudinal oscillator strength $f_{0n}(\mathbf{q})$ is defined as

$$f_{0n}(\mathbf{q})=\frac{2m}{q^2}\omega_{0n}|\rho(\mathbf{q})_{0n}|^2=\frac{2m}{\omega_{0n}}\left|\frac{\mathbf{q}}{q}\cdot\mathbf{j}(\mathbf{q})_{0n}\right|^2.\qquad(2.22)$$

Here the subscript 0 indicates the ground state of the insulator and n some excited state; ω_{0n} is the difference of energy between these states and $\rho(\mathbf{q})_{0n}$ is the matrix element of $\rho(\mathbf{q})$ between them. Taking the expectation value of both sides of Eq. (2.20) in the ground state of the insulator, one has

$$\tfrac{1}{2}\textstyle\sum_n[f_{0n}(\mathbf{q})+f_{0n}(-\mathbf{q})]=\sum_n f_{0n}(\mathbf{q})=N\qquad(2.23)$$

where the most general reason for the equality between the first and second expressions in (2.23) is the invariance under time reversal of the insulator Hamiltonian (2.1).

The complex polarizability, $\alpha(\omega)$, [see Eqs. (2.13) and (2.15)] may be written directly in terms of the many-particle wave functions of the insulator as

$$\alpha(\omega)=-\lim_{q\to 0}\frac{4\pi e^2}{q^2\Omega}\sum_n\left(\frac{\rho(-\mathbf{q})_{0n}\rho(\mathbf{q})_{n0}}{\omega_{0n}-\omega-is}+\frac{\rho(\mathbf{q})_{0n}\rho(-\mathbf{q})_{n0}}{\omega_{0n}+\omega+is}\right)=-\frac{4\pi e^2}{m\Omega}\lim_{q\to 0}\sum_n\frac{f_{0n}(\mathbf{q})}{2\omega_{0n}}\times\left(\frac{1}{\omega_{0n}-\omega-is}+\frac{1}{\omega_{0n}+\omega+is}\right).\qquad(2.24)$$

We now show that the quantities $f_{0n}(\mathbf{q})$ behave discontinuously at $q=0$, and that a relation very similar to (2.24) holds for $\alpha_P(\omega)$. Since (2.24) is independent of the direction of $\mathbf{q}$, we may set $\mathbf{q}=\mathbf{n}q$ where $\mathbf{n}$ is an

arbitrary unit vector. Then we have from Eq. (2.22) that

$$f_{0n}(\mathbf{q})=f_{0n}(\mathbf{n}q)=\frac{2m}{\omega_{0n}}|\mathbf{n}\cdot\mathbf{j}(\mathbf{n}q)_{0n}|^2. \quad (2.25)$$

When (2.25) is substituted into (2.24) the resulting expression may be written as a sum of graphs. The details of this expansion will be made clear in the next section. [See Eqs. (3.10), (3.9), and the discussion following Eq. (3.11).] The only point that is relevant here is that for q small but finite one has in the graphical expansion both proper and improper graphs, whereas if one replaces $f_{0n}(\mathbf{q})$ in (2.24) by

$$f_{0n}(0)\equiv\frac{2m}{\omega_{0n}}|\mathbf{n}\cdot\mathbf{j}(0)_{0n}|^2, \quad (2.26)$$

the charge neutrality of the system ensures *no* improper graphs. Thus the limit as $q\rightarrow 0$ and $q=0$ give quite different results. Now $\alpha_P(\omega)$ differs from $\alpha(\omega)$ only in that all improper graphs are omitted from the former. Thus, by comparison with (2.24) one has

$$\alpha_P(\omega)=-\frac{4\pi e^2}{m\Omega}\sum_n\frac{f_{0n}(0)}{2\omega_{0n}}\times\left(\frac{1}{\omega_{0n}+\omega+is}+\frac{1}{\omega_{0n}-\omega-is}\right). \quad (2.27)$$

We shall show in the next section that $\alpha_P(\omega)$ describes the response of the insulator to a *transverse* electric field of long wavelength. We shall thus be able to interpret $f_{0n}(0)$ as the transverse oscillator strengths.

3. RESPONSE TO A GENERAL FIELD

Let us now discuss the response of the insulator to a long wavelength field of arbitrary polarization. We shall describe this field by a vector potential

$$\mathbf{A}(\mathbf{x},t)=\int\mathbf{A}(\mathbf{q},\omega)e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}d\mathbf{q}d\omega, \quad (3.1)$$

and calculate the induced current to first order in $\mathbf{A}$. The linear relation between the Fourier coefficient, $\mathbf{j}(\mathbf{q},\omega)$, of the induced current and $\mathbf{A}(\mathbf{q},\omega)$ may be written as

$$j_\mu(\mathbf{q},\omega)=T_{\mu\nu}(\mathbf{q},\omega)A_\nu(\mathbf{q},\omega), \quad (3.2)$$

where the subscripts μ,ν indicate Cartesian components. We shall examine the structure of the kernel $T_{\mu\nu}$ in the limit of small $\mathbf{q}$ and show that it has the form

$$\lim_{\mathbf{q}\rightarrow 0}T_{\mu\nu}(\mathbf{q},\omega)=\frac{\omega^2}{4\pi c}[\kappa(\omega)-1]\times\left[\delta_{\mu\nu}+\frac{q_\mu q_\nu}{q^2}\left(\frac{1}{\kappa(\omega)}-1\right)\right]. \quad (3.3)$$

Here $\kappa(\omega)$ is the complex dielectric constant which is defined in terms of the quantity $\alpha(\omega)$ of the last section as

$$1/\kappa(\omega)=1+\alpha(\omega), \quad (3.4)$$

or equivalently [see Eq. (2.18)] in terms of $\alpha_P(\omega)$ as[11]

$$\kappa(\omega)=1-\alpha_P(\omega). \quad (3.5)$$

Equation (3.3) is the constitutive equation which determines the response of the insulator to long wavelength fields of arbitrary polarization.

We now derive Eq. (3.3). The Hamiltonian describing the interaction of the external vector potential (3.1) and the system is, to first-order in $\mathbf{A}$,

$$H(t)=-\frac{e}{2mc}\left(\sum_i \mathbf{p}_i\cdot\mathbf{A}(\mathbf{x}_i,t)+\mathbf{A}(\mathbf{x}_i,t)\cdot\mathbf{p}_i\right)e^{st}$$

$$=-\frac{e}{c}\int\mathbf{A}(\mathbf{q},\omega)\cdot\mathbf{j}(\mathbf{q})e^{-i\omega t}e^{st}d\mathbf{q}d\omega. \quad (3.6)$$

The operator $\mathbf{j}(\mathbf{q})$ was defined by Eq. (2.21). In Eq. (3.6) we imagine, as in the last section that the perturbation is turned on with a time factor e^{st}. The current induced in the insulator is given by the expectation value of the current density operator in the wave function produced from the ground state of the insulator by the perturbation (3.6). The current density operator is

$$\mathbf{j}(\mathbf{x},t)=\frac{e}{m}\sum_i\left(\mathbf{p}_i-\frac{e}{c}\mathbf{A}(\mathbf{x}_i,t)\right)\delta(\mathbf{x}-\mathbf{x}_i)$$

$$=\frac{e}{\Omega}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}\mathbf{j}(-\mathbf{k})-\frac{e^2}{mc}\frac{\mathbf{A}(\mathbf{x},t)}{\Omega}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}\rho(-\mathbf{k}). \quad (3.7)$$

The tensor $T_{\mu\nu}$ of Eq. (3.2) is then easily seen to be

$$T_{\mu\nu}(\mathbf{q},\omega)=\frac{e^2}{c\Omega}\sum_n\left(\frac{j_\mu(-\mathbf{q})_{0n}j_\nu(\mathbf{q})_{n0}}{\omega_{0n}-\omega-is}+\frac{j_\nu(\mathbf{q})_{0n}j_\mu(-\mathbf{q})_{n0}}{\omega_{0n}+\omega+is}\right)-\frac{e^2}{mc}\frac{N}{\Omega}\delta_{\mu\nu}. \quad (3.8)$$

The quantity $q_\mu T_{\mu\nu}q_\nu/q^2$ may be directly related to the oscillator strengths of the last section. Using the definition (2.22) of $f_{0n}(\mathbf{q})$ and the sum rule (2.23), one

[11] Equations (3.4) and (3.5) define the longitudinal and transverse dielectric constants, respectively. In reference 5, Nozières and Pines assert that the equality between these two dielectric constants only holds in the random phase approximation. In fact this equality is exact, provided only that the external fields are of sufficiently long wavelength ($\mathbf{q}\ll\mathbf{K}_\nu$). This condition is satisfied both for optical absorption and the forward inelastic scattering of kilovolt electrons. The arguments that establish Eqs. (2.18) and (3.3) apply equally well to metals.

has from Eq. (3.8)

$$q_\mu T_{\mu\nu} q_\nu/q^2 = \frac{e^2}{q^2 c\Omega}\sum_n\left(\frac{|\mathbf{q}\cdot\mathbf{j}(-\mathbf{q})_{0n}|^2}{\omega_{0n}-\omega-is}+\frac{|\mathbf{q}\cdot\mathbf{j}(\mathbf{q})_{0n}|^2}{\omega_{0n}+\omega+is}\right)-\frac{e^2}{mc}\frac{N}{\Omega}$$
$$=\frac{e^2}{mc\Omega}\sum_n f_{0n}(\mathbf{q})\left(\frac{\omega_{0n}}{2(\omega_{0n}-\omega-is)}+\frac{\omega_{0n}}{2(\omega_{0n}+\omega+is)}-1\right)$$
$$=\frac{e^2(\omega+is)^2}{mc\Omega}\sum_n\frac{f_{0n}(\mathbf{q})}{2\omega_{0n}}\left(\frac{1}{\omega_{0n}-\omega-is}+\frac{1}{\omega_{0n}+\omega+is}\right). \quad (3.9)$$

Comparing the last equality with the expression (2.24) for $\alpha(\omega)$, one sees that

$$\lim_{q\to 0} q_\mu T_{\mu\nu} q_\nu/q^2 = -(\omega^2/4\pi c)\alpha(\omega). \quad (3.10)$$

(The infinitesimal quantity s has only been retained in the energy denominators.) Equation (3.10) expresses the gauge invariance of the induced polarization current. It simply states that the same longitudinal electric field described either by a vector potential or a scalar potential gives rise to the same current. However it is possible, as we now show, to deduce the complete form of $T_{\mu\nu}$ to lowest order in $\mathbf{q}$ from Eq. (3.10).

Because of the assumed cubic symmetry of the lattice, $T_{\mu\nu}$ must have the form

$$\lim_{q\to 0} T_{\mu\nu} = a(\omega)\delta_{\mu\nu} + b(\omega) q_\mu q_\nu/q^2. \quad (3.11)$$

A further insight into $\lim_{q\to 0} T_{\mu\nu}$ may be obtained by a graphical expansion. The first two terms of $T_{\mu\nu}$, Eq. (3.8), can be calculated as an expansion in powers of the Coulomb interaction in a manner quite analogous to the calculation of $\alpha(\omega)$ in Sec. 2: one expands the wave function to all orders in the Coulomb interaction and to first-order in the interaction (3.6) with the external field, and then takes the expectation value of the first part of the current operator, Eq. (3.7), in this wave function. The resulting perturbation expansion can also be described by graphs. These graphs have the same structure as those that occurred in the expansion (2.16) of $\alpha(\omega)$, except that here matrix elements of j_μ and j_ν occur at the external interaction lines. Among them are both proper and improper ones. It is shown in Appendix B that the proper graphs give a contribution of the form of the first term on the right of Eq. (3.11) while the improper graphs give a contribution of the form of the second term. The third term of $T_{\mu\nu}$, Eq. (3.8), arises directly on taking the expectation value of the second part of the current operator, Eq. (3.7).

Now consider the response to the vector potential (3.1) of the *hypothetical* medium introduced in the last section in which the interactions between charged particles are described by a cutoff Coulomb potential. Let the response of this medium be characterized by $T_{\mu\nu}'$ which, from our previous discussion, differs from $T_{\mu\nu}$ only in the omission of improper graphs. As the latter contributed the second term of Eq. (3.11), one has

$$\lim_{q\to 0} T_{\mu\nu}' = a(\omega)\delta_{\mu\nu}. \quad (3.12)$$

Further, in analogy with Eq. (3.10), we now find

$$\lim_{q\to 0} q_\mu T_{\mu\nu}' q_\nu/q^2 = -(\omega^2/4\pi c)\alpha_P(\omega), \quad (3.13)$$

since the longitudinal polarizability of this hypothetical medium is α_P. From these two equations we see that

$$a(\omega) = -(\omega^2/4\pi c)\alpha_P(\omega). \quad (3.14)$$

Now, Eq. (3.10) as it stands says

$$a(\omega)+b(\omega) = -(\omega^2/4\pi c)\alpha(\omega). \quad (3.15)$$

Remembering the relation (2.18) between $\alpha(\omega)$ and $\alpha_P(\omega)$, we thus have for the real insulator

$$\lim_{q\to 0} T_{\mu\nu} = -(\omega^2/4\pi c)\alpha_P(\omega)[\delta_{\mu\nu}+\alpha(\omega) q_\mu q_\nu/q^2]. \quad (3.16)$$

When one now expresses $\alpha_P(\omega)$ and $\alpha(\omega)$ in terms of $\kappa(\omega)$ from Eqs. (3.4) and (3.5) one gets the result (3.3).

The second term in the square bracket in Eq. (3.16) plays a role only in the case of a longitudinal field and contains the long range effects of the Coulomb interactions. It has the effect of reducing the amplitude of an external longitudinal electric field, $E(\omega)=i(\omega/c)A(\omega)$. by a factor of $\kappa(\omega)$. In both the longitudinal and transverse cases, however, one gets the same local relation (1.1) between the induced current and the total electric field.

4. OPTICAL PROPERTIES AND SUM RULES

In this section we shall recall the relation of the dielectric constant $\kappa(\omega)$ to physically observable properties.

To discuss the propagation of light through our system, we may use Maxwell's equations in the transverse gauge, $\nabla\cdot\mathbf{A}=0$, namely

$$\Box\mathbf{A} = -\frac{4\pi}{c}\mathbf{j}_\perp, \quad \mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} - \nabla\varphi,$$
$$\nabla^2\varphi = -4\pi\rho, \quad \mathbf{B} = \nabla\times\mathbf{A}, \quad (4.1)$$

where $\mathbf{j}_\perp$ is the solenoidal part of the current density.

We see from the discussion of the last section that a transverse vector potential excites only a transverse current and thus we can find transverse wave solutions for the electromagnetic field in the insulator:

$$\mathbf{A}=\mathbf{A}_0 e^{i[\mathbf{q}(\omega)\cdot\mathbf{x}-\omega t]},\quad \varphi=0. \tag{4.2}$$

Substituting (4.2) into (4.1) and using the constitutive equation of the last section [see Eqs. (3.2), (3.3)] we have

$$\mathbf{A}_0(-q^2+\omega^2/c^2) = -(4\pi/c)\{(\omega^2/4\pi c)[\kappa(\omega)-1]\}\mathbf{A}_0. \tag{4.3}$$

The usual dispersion relation $\mathbf{q}(\omega)$ in the medium results from (4.3), namely

$$q^2=(\omega^2/c^2)\kappa(\omega). \tag{4.4}$$

The complex dielectric constant $\kappa(\omega)$ may as usual be written

$$\kappa(\omega)=\epsilon(\omega)+(4\pi i/\omega)\sigma(\omega), \tag{4.5}$$

where $\epsilon(\omega)$ is the real dielectric constant and $\sigma(\omega)$ the real conductivity. From Eqs. (3.5) and (2.27) we see that

$$\sigma(\omega)=-\frac{\omega}{4\pi}\,\mathrm{Im}\alpha_P(\omega)=\frac{\pi e^2}{2m\omega}\sum_n f_{0n}(0)\delta(\omega-\omega_{0n}), \tag{4.6}$$

where a term containing $\delta(\omega+\omega_{0n})$ has been omitted for obvious reasons. Integrating over ω and using the sum rule (2.23) (for $q=0$) gives

$$\int_0^\infty \sigma(\omega)d\omega=\pi e^2N/2m\Omega. \tag{4.7}$$

The alternative definition (3.4) of $\kappa(\omega)$, namely $\kappa(\omega)=[1+\alpha(\omega)]^{-1}$, is the natural definition for the discussion of the response to longitudinal fields. In the limit of zero frequency $\kappa(\omega)$ becomes the static dielectric constant which is real and finite for the perfect insulator.[12] We see from the definitions (2.13) and (2.15) of $\alpha(\omega)$ that $\kappa(0)$ describes, in the usual way, the partial neutralization of a static external charge embedded in the insulator.[13]

Another sum rule follows from Eqs. (3.4), (2.24), and (2.23),

$$\mathrm{Im}\int_0^\infty \frac{\omega}{\kappa(\omega)}d\omega=-\frac{2\pi^2e^2}{m\Omega}\int_0^\infty d\omega \lim_{q\to 0}\sum_n f_{0n}(\mathbf{q})\delta(\omega-\omega_{0n}) = -\frac{2\pi^2e^2N}{m\Omega}. \tag{4.8}$$

This relation has been used to discuss the energy loss {proportional to $\mathrm{Im}[\omega/\kappa(\omega)]$} of fast particles traversing a solid.[14,5]

It may be worth noting that [using Eq. (4.5)] this longitudinal sum rule can also be written in the form

$$\int_0^\infty \frac{\sigma(\omega)}{[4\pi\sigma(\omega)/\omega]^2+\epsilon^2(\omega)}d\omega=\frac{\pi e^2N}{2m\Omega}, \tag{4.9}$$

where it refers explicitly to the optical properties of the medium.

5. STATIC MAGNETIC PERMEABILITY

In the preceding sections the only restriction that has been made is to long wavelengths. The constitutive equation (3.3) is the first term in an expansion of the kernel $T_{\mu\nu}$ in powers of q. We wish to remark here that if the further restriction to low frequencies is made, one can deduce the form of the next term in the expansion of $T_{\mu\nu}$. This term contains the static magnetic permeability of the medium.

Let us make a schematic order of magnitude expansion of the explicit relation (3.8) for $T_{\mu\nu}$:

$$T(\mathbf{q},\omega)=\frac{e^2N}{mc\Omega}\left[O\left(\frac{\omega^2}{\omega_e^2}\right)+O\left(\frac{q^2}{q_e^2}\right)+O\left(\frac{\omega^2q^2}{\omega_e^2q_e^2}\right)+\cdots\right]. \tag{5.1}$$

Here ω_e is a typical electronic frequency (of the order of volts) and q_e a typical electronic wave number (of the order of reciprocal angstroms). The first term in the square bracket in (5.1) has been dealt with in detail in the preceding sections. It is clear from symmetry that there can be no term linear in q. The second and third terms in (5.1) are quadratic in q and are negligible compared to the first term in the long wavelength limit ($q/q_e\ll 1$). The second term does not involve the frequency ω and may thus be clearly identified as describing a current induced by the magnetic field, $\mathbf{B}=\nabla\times\mathbf{A}$, associated with the external vector potential (3.1). Since there is no magnetic field associated with a longitudinal field, the complete tensor form of this term must be[15]

$$C(q^2\delta_{\mu\nu}-q_\mu q_\nu). \tag{5.2}$$

The current described by (5.2) may be related to the usual magnetization current of macroscopic electrodynamics by writing

$$C=c\frac{\mu(0)-1}{4\pi\mu(0)}, \tag{5.3}$$

where $\mu(0)$ is the static magnetic permeability. The third term of (5.1) becomes comparable to the second

[12] This is seen from Eq. (2.24) using the fact that there is an energy gap between the ground state and the first excited state of the perfect insulator.

[13] $\kappa(0)$ is the static dielectric constant introduced in reference 4 in terms of the energy of interaction of two distant point changes.

[14] J. Hubbard, Proc. Phys. Soc. (London) **A68**, 976 (1955). See also E. Fermi, Phys. Rev. **57**, 485 (1940); and H. Fröhlich and H. Pelzer, Proc. Phys. Soc. (London) **A68**, 525 (1955).

[15] M. R. Schafroth, Helv. Phys. Acta **24**, 645 (1951).

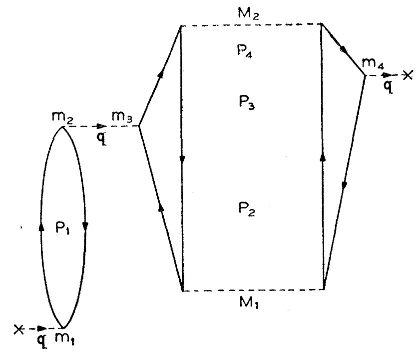


FIG. 4. An improper polarization graph used in the discussion of the factorization of these graphs.

term when the external frequency becomes comparable to an electronic frequency. It is not possible to deduce the structure of this term from simple arguments. However, if we restrict ourselves to low frequencies ($\omega\ll\omega_e$) the dominant terms of the expansion of $T_{\mu\nu}$ are, using (5.2), (5.3) and (3.3),

$$\lim_{\substack{q\to 0\\ \omega\to 0}} T_{\mu\nu}(\mathbf{q},\omega)=\frac{\omega^2}{4\pi c}[\kappa(0)-1]\left[\delta_{\mu\nu}+\frac{q_\mu q_\nu}{q^2}\left(\frac{1}{\kappa(0)}-1\right)\right] +c\frac{\mu(0)-1}{4\pi\mu(0)}(q^2\delta_{\mu\nu}-q_\mu q_\nu). \quad (5.4)$$

When the constitutive equation (5.4) is used with Maxwell's equations, as in Sec. 4, the induced currents may be interpreted, in the usual manner of macroscopic electrodynamics, as the sum of induced polarization and magnetization currents; and the dispersion relation for low-frequency light can easily be seen to be

$$q^2=(\omega^2/c^2)\kappa(0)\mu(0). \quad (5.5)$$

This completes our derivation of the macroscopic electromagnetic properties of an insulator from the microscopic Schrödinger equation, including the electron-electron interaction.

APPENDIX A

We wish here to consider the following theorem. Consider any improper polarization graph which occurs in the expansion (2.16) of $\alpha(\omega)$. Call it $\mathfrak{D}$. It will consist of a number of proper graphs connected by Coulomb interaction lines carrying momentum $\mathbf{q}$. Focus attention on any one of these lines. Call it L. Let $\mathfrak{D}_L$ be the part of the graph on the left of L and $\mathfrak{D}_R$ the part on the right. Consider all graphs $\mathfrak{D}',\mathfrak{D}'',\cdots$ etc., obtained from $\mathfrak{D}$ by keeping L fixed and $\mathfrak{D}_L$ and $\mathfrak{D}_R$ unchanged, but arranging those interaction lines of $\mathfrak{D}_L$ that are above L in all possible positions relative to the interaction lines of $\mathfrak{D}_R$ above L, and similarly arranging the interaction lines of $\mathfrak{D}_L$ and $\mathfrak{D}_R$ below L. Now consider the separate graphs $\bar{\mathfrak{D}}_L$ and $\bar{\mathfrak{D}}_R$ obtained from $\mathfrak{D}$ by removing L and in its place attaching to the two parts of $\mathfrak{D}$ external interaction lines that preserve the sense of the momentum transfer. Then the sum of the contributions to $\alpha(\omega)$ of $\mathfrak{D},\mathfrak{D}',\mathfrak{D}''$etc. is equal to the product of the contributions of $\bar{\mathfrak{D}}_L$ and $\bar{\mathfrak{D}}_R$.

We shall illustrate this theorem by a simple example which exhibits its complete generality. In Fig. 4 the quantities m_1,m_2,m_3,m_4 represent the matrix elements (between Bloch states) of $e^{\pm i\mathbf{q}\cdot\mathbf{x}}/q$ which occur at the verticies adjacent to these symbols. Note that the matrix element of the Coulomb interaction (2.3) which occurs at the interaction line connecting the two parts of the diagram has been split up into separate matrix elements of $e^{-i\mathbf{q}\cdot\mathbf{x}}/q$ and $e^{i\mathbf{q}\cdot\mathbf{x}}/q$ called m_2 and m_3, respectively. At the two other Coulomb interaction lines the matrix elements are indicated, with sufficient generality for our purposes, as M_1 and M_2. P_1,P_2 etc., are differences between hole and electron energies. P_1 refers to the electron and hole in the left-hand portion of the diagram; P_2,P_3 etc., refer to the particles and holes in the appropriate sections of the right-hand part. The contribution of Fig. 4 to $\alpha(\omega)$ is

$$-\left(\frac{4\pi e^2}{\Omega}\right)^2 M_2\frac{1}{P_4}m_4\frac{1}{P_3+\omega+is}m_3m_2 \times\frac{1}{P_1+P_2+\omega+is}M_1\frac{1}{P_1+\omega+is}m_1. \quad (A.1)$$

In (A.1) the sign can be obtained from the rule[6] $(-1)^{h+l}$ where h is the number of hole lines and l the number of closed loops; one of the factors $4\pi e^2/\Omega$ comes from the definition (2.16) of $\alpha(\omega)$, the other occurs because $(4\pi e^2/\Omega)m_1m_2$ is the Coulomb matrix element.

Consider now the graph Fig. 5. Its contribution is

$$-\left(\frac{4\pi e^2}{\Omega}\right)^2 M_2\frac{1}{P_4}m_4\frac{1}{P_3+\omega+is}m_3m_2 \times\frac{1}{P_1+P_2+\omega+is}m_1\frac{1}{P_2}M_1. \quad (A.2)$$

Using the identity[16]

$$\frac{1}{P_1+\omega+is}\,\frac{1}{P_2}=\frac{1}{P_1+P_2+\omega+is}\,\frac{1}{P_1+\omega+is} +\frac{1}{P_1+P_2+\omega+is}\,\frac{1}{P_2} \quad (A.3)$$

the sum of the expressions (A.1) and (A.2) is

$$\left[-\left(\frac{4\pi e^2}{\Omega}\right)M_2\frac{1}{P_4}m_4\frac{1}{P_3+\omega+is}m_3\frac{1}{P_2}M_1\right] \times\left[\left(\frac{4\pi e^2}{\Omega}\right)m_2\frac{1}{P_1+\omega+is}m_1\right]. \quad (A.4)$$

[16] N. M. Hugenholtz, Physica 23, 481 (1957).

The first square bracket in (A.4) is the contribution of the graph on the right of Fig. 6, the second that of the graph on the left.

By applying a succession of identities of the form (A.3), and following the prescription given in the first paragraph of this appendix, the most general improper diagram can be factored as in the above example.

APPENDIX B

In this appendix we consider the graphical expansion of the tensor $T_{\mu\nu}$ [see the explicit expression (3.8)] and discuss the tensor form of the graphs which describe the first two terms of $\lim_{q\to 0} T_{\mu\nu}$, namely

$$\frac{e^2}{c\Omega}\lim_{q\to 0}\sum_n\left[\frac{j_\mu(-\mathbf{q})_{0n}j_\nu(\mathbf{q})_{n0}}{\omega_{0n}-\omega-is}+\frac{j_\nu(\mathbf{q})_{0n}j_\mu(-\mathbf{q})_{n0}}{\omega_{0n}+\omega+is}\right]. \quad \text{(B.1)}$$

Comparing these terms with the expression (2.24) for $\alpha(\omega)$, it is clear that the graphs which occur here have the same form as those that describe the expansion (2.16) of $\alpha(\omega)$ except that here the operators j_μ and j_ν occur at the external interaction lines.

The one particle matrix element of $j_\mu(\mathbf{q})$ is

$$\frac{1}{m}(\psi_{n,\mathbf{k}+\mathbf{q}},\, e^{i\mathbf{q}\cdot\mathbf{x}}(p_\mu+q_\mu/2)\psi_{m,\mathbf{k}}), \quad \text{(B.2)}$$

where $\psi_{n,\mathbf{k}+\mathbf{q}}$, and $\psi_{m,\mathbf{k}}$ are Bloch functions. This matrix element approaches a finite limit as q approaches zero. As a result, in the calculation of the contribution of a proper graph to (B.1) one finds to lowest order in q a second rank tensor independent of $\mathbf{q}$. It follows from the assumed cubic symmetry of our system that this tensor must be diagonal. Thus the contribution of all proper graphs has the tensor form $\delta_{\mu\nu}$.

Consider, now, an arbitrary improper graph that

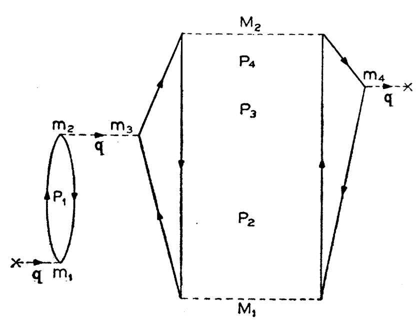


FIG. 5. A graph closely related to that of Fig. 4.

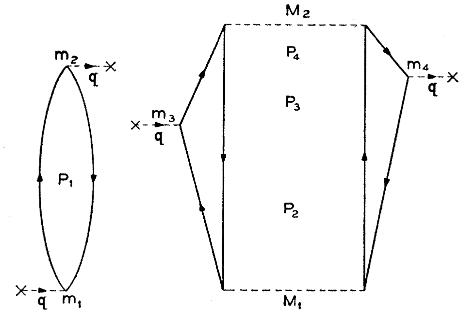


FIG. 6. Two graphs the product of whose contributions equals the sum of the contributions of Figs. 4 and 5.

occurs in the expansion of (B.1). (See the schematic graph of Fig. 1.) It can be factored as in Appendix A into the product of proper parts. The *inner* proper parts, namely those which have one-particle matrix elements of $q^{-1}\rho(\pm\mathbf{q})$ at both their external lines make a contribution which in the limit of small q is a scalar function of frequency. The two *outer* proper graphs, each of which has a $\mathbf{j}$ operator at one external line and a ρ operator at the other, make contributions which transform like vectors under rotations.

Consider any outer proper graph in which the matrix element of $q^{-1}\rho(\mathbf{q})$ occurs at one external line. This matrix element has, in the limit of small q, the form

$$(\psi_{n,\mathbf{k}+\mathbf{q}},q^{-1}e^{i\mathbf{q}\cdot\mathbf{x}}\psi_{m,\mathbf{k}}) = q^{-1}\delta_{nm}+q^{-1}\mathbf{q}\cdot\left(\frac{\partial}{\partial\mathbf{k}}u_{n,\mathbf{k}},u_{m,\mathbf{k}}\right), \quad \text{(B.3)}$$

where $u_{n,\mathbf{k}}$ is the modulating function of the Bloch wave. If an *inter*band transition takes place at the vertex where the above matrix element occurs, the δ_{nm} gives zero. Then one finds, to lowest order in $\mathbf{q}$, a contribution from the graph of the form $q^{-1}q_\lambda U_{\lambda\nu}(\omega)$ where $U_{\lambda\nu}(\omega)$ is a tensor with no $\mathbf{q}$ dependence and ν indicates the Cartesian component of the $\mathbf{j}$ operator which acts at the other external interaction line. From cubic symmetry $U_{\lambda\nu}(\omega)$ must be diagonal, and, thus, the vector dependence of this outer graph has the form $q^{-1}q_\nu$. That the same vector dependence occurs for an outer proper part in which an *intra*band transition takes place at the external ρ vertex follows from arguments given in reference 4, Sec. 2.

Similarly, the vector form of the other outer proper graph which multiplies the contribution of the part discussed in the last paragraph is q_μ/q. Thus the tensor form of the sum of all improper graphs is $q_\mu q_\nu/q^2$.