Electromagnetic Properties of Insulators. II*

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This paper is a continuation of an earlier study, from a many particle point of view, of the electromagnetic properties of insulators. Here the system of an insulator and one electron is treated. The Coulomb interactions between all the electrons in the system are allowed for to all orders of perturbation theory. The true effective mass m^* of the extra particle is defined as the curvature in wave vector space of the energy surface connecting the ground state and the low-lying excited states of the interacting system. The central result then obtained is that the response of the system to long-wavelength, low-frequency electric fields is exactly that of a free electron of mass m^* moving in a medium characterized by the dielectric constant of the perfect insulator. The energy levels of the system in a static magnetic field are also discussed. An alternative derivation of a single-particle effective-mass equation, previously obtained by Klein, is given. The eigenvalues of this equation are under certain conditions the energy levels of the interacting system in a magnetic field. In an Appendix a Kramers-Kronig relation connecting the difference in optical absorption of the present system and the perfect insulator with m^* is derived. These results indicate that the usual effective-mass theory of semiconductors of low carrier concentration includes the effects of the electron-electron interactions to an excellent approximation.

1. INTRODUCTION

EXPERIMENTS on semiconductors containing a few carriers, such as those dealing with shallow impurity states, optical absorption and cyclotron resonance, have long been interpreted with quantitative success in terms of an effective mass model.[1] In this model, the carriers are treated as free particles having an effective mass m^* (in the simplest cases a scalar), moving in a medium characterized by a macroscopic dielectric constant. Effective-mass theory is customarily justified from the standpoint of the independent-particle approximation.[2] In view of the experimental success of the theory, however, one is led to suspect that the assumption of weak electron-electron interactions is sometimes not necessary for its derivation. Recent theoretical work, mentioned below, has shown that this is in fact the case. In the present paper we further investigate this question. We consider the system of an insulator plus one electron. We study the response of this system to weak electromagnetic fields using methods very similar to those applied in an earlier paper[3] to the perfect insulator. The main result we then prove is an inertial theorem which states that the response of the system to *long-wavelength, low-frequency* electric fields is exactly that of a free electron of mass m^* moving in a medium having the dielectric constant of the perfect insulator. This result includes Coulomb interactions to all orders of perturbation theory. Kohn [4,5] has previously shown that the bound states which occur when a small positive charge is embedded in this system have a hydrogenlike spectrum given by

$$E_n=-\frac{m^*e^2Q^2}{2[\kappa^I(0)]^2}\frac{1}{n^2},\quad n=1,2\cdots, \tag{1.1}$$

where Q is the embedded charge and $\kappa^I(0)$ the static dielectric constant of the perfect insulator.[6] Furthermore, Klein[7] has shown, and we shall also show, that the spacing of the low-lying energy levels of this system in a constant not too strong magnetic field is

$$\omega_C=e\mathfrak{H}/m^*c, \tag{1.2}$$

where $\mathfrak{H}$ is the magnetic field. The results (1.1) and (1.2), like the inertial theorem to be proved here, are exactly what one expects on the basis of the above-mentioned effective-mass theory. They show that this theory is exact for gently varying perturbations of the system of an insulator and one electron. Consequently, it is very nearly exact for semiconductors of low carrier concentration.

In outline, the program of this paper is as follows. In Sec. 2 we discuss the form of the many-particle wave functions of our system, and define the true effective mass m^*. We also derive a longitudinal sum rule satisfied by our system. In Sec. 3, we calculate the response of our system to long-wavelength electric fields of arbitrary polarization. In Sec. 4 we show that the low-frequency response may be interpreted as the inertial theorem stated above, and make some comments about the response at higher frequencies and about the case of more than one extra particle. Finally, in Sec. 5 we discuss the response to a static magnetic

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[1] W. Kohn, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1957), Vol. V, p. 257; H. Y. Fan, *Reports on Progress in Physics* (The Physical Society, London, 1956), Vol. 19, p. 107; G. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev. **98**, 368 (1955).

[2] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955). Other references are given here.

[3] V. Ambegaokar and W. Kohn, Phys. Rev. **117**, 423 (1960).

[4] W. Kohn, Phys. Rev. **105**, 509 (1957).

[5] W. Kohn, Phys. Rev. **110**, 857 (1957).

[6] Throughout this paper the superscript I indicates a property of the perfect insulator and $\hbar=1$.

[7] A. Klein, Phys. Rev. **115**, 1136 (1959).

field. Appendixes A and C clarify some details of the argument. In Appendix B we show that a Kramers-Kronig relation[8] between the true effective mass and the integrated electrical conductivity follows quite generally from the inertial theorem.

2. EIGENSTATES, TRUE EFFECTIVE MASS, AND SUM RULE

As our model we consider a lattice of nuclei (supposed rigid and of cubic symmetry) and electrons which interact with these nuclei as well as with each other at the absolute zero of temperature. Our system is obtained by adding one electron to the perfect insulator of reference 3. The Hamiltonian that describes this system of $(N+1)$ electrons is

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

where

$$H_0=\sum_{i=1}^{N+1}(T_i+V_i), \tag{2.2}$$

and

$$H_C=\frac{4\pi e^2}{\Omega}\sum_{i<j}\sum_{k\neq 0}\frac{e^{i\mathbf{k}\cdot\mathbf{x}_i-\mathbf{x}_j}}{k^2}. \tag{2.3}$$

Here T_i is the kinetic energy of the ith electron and V_i its interaction with the lattice. H_C describes the Coulomb interactions between the electrons (Ω is the volume of the normalization box) and H_L the electrostatic energy of the lattice. Because of the translational symmetry of the lattice, the eigenstates of (2.1) may be characterized by a wave vector $\mathbf{k}$ (confined to a unit cell of the reciprocal lattice) such that

$$\begin{aligned}T_\alpha\Psi_{n,\mathbf{k}}(\mathbf{x}_1,\mathbf{x}_2,\cdots)&=\Psi_{n,\mathbf{k}}(\mathbf{x}_1+\boldsymbol{\tau}_\alpha,\mathbf{x}_2+\boldsymbol{\tau}_\alpha,\cdots)\\&=\exp(i\mathbf{k}\cdot\boldsymbol{\tau}_\alpha)\Psi_{n,\mathbf{k}}(\mathbf{x}_1,\mathbf{x}_2,\cdots),\end{aligned} \tag{2.4}$$

where

$$H\Psi_{n,\mathbf{k}}=E_{n,\mathbf{k}}\Psi_{n,\mathbf{k}}. \tag{2.5}$$

Here T_α is the operator which translates all electrons through the lattice vector $\boldsymbol{\tau}_\alpha$ and n denotes all quantum numbers needed in addition to $\mathbf{k}$ to specify the state $\Psi_{n,\mathbf{k}}$ of energy $E_{n,\mathbf{k}}$. Let us assume for simplicity that the ground state corresponds to $\mathbf{k}=0$ and call the n associated with this state $n=0$. We also require that in the neighborhood of the ground-state (energy $E_{0,0}$) there be a set of states of energy $E_{0,\mathbf{k}}$, and that for small enough $\mathbf{k}$ all other states $E_{n,\mathbf{k}}$ $(n\neq 0)$ satisfy the inequality

$$E_{n,\mathbf{k}}-E_{0,0}>\Delta E, \tag{2.6}$$

where ΔE is a characteristic energy of the order of electron volts. The foregoing requirements incorporate the notion of an energy gap against all excitations in our interacting system except those corresponding to "intra-band" transitions of the "extra particle."[4] They, furthermore, make the unimportant simplifying assumption that, except for direction of $\mathbf{k}$, degeneracies due to the point group symmetry of the lattice do not occur near $E_{0,0}$. The eigenstates $\Psi_{0,\mathbf{k}}$, for small $\mathbf{k}$, are then the one-particle like states which may be put into one-to-one correspondence with the set of Slater determinants corresponding to N electrons filling a certain integral number of Brillouin zones and one electron near the bottom of a simple conduction band. The true effective mass is defined by the expansion[9]

$$E_{0,\mathbf{k}}=E_{0,0}+(k^2/2m^*)+\cdots, \tag{2.7}$$

where we have used the assumed cubic symmetry of the system. Let us also note for future reference that, because of the invariance of the Hamiltonian (2.1) under time reversal, the energy levels $E_{n,k}$ satisfy

$$E_{n,\mathbf{k}}=E_{n,-\mathbf{k}}, \tag{2.8}$$

and the states $\Psi_{n,\mathbf{k}}$ may be chosen to have the property

$$\Psi_{n,\mathbf{k}}{}^*(\mathbf{x}_1,\mathbf{x}_2,\cdots)=\Psi_{n,-\mathbf{k}}(\mathbf{x}_1,\mathbf{x}_2,\cdots). \tag{2.9}$$

We now proceed to derive a longitudinal f-sum rule satisfied by our system of $N+1$ electrons. We start from the identities

$$[H,\rho(\mathbf{q})]=\mathbf{q}\cdot\mathbf{j}(\mathbf{q}), \tag{2.10}$$

$$[[H,\rho(\mathbf{q})],\rho(-\mathbf{q})]=-\frac{(N+1)q^2}{m}, \tag{2.11}$$

where the operators $\rho(\mathbf{q})$ and $\mathbf{j}(\mathbf{q})$ are defined as follows:

$$\rho(\mathbf{q})=\sum_{i=1}^{N+1}e^{i\mathbf{q}\cdot\mathbf{x}_i}, \tag{2.12}$$

$$\mathbf{j}(\mathbf{q})=\frac{1}{2m}\sum_{i=1}^{N+1}(\mathbf{p}_i e^{i\mathbf{q}\cdot\mathbf{x}_i}+e^{i\mathbf{q}\cdot\mathbf{x}_i}\mathbf{p}_i). \tag{2.13}$$

Here $\mathbf{p}_i$ is the momentum operator for the ith electron.

Taking the expectation value of (2.11) in the ground state $\Psi_{0,0}$, we have

$$\begin{aligned}&(E_{0,\mathbf{q}}-E_{0,0})\,|\,(0,\mathbf{q}\,|\,\rho(\mathbf{q})\,|\,0,0)\,|^2\\&\quad+(E_{0,-\mathbf{q}}-E_{0,0})\,|\,(0,-\mathbf{q}\,|\,\rho(-\mathbf{q})\,|\,0,0)\,|^2\\&\quad+\sum_{n\neq 0}(E_{n,\mathbf{q}}-E_{0,0})\,|\,(n,\mathbf{q}\,|\,\rho(\mathbf{q})\,|\,0,0)\,|^2\\&\quad+\sum_{n\neq 0}(E_{n,-\mathbf{q}}-E_{0,0})\,|\,(n,-\mathbf{q}\,|\,\rho(-\mathbf{q})\,|\,0,0)\,|^2\\&\qquad=\frac{(N+1)q^2}{m}.\end{aligned} \tag{2.14}$$

Using time-reversal invariance (2.8) and (2.9) and the definition (2.7) of the effective mass, we have[10]

$$\lim_{q\to 0}\frac{m}{m^*}\,|\,(0,\mathbf{q}\,|\,\rho(\mathbf{q})\,|\,0,0)\,|^2+\sum_{n\neq 0}f_{0n}{}^l=(N+1), \tag{2.15}$$

[8] V. Ambegaokar and W. Kohn, Phys. Rev. Letters **2**, 385 (1959).

[9] This is the same definition as that used by Kohn[4] and Klein.[7]

[10] This relation is also a direct consequence of gauge invariance. See reference 16.

where $f_{0n}{}^{l}$ is defined by

$$f_{0n}{}^{l}=\lim_{q\to 0}\frac{2m}{q^2}(E_{n,\mathbf{q}}-E_{0,0})\,|\,(n,\mathbf{q}|\rho(\mathbf{q})|0,0)\,|^2$$

$$=\lim_{q\to 0}\frac{2m}{E_{n,q}-E_{0,0}}\left|\left(n,\mathbf{q}\left|\frac{\mathbf{q}}{q}\cdot\mathbf{j}(\mathbf{q})\right|0,0\right)\right|^2 \quad (2.16)$$

and the last equality follows from (2.10). The matrix element $\lim_{q\to 0}(0,\mathbf{q}|\rho(\mathbf{q})|0,0)$ has been discussed by Kohn.[5] He has shown that

$$\lim_{q\to 0}(0,\mathbf{q}|\rho(\mathbf{q})|0,0)=\frac{1}{\kappa^I(0)}, \quad (2.17)$$

where $\kappa^I(0)$ is the static dielectric constant of the perfect insulator. Substituting (2.17) into (2.15), we get the sum rule

$$\frac{m}{m^*}\left(\frac{1}{\kappa^I(0)}\right)^2+\sum_{n\neq 0} f_{0n}{}^{l}=(N+1). \quad (2.18)$$

Since this sum rule contains the static dielectric constant of the perfect insulator, a characteristic many-particle effect, it cannot be derived in the independent-particle model.

We shall see in the next section that the longitudinal oscillator strengths introduced here characterize the response of our system to perturbing long-wavelength longitudinal electric fields. We shall also see that a transverse sum rule having exactly the form of the usual f-sum rule of the Bloch theory holds for our system as well.[11] This sum rule will characterize the response to transverse fields.

3. RESPONSE TO FIELDS OF ARBITRARY POLARIZATION

The program of this section is very similar to that of reference 3, Secs. 2 and 3. We start by calculating the longitudinal long-wavelength polarizability of our system in terms of the exact many-particle wave functions. We then make an expansion of this quantity in powers of the Coulomb interaction and represent the terms by graphs. As a result of the graphical expansion we are able to isolate the long-range effects of the Coulomb interactions which do not occur in the response to a transverse field. Finally, we calculate the complete tensor form of the kernel $T_{\mu\nu}$ which relates the induced current to a perturbing vector potential. The low-frequency form of $T_{\mu\nu}$ which we explicitly exhibit here leads at once in the next section to the inertial theorem mentioned in Sec. 1.

Let us start, then, by calculating the long-wavelength longitudinal polarizability, $\alpha(\omega)$, of our system. We define this quantity by the relations

$$\rho_{\text{ind}}(\mathbf{q},\omega)=\alpha(\mathbf{q},\omega)\rho_{\text{ext}}(\mathbf{q},\omega), \quad (3.1)$$

$$\alpha(\omega)=\lim_{q\to 0}\alpha(\mathbf{q},\omega). \quad (3.2)$$

Here $\rho_{\text{ext}}(\mathbf{q},\omega)$ and $\rho_{\text{ind}}(\mathbf{q},\omega)$ are, respectively, the Fourier coefficients of an external charge density embedded in the system and the induced charge density. To calculate $\alpha(\omega)$ we suppose the external perturbation to be slowly turned on with a time factor e^{st}, find the perturbed wave function of the $(N+1)$-particle system to first order in the external potential, and take the expectation value of the electronic charge density operator in this wave function.[3] As a result we find[12]

$$\alpha(\omega)=\lim_{q\to 0}\left(\frac{4\pi e^2}{q^2\Omega}\right)(-i)\times\int_{-\infty}^{0}dt\langle[\rho(-\mathbf{q},0),\rho(\mathbf{q},t)]\rangle_0 e^{-i\omega t}e^{st}. \quad (3.3)$$

Here $\rho(\mathbf{q},t)$ is the operator $\rho(\mathbf{q})$ [Eq. (2.12)] in the Heisenberg representation, i.e.,

$$\rho(\mathbf{q},t)=e^{iHt}\rho(\mathbf{q})e^{-iHt}, \quad (3.4)$$

with H given by (2.1). In (3.3) the subscript 0 indicates that the expectation value of the commutator is to be taken in the ground state $\Psi_{0,0}$. Performing the time integration indicated in (3.3) and introducing the oscillator strengths of the last section, we have

$$\begin{aligned}\alpha(\omega)&=\lim_{q\to 0}-\frac{4\pi e^2}{q^2\Omega}\sum_n\left(\frac{\rho(-\mathbf{q})_{0n}\rho(\mathbf{q})_{n0}}{\omega_{0n}-\omega-is}+\frac{\rho(\mathbf{q})_{0n}\rho(-\mathbf{q})_{n0}}{\omega_{0n}+\omega+is}\right)\\&=-\frac{4\pi e^2}{\Omega}\lim_{q\to 0}\left\{\frac{1}{[\kappa^I(0)]^2q^2}\left[\frac{1}{(q^2/2m^*)-\omega-is}\right.\right.\\&\qquad\left.\left.+\frac{1}{(q^2/2m^*)+\omega+is}\right]\right\}\\&\quad-\frac{4\pi e^2}{m\Omega}\sum_{n\neq 0}\frac{f_{0n}{}^{l}}{2\omega_{0n}}\left(\frac{1}{\omega_{0n}-\omega-is}+\frac{1}{\omega_{0n}+\omega+is}\right)\\&=\frac{4\pi e^2}{\Omega\omega^2}\frac{1}{m^*[\kappa^I(0)]^2}-\frac{4\pi e^2}{m\Omega}\sum_{n\neq 0}\frac{f_{0n}{}^{l}}{2\omega_{0n}}\left(\frac{1}{\omega_{0n}-\omega-is}\right.\\&\qquad\left.+\frac{1}{\omega_{0n}+\omega-is}\right).\end{aligned} \quad (3.5)$$

[11] It is easily seen from the explicit form (3.11) of $T_{\mu\nu}$ that Eq. (3.22) implies the following transverse sum rule

$$\frac{m}{m^*}+\sum_{n\neq 0} f_{0n}{}^{t}=N+1,$$

where

$$f_{0n}{}^{t}\equiv\lim_{q\to 0}\frac{2m}{E_{n,\mathbf{q}}-E_{0,0}}|\,(n,\mathbf{q}|\mathbf{j}(\mathbf{q})\cdot\mathbf{t}_{\mathbf{q}}|0,0)\,|^2,$$

where $\mathbf{t}_{\mathbf{q}}$ is a unit vector perpendicular to $\mathbf{q}$. A sum rule of the same form is well known in the Bloch theory. Here, however, the excited states indicated by the sum over n include states not obtainable in the independent-particle approximation.

[12] This is a special case of the type of result discussed by R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).

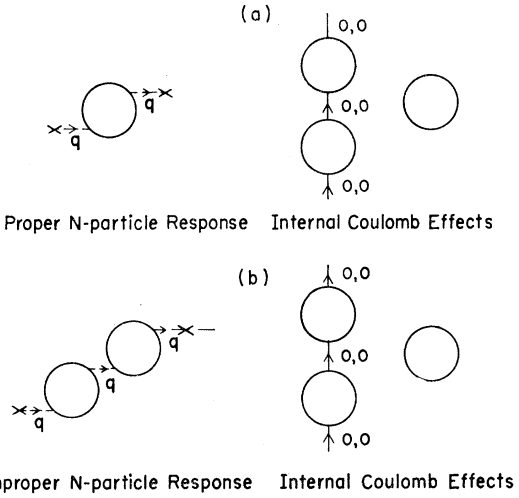

FIG. 1. Graphs corresponding to the polarization of the perfect insulator by a charge embedded in the $(N+1)$-particle system.

The subscripts in (3.5) refer to the exact $(N+1)$-particle eigenstates, the wave vector index has been suppressed for brevity, and $\omega_{0n}=E_n-E_0$.

The quantity $\alpha(\omega)$ may also be calculated as an expansion in powers of the Coulomb interaction. This was done in detail in reference 3 for the perfect insulator. We imagine the Coulomb interactions to be turned on with a time factor $e^{\eta t}$ and go over in (3.3) from the Heisenberg representation to the interaction representation, in which the time dependence of operators is determined by H_0.[13] The terms of the resulting perturbation series may be represented by graphs.[14] In this graphical representation we take the one particle ground state of the perfect insulator as "vacuum." Then the graphs that occur start and end with one line traveling upward and labelled with the one-particle quantum numbers, 0,0 (band 0, wave vector 0). The classes of graphs illustrated in Figs. 1 and 2 occur. Here the dashed horizontal lines starting at the crosses represent interactions with the external charge, those ending at crosses represent measurements of the induced charge. The solid line traveling upward represents the one particle state 0,0 occurring as the initial, intermediate or final state. The dashed horizontal internal lines indicate Coulomb matrix elements of wave vector $\mathbf{q}$. The circles schematically represent arbitrary graphs of interacting electrons with the restriction that they cannot be split into two parts by cutting either a single electron line labelled 0,0 or a single Coulomb interaction line carrying momentum $\mathbf{q}$. In the graphs of Fig. 1, the external interaction lines are not attached to the part of the graph that starts and ends with one line. The contribution of these graphs to the polarizability $\alpha(\omega)$ of (3.5) is exactly that of the perfect insulator which we here call $\alpha^I(\omega)$. (The parts of Fig. 1 labelled "internal Coulomb effects" correspond to the normalization sum of the clothed state $\Psi_{0,0}$, make a multiplicative contribution of 1, and may thus be omitted.[3]) The graphs of Fig. 2 represent the contribution of the extra particle to the polarizability. (Here again the vacuum parts may be omitted.) Let us call the contribution of graphs of the form of Fig. 2, $\beta(\omega)$. Then by our definition

$$\alpha(\omega)=\alpha^I(\omega)+\beta(\omega). \tag{3.6}$$

We now consider the connection between the totality of graphs and those of the form of Figs. 1(a) and 2(a). The latter cannot be split into two parts by cutting a single Coulomb line carrying momentum $\mathbf{q}$. Such graphs we call *proper* polarization graphs. Graphs of the form of Figs. 1(b) and 2(b), on the other hand, we call *improper* polarization graphs. For $\alpha^I(\omega)$ we have a relation between proper and improper graphs. This was discussed in detail in reference 3 and is

$$\alpha^I(\omega)=\alpha_P{}^I(\omega)[1+\alpha^I(\omega)]. \tag{3.7}$$

Here $\alpha_P{}^I$ is the sum of the contributions of all graphs of the form of Fig. 1(a). A similar relation connects $\beta(\omega)$ and graphs of the form of Fig. 2(a) whose contribution we call $\beta_P(\omega)$. It is

$$\beta(\omega)=[1+\alpha^I(\omega)]\beta_P(\omega)[1+\alpha^I(\omega)]. \tag{3.8}$$

Equation (3.8) follows from the fact that the contribution of the most general β graph may be factored into the parts obtained by cutting the Coulomb interaction lines carrying momentum $\mathbf{q}$. (See Appendix A where the question of taking the limit $q\rightarrow 0$ is also discussed.) Since a general improper β graph is obtained by attaching an N-particle polarization graph to one or other or both of the external lines of a β_P graph, Eq. (3.8) is proved. The relations (3.7) and (3.8) will prove useful in calculating the response to transverse fields since in this case, as we shall see, the long-wavelength Coulomb effects represented by the factors $[1+\alpha^I(\omega)]$ do not occur.

We now calculate the response of our system to fields of arbitrary polarization. To do this we calculate the tensor $T_{\mu\nu}(\mathbf{q},\omega)$ defined by the relation

$$j_\mu(\mathbf{q},\omega)=T_{\mu\nu}(q,\omega)A_\nu(\mathbf{q},\omega), \tag{3.9}$$

where $A_\nu(\mathbf{q},\omega)$ is the Fourier coefficient of the per-

[13] Explicitly, the first term in the commutator of (3.3) now becomes

$$\lim_{q\rightarrow 0}\frac{4\pi e^2}{q^2\Omega}(-i)\int_{-\infty}^{0}dt\lim_{\eta\rightarrow 0}(\Psi_{0,0}{}^{(0)}|U_\eta(-\infty,0)\rho(-q,0)\times P[U_\eta(0,-\infty)\rho_0(\mathbf{q},t)]|\Psi_{0,0}{}^{(0)})e^{-i\omega t}e^{st},$$

where

$$U_\eta(0,-\infty)=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}P\int_{-\infty}^{0}dt_1\cdots dt_n\,H_C(t_1)e^{\eta t_1}\cdots H_C(t_n)e^{\eta t_n}.$$

Here P is the usual chronological operator; $H_C(t)$ and $\rho_0(q,t)$ are interaction representation operators, i.e., $e^{iH_0t}H_Ce^{-iH_0t}$ and $e^{iH_0t}\rho(\mathbf{q})e^{-iH_0t}$, and $\Psi_{0,0}{}^{(0)}$ is the independent-particle ground state of the system.

[14] For more details on the graphical representation see J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957); J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957).

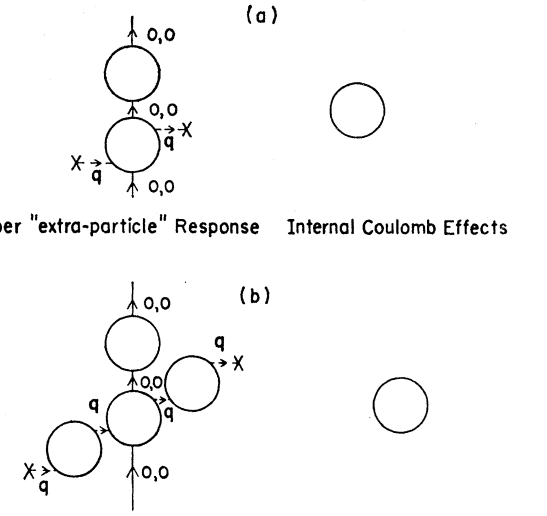

FIG. 2. Graph (a) represents the charge induced by the direct esponse of the "extra particle" to an embedded charge. Graph (b) shows the "extra particle" responding to the polarized medium and thereby further polarizing the medium.

turbing vector potential[15] and $j_\mu(\mathbf{q},\omega)$ that of the induced current.[3] The method of calculating $T_{\mu\nu}$ is similar to that described before Eq. (3.3). The result is[12]

$$T_{\mu\nu}(\mathbf{q},\omega)=\frac{ie^2}{c\Omega}\int_{-\infty}^{0}dt\langle[j_\mu(-\mathbf{q},0),j_\nu(\mathbf{q},t)]\rangle_0 e^{-i\omega t}e^{st} -\frac{e^2}{mc}\frac{(N+1)}{\Omega}\delta_{\mu\nu}. \quad (3.10)$$

Here $\mathbf{j}(\mathbf{q},t)$ is the operator $\mathbf{j}(\mathbf{q})$ [Eq. (2.13)] in the Heisenberg representation.

Performing the time integration in (3.10), we get[16]

$$T_{\mu\nu}(\mathbf{q},\omega)=\frac{e^2}{c\Omega}\sum_n j_\mu(-\mathbf{q})_{0n}j_\nu(\mathbf{q})_{n0}\left(\frac{1}{\omega_{0n}-\omega-is}+\frac{1}{\omega_{0n}+\omega+is}\right)-\frac{e^2}{mc}\frac{(N+1)}{\Omega}\delta_{\mu\nu}. \quad (3.11)$$

Here again the subscripts refer to exact $(N+1)$-particle eigenstates and the wave vector index has been suppressed. Note that the terms in the sum on n corresponding to $n=0$ (namely, those that refer to the transition from $\Psi_{0,0}$ to $\Psi_{0,\mathbf{q}}$) give no contribution in the limit of small q since then ω_{0n} approaches zero and the two terms in the large bracket have opposite sign.

By transforming (3.11) using the sum rule (2.18), the long-wavelength longitudinal part of $T_{\mu\nu}$ may be seen to be related to $\alpha(\omega)$ as follows:

$$T_l(\omega)\equiv\lim_{q\to0}q_\mu T_{\mu\nu}q_\nu/q^2 =-\frac{\omega^2}{4\pi c}\alpha(\omega). \quad (3.12)$$

Equation (3.12) is a statement of gauge invariance, namely, that the same longitudinal electric field described either by a vector or scalar potential induces the same charge.

Here, as in reference 3, we may use (3.12) to derive also the transverse part of $T_{\mu\nu}$. The first term of this quantity [Eq. (3.10)] may be expanded in powers of the Coulomb interaction. The graphs which represent this expansion have the same form as Figs. 1 and 2. It can be shown[17] that the improper graphs, i.e., Figs. 1(b) and 2(b), in the limit of small q have the tensor form $q_\mu q_\nu/q^2$ whereas the proper graphs have the form $\delta_{\mu\nu}$. Thus only the latter contribute to the transverse part of $T_{\mu\nu}$. Now the equality (3.12) also holds for the subseries represented by proper graphs in the expansions of the right and left sides.[18] Thus we conclude that

$$T_t(\omega)\equiv\lim_{q\to0}t_\mu T_{\mu\nu}(\mathbf{q},\omega)t_\nu=-\frac{\omega^2}{4\pi c}\alpha_P(\omega), \quad (3.13)$$

where α_P is the sum of graphs of the form of Figs. 1(a) and 2(a), i.e.,

$$\alpha_P(\omega)=\alpha_P{}^I(\omega)+\beta_P(\omega), \quad (3.14)$$

and $\mathbf{t}$ is a vector perpendicular to $\mathbf{q}$. Thus the complete tensor form of $T_{\mu\nu}$ is

$$\lim_{q\to0}T_{\mu\nu}(\mathbf{q},\omega)=-\frac{\omega^2}{4\pi c}\{\alpha_P(\omega)\delta_{\mu\nu} +[\alpha(\omega)-\alpha_P(\omega)]q_\mu q_\nu/q^2\}. \quad (3.15)$$

In the next section we shall discuss the physical interpretation of (3.15). Before doing this, however, it is convenient to display the low-frequency forms of the response more explicitly. For the longitudinal case we have, from (3.12) and (3.5), that

$$\lim_{\omega\to0}T_l(\omega)=-\frac{e^2}{m^*c\Omega}\frac{1}{[\kappa^I(0)]^2}. \quad (3.16)$$

[15] Since only the Coulomb interactions have been included in the Hamiltonian H, we mean here the *total* transverse vector potential and the longitudinal vector potential due to *external* sources. As in reference 3, we treat the long-wavelength part of the transverse field self-consistently.

[16] The relation (2.15) is equivalent to the statement $q_\mu T_{\mu\nu}(q,0)q_\nu/q^2=0$ as may be readily verified from the explicit expression (3.11) and the definition (2.16) of the oscillator strengths. Thus (2.15), and consequently the sum rule (2.18), follows from a requirement of gauge invariance, namely, that a longitudinal time-independent vector potential induce no polarization, since it describes no physical fields.

[17] See reference 3, Appendix B.

[18] This was shown in reference 3 by the mathematical artifice of applying the gauge invariance relation (3.12) to a hypothetical medium in which the electron-electron interaction had no q^{-2} divergence in the long-wavelength limit. For, in such a medium the contribution of improper graphs approaches zero with q. It is also possible, though tedious, to prove (3.13) directly by explicitly examining the contributions of certain related proper graphs to the right- and left-hand sides of (3.12) and showing these contributions to be equal.

To find the form of the response to a low-frequency transverse field we note that from (3.5)

$$\lim_{\omega\to 0}\omega^2\alpha(\omega)=\frac{4\pi e^2}{m^*\Omega}\frac{1}{[\kappa^I(0)]^2}. \tag{3.17}$$

Now, for the perfect insulator

$$\lim_{\omega\to 0}\omega^2\alpha^I(\omega)=0, \tag{3.18}$$

and, thus, from the definition (3.6) of $\beta(\omega)$

$$\lim_{\omega\to 0}\omega^2\beta(\omega)=\frac{4\pi e^2}{m^*\Omega}\frac{1}{[\kappa^I(0)]^2}. \tag{3.19}$$

Using the connection (3.8) between β and β_P and the definition,[3]

$$\kappa^I(\omega)=\frac{1}{1+\alpha^I(\omega)}=1-\alpha_P{}^I(\omega), \tag{3.20}$$

of the dielectric constant of the perfect insulator, we then find

$$\lim_{\omega\to 0}\omega^2\beta_P(\omega)=\lim_{\omega\to 0}\frac{\omega^2\beta(\omega)}{[1+\alpha^I(\omega)]^2}=\lim_{\omega\to 0}\omega^2\beta(\omega)[\kappa^I(\omega)]^2 =\frac{4\pi e^2}{m^*\Omega}. \tag{3.21}$$

Thus finally from (3.13), (3.14), and the fact that (3.18) holds for $\alpha_P{}^I(\omega)$, we see that[11]

$$\lim_{\omega\to 0}T_t(\omega)=-\frac{e^2}{m^*c\Omega}. \tag{3.22}$$

We shall see in the next section that the response calculated here is physically readily understandable.

4. PHYSICAL INTERPRETATION

We begin this section by showing that the low-frequency limits of the expressions for $T_l(\omega)$ and $T_t(\omega)$ which were derived in the last section [Eqs. (3.16) and (3.22)] are identical to those one finds for a classical system of an electron of mass m^* moving in a medium of dielectric constant $\kappa^I(\omega)$.

What is the response of the classical system mentioned above to a perturbing electric field? Consider first a transverse field. Let $\mathbf{A}(\mathbf{x},t)$ describe the total transverse field in the system. The motion of the single electron is determined by the equation of motion,

$$m^*d^2\mathbf{x}/dt^2=e\mathbf{E}'(\mathbf{x},t)=-(e/c)\mathbf{A}'(\mathbf{x},t), \tag{4.1}$$

where $\mathbf{x}$ is the position of the particle, $\mathbf{E}'$ the electric field it sees (i.e., the total field less its own), and $\mathbf{A}'$ the corresponding vector potential. The motion (4.1) gives rise to an average current density

$$\mathbf{j}'=(e/\Omega)d\mathbf{x}/dt=-(e^2/m^*c\Omega)\mathbf{A}'(x',t). \tag{4.2}$$

Consider the long-wavelength Fourier transform of (4.2). Since the difference between $\mathbf{A}$ and $\mathbf{A}'$ is of order A/N, we may neglect the contribution of this difference. Thus we have

$$\mathbf{j}'(\omega)=-(e^2/m^*c\Omega)\mathbf{A}(\omega), \tag{4.3}$$

where, as in previous sections,

$$\mathbf{j}'(\omega)=\lim_{q\to 0}\mathbf{j}'(\mathbf{q},\omega),\quad \mathbf{A}(\omega)=\lim_{q\to 0}\mathbf{A}(\mathbf{q},\omega). \tag{4.4}$$

The classical dielectric medium responds to the total field $\mathbf{A}$ according to

$$\mathbf{j}_d(\omega)=(\omega^2/4\pi c)[\kappa^I(\omega)-1]\mathbf{A}(\omega). \tag{4.5}$$

Thus the Fourier coefficient of the total current induced in our classical system is

$$\mathbf{j}(\omega)=\left[-\frac{e^2}{m^*c\Omega}+\frac{\omega^2}{4\pi c}[\kappa^I(\omega)-1]\right]\mathbf{A}(\omega). \tag{4.6}$$

At low frequencies the first term in (4.6) dominates. This term corresponds exactly to the response of the interacting system described by (3.22).

Consider now that an external time dependent charge density is embedded in the classical system. Let $\mathbf{A}(\omega)$ now describe the longitudinal field due to the *external* source. The induced current may be broken up into the following three parts: first, the response of the "extra particle" to the external field as modified by the medium; second, the current carried by the dielectric medium in responding to and modifying the external field; and third, the additional current induced in the medium as a result of the motion of the extra particle. The first current described above has, in analogy with (4.3), the form

$$\mathbf{j}'(\omega)=-(e^2/m^*c\Omega)\mathbf{A}(\omega)/\kappa^I(\omega). \tag{4.7}$$

The sum of the second and third currents is

$$\mathbf{j}_d(\omega)=\frac{\omega^2}{4\pi c}\left(\frac{\kappa^I(\omega)-1}{\kappa^I(\omega)}\right)[\mathbf{A}(\omega)+\mathbf{A}'(\omega)], \tag{4.8}$$

where $\mathbf{A}'(\omega)$ is the longitudinal vector potential set up by the current $\mathbf{j}'(\omega)$ and is given by

$$\mathbf{A}'(\omega)=-(4\pi c/\omega^2)\mathbf{j}'(\omega). \tag{4.9}$$

Thus the total response current is

$$\begin{aligned}\mathbf{j}(\omega)&=\mathbf{j}'(\omega)+\mathbf{j}_d(\omega)\\ &=-\frac{e^2}{m^*c\Omega}\frac{\mathbf{A}(\omega)}{\kappa^I(\omega)}+\frac{\omega^2}{4\pi c}\left(\frac{\kappa^I(\omega)-1}{\kappa^I(\omega)}\right)\\ &\qquad\times\left[1+\frac{4\pi c}{\omega^2}\frac{e^2}{m^*c\Omega}\frac{1}{\kappa^I(\omega)}\right]\mathbf{A}(\omega)\\ &=-\frac{e^2}{m^*c\Omega}\frac{\mathbf{A}(\omega)}{[\kappa^I(\omega)]^2}+\frac{\omega^2}{4\pi c}\left(\frac{\kappa^I(\omega)-1}{\kappa^I(\omega)}\right)\mathbf{A}(\omega).\end{aligned} \tag{4.10}$$

For an external source whose significant Fourier coefficients occur for very low frequencies. (4.10) reduces to

$$\mathbf{j}(\omega)=-\frac{e^2}{m^*c\Omega}\frac{1}{[\kappa^I(0)]^2}\mathbf{A}(\omega), \tag{4.11}$$

in exact agreement with the explicit form (3.16) of the low-frequency longitudinal response function calculated in the last section. We have thus proved that an effective-mass picture of the response of the interacting system of insulator plus one electron to low-frequency, long-wavelength perturbations is exactly correct.

It is interesting that the decomposition of the induced current according to the above classical discussion exactly corresponds to a separation into topological classes of the graphs which occurred in the quantum mechanical discussion of the last section. Consider the graphs which describe the expansion of the transverse response function $T_t(\omega)$. These have the form of Figs. 1(a) and 2(a). They correspond, respectively, to the response of the medium and the "particle" to the total transverse field. The case of a longitudinal field is more interesting. The graphs which occur in the expansion of $T_l(\omega)$ have the form of Figs. 1 and 2. Figure 1 shows the perfect insulator responding to and modifying the external field as discussed in reference 3. Figure 2(a) and those graphs of the form of Fig. 2(b) that have N-particle polarization graphs only between the incoming interaction line (corresponding to the interaction with the external source) and the proper extra particle part show the "extra particle" responding to the external field as modified by the medium. The remaining graphs of the form of Fig. 2(b) show the medium in turn responding to the field set up by the extra particle.

It is only, of course, at extremely low frequencies that the effective-mass picture of the interacting system is exact.[19] At higher frequencies, Eqs. (4.6) and (4.10) no longer hold for this system. It may be readily verified, however, that when the quantity $(e^2/m^*c\Omega)$ is replaced by $(-\omega^2/4\pi c)\beta_P(\omega)$ [20] in these equations they correspond to the exact results (3.13) and (3.12). [Use Eqs. (3.14), (3.6–8), and (3.20).] Since the expansion represented by Figs. 1 and 2 corresponds to these exact results, we see that the classical decomposition of the response current discussed above still applies.

It should also be remarked that in so far as interactions between carriers may be neglected, results of the form of (3.16) and (3.22) will continue to hold for the system of insulator plus a *few* carriers. The response of such a system would be described by N-particle polarization graphs (Fig. 1) plus extra particle polarization graphs (Fig. 2) for each carrier. Thus, apart from terms smaller by a factor of (n/N), where n is the number of carriers, we would have

$$\lim_{\omega\to 0} T_l^{(n)}(\omega)=-\frac{e^2}{m^*c\Omega}\frac{n}{[\kappa^I(0)]^2}, \tag{4.12}$$

and

$$\lim_{\omega\to 0} T_t^{(n)}(\omega)=-\frac{e^2}{m^*c\Omega}n. \tag{4.13}$$

Physically these results mean that such a system would respond to low-frequency, long-wavelength perturbations like a system of n free particles of mass m^* moving in a dielectric medium.

5. EFFECTIVE HAMILTONIAN FOR STATIC MAGNETIC FIELDS

In this final section we consider the effects of a static magnetic field on the system of an insulator and one electron. Klein,[7] as mentioned in Sec. 1, has previously derived the results we shall obtain here. We include this discussion both because it is a little more explicit than Klein's and, also, because it follows quite naturally from the preceding considerations.

What will be shown here is that the low-lying energy levels of the interacting $(N+1)$-particle system in a magnetic field may be very accurately obtained from a one-particle Schrödinger equation, namely,

$$\frac{1}{2m^*}\left(\frac{1}{i}\nabla-\frac{e}{c}\mu^I\mathbf{A}_{\rm ext}(\mathbf{x})\right)^2F(\mathbf{x})=WF(\mathbf{x}). \tag{5.1}$$

Here m^* is the effective mass defined by Eq. (2.7), $\mathbf{A}_{\rm ext}(\mathbf{x})$ is the vector potential describing the external magnetic field, μ^I is the static magnetic permeability of the perfect insulator,[21] and W the energy measured relative to the ground state of the $(N+1)$-particle system. The conditions under which (5.1) is valid are as follows:

$$\omega_C\ll\Delta E,\quad \frac{1}{A_{\rm ext}}|\nabla A_{\rm ext}|\ll(m\omega_C)^{\frac{1}{2}}\ll\frac{1}{a}, \tag{5.2}$$

where ω_C is the cyclotron resonance frequency, $(e\mathfrak{H}C/m^*c)$ ($\mathfrak{H}C$ is a representative value of the magnetic field), ΔE is the energy gap, and a is the lattice parameter. Under ordinary experimental conditions these requirements are extremely well satisfied.

[19] In the limit of high frequencies our system behaves like a system of $(N+1)$ free particles of mass m. For from (3.11) we have

$$\lim_{\omega\to\infty} T_{\mu\nu}(\mathbf{q},\omega)=-\frac{e^2}{mc}\frac{N+1}{\Omega}\delta_{\mu\nu}.$$

[20] The function $\beta_P(\omega)$ describes the transition from the low-frequency region where the motion of the extra particle is most strongly influenced by interactions with the lattice and the other electrons ($\beta_P\propto 1/m^*\omega^2$) to the high-frequency region where the particle behaves essentially as though free. (It is easy to deduce from reference 19 that for high frequencies $\beta_P(\omega)\propto 1/m\omega^2$.)

[21] In reality, the correction obtained by taking into account the modification of the external magnetic field by the permeability of the system is of the order of the accuracy of (5.1). We include this correction, however, for formal completeness.

We now derive Eq. (5.1). The Hamiltonian describing our system in an external magnetic field is $H+H'$. Here H is the unperturbed Hamiltonian (2.1). It contains all the Coulomb interactions. H' describes the interaction with a magnetic field. We shall see later from a self-consistency argument that the magnetic field which contributes to H' is the sum of the external field and the long-wavelength field it induces in the medium. Let this total magnetic field be described by a vector potential $\mathbf{A}(\mathbf{x})$. We Fourier-analyze this quantity as follows:

$$\mathbf{A}(\mathbf{x})=\sum_{\mathbf{q}}\mathbf{A}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}. \tag{5.3}$$

We choose $\nabla\cdot\mathbf{A}=0$ so that

$$\mathbf{A}(\mathbf{q})=\mathbf{t}_{\mathbf{q}}A(\mathbf{q}), \quad \text{where} \quad \mathbf{t}_{\mathbf{q}}\cdot\mathbf{q}=0. \tag{5.4}$$

Then we have

$$H'=H_1'+H_2', \tag{5.5}$$

where

$$H_1'=-\frac{e}{mc}\sum_i \mathbf{p}_i\cdot\mathbf{A}(\mathbf{x}_i)=-\frac{e}{c}\sum_{\mathbf{q}} A(\mathbf{q})\mathbf{t}_{\mathbf{q}}\cdot\mathbf{j}(\mathbf{q}), \tag{5.6}$$

and

$$\begin{aligned}H_2'&=\frac{e^2}{2mc^2}\sum_i A^2(x_i)\\&=\frac{e^2}{2mc^2}\sum_{\mathbf{q},\mathbf{q}'}\mathbf{t}_{\mathbf{q}}\cdot\mathbf{t}_{\mathbf{q}'}A(\mathbf{q})A(\mathbf{q}')\rho(\mathbf{q}+\mathbf{q}').\end{aligned} \tag{5.7}$$

The operators $\mathbf{j}(\mathbf{q})$ and $\rho(\mathbf{q})$ were defined in Eqs. (2.12–.13). We wish to solve the equation

$$(H+H')\Psi=E\Psi. \tag{5.8}$$

Let us expand Ψ as follows:

$$\Psi=\sum_{n,\mathbf{k}} a_{n,\mathbf{k}}\Psi_{n,\mathbf{k}}, \tag{5.9}$$

where the $\Psi_{n,\mathbf{k}}$'s are the eigenstates of H and were discussed in Sec. 2. The wave vector $\mathbf{k}$ runs over a single Brillouin zone. In the $\Psi_{n,\mathbf{k}}$ representation the Schrödinger equation (5.8) is

$$\sum_{n',\mathbf{k}'}(n,\mathbf{k}|H'|n',\mathbf{k}')a_{n',\mathbf{k}'}=(E-E_{n,\mathbf{k}})a_{n,\mathbf{k}}. \tag{5.10}$$

Explicitly exhibiting the terms corresponding to $n=0$, we have

$$\sum_{\mathbf{k}'}(0,\mathbf{k}|H'|0,\mathbf{k}')a_{0,\mathbf{k}'}+\sum_{\substack{n'\neq 0\\ \mathbf{k}'}}(0,\mathbf{k}|H'|n',\mathbf{k}')a_{n',\mathbf{k}'}=(E-E_{0,\mathbf{k}})a_{0,\mathbf{k}}, \tag{5.11}$$

and

$$\sum_{\mathbf{k}'}(n,\mathbf{k}|H'|0,\mathbf{k}')a_{0,\mathbf{k}'}+\sum_{\substack{n'\neq 0\\ \mathbf{k}'}}(n,\mathbf{k}|H'|n',\mathbf{k}')a_{n',\mathbf{k}'}=(E-E_{n,\mathbf{k}})a_{n,\mathbf{k}}. \tag{5.12}$$

We shall see later that, under the conditions (5.2), the low-lying solutions of the Schrödinger equation (5.8) satisfy

$$|E-E_{0,0}|<\Delta E; \quad a_{n,\mathbf{k}}\neq 0 \quad \text{only for} \quad ka<1. \tag{5.13}$$

Then, solving for $a_{n,\mathbf{k}}$ $(n\neq 0)$ from (5.12) to lowest order in H', we obtain

$$a_{n,\mathbf{k}}=\frac{1}{E_{0,0}-E_{n,0}}\sum_{\mathbf{k}'}(n,\mathbf{k}|H'|0,\mathbf{k}')a_{0,\mathbf{k}'}. \tag{5.14}$$

Substituting (5.14) into (5.11), and retaining only terms quadratic or of lower order in A, we find

$$\sum_{\mathbf{k}'}\left[(0,\mathbf{k}|H'|0,\mathbf{k}')+\sum_{\substack{\mathbf{k}''\\ n\neq 0}}\frac{(0,\mathbf{k}|H_1'|n,\mathbf{k}'')(n,\mathbf{k}''|H_1'|0,\mathbf{k}')}{E_{0,0}-E_{n,0}}\right]a_{0,\mathbf{k}'}=(E-E_{0,\mathbf{k}})a_{0,\mathbf{k}}. \tag{5.15}$$

We shall see that Eq. (5.15) is equivalent to the effective-mass equation (5.1).

Let us, then, explicitly consider the matrix elements that have been retained in (5.15). In evaluating these matrix elements we impose the second set of inequalities stated in (5.2). We shall see later that the spread of the wave packet (5.9) for the states of interest is of the order of the fundamental cyclotron length $(1/m\omega_C)^{\frac{1}{2}}$. Thus the above inequalities require that the magnetic field vary gently over lengths comparable to the spread of the wave packet and that this spread itself be large compared to the lattice parameter. Under these circumstances the contribution of H_1' to the first term in the square bracket in (5.15) is

$$\begin{aligned}&(0,\mathbf{k}|H_1'|0,\mathbf{k}')\\&\quad=-(e/c)\sum_{\mathbf{q}}A(\mathbf{q})(0,\mathbf{k}|\mathbf{t}_{\mathbf{q}}\cdot\mathbf{j}(\mathbf{q})|0,\mathbf{k}')\\&\quad=-(e/c)A(\mathbf{k}-\mathbf{k}')\mathbf{t}_{\mathbf{k}-\mathbf{k}'}\cdot(0,\mathbf{k}|\mathbf{j}(\mathbf{k}-\mathbf{k}')|0,\mathbf{k}').\end{aligned} \tag{5.16}$$

It is proved in Appendix C, to all orders of perturbation theory, that for $k,\ k'\ll 1/a$

$$\lim_{\mathbf{k}\to\mathbf{k}'}(0,\mathbf{k}|\mathbf{t}_{\mathbf{k}-\mathbf{k}'}\cdot\mathbf{j}(\mathbf{k}-\mathbf{k}')|0,\mathbf{k}')\to\mathbf{t}_{\mathbf{k}-\mathbf{k}'}\cdot\mathbf{k}'/m^*. \tag{5.17}$$

Thus under our conditions

$$(0,\mathbf{k}|H_1'|0,\mathbf{k}')=-(e/c)A(\mathbf{k}-\mathbf{k}')\mathbf{t}_{\mathbf{k}-\mathbf{k}'}\cdot\mathbf{k}'/m^*. \tag{5.18}$$

The contribution of H_2' to the first term in the square bracket in (5.15) is

$$\begin{aligned}(0,\mathbf{k}|H_2'|0,\mathbf{k}')&=\frac{e^2}{2mc^2}\sum_{\mathbf{q},\mathbf{q}'}\mathbf{t}_{\mathbf{q}}\cdot\mathbf{t}_{\mathbf{q}'}A(\mathbf{q})A(\mathbf{q}')\\&\quad\times(0,\mathbf{k}|\rho(\mathbf{q}+\mathbf{q}')|0,\mathbf{k}')\\&=\frac{e^2}{2mc^2}\sum_{\mathbf{q}}\mathbf{t}_{\mathbf{q}}\cdot\mathbf{t}_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}A(\mathbf{q})A(\mathbf{k}-\mathbf{k}'-\mathbf{q})\\&\quad\times(0,\mathbf{k}|\rho(\mathbf{k}-\mathbf{k}')|0,\mathbf{k}').\end{aligned} \tag{5.19}$$

The contribution of H_1' to the second term in the square bracket in (5.15) is

$$\sum_{n\neq 0}(0,\mathbf{k}|H_1'|n,\mathbf{k}'')(n,\mathbf{k}''|H_1'|0,\mathbf{k}')/(E_{0,0}-E_{n,0})$$
$$=-\frac{e^2}{2c^2}\sum_{\substack{\mathbf{q}\\ n\neq 0}}\frac{A(\mathbf{q})A(\mathbf{k}-\mathbf{k}'-\mathbf{q})}{E_{n,0}-E_{0,0}}$$
$$\times[(0,\mathbf{k}|\mathbf{t}_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}\cdot\mathbf{j}(\mathbf{k}-\mathbf{k}'-\mathbf{q})|n,\mathbf{k}'+\mathbf{q})$$
$$\times(n,\mathbf{k}'+\mathbf{q}|\mathbf{t}_{\mathbf{q}}\cdot\mathbf{j}(\mathbf{q})|0,\mathbf{k}')$$
$$+(0,\mathbf{k}|\mathbf{t}_{\mathbf{q}}\cdot\mathbf{j}(\mathbf{q})|n,\mathbf{k}-\mathbf{q})$$
$$\times(n,\mathbf{k}-\mathbf{q}|\mathbf{t}_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}\cdot\mathbf{j}(\mathbf{k}-\mathbf{k}'-\mathbf{q})|0,\mathbf{k}')]. \quad (5.20)$$

The following transverse sum rule is also proved in Appendix C.

$$m\sum_{n\neq 0}[(0,\mathbf{k}|\mathbf{t}_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}\cdot\mathbf{j}(\mathbf{k}-\mathbf{k}'-\mathbf{q})|n,\mathbf{k}'+\mathbf{q})$$
$$\times(n,\mathbf{k}'+\mathbf{q}|\mathbf{t}_{\mathbf{q}}\cdot\mathbf{j}(\mathbf{q})|0,\mathbf{k}')$$
$$+(0,\mathbf{k}|\mathbf{t}_{\mathbf{q}}\cdot\mathbf{j}(\mathbf{q})|n,\mathbf{k}-\mathbf{q})$$
$$\times(n,\mathbf{k}-\mathbf{q}|\mathbf{t}_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}\cdot\mathbf{j}(\mathbf{k}-\mathbf{k}'-\mathbf{q})|0,\mathbf{k}')]/$$
$$(E_{n,0}-E_{0,0})+\mathbf{t}_{\mathbf{q}}\cdot\mathbf{t}_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}\left(\frac{m}{m^*}\right)$$
$$=\mathbf{t}_{\mathbf{q}}\cdot\mathbf{t}_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}(0,\mathbf{k}|\rho(\mathbf{k}-\mathbf{k}')|0,\mathbf{k}'). \quad (5.21)$$

(For $\mathbf{k}'=\mathbf{k}$, this reduces to the transverse sum rule of reference 18.) Using (5.21), the terms (5.19) and (5.20) can be combined. Then Eq. (5.15) reduces to

$$\sum_{\mathbf{k}'}a_{0,\mathbf{k}'}\left[-\frac{e}{c}\mathbf{A}(\mathbf{k}-\mathbf{k}')\cdot\frac{\mathbf{k}'}{m^*}+\frac{e^2}{2m^*c^2}\sum_{\mathbf{q}}\mathbf{A}(\mathbf{q})\cdot\mathbf{A}(\mathbf{k}-\mathbf{k}'-\mathbf{q})\right]$$
$$=\left[E-E_{0,0}-\frac{k^2}{2m^*}\right]a_{0,\mathbf{k}}, \quad (5.22)$$

where we have used the expansion (2.7) for the energy $E_{0,\mathbf{k}}$. Equation (5.22) is in fact the effective-mass equation (5.1), written however in "momentum" space. To obtain (5.1) we form a wave function $F(\mathbf{x})$ as follows:

$$F(\mathbf{x})=\sum_{\mathbf{k}}a_{0,\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (5.23)$$

where the sum on $\mathbf{k}$ runs of course over one Brillouin zone. Multiplying Eq. (5.22) by $e^{i\mathbf{k}\cdot\mathbf{x}}$ and summing over $\mathbf{k}$, we obtain

$$(E-E_{0,0})F(\mathbf{x})=-\frac{1}{2m^*}\nabla^2F(\mathbf{x})$$
$$-\frac{e}{m^*c}\sum_{\mathbf{k},\mathbf{k}'}\mathbf{A}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{k}'a_{0,\mathbf{k}'}e^{i\mathbf{k}\cdot\mathbf{x}}$$
$$+\frac{e^2}{2m^*c^2}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'}\mathbf{A}(\mathbf{q})\cdot\mathbf{A}(\mathbf{k}-\mathbf{k}'-\mathbf{q})a_{0,\mathbf{k}'}e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (5.24)$$

Now

$$\mathbf{A}(\mathbf{q})=\frac{1}{\Omega}\int\mathbf{A}(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}}d\mathbf{x}, \quad (5.25)$$

and

$$\frac{1}{\Omega}\sum_{\mathbf{k}\subset\text{B.Z.}}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}=\Delta(\mathbf{x}-\mathbf{x}'), \quad (5.26)$$

where Δ is a spread-out δ function having the dimensions of a unit cell of the lattice. Using (5.25) and (5.26), we obtain

$$WF(\mathbf{x})=-\frac{1}{2m^*}\nabla^2F(\mathbf{x})$$
$$-\frac{e}{m^*c}\int d\mathbf{x}'\,\Delta(\mathbf{x}-\mathbf{x}')\mathbf{A}(\mathbf{x}')\cdot\frac{1}{i}\nabla'F(\mathbf{x}')$$
$$+\frac{e^2}{2m^*c^2}\int d\mathbf{x}'\,A^2(\mathbf{x}')\Delta(\mathbf{x}-\mathbf{x}')F(\mathbf{x}'), \quad (5.27)$$

where $W=E-E_{0,0}$. Since $A(\mathbf{x})$ varies extremely little over the dimensions of a unit cell, we have

$$\left[-\frac{1}{2m^*}\nabla^2-\frac{e}{m^*c}\mathbf{A}(\mathbf{x})\cdot\frac{1}{i}\nabla+\frac{e^2}{2m^*c^2}A^2(\mathbf{x})\right]F(\mathbf{x})$$
$$=WF(\mathbf{x}). \quad (5.28)$$

To complete the derivation of (5.1) we must relate $\mathbf{A}(\mathbf{x})$ to $\mathbf{A}_{\text{ext}}(\mathbf{x})$. Now for consistency the field $\mathbf{A}(\mathbf{x})$ must satisfy

$$\nabla^2\mathbf{A}(\mathbf{x})=-(4\pi/c)[\langle\mathbf{j}_{\text{el}}\rangle+\mathbf{j}_{\text{ext}}], \quad (5.29)$$

where $\mathbf{j}_{\text{ext}}$ is the source of the external field and $\langle\mathbf{j}_{\text{el}}\rangle$ the average current density induced by $\mathbf{A}$ in the N-particle system. As discussed in reference 3, it must be possible in the long-wavelength limit to write this current to lowest order in A in the form

$$\langle\mathbf{j}_{\text{el}}\rangle=-\frac{c}{4\pi}\left(\frac{\mu^I-1}{\mu^I}\right)\nabla^2\mathbf{A}. \quad (5.30)$$

Here μ^I may be interpreted as the static magnetic permeability of the perfect insulator. Substituting (5.30) into (5.29) and using the fact that $\nabla^2\mathbf{A}_{\text{ext}}=-(4\pi/c)\mathbf{j}_{\text{ext}}$, we find

$$\mathbf{A}(\mathbf{x})=\mu^I\mathbf{A}_{\text{ext}}(\mathbf{x}). \quad (5.31)$$

When (5.31) is substituted in (5.28), the result is

$$\frac{1}{2m^*}\left(\frac{1}{i}\nabla-\frac{e}{c}\mu^I\mathbf{A}_{\text{ext}}\right)^2F(\mathbf{x})=WF(\mathbf{x}). \quad (5.32)$$

This is the effective-mass equation (5.1).

We conclude with some comments on the consistency and accuracy of (5.32). First, we note that, for the low-lying states, $W\sim\omega_C$ and the spread of the wave func-

tions is indeed of the order of $(1/m\omega_C)^{\frac{1}{4}}$. Thus the inequalities (5.13) which we assumed in deriving (5.32) are in fact implied by the conditions (5.2). Since, under typical conditions for a cyclotron resonance experiment, $(\omega_C/\Delta E)\sim 10^{-5}$ and $(m\omega_C)^{\frac{1}{4}}a\sim 10^{-3}$, the latter conditions are well satisfied. Second, we note that the spread of the wave functions implies that for the states of interest the quantity eA/c effectively has the value $m\omega_C/\bar{k}$, where $\bar{k}$ is a representative wave number, i.e., $\bar{k}\sim(m\omega_C)^{\frac{1}{2}}$. Thus, effectively $eA/c\sim\bar{k}$ and our procedure of retaining terms up to the second order in these two quantities is consistent. Finally, we remark that it can be shown for crystals having a center of symmetry that the terms omitted in deriving (5.32) are effectively smaller by a factor of $(\omega_C/\Delta E)$.[22] As mentioned above, this factor is extremely small under typical conditions. Thus the simple effective-mass equation (5.32) in fact includes the effects of electronic correlation to an excellent approximation.

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APPENDIX A

Here we discuss the factorization of graphs of the form of Figs. 2(b) into proper parts. We refer to the discussion of reference 3, Appendix A. The procedure for factorization described there amounted to first performing the time integrations[23] associated with the part of a graph on one side of a Coulomb interaction carrying momentum $\mathbf{q}$ while preserving their relative order. When this was done the contribution of the complete graph factored into those of the two parts obtained by removing the interaction line carrying momentum q and in its place attaching two external lines that preserve the sense of the momentum transfer. In applying this procedure to graphs of the form of Fig. 2(b) a slight complication arises. The complication is due to the occurrence of the initial one-particle state 0,0 as an intermediate state, leading to energy denominators which vanish with η (the rate of turning on the interactions). This, as is well known,[24] contributes only a phase factor, undefined as η approaches zero, which corresponds to the energy shift induced by the interactions. Since both this phase factor and its complex conjugate occur in the calculation of the expectation value $\alpha(\omega)$, no real difficulty is caused. In the discussion of the perfect insulator, in fact, the corresponding phase factor and its complex conjugate were explicitly removed by the elimination of unlinked parts. However, even after the internal Coulomb effects are eliminated in the graphs of Fig. 2, the possibility remains of returning to the state 0,0. Thus the limit $\eta\rightarrow 0$ cannot be taken in these graphs until the contribution of all of them are summed. This causes an apparent difficulty. For, the factorization procedure discussed above does not preserve the η dependence of the factored parts. In carrying out the intermediate integrations, the time factors $e^{\eta t}$ (due to the turning on of the Coulomb interactions) accumulate at the limits of integration. In general, one finds that, if there are l internal Coulomb interaction lines in the portion of a graph between the incoming *external* interaction line and the *internal* line carrying momentum $\mathbf{q}$ about which the factorization is to be performed, this line effectively carries an energy $[\omega+is+i(l+1)\eta]$. In other words, the contribution of the factored part, in which half the erstwhile internal line is now the incoming external line, is that of the complete graph of the same form in which, however, the *exterenal* perturbation is turned on with a time factor $e^{[s+(l+1)\eta]t}$ instead of e^{st}. This fact causes no real difficulty, however. For, the only factored parts which depend crucially on η are those which start and end with one line. But when all such parts are included in turn in a particular improper graph, and the factorization performed, the limit $\eta=0$ may be taken with impunity for the reasons given above. The result (3.8) then follows.

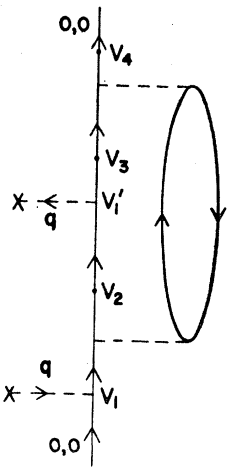

FIG. 3. A simple "extra-particle" polarization graph.

One other point requiring special discussion is the question of taking the limit $q\rightarrow 0$ in the contributions of β graphs, Fig. 2. An explicit factor q^{-2} occurs in their contributions [see Eq. (3.3)]. It is important to note that this causes no difficulty as $q\rightarrow 0$. When *inter*band transitions take place at the external vertices it is

[22] Since many-particle effects do not enter into the order of magnitude arguments which give this result we refer to studies of the motion of Bloch electrons in a magnetic field, i.e., reference 2.

[23] See reference 13. This factorization has also been discussed by J. Hubbard, reference 14.

[24] M. Gell-Mann and F. Low, Phys. Rev. 84, 350 (1951), Appendix.

obvious that no divergence occurs. For the matrix elements between Bloch functions of $e^{\pm iq\cdot x}$ which then occur there are themselves linear in q. It is when *intra*-band transitions occur at the external vertices that a special discussion is required. For the perfect insulator this was given in reference 5, Sec. 2. The point there was that the terms singular in q occurred in pairs: one had to consider together graphs in which each of the troublesome intraband vertices was associated in turn with the other point on the same electron-hole loop at the same horizontal level. Then because the sign[14] that goes with these graphs is $(-1)^{l+h}$, where l is the number of closed loops and h the number of internal hole lines, a cancellation occurred. Now for the graphs which occur in Fig. 2 this method of eliminating the divergence as $q\rightarrow 0$ sometimes does not apply since it is possible that the external vertices do not lie on a closed loop. However, the procedure exemplified below applies to such cases. In Fig. 3, if an interband transition occurs at V_1', and an intraband one at V_1, the singular part of the contribution (proportional to q^{-1}) is removed by adding together graphs in which this vertex is replaced by intraband vertices at the points V_2, V_3, and V_4. If the vertex V_1' is also intraband, the graphs obtained by attaching the outgoing interaction line at all possible distinct points along the single particle-hole line traveling from the bottom to the top of the page, and causing intraband transitions at these points must also be included. When the contributions of all the above graphs are added together, the result approaches a finite limit as $q\rightarrow 0$.

APPENDIX B

The inertial theorem discussed in Sec. 4 may be equivalently stated as the following Kramers-Kronig relation between the true effective mass m^* and optically measurable parameters:

$$1-\frac{2m\Omega}{\pi e^2}\int_{0+}^{\infty}[\sigma(\omega)-\sigma^I(\omega)]d\omega=\frac{m}{m^*}. \tag{B.1}$$

Here $\sigma(\omega)$ is the real part of the complex conductivity of the system of insulator plus one electron and $\sigma^I(\omega)$ that of the perfect insulator. The lower limit of the integration indicates that the principal value is intended at $\omega=0$ (i.e., $\lim_{\epsilon\rightarrow 0}\int_{\epsilon}^{\infty}$). Equation (B.1) can be shown to follow from the transverse sum rule (reference 11) in the explicit model considered in the preceding sections. However, it also follows independently of that model from the low-frequency form of the transverse response function for very general reasons. This will be shown here.

Consider a system of (N+1) interacting particles described by a response function, which relates a transverse vector potential to the current it induces, of the form

$$T_t(\omega)=-e^2/m^*c\Omega+\omega^2B(\omega), \tag{B.2}$$

where $B(\omega)$ is a complex function of ω whose real part is finite at $\omega=0$. The system discussed in Chapter II is a special case of (B.2). A result of the form (B.1) follows from (B.2) if

$$\lim_{\omega\rightarrow\infty}T_t(\omega)=-\frac{e^2(N+1)}{mc\Omega}. \tag{B.3}$$

Physically (B.3) implies that the response of the system of $(N+1)$ interacting particles to fields of high frequency should asymptotically approach that of $(N+1)$ free particles of mass m. (This physical requirement is of course satisfied for our explicit model.[19]) Now $-(ic/\omega)T_t(\omega)\equiv S(\omega)$ is the complex conductivity which relates the induced current to an electric field. Since this must be a *causal* connection, it follows that[25] (i) $S(\omega)$ considered as a function of the complex variable ω is analytic in the upper half ω plane, and (ii) $S(-\omega)=S^*(\omega)$.

Using requirement (i), we have

$$\int_c\frac{\omega S(\omega)}{\omega-\omega'}d\omega=0, \tag{B.4}$$

where ω' is a real number and c is any closed finite contour in the upper half ω plane. If this contour is deformed to run parallel to an infinitesimally above the real axis from $-\infty$ to $+\infty$, and then along a large semicircle in the upper half plane, we get

$$P_{\omega'}\int_{-\infty}^{\infty}\frac{\omega S(\omega)}{\omega-\omega'}d\omega-i\pi\omega' S(\omega')-\frac{\pi e^2}{m\Omega}(N+1)=0, \tag{B.5}$$

where the first two terms come from the integration along the real axis ($P_{\omega'}$ means that the principal part of the integral must be taken at $\omega=\omega'$), and the third term is the contribution of the large semicircle along which $T_t(\omega)$ has the asymptotic form (B.3). Taking the real part of (B.5), we have

$$P_{\omega'}\int_{-\infty}^{\infty}\frac{\omega\,\mathrm{Re}[S(\omega)]}{\omega-\omega'}d\omega+\pi\omega'\,\mathrm{Im}[S(\omega')]-\frac{\pi e^2}{m\Omega}(N+1)=0. \tag{B.6}$$

Let us now let $\omega'\rightarrow 0$ and substitute the assumed low-frequency form of the response. Then, defining $\sigma(\omega)=\mathrm{Re}[S(\omega)]$, we have

$$P_0\int_{-\infty}^{\infty}\sigma(\omega)d\omega=\frac{\pi e^2}{m\Omega}\left[N+1-\frac{m}{m^*}\right]. \tag{B.7}$$

The symmetry requirement (ii) implies that $\sigma(\omega)=$

[25] See, e.g., L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1958), Sec. 122.

$\sigma(-\omega)$, and thus

$$\int_{0+}^{\infty}\sigma(\omega)d\omega=\frac{\pi e^2}{2m\Omega}\left[N+1-\frac{m}{m^*}\right]. \tag{B.8}$$

If the N-particle system has a finite dielectric constant at $\omega=0$, as will be true for an insulator, we have from arguments similar to those given above that

$$\int_{0}^{\infty}\sigma^I(\omega)d\omega=\frac{\pi e^2}{2m\Omega}N. \tag{B.9}$$

Introducing (B.9) into (B.8), we get the result (B.1). If a system of $(N+n)$ particles has a low-frequency response of the form (4.13), we similarly find that

$$1-\frac{2m\Omega}{\pi ne^2}\int_{0+}^{\infty}[\sigma^n(\omega)-\sigma^I(\omega)]d\omega=\frac{m}{m^*}. \tag{B.10}$$

Since (4.13) has been shown to be very nearly exact for the system of insulator plus n particles, it follows that (B.10) is also.

For the system of insulator plus one electron described in Chapter II, $\sigma(\omega)$ has no singularity at $\omega=0$. This, as is well known from similar treatments of the Bloch model,[26] is due to the neglect of damping. The integral in (B.1) must be understood to omit the low-frequency peak in the conductivity of the $(N+1)$ system which would be experimentally observed and which a more realistic treatment would predict.

It is possible to define an effective mass for a semiconductor of large carrier concentration, for which the theory of the main body of this paper does not apply, by requiring that the low-frequency electric susceptibility lead to a response of the form of Eq. (4.13).[27] We see that the effective mass so calculated will also characterize, according to (B.10), the difference in the optical absorption of pure and doped material. However, it is not, of course, obvious that the same value for the effective mass would be measured by some other means (e.g., cyclotron resonance). What we have shown in the main body of this paper is that for low carrier concentrations this is in fact so.

APPENDIX C

In this Appendix we evaluate some matrix elements needed in Sec. 5. We first consider the quantity

$$\lim_{q\to 0}(0,\mathbf{k}+\mathbf{q}|j_\mu(\mathbf{q})|0,\mathbf{k}),\quad k\ll\frac{1}{a}. \tag{C.1}$$

Now from the identity (2.10), i.e., $[H,\rho(\mathbf{q})]=\mathbf{q}\cdot\mathbf{j}(\mathbf{q})$, we have

$$\begin{aligned}\lim_{q\to 0}&(0,\mathbf{k}+\mathbf{q}|\hat{q}\cdot\mathbf{j}(\mathbf{q})|0,\mathbf{k})\\&=\lim_{q\to 0}\frac{1}{q}(E_{0,\mathbf{k}+\mathbf{q}}-E_{0,\mathbf{k}})(0,\mathbf{k}+\mathbf{q}|\rho(\mathbf{q})|0,\mathbf{k})\\&=\lim_{q\to 0}\frac{1}{q}[(\mathbf{k}+\mathbf{q})^2-k^2]\frac{1}{2m^*\kappa^I(0)}\\&=\mathbf{k}\cdot\hat{q}/m^*[\kappa^I(0)].\end{aligned} \tag{C.2}$$

Here we have used the identity[5]

$$\lim_{q\to 0}(0,\mathbf{k}+\mathbf{q}|\rho(\mathbf{q})|0,\mathbf{k})=1/[\kappa^I(0)], \tag{C.3}$$

and the expansion (2.7), valid for small k, for the effective mass m^*. In (C.2) and in what follows, $\hat{q}$ is a unit vector in the direction of $\mathbf{q}$. To calculate (C.1) in an arbitrary direction we make an expansion in powers of the Coulomb interaction of the exact states $|0,\mathbf{k}\rangle$ and $|0,\mathbf{k}+\mathbf{q}\rangle$.[5] When the resulting series for (C.1) is represented by graphs, one finds that these fall into two classes symbolized by Fig. 4(a) and Fig. 4(b). In these graphs the operator $j_\mu(\mathbf{q})$ occurs at the interaction line starting at the cross. The circles have the same significance as those in Figs. 1 and 2. The solid lines represent the one-particle states $0,\mathbf{k}$ and $0,\mathbf{k}+\mathbf{q}$, (filled zones and one electron with wave vector $\mathbf{k}$, $\mathbf{k}+\mathbf{q}$ in the lowest conduction band). By examining the contributions of these graphs, one sees that

$$\lim_{q\to 0}(0,\mathbf{k}+\mathbf{q}|j_\mu(\mathbf{q})|0,\mathbf{k})=\hat{q}_\mu a(\mathbf{k})+k_\mu b(\mathbf{k}), \tag{C.4}$$

where the first term is the contribution of the improper graphs, Fig. 4(b), and the second that of the proper graphs, Fig. 4(a). To calculate (C.1) we must now determine the quantitites $a(\mathbf{k})$ and $b(\mathbf{k})$. One relation for this purpose is given by (C.2). Another may be most easily obtained by the artifice used in reference 3. and in Sec. 3 of this paper. We examine the content of the identity (2.10) in a hypothetical medium in which the electron-electron interaction does not have a $1/q^2$ singularity for small q. In such a medium the contribution of the *improper* graphs goes to zero with q, while

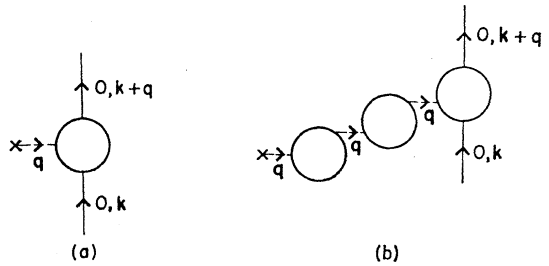

FIG. 4. The two classes of graphs which occur in the expansion of the matrix element $(0,\mathbf{k}+\mathbf{q}|j_\mu(q)|0,\mathbf{k})$.

[26] F. Seitz, *Modern Theory of Solids* (McGraw-Hill Book Company, New York, 1940).
[27] W. G. Spitzer and H. Y. Fan, Phys. Rev. **106**, 882 (1957).

that of the *proper* graphs remains unchanged. We then conclude that[28] (the subscript P means the contribution of proper graphs alone)

$$\lim_{q\to 0}(0,\mathbf{k}+\mathbf{q}|\hat{q}\cdot\mathbf{j}(\mathbf{q})|0,\mathbf{k})_P$$
$$=\lim_{q\to 0}\frac{1}{q}(E_{0,\mathbf{k}+\mathbf{q}}-E_{0,\mathbf{k}})(0,\mathbf{k}+\mathbf{q}|\rho(\mathbf{q})|0,\mathbf{k})_P$$
$$=\mathbf{k}\cdot\hat{q}/m^*, \tag{C.5}$$

since[5]

$$\lim_{q\to 0}(0,\mathbf{k}+\mathbf{q}|\rho(\mathbf{q})|0,\mathbf{k})_P=(0,\mathbf{k}|0,\mathbf{k})=1. \tag{C.6}$$

Using (C.4), (C.5), (C.2) and the fact that proper graphs contributed the second term in (C.4), we see that

$$a(\mathbf{k})+\mathbf{k}\cdot\hat{q}b(\mathbf{k})=\frac{\mathbf{k}\cdot\hat{q}}{m^*}[1+\alpha^I(0)], \tag{C.8}$$

and

$$\mathbf{k}\cdot\hat{q}b(\mathbf{k})=\mathbf{k}\cdot\hat{q}/m^*. \tag{C.9}$$

In (C.8) we have written the dielectric constant $\kappa^I(0)$ in terms of the polarizability $\alpha^I(0)$ [Eq. (3.20)]. From (C.8), (C.9) and (C.4) we conclude that

$$\lim_{q\to 0}(0,\mathbf{k}+\mathbf{q}|j_\mu(\mathbf{q})|0,\mathbf{k})=\frac{k_\nu}{m^*}(\delta_{\mu\nu}+\hat{q}_\mu\hat{q}_\nu\alpha^I(0)). \tag{C.10}$$

In particular, the transverse part of this vector is given by

$$\lim_{q\to 0}(0,\mathbf{k}+\mathbf{q}|\mathbf{t}_\mathbf{q}\cdot\mathbf{j}(\mathbf{q})|0,\mathbf{k})=\mathbf{t}_\mathbf{q}\cdot\mathbf{k}/m^*. \tag{C.11}$$

This is equivalent to the identity (5.17).

Finally, we wish to derive the transverse sum rule (5.21). This is the transverse analog of the longitudinal sum rule which arises from the following identity:

$$[[H,\rho(\mathbf{q})],\rho(-\mathbf{q}')]=-\mathbf{q}\cdot\mathbf{q}'\rho(\mathbf{q}-\mathbf{q}')/m^*. \tag{C.12}$$

Taking the matrix element of the right and left sides of (C.11) between the exact states $|0,\mathbf{k}\rangle$ and $|0,\mathbf{k}+\mathbf{q}-\mathbf{q}'\rangle$, we obtain for small $\mathbf{q}$ and $\mathbf{q}'$

$$\hat{q}\cdot\hat{q}'/m^*[\kappa^I(0)]^2+\sum_{n\neq 0}\frac{(0,\mathbf{k}+\mathbf{q}-\mathbf{q}'|\hat{q}'\cdot\mathbf{j}(-\mathbf{q}')|n,\mathbf{k}+\mathbf{q})(n,\mathbf{k}+\mathbf{q}|\hat{q}\cdot\mathbf{j}(\mathbf{q})|0,\mathbf{k})}{E_{n,\mathbf{k}}-E_{0,\mathbf{k}}}$$
$$+\sum_{n\neq 0}\frac{(0,\mathbf{k}+\mathbf{q}-\mathbf{q}'|\hat{q}\cdot\mathbf{j}(\mathbf{q})|n,\mathbf{k}-\mathbf{q}')(n,\mathbf{k}-\mathbf{q}'|\hat{q}'\cdot\mathbf{j}(-\mathbf{q}')|0,\mathbf{k})}{E_{n,\mathbf{k}}-E_{0,\mathbf{k}}}=\hat{q}\cdot\hat{q}'(0,\mathbf{k}+\mathbf{q}-\mathbf{q}'|\rho(\mathbf{q}-\mathbf{q}')|0,\mathbf{k})/m, \tag{C.13}$$

where we have used (C.3) and the expansion (2.7) to transform the terms on the left-hand side of (C.13) corresponding to intermediate states with $n=0$.

A transverse sum rule follows from (C.13) in the same way as the transverse sum rule of reference 11 followed from (2.18). We start by constructing the tensor

$$K_{\mu\nu}(\mathbf{q},\mathbf{q}',\omega)\equiv\left\{\frac{i}{2}\int_{-\infty}^{0}dt\,e^{-i\omega t}e^{st}\right.$$
$$\times(0,\mathbf{k}+\mathbf{q}-\mathbf{q}'|[j_\mu(-\mathbf{q}',0)j_\nu(\mathbf{q},t)]$$
$$\left.+[j_\nu(\mathbf{q},0),j_\mu(-\mathbf{q}',t)]|0,\mathbf{k})\right\}$$
$$-\frac{1}{m}\delta_{\mu\nu}(0,\mathbf{k}+\mathbf{q}-\mathbf{q}'|\rho(\mathbf{q}-\mathbf{q}')|0,\mathbf{k}). \tag{C.14}$$

We now consider $\hat{q}'\cdot\mathbf{K}(\mathbf{q},\mathbf{q}',\omega)\cdot\hat{q}$. Using the sum rule (C.13), one then sees that in the limit $q,\ q'\to 0$

$$\lim_{\omega\to 0}\hat{q}'\cdot\mathbf{K}\cdot\hat{q}=-\hat{q}\cdot\hat{q}'/m^*[\kappa^I(0)]^2. \tag{C.15}$$

This relation is analogous to (3.16). Now, by a line of reasoning similar to that which lead to (3.22) from (3.16), one can show that

$$\lim_{\omega\to 0}\mathbf{t}_{q'}\cdot\mathbf{K}\cdot\mathbf{t}_\mathbf{q}=-\mathbf{t}_\mathbf{q}\cdot\mathbf{t}_{q'}/m^*. \tag{C.16}$$

Calculating the left-hand side of (C.16) explicitly from (C.14), one finally obtains[29]

$$\mathbf{t}_\mathbf{q}\cdot\mathbf{t}_{q'}/m^*+\sum_{n\neq 0}\frac{(0,\mathbf{k}+\mathbf{q}-\mathbf{q}'|\mathbf{t}_{q'}\cdot\mathbf{j}(-\mathbf{q}')|n,\mathbf{k}+\mathbf{q})(n,\mathbf{k}+\mathbf{q}|\mathbf{t}_\mathbf{q}\cdot\mathbf{j}(\mathbf{q})|0,\mathbf{k})}{E_{n,\mathbf{k}}-E_{0,\mathbf{k}}}$$
$$+\sum_{n\neq 0}\frac{(0,\mathbf{k}+\mathbf{q}-\mathbf{q}'|\mathbf{t}_\mathbf{q}\cdot\mathbf{j}(\mathbf{q})|n,\mathbf{k}-\mathbf{q}')(n,\mathbf{k}-\mathbf{q}'|\mathbf{t}_{q'}\cdot\mathbf{j}(-\mathbf{q}')|0,\mathbf{k})}{E_{n,\mathbf{k}}-E_{0,\mathbf{k}}}=\mathbf{t}_\mathbf{q}\cdot\mathbf{t}_{q'}(0,\mathbf{k}+\mathbf{q}-\mathbf{q}'|\rho(\mathbf{q}-\mathbf{q}')|0,\mathbf{k})/m. \tag{C.17}$$

To lowest order in k, we may neglect the k dependence of the energy denominators in (C.17). The result is then equivalent to (5.21).

[28] The energies $E_{0,\mathbf{k}}$ and $E_{0,\mathbf{k}+\mathbf{q}}$ are not affected by the removal of the extreme long-range tail of the Coulomb interaction. These energies are related to the proper electron self-energy parts. [See M. N. Hugenholtz, Physica **23**, 481 (1957) and D. F. Du Bois, Ann. Phys. **7**, 174 (1959).] In the calculation of such parts the Coulomb interactions lines are integrated over *all* momenta.

[29] In the limit of small q, q' the contributions of intermediate states with $n=0$ cancel in the same way that they did in (3.11).