region.[5] Extrapolation to low strains suggests that the high-temperature rise in "unstrained" crystals measured by the composite oscillator technique can be attributed to loss in the joint-stressed region.

It should be pointed out that these new determinations do not invalidate the "vacancy-drag" model proposed by Kessler. There are three factors in this model causing a variation of internal friction as the temperature rises: (i) the decrease of vacancy jump time, (ii) dispersion of the vacancy atmosphere from the dislocations, and (iii) increase in equilibrium vacancy concentration. These results indicate that the first two factors dominate the third in undistorted crystals, causing a decrease in decrement at temperatures above the "freezing-in" temperature which was postulated. The quenching experiment shows that, on this model, excess vacancies have probably diffused to inactive points within 4 minutes. This is in accordance with derived values of the diffusion coefficient of vacancies[6] if it is assumed that the maximum diffusion distance is of the order 10^{-4} cm.

The vacancy-drag model has the weakness, however, that the Peierls force on the dislocation has been ignored. This force is high in diamond-structure lattices, as is demonstrated by the tendency of dislocations to lie in preferred orientations.[7] It is probable that a dislocation relaxation mechanism such as that developed by Seeger *et al.*[8] is operating concurrently with the vacancy drag. Application of this theory to the lower-temperature peak yields an expected activation energy of rather less than 1 ev. There is some doubt whether this peak can be directly attributed to dislocations, as the plastic straining experiments indicate that the high-temperature rise is more directly affected by introduced dislocations. A more reasonable postulate might be that the high-temperature rise is part of a dislocation relaxation peak. In this case the theory gives an activation energy of 1.2 ev. This is not in disaccord with experiment as some spread of energies must be allowed for.

ACKNOWLEDGMENTS

The author wishes to extend his thanks to Dr. H. G. van Beuren for providing the plastically strained crystal used in the present work, and to Dr. J. O. Kessler for kindly making available the crystal he had measured.

[5] H. G. van Beuren (private communication).
[6] Letaw, Portnoy, and Slifkin, Phys. Rev. **102**, 636 (1956).
[7] W. C. Dash, J. Appl. Phys. **27**, 1193 (1956).
[8] Seeger, Donth, and Pfaff, Discussions Faraday Soc. No. 23, 19 (1957).

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Interaction of Charged Particles in a Dielectric*

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This paper is a sequel to an earlier study, from a many-particle standpoint, of the motion of an electron (or hole) in an insulator. We consider an insulator (whose nuclei are taken as fixed), including the electron-electron interaction. It is then shown that the static dielectric constant κ defined in terms of the force between two distant point charges immersed in the medium, and the effective dielectric constant κ^*, which determines the force between an extra electron (or hole) and a distant point charge, are equal. These results may be summarized by the statement that, if sufficiently distant, external charges in a dielectric interact with each other and with the charge of an extra electron or hole as if all charges were renormalized according to the prescription $Q \rightarrow Q/\kappa^{\frac{1}{2}}$. The method of proof is to treat the Coulomb interactions between the electrons and between the electrons and external charges by perturbation theory and to establish a correspondence, to all orders, between the Feynman graphs which define κ and those which define κ^*. The result is therefore exact, at least as long as the perturbation series converge.

1. INTRODUCTION

ONE of the simplest many-body systems in solid state physics is the following: We begin with the ground state of a perfect large insulator (of cubic symmetry) whose nuclei are regarded as fixed and which contains N electrons, moving under the action of the Coulomb field of the nuclei and of their mutual repulsion. Into this system we introduce a small number of electrons and (or) holes. We are then interested in the behavior of the resulting $(N+n)$-electron system $(n \ll N)$ under the influence of its internal interactions and of applied electromagnetic fields.

It is well known that experiments on such systems have been interpreted in great detail and with considerable quantitative success in terms of an effective single-particle model. According to this model the system behaves quite analogously to a collection of negatively and positively charged particles in a vacuum. Only the following modifications are necessary. The kinetic energy of these particles must be taken as

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$E_n(\mathbf{k})$, the appropriate energy band function, and their pairwise interaction at large distances as

$$V=Q_1Q_2/\kappa r, \tag{1.1}$$

where Q_1, Q_2 are their charges and κ is the static dielectric constant. In this model the same interaction (1.1) is also appropriate when one or both of the charges is an "external" charge such as a classical point charge or proton.

Because of its long and successful history, most physicists regard this model as plausible beyond reasonable doubt. However, the question of why and under what circumstances it is a consequence of the full Schrödinger equation for the $(N+n)$ electrons, including all their rather substantial interactions, has not yet been fully clarified.

In a previous paper[1] we have begun a study of these questions. We considered the case of a perfect insulator with a single extra electron (or hole) and a small external charge q embedded in it. It was shown that under the single assumption that q is small, and without in any way treating the electron-electron interaction as weak, the $(N\pm1)$-particle Schrödinger equation could be reduced—for the low-lying states—to a single-particle equation of the form

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2\mp\frac{eq}{\kappa^* r}\right)F=EF, \tag{1.2}$$

where m^* and κ^* were certain constants. This is just the form one would expect on the basis of the above-mentioned single-particle model, which further suggests that the constant κ^* must equal the ordinary static dielectric constant κ. In reference 1, the identity of κ and κ^* was however not completely established. All that was done was to give a strong plausibility argument[2] and to prove the identity explicitly in lowest order of perturbation theory in the electron-electron interaction (Appendix). The bulk of the present paper is devoted to a demonstration of the equality,

$$\kappa^*=\kappa, \tag{1.3}$$

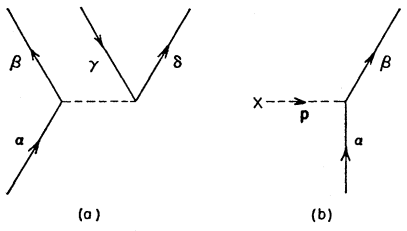

FIG. 1. Two elementary graphs. (a) shows creation of an electron-hole pair, (b) the interaction of an electron with the external potential, X.

[1] W. Kohn, Phys. Rev. **105**, 509 (1957).
[2] See reference 1, p. 513, footnote 8.

to all orders in the electron-electron interaction, H' (Secs. 2 and 3). This demonstration makes essential use of Feynman diagrams and the linked-cluster theory of Brueckner[3] and Goldstone.[4]

In Sec. 4 we show that the results of Secs. 2 and 3 apply also to finite external charges, provided they are sufficiently distant. In Sec. 5 the results of Sec. 3 are generalized to electrons and holes of finite excitation energy. Section 6 contains comments concerning convergence, and Sec. 7 some concluding remarks.

It is hardly necessary to point out the close relationship of this paper with recent studies of charge renormalization in field theory.[5]

2. DIELECTRIC CONSTANT κ

Consider a perfect insulator with N electrons described by the Hamiltonian

$$H=H_0+H', \tag{2.1}$$

where

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

represents the kinetic and interaction with the nuclei of the lattice, and

$$H'\equiv e^2\sum_{i>j}\sum_{\mathbf{K}}{}'\frac{4\pi}{\Omega}\frac{e^{i\mathbf{K}\cdot(\mathbf{r}_i-\mathbf{r}_j)}}{K^2} \tag{2.3}$$

describes the Coulomb repulsion of the electrons. Ω is the volume of the insulator and $\sum'$ means summation with $K=0$ omitted.

To define the dielectric constant κ we now consider the effect on the energy of this system of a long-wavelength sinusoidal perturbing potential of the form

$$U=U_0(\rho_{\mathbf{p}}+\rho_{-\mathbf{p}}), \tag{2.4}$$

where

$$\rho_{\mathbf{p}}\equiv\sum_{i=1}^{N}e^{i\mathbf{p}\cdot\mathbf{r}_i}. \tag{2.5}$$

Let us call the second-order energy change produced by U, ΔE_2. Then κ is defined by the equation[6]

$$1/\kappa=1+\alpha, \tag{2.6}$$

where

$$\alpha=\lim_{\mathbf{p}\to0}\frac{4\pi e^2}{\Omega}\frac{\Delta E_2}{U_0^2p^2}. \tag{2.7}$$

Our total Hamiltonian can now be written as

$$H_T=H_0+H_1, \tag{2.8}$$

[3] K. A. Brueckner, Phys. Rev. **100**, 36 (1955).
[4] J. Goldstone, Proc. Roy. Soc. (London) **A293**, 267 (1957).
[5] F. J. Dyson, Phys. Rev. **75**, 1736 (1949); A. Salam, Phys. Rev. **82**, 217 (1951); J. C. Ward, Proc. Phys. Soc. (London) **A64**, 54 (1951).
[6] It is elementary to verify that this definition of κ is identical with that given in reference 1, in terms of the interaction between two small and distant point charges immersed in the medium. See Sec. 4.

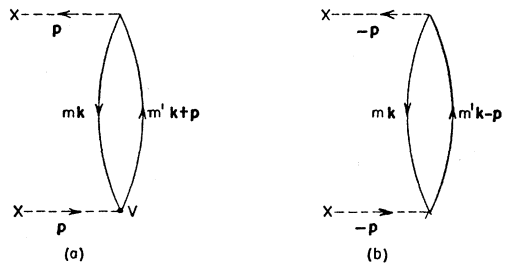

FIG. 2. Lowest order graphs in the dielectric constant expansion.

where

$$H_1=H'+U, \tag{2.9}$$

and includes both the Coulomb repulsion between the electrons and their interaction with the perturbing field. To obtain ΔE_2 we must find the energy corresponding to H_T to all orders in H' but only to second order in U.

The total energy shift due to H_1 can be written conveniently by means of Goldstone's linked-cluster perturbation formula[7]

$$\Delta E=\sum_L\left(\Psi_0\left|H_1\left(\frac{1}{E_0-H_0}H_1\right)^n\right|\Psi_0\right), \tag{2.10}$$

where Ψ_0 is the ground state (Slater determinant) of H_0, with unperturbed energy E_0, and $\sum_L$ signifies summation over all linked clusters leading from Ψ_0 to Ψ_0. To obtain ΔE_2 we select from these graphs that subset in which U acts only twice and denote it by L_2. Thus

$$\Delta E_2=\sum_{L_2}\left(\Psi_0\left|H_1\left(\frac{1}{E_0-H_0}H_1\right)^n\right|\Psi_0\right). \tag{2.11}$$

We shall use the same graphical representation as Goldstone, which is exemplified by the elementary graphs of Fig. 1. A Greek symbol represents all quantum numbers of a one-electron wave function, that is band index, crystal momentum, and spin direction. Lines with arrows pointing up refer to states which are not occupied in the unperturbed state Ψ_0, those with arrows pointing down to states occupied in Ψ_0. Figure 1(a) shows an electron in the normally empty state α going into the normally empty state β as a result of a Coulomb collision (H') with an electron in the normally filled state γ which is scattered into the normally empty state δ, leaving a hole in γ. Figure 1(b) shows an electron being scattered by the external potential (U), from which it absorbs crystal momentum $\mathbf{p}$. It is of great importance that also graphs violating the exclusion principle must be included. For example, β and δ in Fig. 1(a) can be identical states.

The graphs for ΔE_2 of zeroth order in the electron-electron interaction are shown in Fig. 2. Right to left in Eq. (2.11) corresponds to an upward direction in our graphs. m and m' are the indices of bands which are, respectively, filled and unfilled in Ψ_0. Let us denote the single-particle normalized Bloch waves by

$$\psi_{n\mathbf{k}}=u_{n\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{2.12}$$

and their energies by $\epsilon_{n\mathbf{k}}$. Then the contribution of these graphs to ΔE_2 is

$$\begin{aligned}\Delta E_2^{(0)}&=\left(\Psi_0\left|U\frac{1}{E_0-H_0}U\right|\Psi_0\right)\\&=\sum_{m,m'}\sum_{\mathbf{k}}\frac{(\psi_{m\mathbf{k}}|U_0e^{-i\mathbf{p}\cdot\mathbf{r}}|\psi_{m'\mathbf{k}+\mathbf{p}})(\psi_{m'\mathbf{k}+\mathbf{p}}|U_0e^{i\mathbf{p}\cdot\mathbf{r}}|\psi_{m\mathbf{k}})}{\epsilon_{m\mathbf{k}}-\epsilon_{m'\mathbf{k}+\mathbf{p}}}\\&\qquad+(\mathbf{p}\rightarrow-\mathbf{p}),\end{aligned} \tag{2.13}$$

where $(\mathbf{p}\rightarrow-\mathbf{p})$ means a similar term [corresponding to Fig. 2(b)] with $\mathbf{p}$ replaced by $-\mathbf{p}$. In the limit of small $\mathbf{p}$, and with the use of the cubic symmetry of the crystal, (2.13) becomes

$$\begin{aligned}\Delta E_2^{(0)}&=2U_0^2\sum_{m,m'}\frac{[\mathbf{p}\cdot(u_{m\mathbf{k}},\nabla_{\mathbf{k}}u_{m'\mathbf{k}})][\mathbf{p}\cdot(\nabla_{\mathbf{k}}u_{m'\mathbf{k}},u_{m\mathbf{k}})]}{\epsilon_{m\mathbf{k}}-\epsilon_{m'\mathbf{k}}}\\&=2U_0^2\frac{\Omega}{(2\pi)^3}p^2\sum_{m,m'}\int d\mathbf{k}\frac{|(u_{m\mathbf{k}},\partial u_{m'\mathbf{k}}/\partial k_1)|^2}{\epsilon_{m\mathbf{k}}-\epsilon_{m'\mathbf{k}}}.\end{aligned} \tag{2.14}$$

The corresponding contribution to α, and hence to $1/\kappa$ is, by (2.7),

$$\alpha^{(0)}=\frac{e^2}{\pi^2}\sum_{m,m'}\int d\mathbf{k}\frac{|(u_{m\mathbf{k}},\partial u_{m'\mathbf{k}}/\partial k_1)|^2}{\epsilon_{m\mathbf{k}}-\epsilon_{m'\mathbf{k}}}. \tag{2.15}$$[8]

It is important to note the reason for the factor p^2 in $\Delta E_2^{(0)}$. It arises from the fact that at each vertex such as V, Fig. 2(a), where an electron makes an *inter*band transition, the corresponding matrix element,

$$(\psi_{n_1\mathbf{k}+\mathbf{p}}|U_0e^{i\mathbf{p}\cdot\mathbf{r}}|\psi_{n_2k})=U_0\,\mathbf{p}\cdot(u_{n_1\mathbf{k}},\nabla_{\mathbf{k}}u_{n_2\mathbf{k}}), \tag{2.16}$$

is linear in $\mathbf{p}$.

Other types of graphs occur in higher orders, for instance those shown in Fig. 3.

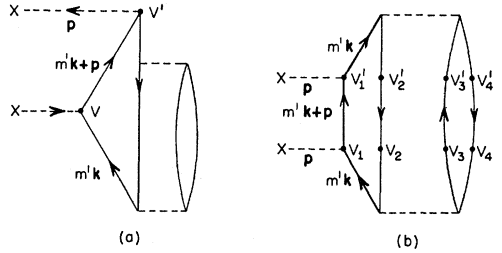

FIG. 3. Some higher order graphs in the dielectric constant expansion.

[7] Reference 3, Eq. (3.3).

[8] This corresponds to Eq. (A.17) of reference 1.

In Fig. 3(a), the collision at V is *intra*band and for small p the corresponding matrix element is

$$(\psi_{m'\mathbf{k}+\mathbf{p}}|\,U_0e^{i\mathbf{p}\cdot\mathbf{r}}|\psi_{m'\mathbf{k}})=U_0+O(\mathbf{p}), \qquad (2.17)$$

i.e., of degree zero in $\mathbf{p}$. The matrix element at V' is of course linear in $\mathbf{p}$, so that this entire graph makes a contribution linear in $\mathbf{p}$ to ΔE_2. However, when this graph is combined with that obtained by replacing $\mathbf{p}$ by $-\mathbf{p}$, the linear terms cancel and one is left with a quadratic contribution to ΔE_2.

In Fig. 3(b), the vertices V_1 and V_1' are both intraband, so that this graph contributes a term of degree zero in $\mathbf{p}$. Now consider the graph obtained from Fig. 3(b) by replacing the vertex V_1 by V_2, causing an intraband collision at V_2. This graph contributes the same term of degree zero to ΔE_2 as Fig. 3(b), but with the opposite sign. For according to the rules of evaluating the contributions of these graphs,[4] each must be multiplied by a factor $(-1)^{l+h}$, where l is the number of closed loops and h the number of internal hole lines. In this way the leading terms of the 16 graphs obtained by taking one of the vertices from the group $V_1\cdots V_4$ and the other from $V_1'\cdots V_4'$ cancel in pairs. Any remaining terms linear in $\mathbf{p}$ cancel on replacing $\mathbf{p}$ by $-\mathbf{p}$.

It is clear that these examples are representative of all graphs, since any graph is cut by any horizontal line in an equal number of electrons and hole-lines. The total ΔE_2 is obtained by adding up the contributions of all relevant graphs, and the dielectric constant κ is then obtained from Eqs. (2.6) and (2.7).

3. EXTRA ELECTRON (OR HOLE): EFFECTIVE DIELECTRIC CONSTANT κ^*

We consider now the system consisting of the perfect insulator plus one extra electron. The wave functions of this system will be denoted by $\Psi_{n\mathbf{K}}$, where $\mathbf{K}$ is the total propagation vector and n is an additional set of quantum numbers. The corresponding energies will be called $E_{n\mathbf{K}}$. The Hamiltonian of the system is given by

$$H=H_0+H', \qquad (3.1)$$

where

$$H_0=\sum_{i=1}^{N+1}(T_i+V_i), \qquad (3.2)$$

and

$$H'=e^2\sum_{i>j}\sum_{\mathbf{K}}{}'\frac{4\pi}{\Omega}\frac{e^{i\mathbf{K}\cdot(\mathbf{r}_i-\mathbf{r}_j)}}{K^2}. \qquad (3.3)$$

Let now $\Psi_{0\mathbf{K}}$ be that eigenfunction of H which corresponds to the unperturbed function $\Psi_{0\mathbf{K}}{}^{(0)}$ describing the perfect insulator plus an extra electron in the one-electron state $\psi_{0\mathbf{K}}$ of the lowest empty band. We shall sometimes call $\Psi_{0\mathbf{K}}$ the wave function of the "clothed" electron.

Suppose we want to describe the scattering of the "clothed" electron by a small external charge q immersed in the medium. We then require the matrix element

$$M_{\mathbf{K}'\mathbf{K}}\equiv\left(\Psi_{0\mathbf{K}'}\left|\sum_{i=1}^{N+1}-\frac{eq}{r_i}\right|\Psi_{0\mathbf{K}}\right). \qquad (3.4)$$

Now we may Fourier analyze the perturbation and write

$$\sum_i\frac{1}{r_i}=\frac{4\pi}{\Omega}\sum_{\mathbf{p}}{}'\frac{1}{p^2}\rho_{\mathbf{p}}, \qquad (3.5)$$

where $\rho_{\mathbf{p}}$ was defined in Eq. (2.5). Then for sufficiently small $\mathbf{K}$ and $\mathbf{K}'$, (3.4) becomes

$$M_{K'K}=\frac{4\pi}{\Omega}\frac{-eq}{\kappa^*}\frac{1}{|\mathbf{K}-\mathbf{K}'|^2}, \qquad (3.6)$$

where κ^* is defined by the following equation:

$$\frac{1}{\kappa^*}\equiv\lim_{\substack{\mathbf{K},\mathbf{K}'\to 0\\ \mathbf{K}\neq\mathbf{K}'}}(\Psi_{0\mathbf{K}'}|\rho_{\mathbf{K}'-\mathbf{K}}|\Psi_{0\mathbf{K}}). \qquad (3.7)$$

The quantity κ^* is called the effective dielectric constant. It is the same constant which describes the interaction of the "clothed" electron with q in a bound state of large orbit [see Eq. (1.2)].

Clearly (3.6) is just the matrix element for the interaction of the extra electron and q in vacuum except that both charges have effectively been renormalized by the factor $\kappa^{*-\frac{1}{2}}$.

We now wish to demonstrate the equality of this constant κ^* and the static dielectric constant κ defined in the previous section, to all orders in the electron-

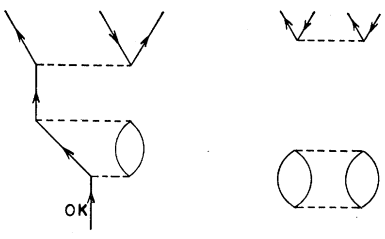

FIG. 4. A typical graph in the perturbation expansion of the wave function $\Psi_{0\mathbf{K}}$, Eq. (3.10).

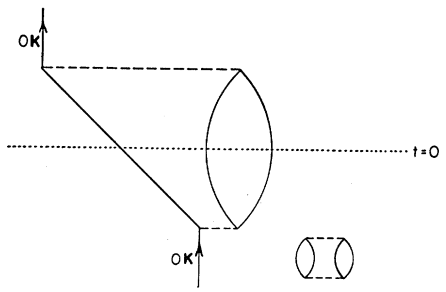

FIG. 5. A graph occurring in the normalization sum, Eq. (3.11).

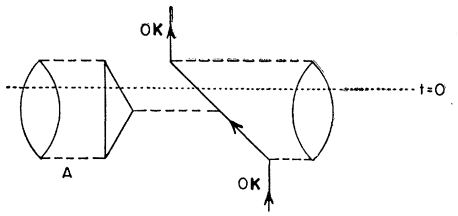

FIG. 6. A graph which *cannot* occur in (3.11) because it violates conservation of total crystal momentum.

electron interaction H'. For this purpose we require first the wave functions $\Psi_{0\mathbf{K}}$. Let us imagine that at time $t=-\infty$ our system is in the unperturbed state $\Psi_{0\mathbf{K}}{}^{(0)}$ and that the interaction H' is slowly turned on according to the factor $\exp(\eta t/\hbar)$.[9] Then at time $t=0$, the normalized wave function is given by

$$\Psi_{0\mathbf{K}}=\left[\sum_{l=0}^{\infty}\left(\frac{-i}{\hbar}\right)^{l}\int H'(t_1)\cdots H'(t_l)dt_1\cdots dt_l\right]\Psi_{0\mathbf{K}}{}^{(0)},$$

$$t_l<\cdots<t_1<0, \quad (3.8)$$

where

$$H'(t)=e^{iH_0t/\hbar}H'e^{-iH_0t/\hbar}e^{\eta t/\hbar}. \quad (3.9)$$

On performing the time integrations, one obtains[10]

$$\Psi_{0\mathbf{K}}=\left[\sum_{l=0}\frac{1}{E_{0\mathbf{K}}{}^{(0)}-H_0+il\eta}H'\cdots\times\frac{1}{E_{0\mathbf{K}}{}^{(0)}-H_0+i\eta}H'\right]\Psi_{0\mathbf{K}}{}^{(0)}. \quad (3.10)$$

A typical graph representing one of the terms of (3.10) is shown in Fig. 4.

The normalization of (3.10) is expressed by the equation

$$(\Psi_{0\mathbf{K}},\Psi_{0\mathbf{K}})=\sum_{ll'}\left(\Psi_{0\mathbf{K}}{}^{(0)}\left|H'\frac{1}{E_{0\mathbf{K}}{}^{(0)}-H_0-i\eta}\cdots H'\frac{1}{E_{0\mathbf{K}}{}^{(0)}-H_0-il\eta}\times\frac{1}{E_{0\mathbf{K}}{}^{(0)}-H_0+il'\eta}H'\cdots\frac{1}{E_{0\mathbf{K}}{}^{(0)}-H_0+i\eta}H'\right|\Psi_{0\mathbf{K}}{}^{(0)}\right)=1. \quad (3.11)$$

A typical graph representing one term in the normalization sum (3.11) is shown in Fig. 5. The dotted line indicates the place where the two propagators follow each other directly in (3.11). The portion below it is one graph in $\Psi_{0\mathbf{K}}$, that above it one graph of $\Psi_{0\mathbf{K}}{}^{*}$ with matching external lines.

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

[10] It is well known that because $\Psi_{0\mathbf{K}}{}^{(0)}$ re-occurs among the intermediate states, the phase—but only the phase—of $\Psi_{0\mathbf{K}}$ depends critically on the value of η. This does not cause any difficulties in what follows.

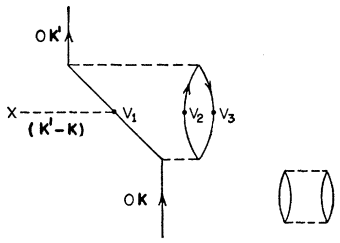

FIG. 7. A graph of class I, occurring in the evaluation of $1/\kappa^{*}$, Eq. (3.12).

It may be noted here for later use that graphs of the structure of Fig. 6, in which one portion (marked A) can be completely unlinked by breaking a single interaction line, in general *cannot* occur. For such graphs evidently violate the conservation of total crystal momentum during the interactions, except in the special case (which will not be relevant in the following) where the crystal momentum carried by the linking line just equals a reciprocal lattice vector.

Next consider the expression (3.7) for $1/\kappa^{*}$ with $\Psi_{0\mathbf{K}}$ and $\Psi_{0\mathbf{K}'}$ expressed by means of Eq. (3.10)

$$\frac{1}{\kappa^{*}}=\lim_{\substack{\mathbf{K},\mathbf{K}'\to 0\\ \mathbf{K}\neq\mathbf{K}'}}\sum_{l,l'}\left(\Psi_{0\mathbf{K}'}{}^{(0)}\left|H'\frac{1}{E_{0\mathbf{K}'}{}^{(0)}-H_0-i\eta}\cdots\times H'\frac{1}{E_{0\mathbf{K}'}{}^{(0)}-H_0-il'\eta}\rho_{\mathbf{K}'-\mathbf{K}}\times\frac{1}{E_{0\mathbf{K}}{}^{(0)}-H_0+il\eta}H'\cdots\times\frac{1}{E_{0\mathbf{K}}{}^{(0)}-H_0+i\eta}H'\right|\Psi_{0\mathbf{K}}{}^{(0)}\right). \quad (3.12)$$

There are only two classes of graphs which make finite contributions to (3.12) in the limit $\mathbf{K}'-\mathbf{K}\to 0$:

Class I is obtained by attaching an external line $\mathbf{K}'-\mathbf{K}$ [representing a Fourier component of the external potential, Eq. (3.5)] at $t=0$ to a normalization graph, such as Fig. 5, and adjusting the crystal momenta in the latter by the small momentum transfer $\mathbf{K}'-\mathbf{K}$ in accordance with the conservation laws. For example, one of the graphs corresponding to Fig. 5 is shown in Fig. 7. The interaction at V_1 is *intra*band and in the limit $\mathbf{K}'-\mathbf{K}\to 0$, the corresponding matrix element of $\rho_{\mathbf{K}'-\mathbf{K}}$ is 1. Consequently Fig. 7 contributes to $1/\kappa^{*}$ the same as Fig. 5 does to the normalization. The two similar graphs, obtained from Fig. 7 by replacing V_1 by V_2 and V_3, cancel in the limit $\mathbf{K}'-\mathbf{K}\to 0$ (different number of hole lines). Thus clearly all the graphs of class I together contribute 1 to $1/\kappa^{*}$.

The second class of graphs is split into two halves, classes IIA and IIB. Consider first class IIA. It is constructed as follows (see Fig. 8). We take a normalization graph, such as Fig. 5, which we shall call the $\mathfrak{N}$ graph, and a dielectric constant graph, such as Fig. 2(a), with two external lines $\mathbf{p}=\mathbf{K}'-\mathbf{K}$, which we shall call the $\mathfrak{D}$ graph. The "later" of the external lines is attached to the $\mathfrak{N}$ graph at all possible points with $t>0$ [Figs. 8(a) and 8(b)] thus becoming an internal

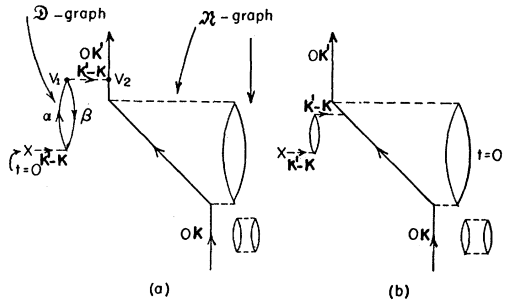

FIG. 8. Two closely related graphs of class IIA, occurring in the evaluation of $1/\kappa^*$, Eq. (3.12).

line of the graph, while the other external line remains external at $t=0$. In contrast to class I, when the external line is deleted from one of the present graphs, the resulting graph is topologically different from any $\mathfrak{N}$ graph (see Fig. 6).

The interaction V_1V_2 causes an *intra*band scattering at V_2, with the momentum transfer $\mathbf{K}'-\mathbf{K}$. The corresponding matrix element M' is therefore

$$M'=\frac{4\pi e^2}{\Omega}\frac{1}{|\mathbf{K}'-\mathbf{K}|^2}(\beta|e^{-i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{r}}|\alpha). \qquad (3.13)$$

When we sum over all graphs of class IIA arising from a given $\mathfrak{N}$ graph and $\mathfrak{D}$ graph, by taking all possible times ($t>0$) for the point of attachment and all possible time relationships between the interactions occurring in the $\mathfrak{N}$ graph and those occurring in the $\mathfrak{D}$ graph [see Figs. 8(a) and 8(b)], the resulting contribution to $1/\kappa^*$ is exactly a product of three factors[11]:

(1) The contribution of the $\mathfrak{N}$ graph to the normalization sum Eq. (3.11), say $C(\mathfrak{N})$.

(2) The factor $(4\pi e^2/\Omega)|\mathbf{K}'-\mathbf{K}|^{-2}$ coming from the matrix element M', Eq. (3.13), and describing the *intra*band scattering taking place at V_2, Fig. 8(a), in the $\mathfrak{N}$ graph.

(3) The contribution of the $\mathfrak{D}$ graph to the second order energy ΔE_2 encountered in the calculation of κ, with U_0 set equal to 1 [see Eqs. (2.4)ff.].[12]

The product of (2) and (3) is just the contribution of the $\mathfrak{D}$ graph to the quantity α, Eq. (2.7).

Holding fixed our original $\mathfrak{N}$ graph, we now construct the graphs of class IIB, which differ from those of class IIA only by having the interaction between the $\mathfrak{N}$ and $\mathfrak{D}$ parts occur at time $t<0$. (A typical $\mathfrak{D}$ part in class IIB will be Fig. 2b, with $\mathbf{p}=\mathbf{K}'-\mathbf{K}$.) Then, by adding all graphs of classes IIA and IIB corresponding to a given $\mathfrak{N}$ graph we clearly obtain $C(\mathfrak{N})\alpha$. Now we sum over all $\mathfrak{N}$ graphs and since $\sum C(\mathfrak{N})=1$, we obtain simply α. Finally, by adding the contribution 1 from class I we obtain the desired result:

$$\frac{1}{\kappa^*}=1+\alpha=\frac{1}{\kappa}. \qquad (3.14)$$

The physical meaning of the two classes of graphs can be seen from Figs. 7 and 8. Class I is of the structure of Fig. 9 which shows a "clothed" electron interacting directly with the external potential. [The portion marked "clothed" electron does not contain any part which can be completely unlinked from it by breaking a single interaction line carrying crystal momentum $\mathbf{K}'-\mathbf{K}$ (see Fig. 6).]

Class IIA is of the structure of Fig. 10, in which the clothed electron is scattered by the electrons of the medium which has been polarized by the external potential. In class IIB the time order of the two momentum transfer lines shown in Fig. 10 is inverted.

The case of an insulator with a single *hole* is completely analogous to that of an insulator with a single electron. We can define wave functions $\bar{\Psi}_{0\mathbf{K}}$ for the entire system, corresponding to the functions $\Psi_{0\mathbf{K}}$ of Eq. (3.10). Graphs representing $\bar{\Psi}_{0\mathbf{K}}$ are similar to those for $\Psi_{0\mathbf{K}}$, except that the initial electron line, running upwards, is replaced by a hole line, running down. In analogy with Eqs. (3.7) and (3.14), one then finds readily

$$\lim_{\substack{\mathbf{K},\mathbf{K}'\to 0\\ \mathbf{K}\neq\mathbf{K}'}}(\bar{\Psi}_{0\mathbf{K}'}|\rho_{\mathbf{K}'-\mathbf{K}}|\bar{\Psi}_{0\mathbf{K}})=-\frac{1}{\kappa}. \qquad (3.15)$$

The change of sign, which is a direct consequence of the algebra of these graphs, reflects the opposite charge of this "particle."

4. FINITE EXTERNAL CHARGE

In the preceding sections we have restricted ourselves to infinitesimal external fields. We shall now show that the constant κ also determines the interaction between *finite* external charges and between a finite external charge and an extra electron (or hole), provided only that they are far enough apart.

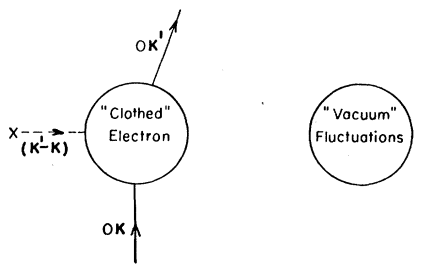

FIG. 9. Direct scattering of the "clothed" electron by the external potential.

[11] See reference 3, paragraph 3.

[12] Actually some η's will occur in the denominators of (3), whereas in (2.11) the limit $\eta\to 0$ has already been taken. Since *this* limit is well defined, no difficulty is caused. The important thing is that (1) is *exactly* equal to the contribution of the $\mathfrak{N}$ graph to (3.11), including its dependence on η, which is critical. (See reference 10.)

We begin by considering two finite charges in a perfect insulator, q_1 placed at the origin and q_2 at $\mathbf{R}$. The resulting perturbing potential is

$$U=-eq_1\sum_i\frac{1}{r_i}-eq_2\sum_i\frac{1}{|\mathbf{r}_i-\mathbf{R}|}$$
$$=-\frac{4\pi e}{\Omega}\sum_i\left[q_1\sum_{\mathbf{p}_1}{}'\frac{e^{i\mathbf{p}_1\cdot\mathbf{r}_i}}{p_1^2}+q_2\sum_{\mathbf{p}_2}{}'\frac{e^{-i\mathbf{p}_2\cdot\mathbf{r}_i}e^{i\mathbf{p}_2\cdot\mathbf{R}}}{p_2^2}\right]. \quad (4.1)$$

Let $\delta E(R)$ be the energy change of the dielectric caused by U. Then the force acting on q_2 is of course given by

$$\mathbf{F}=\frac{q_1q_2}{R^2}-\nabla_{\mathbf{R}}\delta E(\mathbf{R}), \quad (4.2)$$

apart from the irrelevant force exerted by the unperturbed medium on q_2.

Now $\delta E(\mathbf{R})$ can be calculated by means of the linked-cluster perturbation formula, (2.10). Graphs of order $q_1{}^nq_2{}^0$ are independent of $\mathbf{R}$ and so do not contribute to $\mathbf{F}$, and graphs of order $q_1{}^0q_2{}^n$ are periodic in $\mathbf{R}$ and describe the interaction energy of q_2 alone with the medium. They are not of interest here.

The graphs of order q_1q_2 are exactly those encountered in Sec. 2. (A typical one is shown in Fig. 11.) We can write the contribution of these graphs to $\delta E(\mathbf{R})$ as

$$\delta E_{11}(\mathbf{R})=\frac{4\pi q_1q_2}{\Omega}\sum{}'G_{11}(\mathbf{p}_2)e^{i\mathbf{p}_2\cdot\mathbf{R}}.^{13} \quad (4.3)$$

For small p_2 one obtains, by comparison with the definition of α given in Eq. (2.7),

$$\lim_{\mathbf{p}_2\to0}G_{11}(\mathbf{p}_2)=\frac{\alpha}{p_2^2}. \quad (4.4)$$

From (4.3) and (4.4) we see then at once that, for large $\mathbf{R}$,

$$\delta E_{11}(\mathbf{R})\to\alpha(q_1q_2/R). \quad (4.5)$$

Let us next look at terms of higher order, say of order $q_1{}^2q_2$. In analogy with (4.3) we may write the contribution of these terms to $\delta E(\mathbf{R})$ in the form

$$\delta E_{21}(\mathbf{R})=\frac{4\pi q_1{}^2q_2}{\Omega}\sum{}'G_{21}(\mathbf{p}_2)e^{i\mathbf{p}_2\cdot\mathbf{R}}. \quad (4.6)$$

A typical graph contributing to $G_{21}(\mathbf{p}_2)$ is shown in Fig. 12. For fixed $\mathbf{p}_2$, all graphs of this structure contribute to $G_{21}(\mathbf{p}_2)$ for which (to within a reciprocal lattice vector)

$$\mathbf{p}_1{}'+\mathbf{p}_1{}''=\mathbf{p}_2. \quad (4.7)$$

In adding up their contributions an integration, say over $\mathbf{p}_1{}'-\mathbf{p}_1{}''$, remains. Thus, whereas the vertex V in Fig. 11 contributed a singular matrix element of order $p_2{}^{-1}$, pairs of vertices such as V and V' in Fig. 12 do not. Consequently one finds that

$$\lim_{\mathbf{p}_2\to0}p_2{}^2G_{21}(\mathbf{p}_2)=0, \quad (4.8)$$

and hence

$$\lim_{R\to\infty}R\delta E_{21}(\mathbf{R})=0. \quad (4.9)$$

In other words, the terms of order $q_1{}^2q_2$ give an interaction of shorter range than those of order q_1q_2. The same is true, for similar reasons, of all higher order terms.

Therefore (on neglecting terms periodic in $\mathbf{R}$) we obtain for large $\mathbf{R}$

$$\delta E(\mathbf{R})=\delta E_{11}(\mathbf{R})=\alpha q_1q_2/R, \quad (4.10)$$

which, when combined with (4.2) and the definition $\kappa^{-1}=(1+\alpha)$, gives

$$\mathbf{F}=\frac{q_1q_2}{\kappa R^2}\left(\frac{\mathbf{R}}{R}\right). \quad (4.11)$$

The case of a finite external charge interacting with a distant electron (or hole) is exactly similar. For small momentum transfer $\mathbf{K}'-\mathbf{K}$, the graphs linear in q give a matrix element of order $|\mathbf{K}'-\mathbf{K}|^{-2}$, all higher order graphs being less singular.

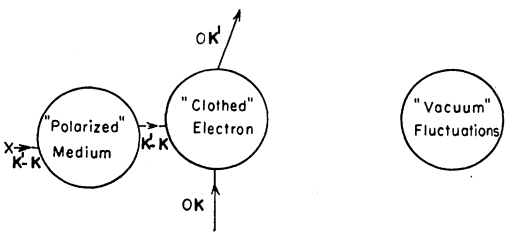

FIG. 10. Scattering of the "clothed" electron by the medium which has been polarized by the external potential.

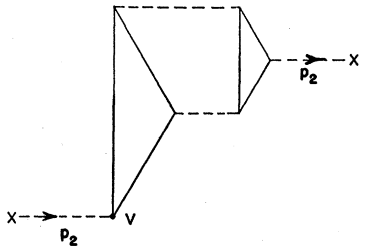

FIG. 11. A graph of order q_1q_2 referring to the interaction energy between the charges q_1 and q_2.

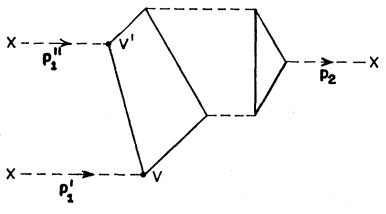

FIG. 12. A graph of order $q_1{}^2q_2$ referring to the interaction energy between the two charges q_1 and q_2.

[13] The subscripts $_{11}$ refer to the linearity in q_1 and q_2.

One remark should however be made. The arguments just given depend of course on the covergence of the power series in the q's. The following physical consideration shows that this power series must have a finite radius of convergence. For as we increase the magnitude of q there will come a point when the electric field produced by it is so large that the dielectric will break down. For example, the vicinity of an As impurity in silicon may be considered as such a broken-down dielectric, produced by placing a charge of $(Z_{\mathrm{As}}-Z_{\mathrm{Si}})e$ on a silicon nucleus. The results we have proved will then not be applicable.

5. ELECTRONS (OR HOLES) IN STATES OF FINITE EXCITATION

In Sec. 3 we have considered an electron or hole in states infinitesimally near the lowest possible state ($n=0$, $\mathbf{K}$, $\mathbf{K}'\rightarrow 0$). Those were the states which were encountered in the discussion of impurity states in reference 1. However, while our arguments in Sec. 3 depended critically on the assumption of small momentum transfer,

$$\mathbf{K}'-\mathbf{K}\rightarrow 0, \tag{5.1}$$

no explicit use was made of the fact that $n=0$ or that $\mathbf{K}$ and $\mathbf{K}'$ are separately small.

For sufficiently highly excited states a delicate difficulty arises, because the unperturbed state $\Psi_{n\mathbf{K}}{}^{(0)}$ describing a perfect insulator and one fairly highly excited electron then becomes degenerate with other states $\Psi_{n'\mathbf{K}}{}^{(0)}$ describing a perfect insulator, a conduction electron, and one or several electron-hole pairs. This situation requires separate discussion into which we do not want to enter here.[14] But certainly our results continue to hold at least up to energies where this difficulty occurs. Thus we can write, instead of (3.7) and (3.14), the somewhat more general result

$$\lim_{\mathbf{K}'-\mathbf{K}\rightarrow 0}(\Psi_{n\mathbf{K}'}|\rho_{\mathbf{K}'-\mathbf{K}}|\Psi_{n\mathbf{K}})=\frac{1}{\kappa}, \tag{5.2}$$

for all n and $\mathbf{K}$ for which $(E_{n\mathbf{K}}-E_{00})$ is below some critical value.

6. CONVERGENCE OF THE EXPANSION IN THE ELECTRON ELECTRON INTERACTION

In Secs. 2 and 3 we expanded the eigenfunction of our system in powers of the electron electron interaction, H'. It is doubtful if such an expansion would converge for any real dielectric. However, since the equality of κ and κ^* was proved to all orders of perturbation theory, it is likely that it holds even beyond the radius of convergence. Thus if the analytical behavior of our wave functions in their dependence on the electron charge e were known, the general equality of κ and κ^* might be proved by analytic continuation.

Another, and simpler, method of extending the proof of the equality of κ and κ^* is the following well-known procedure. Instead of writing $H=H_0+H'$, as in Eqs. (2.1) and (3.1), we introduce a one-particle potential V', such as the Hartree-Fock potential, which simulates the effects of H' as well as possible, and then write

$$H=\bar{H}_0+\bar{H}', \tag{6.1}$$

where

$$\bar{H}_0=\textstyle\sum_i(T_i+V_i+V_i'), \tag{6.2}$$

and

$$\bar{H}'=H'-\textstyle\sum_i V_i'. \tag{6.3}$$

The graphical analysis given in the preceding sections can be readily extended to cover the new perturbation $\bar{H}'$, and since V_i' does not have divergent long-wavelength components, the result is as before that $\kappa^*=\kappa$. The radius of convergence is, however, much larger now and probably includes real dielectrics.

7. CONCLUDING REMARKS

While this paper accomplishes its immediate purpose of establishing the equality of κ^* and κ, it falls short of proving the following *general* charge renormalization theorem for a dielectric. Any pair of extra charges, provided they are sufficiently far apart, and whether carried by electrons, holes, foreign particles (e.g., protons), or classical charge points, interact with each other via the same Coulomb interaction as in a vacuum, except that each charge Q must be replaced by an effective charge

$$Q_{\mathrm{eff}}=Q/\kappa^{\frac{1}{2}}, \tag{7.1}$$

where κ is the static dielectric constant. We have treated only those cases in which at least one of the charges is classical. The case where both are dynamical particles is complicated by problems of self-energies, adiabatic hypothesis, etc.,[15] and must await further elucidation. From what has been done here, however, there can be little doubt that a general proof of (7.1) must be possible.

ACKNOWLEDGMENTS

It is a pleasure to thank Professor K. A. Brueckner and Professor R. Jost for some stimulating conversations.

[14] We believe that (5.2) holds for any states in which the number of electron-hole pairs is sufficiently small compared to N.

[15] See, e.g., Schweber, Bethe, and de Hoffmann, *Mesons and Fields* (Row, Peterson and Company, Evanston, 1955) Vol. 1, Sec. 16 b.