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Simple Model of Electronic Correlation in Insulators

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To facilitate calculation of the effects of electron-electron interaction in insulators, a dielectric model is developed analogous to one used by Overhauser to discuss correlation in metals. In this model the dynamical many-electron problem is replaced by a field-theoretic problem in which an electron interacts with a "plasmon" field representing the valence-charge distribution. For small wave vector $\vec{q}$ the plasmon dispersion $\omega(\vec{q})$ approaches the bulk plasma frequency; at large $\vec{q}$, $\omega(\vec{q}) \to \hbar\vec{q}^2/2m$, corresponding to single-particle excitations. To determine the electron-plasmon coupling Poisson's equation and the sum rule on oscillator strength are employed. Calculated self-energies of an electron (or hole) due to correlation are large, typically $\frac{1}{3}$ Ry, though substantially reduced by recoil effects if the electron mass is small. Exchange effects lead to further reduction. The crucial importance of short-range (large-$\vec{q}$) dielectric behavior is emphasized.

I. INTRODUCTION

Recent papers have explored the importance of correlation effects on the electronic structure of insulating solids. It has become clear that these effects are large and should be taken into account when interpretations of optical spectra, etc., are attempted. For example, in the case of solid Ar correlation lowers the band gap by 2.5 eV, according to calculations by Lipari and Fowler.[1] This reduction yields an energy gap within 5% of experiment. The latter analysis was based on the "Coulomb-hole-plus-screened-exchange" (COHSEX) approximation introduced by Hedin[2] and used by Brinkman and Goodman[3] to discuss exchange and correlation in semiconductors. Omitting the energy dependence of dielectric screening and local-field corrections, the self-energy operator derived in Ref. 3 contains (i) core exchange, (ii) valence exchange [screened by $\epsilon(\vec{q}, 0)$, the static dielectric function], and (iii) the electrostatic self-energy of an infinitely massive point charge.

An earlier model of correlation effects, due to Toyozawa,[4] replaces the valence-charge distribution by a dispersionless exciton field, coupled to a test electron by a Fröhlich-type interaction representing the macroscopic polarization field. The electron-exciton coupling was chosen by the requirement that a test charge be screened by the static dielectric constant at large distances. No requirement was imposed on the short-range behavior. Haken and Schottky[5] used the Toyozawa model to write an effective electron-hole interaction including the effects of screening within intermediate-coupling theory. Electron and hole self-energies contained in this theory, when computed in a "static approximation," agree closely with the classical Mott-Littleton results, which predict band-gap reductions of several electron volts in large-gap insulators.[6]

A third approach based upon the detailed dielectric response of an insulator is proposed. In this model the valence-electron system is simulated by a single field, as in Ref. 4; however, the collective excitation resembles more closely a plasmon than an exciton. The dispersion $\omega(\vec{q})$ of this field is defined by the zeroes of the longitudinal dielectric function $\epsilon(\vec{q}, \omega)$. For small $\vec{q}$ these are plasmon-type modes, suitably modified by the crystal potential; for large $\vec{q}$ we have single-particle excitations, $\omega(\vec{q}) = \hbar\vec{q}^2/2m$. Moreover the electron-plasmon interaction $V_{\vec{q}}$ is more complicated than q^{-1} (Fröhlich interaction) and reflects (a) the detailed $\vec{q}$ dependence of the dielectric response and (b) the longitudinal sum rule[7] on oscillator strength. The model is analogous to that of Overhauser[8] who investigated electron correlation in metals. Here, as in Ref. 8, it is asserted that

the several important physical constraints underlying our model strengthen the reliability of conclusions derived from it. Section II begins with a derivation of the electron-plasmon interaction. The self-energy calculation, based on Penn's random-phase-approximation (RPA) dielectric function[9] for a model semiconductor, which appears to work well for insulators,[10] is outlined in Sec. III. Finally, a summary and discussion of the results is presented, for self-energies of electrons and holes in fcc alkali halides.

II. ELECTRON-PLASMON INTERACTION

Suppose that the longitudinal dielectric function for an insulator can be represented as

$$\epsilon(\vec{q},\omega) = 1 - \omega_p^2/(\omega^2 - \Delta_q^2) \quad , \tag{1}$$

where $\omega_p = (4\pi Ne^2/m)^{1/2}$ is the free-electron-gas plasma frequency for N electrons per unit volume; umklapp response (local-field corrections[11]) is not considered here, though it may be important in quantitative calculations. Collective excitations of the valence-charge system occur for frequency $\omega(\vec{q})$ and wave vector $\vec{q}$ which satisfy

$$\epsilon(\vec{q},\omega(\vec{q})) = 0$$

or

$$\omega^2(\vec{q}) = \omega_p^2 + \Delta_q^2 \quad . \tag{2}$$

The unknown function $\Delta_{\vec{q}}$ is determined from the requirement that Eq. (1) reduces to the "known" static dielectric function $\epsilon_{\vec{q}} \equiv \epsilon(\vec{q},0)$ as $\vec{q} \to 0$. Thus,

$$\Delta_q^2 = \omega_p^2/(\epsilon_{\vec{q}} - 1) \tag{3}$$

and

$$\omega^2(\vec{q}) = \omega_p^2 \epsilon_{\vec{q}}/(\epsilon_{\vec{q}} - 1) \quad . \tag{4}$$

For an insulator, $\epsilon_{\vec{q}}$ is real; then $\Delta_{\vec{q}}$ and the dispersion $\omega(\vec{q})$ are also real. To ensure that the Kramers-Kronig dispersion relations[12] are satisfied ω must be replaced in (1) by $\omega + i\delta^+$, where δ^+ is a positive infinitesimal. Then the imaginary part of Eq. (1) is, for $\omega > 0$,

$$\epsilon_2(\vec{q},\omega) = \tfrac{1}{2}\pi(\omega_p^2/\Delta_{\vec{q}})\,\delta(\omega - \Delta_{\vec{q}}) \quad , \tag{5}$$

which satisfies the sum rule[13]

$$\int_0^\infty d\omega\ \omega\epsilon_2(\vec{q},\omega) = \tfrac{1}{2}\pi\omega_p^2 \quad . \tag{6}$$

According to Eq. (5), the single-particle excitations of the model insulator have energy $\hbar\Delta_{\vec{q}}$. In particular, as $\vec{q} \to 0$ (the optical wavelength of a typical interband transition is much longer than a lattice parameter) the transverse and longitudinal dielectric functions are identical,[13] and absorption of light takes place in the discrete line

$$\omega = \Delta_0 = \omega_p/(\epsilon_0 - 1)^{1/2} \quad , \tag{7}$$

where ϵ_0 is the macroscopic dielectric constant $\epsilon(0,0)$. Thus Δ_0 may be identified as an average interband energy in the insulator. Further, from Eq. (2) as $\vec{q} \to 0$,

$$\Omega_p = \omega(0) = (\omega_p^2 + \Delta_0^2)^{1/2} = \omega_p[\epsilon_0/(\epsilon_0 - 1)]^{1/2} \tag{8}$$

is the long-wavelength bulk-plasmon frequency; the effect of the crystal potential on Ω_p is completely contained in Δ_0 in our model.[14] Note that while the exciton energy is always less than $\hbar\Delta_0$, the dispersion given by Eq. (2) is always greater than Δ_0, and greater than ω_p. Reference is made to modes for which $\epsilon(\vec{q},\omega) = 0$ as plasmons, following Ref. 8, though for large $\vec{q}$ compared with the Fermi wave vector it would be more accurate to speak of single-particle excitations of frequency $\omega(\vec{q}) = \hbar\vec{q}^2/2m$.

The electron-plasmon interaction is now derived; the discussion closely follows that of Ref. 8. We begin with Poisson's equation for wave vector $\vec{q}$,

$$-\vec{q}^{\,2}\phi_{\vec{q}} = -4\pi e^2\rho_{\vec{q}} \quad , \tag{9}$$

where $\rho_{\vec{q}}$ is the Fourier transform of the valence-electron density,

$$\rho_{\vec{q}} = \sum_{i=1}^{N} e^{-i\vec{q}\cdot\vec{r}_i} \quad , \tag{10}$$

and the corresponding electrostatic potential energy of an electron at $\vec{r}$ is

$$\phi_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} = (4\pi e^2/\vec{q}^{\,2})\rho_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} \quad . \tag{11}$$

Here and in the following discussion the volume of the crystal is set equal to unity. In the usual way[8,15] $\rho_{\vec{q}}$ is regarded as a field variable in a quantum theory, and is written in terms of creation and destruction operators $a_q^\dagger$ and $a_{\vec{q}}$ for the plasmon field as

$$\rho_{\vec{q}} = \gamma_{\vec{q}}(a_q^\dagger + a_{-\vec{q}}) \quad , \tag{12}$$

where the $\gamma_{\vec{q}}$ are real coefficients, to be determined Then the electron-plasmon interaction may be written

$$H_I = \textstyle\sum_{\vec{q}} V_{\vec{q}}(a_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} + a_q^\dagger e^{-i\vec{q}\cdot\vec{r}}) \quad , \qquad V_{\vec{q}} = (4\pi e^2/\vec{q}^{\,2})\gamma_{\vec{q}} \quad . \tag{13}$$

To determine $\gamma_{\vec{q}}$, and hence the electron-plasmon vertex $V_{\vec{q}}$, it is sufficient to invoke the sum rule[13]

$$\textstyle\sum_n E_{n0}\,|\langle n|\rho_{\vec{q}}|0\rangle|^2 = N\hbar^2\vec{q}^{\,2}/2m \quad , \tag{14}$$

where E_{n0} is the transition energy separating the ground state $|0\rangle$ of the valence electrons and the excited state $|n\rangle$. In the model developed here a single "plasmon" mode exhausts the sum rule for a given wave vector $\vec{q}$. That is, since the one-plasmon excited state $|n\rangle = |1_{\vec{q}}\rangle$ has the matrix element $\gamma_{\vec{q}}$ with the ground state, and all other matrix elements vanish, Eq. (14) is simply

$$\hbar\omega_{\vec{q}}\,\gamma_q^2 = N\hbar^2\vec{q}^{\,2}/2m \quad . \tag{15}$$

Thus, in Eq. (13),

$$V_{\vec{q}} = \left(\frac{2\pi e^2 \hbar \omega_p^2}{\vec{q}^2 \omega_{\vec{q}}}\right)^{1/2} = \left(\frac{2\pi e^2}{\vec{q}^2}\hbar\omega_p\right)^{1/2}\left(1-\frac{1}{\epsilon_{\vec{q}}}\right)^{1/4}, \tag{16}$$

which depends only upon the valence-electron density and the static dielectric function.

Note that $V_{\vec{q}}$, derived from Poisson's equation, contains only the electrostatic interaction due to $\rho_{\vec{q}}$; this is appropriate if the electron is a test charge. However, for real electrons we must add an exchange and correlation potential. If the latter is local and proportional to the density[16] it may be written

$$U_{\vec{q}} = -f_{\vec{q}}\rho_{\vec{q}} = -(4\pi e^2/\vec{q}^2)^{-1} f_{\vec{q}} V_{\vec{q}} \tag{17}$$

and the electron-plasmon vertex is replaced by

$$V_q' = V_{\vec{q}} + U_{\vec{q}} = (1-F_{\vec{q}})V_{\vec{q}}\ , \qquad F_{\vec{q}} = (4\pi e^2/\vec{q}^2)^{-1} f_{\vec{q}}\ . \tag{18}$$

Since the effect of exchange and correlation is to lower Coulomb interaction energies, $F_{\vec{q}} > 0$. For example, the Kohn-Sham potential, equal to two-thirds of the oscillatory component of the Slater exchange, leads to

$$F_{\vec{q}} = (e^2 k_F/3\pi N)(4\pi e^2/\vec{q}^2)^{-1} = (\vec{q}/2k_F)^2\ , \tag{19}$$

where $k_F = (3\pi^2 N)^{1/3}$. This relation is not expected to be valid for $\vec{q}$ near k_F.

Since evaluation of electron and hole self-energies below involves consideration of large wave vectors we adopt an approach due to Hubbard, [17] who noted that at large momentum transfers exchange contributions to a given diagram (for the self-energy, say) cancel one-half the direct contributions. In other words, the dominant effect at large $\vec{q}$ is the interaction of antiparallel spins, in consequence of the Pauli principle. Thus Eq. (18) is replaced by[18]

$$(V_{\vec{q}}')^2 = (1-G_{\vec{q}})V_{\vec{q}}^2\ , \tag{20}$$

where $G_{\vec{q}} = \frac{1}{2}\vec{q}^2/(\vec{q}^2 + k_s^2 + k_F^2)$ and $k_s = (2/\pi)k_F$. As $\vec{q}\to 0$, $V_{\vec{q}}' \to V_{\vec{q}}$, while for large $\vec{q}/k_F$, $(V_{\vec{q}}')^2 \to \frac{1}{2}V_{\vec{q}}^2$, as desired. Note that for small $\vec{q}$, Eq. (20) is equivalent to Eq. (18), if we make the identification

$$F_{\vec{q}} = \tfrac{1}{2}G_{\vec{q}} \to [1+(2/\pi)^2]^{-1}(\vec{q}/2k_F)^2\ , \tag{21}$$

which closely approximates Eq. (19).

III. SELF-ENERGY

Consider an electron (or hole) in a parabolic band (extended-zone scheme) with effective mass m^*, interacting with the valence electrons according to Eq. (13). Although this model problem omits the nonparabolic character of real energy bands, it is sufficient to demonstrate the usefulness of the model electron-plasmon interaction in correlating important physical quantities and dielectric behavior. In future work I hope to apply Eq. (13) to other problems in insulators, including collective effects in optical spectra, and the screened electron-hole interaction. Here it is shown that presently accepted theories (RPA) of dielectric response lead to large reductions of the one-electron energy gap, of the order of $\frac{1}{2}$ Ry in fcc alkali halides. The conclusion that band gaps are substantially reduced by polarization effects has already been stated in the literature, [1,3,6] although past estimates for insulators[6] have relied upon classical calculations and a somewhat arbitrary cutoff in momentum space; an exception is found in Ref. 1, for Ar. In the approach used here no cutoff is introduced except that arising naturally out of the specific dielectric response of the solid, and the importance of electronic recoil is demonstrated explicitly.

From second-order perturbation theory the self-energy of an electron of mass m^* and wave vector $\vec{k}$, interacting with the plasmon field according to Eqs. (13) and (20), is given by

$$\Sigma = \sum_{\vec{q}} \frac{-V_{\vec{q}}^2(1-G_{\vec{q}})}{\hbar\omega_{\vec{q}} + \hbar^2\vec{q}^2/2m^* - \hbar^2\vec{k}\cdot\vec{q}/m^*}\ . \tag{22}$$

As in effective-mass theory[19] it is assumed that the wave function $\Psi_{\vec{k}} = e^{i\vec{k}\cdot\vec{r}}\Psi_0$. Note that Eq. (22) differs from Eq. (40) of Ref. 8 for the correlation energy in metals. A second term is present in the latter, corresponding to "vacuum-fluctuation" processes blocked by the Pauli principle.[20] For *intraband* scattering this term is absent in insulators, since the relevant band is either full or empty. *Interband* scattering is ignored in this model, a universal practice in polaron-type theories. Indeed, within effective-mass theory, interband matrix elements of the density operator $e^{i\vec{q}\cdot\vec{r}}$ are zero because of the orthogonality of different Bloch functions at $\vec{k}=0$; the intraband matrix element is unity.

Several applications of this equation suggest themselves, including (i) band-gap renormalization ($\vec{k}=0$) and (ii) the renormalization of the band mass m^*; the latter effect, much less important than electron-phonon mass enhancement, will not be considered here. To establish the energy scale we may omit the recoil terms in Eq. (22). This gives the self-energy of an infinitely massive charge,

$$\Sigma(\infty) = -\textstyle\sum_{\vec{q}}(2\pi e^2/\vec{q}^2)(1-1/\epsilon_{\vec{q}})(1-G_{\vec{q}})\ . \tag{23}$$

The factor $(1-G_{\vec{q}})$, from Eq. (20), contains the exchange effect. Now it is clear that in RPA $\epsilon_q \to 1$ for large $q \sim \kappa = \pi/r_0$, where r_0 is the radius of the appropriate valence shell.[10] Converting the summation to an integral, we have $|\Sigma(\infty)| \sim e^2\kappa/\pi$

$\approx e^2 k_F/\pi$ for alkali halides. The electron-plasmon coupling constant is defined as the ratio of this energy to the free-electron plasmon energy

$$\alpha = e^2 k_F/\pi\hbar\omega_p = 0.17 r_s \quad , \tag{24}$$

where $r_s = (0.521 k_F a_0)^{-1}$ is the average interelectronic spacing in units of the Bohr radius a_0; r_s is about 2 in alkali halides. Thus α is about $\frac{1}{3}$ and $|\Sigma(\infty)|$ is about 5 eV. Some important parameters for fcc alkali halides are given in Table I.

To compute Eq. (22) quantitatively we must specify $\epsilon_{\vec{q}}$; then $\omega(\vec{q})$ follows from Eq. (4). It has been amply demonstrated that Penn's dielectric function for an isotropic two-band semiconductor is a good approximation to the RPA dielectric function of an insulator.[10] An interpolation formula suggested by Penn is

$$\epsilon_{\vec{q}} = 1 + \omega_p^2 (\Delta_0 + \hbar\vec{q}^2/2m)^{-2} \quad , \tag{25}$$

where $\Delta_0 = E_g/F^{1/2}$ and $F \approx 1$.[9] The energy gap is denoted by E_g, and Δ_0 is the average interband energy defined in Eq. (16). Equation (25) has two important limits:

$$\begin{aligned} &\epsilon(\vec{q}=0) = 1 + (\omega_p/\Delta_0)^2 \quad , \\ &\epsilon(\vec{q}\to\infty) \to 1 + (2m\omega_p/\hbar\vec{q}^2)^2 \quad . \end{aligned} \tag{26}$$

In these limits the plasmon dispersion is

$$\begin{aligned} &\omega(\vec{q}=0) = (\omega_p^2 + \Delta_0^2)^{1/2} = \Omega_p \quad , \\ &\omega(\vec{q}\to\infty) \to \hbar\vec{q}^2/2m \quad . \end{aligned} \tag{27}$$

Thus Penn's model yields the bulk-plasma frequency at long wavelengths and gives the correct single-particle excitation energy $\hbar^2\vec{q}^2/2m$ at large $\vec{q}$ compared with $(2m\Delta_0/\hbar)^{1/2}$. It appears that Eq. (25) is the simplest interpolation formula which yields the correct dielectric response in both limits. However, it is necessary to modify $\epsilon(\vec{q})$ in the region $|\vec{q}/k_F| \sim 1$ to include the effects of exchange not contained in RPA. Again following Hubbard[17] we replace Penn's $\epsilon_{\vec{q}}$ by[18]

$$\epsilon_{\vec{q}} = 1 + (1 - G_{\vec{q}})\omega_p^2 (\Delta_0 + \hbar\vec{q}^2/2m)^{-2} \quad . \tag{28}$$

Now

$$\epsilon(\vec{q}\to\infty) \to 1 + \tfrac{1}{2}(2m\omega_p/\hbar\vec{q}^2)^2$$

and $\omega(\vec{q}\to\infty)$ is too large by a factor of $\sqrt{2}$. Nonetheless, Eq. (28) is regarded as superior to Eq. (25) for self-energy calculations since the region $|\vec{q}| \gg (2m\Delta_0/\hbar)^{1/2}$ makes an insignificant contribution to Eq. (22). The preference is slight, however, since $G_{\vec{q}}$ is only about 0.20 even at $|\vec{q}| = \kappa$. As a result, the exchange corrections contained in Eqs. (20) and (28) modify (reduce) calculated self-energies by at most 20% and are not included below in the numerical work, which is intended primarily to demonstrate the scale of self-energies implied by Penn's model.

Before presenting the results the close connection of the simple model developed here and the orthogonalized-plane-wave formulation due to Brinkman and Goodman[3] should be pointed out. The latter authors include exchange and correlation within the random-phase approximation for the self-energy operator.[2] Omitting the energy dependence and nondiagonal terms (local-field corrections[11]) in the dielectric response, they derive the self-energy operator

$$\begin{aligned} M(\vec{k}, \vec{k}+\vec{K}) = {} & V^c_{ex}(\vec{k}, \vec{k}+\vec{K}) + V^v_{ex,s}(\vec{k}, \vec{k}+\vec{K}) \\ & + E_{CH}(\delta_{0\vec{K}} - \langle\vec{k}|P_c|\vec{k}+\vec{K}\rangle) \quad , \end{aligned} \tag{29}$$

where $|\vec{k}\rangle$ and $|\vec{k}+\vec{K}\rangle$ are plane-wave states and the first two terms are the core-exchange and the valence-exchange operators; the latter is screened by the static dielectric function. The core projection operator P_c ensures that the valence and conduction states are orthogonal to the core states, $\vec{K}$ is a reciprocal-lattice vector, and

$$E_{CH} = -\sum_{\vec{q}} (2\pi e^2/\vec{q}^2)(1 - 1/\epsilon_{\vec{q}}) \tag{30}$$

is the "Coulomb-hole" energy. This agrees with Eq. (23), the self-energy of an infinitely massive charge, except that the exchange correction $(1 - G_{\vec{q}})$ is missing. Note also that in the approach of the present paper it would not be appropriate to screen the valence exchange, since plasmon-fluctuation effects are assumed to reside wholly in Eq. (22). To compute an energy gap in this scheme one would (a) solve the one-electron Hartree-Fock problem and (b) calculate the self-energy, Eq. (22), for the electron and hole. Thus, while Eq. (29) is derived from the "Coulomb-hole-plus-screened-exchange" (COHSEX) approximation due

TABLE I. Important parameters for fcc alkali halides. The self-energy of an infinitely massive point charge is of order $\alpha\hbar\omega_p$ in RPA.

	r_s (a.u.)	$\hbar\omega_p$ (Ry)	ϵ_0	α	$\alpha\hbar\omega_p$ (Ry)
LiF	1.63	1.66	1.92	0.28	0.46
NaF	1.87	1.37	1.74	0.32	0.44
KF	2.17	1.09	1.85	0.37	0.40
RbF	2.30	0.99	1.93	0.39	0.39
LiCl	2.08	1.16	2.75	0.35	0.41
NaCl	2.28	1.01	2.25	0.39	0.39
KCl	2.56	0.84	2.13	0.44	0.37
RbCl	2.67	0.78	2.19	0.45	0.35
LiBr	2.24	1.03	3.16	0.38	0.39
NaBr	2.43	0.90	2.62	0.41	0.37
KBr	2.69	0.79	2.33	0.46	0.36
RbBr	2.80	0.73	2.33	0.48	0.35
LiI	2.43	0.90	3.80	0.41	0.37
NaI	2.62	0.81	2.91	0.45	0.36
KI	2.86	0.70	2.69	0.49	0.34
RbI	2.97	0.67	2.63	0.50	0.33

to Hedin,[2] in the theory given here all the dynamical interaction effects reside in the correlation energy, Eq. (22); reference is made here to the latter approach as the "exchange and correlation model" (ECM). COHSEX and ECM differ chiefly in the way exchange and correlation is divided among the various terms representing the quasiparticle energy. It has already been demonstrated by Overhauser, in the case of simple metals,[8] that COHSEX and ECM are equivalent within second-order perturbation theory. In practice it is probably simpler to employ the ECM, since band calculations based on some form of unscreened exchange have already been carried out for a wide class of insulators. Note also that electronic-recoil effects are not included in Eq. (30), which was obtained by neglecting the energy dependence of $\epsilon(\vec{q}, \omega)$.

Here it may be assumed that band gaps including the effect of unscreened exchange are known and the correlation energy from Eq. (22) can be computed, omitting the factor $(1 - G_{\vec{q}})$ which is near unity. The dimensionless parameters

$$\delta = \Delta_0/\omega_p = (\epsilon_0 - 1)^{-1/2}, \quad \eta = m/m^* \tag{31}$$

are introduced, where m is the free-electron mass. From Eqs. (22) and (25) for $\vec{k} = 0$ the result is

$$-\Sigma = (2/\pi)\omega_p^{1/2} I(\delta, \eta) \ , \tag{32}$$

$$I(\delta, \eta) = \int_0^\infty dx[1 + (\delta + x^2)^2]^{-1/2}\{[1 + (\delta + x^2)^2]^{1/2} + x^2\eta\}^{-1}$$

in atomic units, where $x^2 = \hbar\vec{q}^2/2m\omega_p$. To show the dependence of the self-energy on ϵ_0 and m^* $I(\delta, \eta)$ was computed; the results are given in Fig. 1. Note that the self-energy increases with ϵ_0 but decreases with η. Thus, as expected, electronic recoil sharply reduces $|\Sigma|$. The case $\eta = 0$ ($m^* = \infty$) is appropriate to a heavy hole, while $\eta = 3$ ($m^* = \frac{1}{3}m$) describes a typical conduction-band electron. Table II contains the results for the self-energy. To obtain the band-gap reduction in this model, one adds the electron and hole contributions together. Thus, the Penn-model dielectric function leads to renormalizations of about $\frac{1}{2}$ Ry in fcc alkali halides. This is of the order of the energy gap itself, which suggests that the RPA seriously overestimates dielectric response at large $\vec{q}$ (at small $\vec{q}$ the Penn model yields the known ϵ_0). In addition it may be necessary to include nondiagonal response, a difficult proposition.

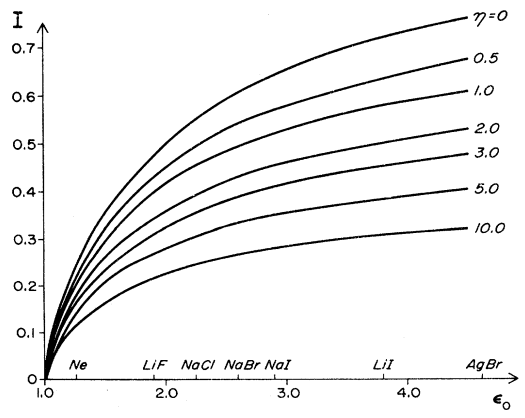

FIG. 1. Phase-space integral $I(\delta, \eta)$ defined by Eq. (32); aside from the factor $-2\omega_p^{1/2}/\pi$ this is the self-energy of an electron with effective mass $m^* = \eta^{-1}m$. The average interband energy is $\hbar\Delta_0 = \delta\hbar\omega_p$, and $\delta = (\epsilon_0 - 1)^{-1/2}$.

TABLE II. RPA self-energies, in rydbergs, of an electron ($m^* = \frac{1}{3}m$) and a hole ($m^* = \infty$) in fcc alkali halides. The energy gap at $\vec{k} = 0$ is renormalized by the energy $\delta E_g = \Sigma_{\text{hole}} + \Sigma_{\text{electron}} < 0$.

	ϵ_0	$\lvert\Sigma_{\text{hole}}\rvert$	$\lvert\Sigma_{\text{electron}}\rvert$	$\lvert\delta E_g\rvert$
LiF	1.92	0.39	0.25	0.64
NaF	1.74	0.32	0.21	0.53
KF	1.85	0.31	0.20	0.51
RbF	1.93	0.30	0.20	0.50
LiCl	2.75	0.43	0.27	0.70
NaCl	2.25	0.35	0.22	0.57
KCl	2.13	0.31	0.20	0.51
RbCl	2.19	0.30	0.19	0.49
LiBr	3.16	0.43	0.27	0.70
NaBr	2.62	0.37	0.23	0.60
KBr	2.33	0.32	0.20	0.52
RbBr	2.33	0.31	0.20	0.51
LiI	3.80	0.44	0.27	0.71
NaI	2.91	0.37	0.23	0.60
KI	2.69	0.33	0.21	0.54
RbI	2.63	0.32	0.20	0.52

IV. SUMMARY AND DISCUSSION

A simple model of electronic correlation in insulators has been developed which requires as input the static dielectric function $\epsilon_{\vec{q}}$. The dimensionless parameters in the theory are r_s, δ, and η; however, the crucial parameter is κ, the scale of dielectric dispersion in $\vec{q}$ space. Indeed, the self-energy of an infinitely massive point charge is of order $e^2\kappa$. Thus, it is of major importance to extend present (RPA) theories of dielectric response to include exchange effects[17] and, especially, short-range correlations. The RPA leads to $\kappa \sim \pi/r_0$, where r_0 is the appropriate valence-shell radius, and resulting self-energies are about $\frac{1}{3}$ Ry. It is emphasized that previous estimates[6] of band-gap renormalization in insulators relied on a poorly justified cutoff $\kappa = \pi/a$, where $2a$ is the lattice parameter. The electronic-polaron theory,[14] though adequately handling long-range correlation effects, is not suited to the calculation of self-en-

ergies, which involve large $\vec{q}$. Indeed, there is no explicit cutoff in the theory and if the "exciton" is dispersionless the self-energy diverges. It is obvious that a cutoff of order π/a must be introduced; however, a microscopic calculation is required to determine its precise value. In particular if we choose $\kappa = \pi/r_0$, the self-energies in Ref. 6 are enhanced by the factor $a/r_0 \approx 3$. This demonstrates the necessity of incorporating the correct dielectric behavior in the calculation. The results given in Table II, are accurate insofar as the Penn dielectric function properly treats short-range dielectric response; however, the RPA is usually considered deficient in this respect. The exchange correction introduced in Eq. (28) is an attempt to improve $\epsilon_{\vec{q}}$; this leads to a reduction of the self-energy of about 20% for the case $m^* = \infty$, and 10% if $m^* = 0.3m$ [recoil diminishes the weight of high-$\vec{q}$ contributions in Eq. (22)].

In rare-gas solids it appears that the Penn model, like a dielectric function developed by the present author,[21] overestimates the RPA response in the large-$\vec{q}$ region.[1,10] In this case the characteristic cutoff $(2m\Delta_0/\hbar)^{1/2} \equiv \kappa_p$ in these models is too large, and computed self-energies in Ar are also too large. The basic flaw in the two-band models seems to be the absence of orthogonalization terms, which cut off the response at $\kappa \approx \pi/r_0 < \kappa_p$ for rare-gas crystals. In case of fcc alkali halides $\kappa_p \approx \pi/r_0$ and the orthogonality corrections are much less important. However, short-range correlation not contained in RPA is probably crucial. Quantitative calculations of the self-energy of an electron or hole in an insulator must await the development of a better dielectric function. In the meantime it is possible to correlate dielectric behavior and various electronic properties of insulating solids, using the model electron-plasmon interaction developed in this paper.

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