# Effective Electron-Hole Interactions in Polar Semiconductors

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We study the problem of an electron and a hole interacting with each other and with longitudinal optical phonons. Our method consists of examining the poles of the $t$ matrix for dressed-particle–hole scattering due to the Coulomb interaction and the exchange of phonons. This approach is carried out in the two limits: (i) $E_B \ll \omega_0$ and (ii) $E_B \gg \omega_0$, where $E_B$ is the binding energy of the exciton state formed and $\omega_0$ is the optical phonon energy. In both cases, we have an effective-mass equation for the electron-hole pair with the same form of nonlocal potential: however, in case (i) the self-energies occurring are polaron self-energies, while in case (ii) the self-energies are eliminated. We find that the first corrections in both limits are more important for the self-energy than for the interaction potential. We make the ansatz that this is true for arbitrary values of $E_B/\omega_0$ so that the potential is left unaltered, but the self-energy scales with the parameter $E_B/\omega_0$. The calculated binding energies obtained from this procedure are in excellent agreement with the measured binding energy of excitons in a variety of ionic semiconductors. The effective nonlocal potential we obtain satisfies the physical requirements of going asymptotically to $(\epsilon_0 r)^{-1}$, where $\epsilon_0$ is the static dielectric constant, for $r \gg$ polaron radius and $E_B/\omega_0 \ll 1$, and to $(\epsilon_\infty r)^{-1}$, where $\epsilon_\infty$ is the high-frequency dielectric constant for $r \ll$ polaron radius, and $E_B/\omega_0 \gg 1$. The first corrections go as $r^{-2}$. We discuss in detail the form of the potential and its nonlocality, etc., as the parameters $E_B/\omega_0$, $\epsilon_\infty/\epsilon_0$, and $m_e/m_h$ (ratio of electron mass to hole mass) vary. We define $E_B'$ as the energy to separate to infinity the electron and the hole without altering the self-energy they have in the bound state. For appreciable electron-phonon coupling strength, $E_B'$ and $E_B$ differ considerably. The exciton radius and the oscillator strength is to be estimated from $E_B'$. For TlCl, the actual exciton radius is estimated to be about three times smaller than one might estimate from $E_B$.

## I. INTRODUCTION

In the 1950's the problem of an electron (or a hole) interacting with longitudinal optical phonons (the polaron problem) received considerable attention.[1] Here was a problem which was the prototype of the general problem of particle-field interactions, and one in which the theoretical predictions could be tested against a body of experimental results in semiconductors. In this work[2] we explore the problem of an electron and a hole interacting with each other and with longitudinal optical (LO) phonons as the prototype of the problem of two particles interacting with a field. Again the problem is made worthwhile by the availability of experimental results on electron-hole bound states (the excitons) in semiconductors.

We confine our attention to the case in which the exciton state has a binding energy $E_B$ that is small compared to the insulating gap $\Delta$ (the Wannier exciton limit). The interaction between the electron or the hole and the LO phonons is represented by the Fröhlich Hamiltonian:

$$H = \sum_{\vec{q}} \gamma_q^{e,h}\, e^{\pm i\vec{q}\cdot\vec{r}_{e,h}}\, a_{\vec{q}} + \text{c. c.}\ , \tag{1.1}$$

where $a_{\vec{q}}$ is the annihilation operator for a phonon of wave vector $\vec{q}$, and $\vec{r}_{e,h}$ are the electron or the hole coordinates, the plus sign in the exponent is associated with $\vec{r}_e$ and the minus sign with $\vec{r}_h$,

$$\gamma_q^{e,h} = (-i\hbar\omega_0/q)\,(4\pi\alpha_{e,h}/\kappa_{e,h}\,V)^{1/2}\ , \tag{1.2}$$

where $\omega_0$ is the LO phonon frequency assumed to be dispersionless, $V$ is the volume of the unit cell, $\alpha_{e,h}$ is the polaron coupling constant

$$\alpha_{e,h} = \tfrac{1}{2}(\epsilon_\infty^{-1} - \epsilon_0^{-1})\, e^2 \kappa_{e,h}/\hbar\omega_0\ , \tag{1.3}$$

and $\kappa_{e,h}$ is the inverse of the polaron radius

$$\kappa_{e,h} = (2m_{e,h}\omega_0/\hbar)^{1/2} = (r^*_{e,h})^{-1}\ . \tag{1.4}$$

In (1.3) $\epsilon_\infty$ and $\epsilon_0$ are the high-frequency and the static dielectric constants, respectively.

### A. Physical Discussion

Let us start by considering an electron and a hole an infinite distance apart. Owing to their interaction with the LO phonons, one has two quasiparticles—the electron polaron and the hole polaron. The polaron is characterized by a self-energy, whose momentum-dependent part is approximately described by an altered mass $m^*_{e,h}$ which

can be related to the bare mass $m_{e,h}$. For example,[3] in the weak and intermediate coupling regime, $\alpha_{e,h} \lesssim 6$,

$$m^*_{e,h} = m_{e,h}(1 + \tfrac{1}{6}\alpha_{e,h}) , \tag{1.5}$$

the momentum-independent part of the self-energy $\sigma_{e,h}$ is given for intermediate coupling by

$$\sigma_{e,h} = -\alpha_{e,h}\hbar\omega_0 . \tag{1.6}$$

The self-energy and the change in the effective mass come about due to the polarization of the lattice. A typical distance over which the lattice is polarized around the electron or the hole defines the polaron radius.

For distances between the electron and the hole large compared to the polaron radii, one expects them to interact due to the Coulomb interaction screened both by the lattice (since their relative angular frequency would in this case be much less than $\omega_0$) and the other electrons, and also to have their self-energies intact. As the distance between the electron and the hole is decreased, their polarization clouds begin to interfere and partially neutralize each other. In field-theory language the virtual phonons emitted by the particle are absorbed by the hole and *vice versa*. The net effect would be to alter the interaction between the electron and the hole, and somewhat loosely speaking, $\sigma_{e,h}$ and $m^*_{e,h}$ are reduced from their free-polaron values. This effect should increase as some function of the ratio of the polaron radii to the distance between the electron and the hole. Finally, when this ratio becomes extremely small, the relative angular frequency of the electron and the hole becomes large compared to $\omega_0$, and, therefore, the pair is not influenced at all by the lattice, i.e., they interact with the Coulomb interaction screened only by the electrons, their effective masses are just the bare masses, and $\sigma_{e,h}$ is completely eliminated.

We have been discussing the problem above as if the distance between the electron and the hole was an independent parameter. Actually, the distribution of this distance is determined by the eigenvalue problem which incorporates the ideas discussed above. Yet another feature of the problem is that since the lattice polarization cannot respond instantaneously, the interaction between the electron and the hole will, in general, be nonlocal in space and in time. We can also guess on physical grounds that in the limit $E_B/\omega_0 \ll 1$ or more precisely $r_{ex}/r^*_{e,h} \gg 1$, where $r_{ex}$ is the exciton radius, the nonlocality is important; in other words, the nonlocality will scale in the same fashion as the self-energies.

The problem is further complicated by the fact that $r^*_e/r^*_h$ or $m_e/m_h$ is also an important parameter. But $r_{ex}$ (or $E_B$) depends parametrically on $m_e/m_h$, since the potential depends upon this parameter. In the text we shall discuss in detail the dependence of the potential on $m_e/m_h$.

### B. Experimental Consequences

From the discussion presented above, we may deduce the experimentally measurable effects of the interaction of the electron and the hole with the LO phonons: (a) The binding energy of the exciton is quite different from that obtained from a Coulomb potential screened either by the static or the optical (high-frequency) dielectric constants, and the distribution of the eigenvalues is nonhydrogenic. (b) There are centrifugal terms in the potential due to the polarization of the lattice. These lead to a splitting, say between the $2s$ and $2p$ states of the exciton, i.e., we have a Lamb shift. (c) Since there is effectively a change in the self-energy of the electron and the hole when they bind, the actual characteristic distance between the electron and the hole is different from that deduced from the experimentally measured binding energy $E_B$, which is the energy released on dissociation into two free polarons. This in turn implies that the actual oscillator strength of the exciton is different from that deduced from the experimentally measured binding energy. (d) Another way of stating the above argument is that the minimum in the energy for the free-polaron states and the exciton states is displaced with respect to each other in a lattice configuration coordinate diagram. The above statement is meant to be only illustrative. Strictly speaking, a configuration coordinate diagram is meaningful only if the adiabatic approximation is valid, i.e., when $E_B \gg \omega_0$, or $\omega_0 \ll E_B$. Nevertheless, we may draw some qualitative conclusions from this argument. If the linewidth of the exciton is much smaller than the optical phonon frequency, we have a Franck-Condon effect, i.e., the emission frequency of the excitons is in general different from the absorption frequency, and the thermal recombination energy is different from the optical recombination energy. The magnitude of all these effects depends upon the two parameters characterizing the problem ($r^*_e$, $r^*_h$) and $r_{ex}$.

There are some other effects due to the optical phonons, which we do not consider here. For example, if the hole is derived from a degenerate valence band, one expects[4] a Jahn-Teller splitting of the exciton, which may be either static or dynamic. Another effect[5] is the resonant interaction between an excited state of the exciton and a state consisting of the ground state of the exciton plus a phonon.

### C. Analytical Procedure

Our method consists in examining the poles of the $t$ matrix for dressed-particle–hole scattering

due to Coulomb interactions and due to the exchange of the phonons. The position of the poles gives the binding energy, and the exciton wave function is obtained from the residue. This method has been outlined by Nozières, [6] and has been employed by Sham and Rice[7] to rigorously derive the effective mass equation for Wannier excitons, and by Sham[8] in the problem of impurity states in semiconductors. We find that this approach can be carried on rigorously only in the two limits (i) $E_B \ll \omega_0$ (or $r_{ex} \gg r_e^*, r_h^*$), and (ii) $E_B \gg \omega_0$ (or $r_{ex} \ll r_e^*, r_h^*$). In both cases we obtain a Schrödinger equation with the *same form of nonlocal potential*; however, in case (i) the masses occurring in the kinetic energy and the effective potential are polaron masses, while in case (ii) they are all bare masses. Further in case (i) the $\sigma_{e,h}$ are completely retained in the Schrödinger equation while in case (ii) they are completely eliminated.

Next we look at the first correction terms to the effective potential and the self-energy in both the limits (i) and (ii) by expanding with respect to the small parameter in each case. We find that in both limits the correction to the effective potential is an order smaller than to the self-energy. We then make the ansatz that the potential remains unchanged for all values of $E_B/\omega_0$, and that the self-energy scales with this parameter and goes appropriately to the two limits and the first corrections. We have no firm theoretical justification for this procedure. However, we find that the binding energies for excitons obtained through such a procedure agree remarkably well with the experimental results. In the two limiting cases mentioned, it is possible to handle the vertex corrections to the particle-hole interactions exactly. In the intermediate case we have found no way of dealing with them properly. Our ansatz amounts to saying that the vertex corrections affect only the self-energy and not the potential. The success of our ansatz poses the theoretical question as to why such a simplification works.

The problem of the interaction between the electron and the hole with the LO phonons has been attempted before, by Haken and Schottky[9] using a variational method, which seems to be valid only for $E_B \ll \omega_0$. The binding energies obtained using Haken and Schottky's potential are in poor agreement with the experimental results.

## II. MANY-BODY DESCRIPTION OF EXCITON STATES

The many-body formalism for treating an exciton state as an excited state of the insulator has been outlined by Nozières.[6] In this section we first present this formalism in its full generality and illustrate its use by considering the simple problem of an electron and a hole interacting through an unscreened Coulomb potential.

The formalism consists in examining the poles of the $t$ matrix for particle-hole scattering. Corresponding to these poles, there are poles in the two-particle Green's function (other than those associated with the particle-hole continuum). The energy of the bound states is given by the isolated poles of the two-particle Green's function, and the corresponding wave functions are obtained from the residue at the pole.

The $t$ matrix satisfies the Bethe-Salpeter (BS) equation (Fig. 1):

$$t(k_1k_2k_3k_4) = I(k_1k_2k_3k_4) + \sum_{k_5,k_6} I(k_5k_2k_3k_6) \times G(k_5)\, G(k_6)\, t(k_1k_6k_5k_4)\,, \qquad (2.1)$$

where $k \equiv (\vec{k}, \zeta)$ is the momentum-energy four vector, $I$ is the irreducible particle-hole interaction,[10] and $G(k)$ is the single-particle Green's function. The irreducible particle-hole interaction conserves energy and momentum; thus we have

$$-k_1 + k_4 = -k_3 + k_2 = -k_5 + k_6 \equiv q\,. \qquad (2.2)$$

Equation (2.2) defines $q \equiv (\vec{Q}, \omega)$ as the total energy momentum carried by the electron-hole pair. We may reduce the number of variables by introducing

$$k = k_2 - \tfrac{1}{2}q\,, \quad k' = k_4 - \tfrac{1}{2}q\,, \quad k'' = k_6 - \tfrac{1}{2}q\,,$$

and we have

$$I(k_1k_2k_3k_4) = I(k, k'; q)\, \delta(k_1 + k_2 - k_3 - k_4)\,.$$

Similarly, we have

$$t(k_1k_2k_3k_4) = t(k, k'; q)\, \delta(k_1 + k_2 - k_3 - k_4)\,.$$

The BS equation then takes the form

$$t(k, k'; q) = I(k, k'; q) + \sum_{k''} I(k, k''; q)\, G(k'' - \tfrac{1}{2}q) \times G(k'' + \tfrac{1}{2}q)\, t(k'', k'; q)\,. \qquad (2.3)$$

Since $I(k, k'; q)$ is well behaved as a function of $\omega$, it may be neglected near the poles of $t(k, k'; q)$. In principle then, given the single-particle Green's function and the irreducible particle-hole interaction, the problem reduces to seeking the poles of $t(k, k'; q)$ as a function of $\omega$ through the solution of the homogeneous equation

$$t(k, k'; q) = \sum_{k''} I(k, k'', q)\, G(k'' - \tfrac{1}{2}q) \times G(k'' + \tfrac{1}{2}q)\, t(k'', k'; q)\,. \qquad (2.4)$$

Since $k'$ and $q$ are fixed parameters (they specify the energy momentum of the initial state), we may use

$$t(k, k'; q) \to T(k)$$

for brevity.

It is easy to specify the single-particle Green's

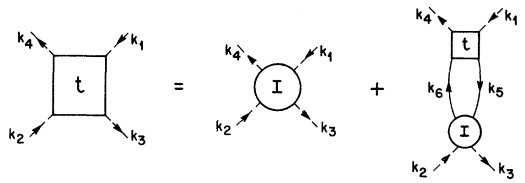


FIG. 1. Bethe-Salpeter equation for the electron-hole $t$ matrix. The external electron and hole lines (dotted lines) are not included in $t$.

function for an insulator, neglecting electron-electron and electron-phonon interactions. Let us for simplicity take a plane wave representation; the generalization to Bloch waves is straightforward. Let us also consider the simple case of a single valence band with maximum at $\vec{k}=0$ and a single conduction band with a minimum, also at $\vec{k}=0$. Then we have

$$G_{e,h}(\vec{k},\zeta)=[\zeta-E_{e,h}(\vec{k})\pm i\delta]^{-1}, \tag{2.5}$$

with

$$E_e(\vec{k})=\Delta+k^2/2m_e$$

and

$$E_h(\vec{k})=-k^2/2m_h, \tag{2.6}$$

where $\Delta$ is the energy of the insulating gap.

To continue with our simple example, if we consider an unscreened Coulomb interaction between the electron and the hole,

$$I(\vec{k},\vec{k}';\vec{q})=-4\pi e^2/|\vec{k}-\vec{k}'|^2,$$

we can perform the energy integration[11] on the right-hand side of (2.4) to get

$$T(k)=\sum_{\vec{k}''}\frac{4\pi e^2}{|\vec{k}-\vec{k}''|^2}\times\left(\Delta+\frac{(\vec{k}''+\frac{1}{2}\vec{Q})^2}{2m_e}+\frac{(\vec{k}''-\frac{1}{2}\vec{Q})^2}{2m_h}-\omega\right)^{-1}T(k''). \tag{2.7}$$

In (2.7) we have neglected a term of $O((\Delta-\omega)/\Delta)$ compared to unity. Since the binding energy $E_B$ is defined as

$$E_B=\Delta-\omega, \tag{2.8}$$

this corresponds to considering Wannier excitons only.

We may write

$$\left(\Delta+\frac{(\vec{k}+\frac{1}{2}\vec{Q})^2}{2m_e}+\frac{(\vec{k}-\frac{1}{2}\vec{Q})^2}{2m_h}-\omega\right)^{-1}T(\vec{k})\equiv\varphi(\vec{k});$$

we can then rewrite Eq. (2.7) as

$$\left(E_B+\frac{(\vec{k}+\frac{1}{2}\vec{Q})^2}{2m_e}+\frac{(\vec{k}-\frac{1}{2}\vec{Q})^2}{2m_h}\right)\varphi(\vec{k})=\sum_{\vec{k}'}\frac{4\pi e^2}{|\vec{k}-\vec{k}'|^2}\varphi(\vec{k}'). \tag{2.9}$$

Now we interpret $\varphi(\vec{k})$ as the exciton wave function, and (2.9) represents the effective-mass equation for the exciton within the stated approximations.

## III. SINGLE-PARTICLE GREEN'S FUNCTION AND IRREDUCIBLE PARTICLE-HOLE INTERACTION

### A. Single-Particle Green's Function

In our treatment of the particle-hole scattering including both Coulomb and phonon exchange effects, we assume that the single-particle spectrum is well understood. The single-particle Green's function differs from the unperturbed function (2.5) by inclusion of the self-energy corrections due to electron-electron and electron-phonon interactions, and the resulting change in the spectral function. For each $\vec{k}$ there are peaks of total weight $Z_e(\vec{k})$ at energy $E_e(\vec{k})$ and $Z_h(\vec{k})$ at energy $E_h(\vec{k})$. The electron and hole energies are given by

$$E_e(k)=\Delta+k^2/2m_e+\Sigma_e(\vec{k},E_e(\vec{k})) \tag{3.1}$$

and

$$E_h(\vec{k})=-k^2/2m_h+\Sigma_h(\vec{k},E_h(\vec{k})), \tag{3.2}$$

where $\Sigma$ is the self-energy. Besides these two peaks which define the quasiparticles, there are two smeared distributions in energy, one associated with the electron and the other with the hole. These smeared distributions which represent the incoherent parts of the single-particle Green's functions are separated from the respective peaks. The quasiparticle amplitude $Z_e(\vec{k})$ for the electron is related[12,8] to its self-energy by

$$Z_e(\vec{k})=\left(1-\frac{\partial\Sigma_e(\vec{k},\zeta)}{\partial\zeta}\right)_{\zeta=E_e(\vec{k})}, \tag{3.3}$$

and a similar relation holds for $Z_h(\vec{k})$. It is reasonable to assume that even in the presence of electron-electron and electron-phonon interaction, one can think in terms of well-defined quasiparticles with long lifetimes, especially for low momentums. In our analysis we shall, therefore, ignore all lifetime effects.

The effects of electron-electron interaction on the single-particle properties in an insulator are quite small for low momentums (because the intermediate state energies are $\gtrsim\Delta$), and we shall neglect them. However, for the case of electrons interacting with dispersionless optical phonons, it is known that[13] the continuum is separated from $E(\vec{k})$ approximately by $\omega_0$. Further, there are several theories which give the real part of the self-energy of the polaron for different regimes of the coupling constant $\alpha_{e,h}$. For intermediate coupling,

the self-energy has been defined by Eqs. (1.5) and (1.6). Thus, the energy of an electron and a hole with bare mass $m_e$ and $m_h$ and momentum $\vec{k}$ are

$$E_e(\vec{k}) = \Delta + k^2/2m_h^* - \alpha_e \omega_0 , \tag{3.4}$$

$$E_h(\vec{k}) = -k^2/2m_h^* - \alpha_h \omega_0 . \tag{3.5}$$

We may also have some knowledge of $Z(\vec{k})$ from the Gellman-Low relation[14]:

$$|\langle \psi_{\vec{k}} | \varphi_{\vec{k}} \rangle|^2 = \exp\left(-\frac{\partial \Sigma(\vec{k}, \zeta)}{\partial \zeta}\right)_{\zeta = E(\vec{k})} = e^{Z(\vec{k})-1} , \tag{3.6}$$

where $\varphi_{\vec{k}}$ and $\psi_{\vec{k}}$ are the unperturbed and perturbed ground-state wave functions, respectively. Theories such as those of Lee, Low, and Pines[3] provide us with reasonable expressions for $\psi_{\vec{k}}$.

We may summarize the above discussion by writing the single-particle Green's function as the sum of a coherent part $G_c$, whose poles are at the quasiparticle energies, and an incoherent part $G_{\mathrm{inc}}(\vec{k}, \zeta)$:

$$G(\vec{k}, \zeta) = G_c(\vec{k}, \zeta) + G_{\mathrm{inc}}(\vec{k}, \zeta) , \tag{3.7}$$

where

$$G_c(\vec{k}, \zeta) = \frac{Z_e(\vec{k})}{\zeta - E_e(\vec{k}) + i\delta} + \frac{Z_h(\vec{k})}{\zeta - E_h(\vec{k}) - i\delta} \tag{3.8}$$

and

$$G_{\mathrm{inc}}(\vec{k}, \zeta) = \int_{E_e(\vec{k})+E_e}^{\infty} \frac{\rho_e(\vec{k}, E)}{\zeta - E}\, dE + \int_{E_h(\vec{k})-E_h}^{-\infty} \frac{\rho_h(\vec{k}, E)}{\zeta - E}\, dE . \tag{3.9}$$

In Eq. (3.9) $\rho_e$ and $\rho_h$ are the spectral weight functions and $E_e$ and $E_h$ are appropriate cuttoff energies which separate the quasiparticle peaks from their respective incoherent parts.

### B. Irreducible Particle-Hole Interaction

The simplest contribution to the irreducible particle-hole interaction $I(k, k'; q)$ comes from the unscreened Coulomb interaction between electron and hole and can be represented by Fig. 2. This diagram and its contribution to the electron-hole interaction have already been discussed in Sec. II. The next important contribution to $I(k, k; q)$ comes from the inclusion of polarization diagrams due to Coulomb interaction alone. In the interaction line of Fig. 2, we may insert the improper polarization part[15] $S(k - k')$. In the long-wavelength limit, $k - k' \to 0$ and to $O(E_B/\Delta)$, the sum of the contributions from Figs. 2 and 3 leads to a screened interaction between the electron and the hole:

$$I_c(\vec{k} - \vec{k}') \equiv (-1/\epsilon_\infty)(4\pi e^2/|\vec{k} - \vec{k}'|^2) , \tag{3.10}$$

a result derived earlier by Sham and Rice.[7]

The inclusion of vertex corrections is expected to alter the above effective electron-hole interaction. However, before discussing the vertex corrections to diagrams 2 and 3, let us consider the contribution to $I(k, k'; q)$ coming from the exchange of LO phonons. The simplest diagram that contributes is shown in Fig. 4, where the wavy line represents a phonon propagator. The contribution from this diagram to irreducible particle-hole interaction is

$$-\omega_0^2 \left(\frac{\alpha_e \alpha_h}{\kappa_e \kappa_h}\right)^{1/2} \frac{4\pi}{|\vec{k} - \vec{k}'|^2} D(\vec{k} - \vec{k}'; \zeta - \zeta') , \tag{3.11}$$

where the phonon propagator $D(\vec{q}, \zeta)$ is given by

$$D(\vec{q}, \zeta) = 1/(\zeta - \omega_0 + i\delta) + 1/(\zeta + \omega_0 - i\delta) . \tag{3.12}$$

We shall use the experimentally measured values of $\omega_0$ and $\alpha_{e,h}$ and ignore phonon lifetime effects. Therefore, we do not consider any polarization insertions in the phonon line. For the same reason the diagrams of Figs. 5 and 6, where both Coulomb and phonon lines are present, need not be considered. The diagrams of the type of Figs. 5 and 6 merely modify the coupling constant and the phonon energy. The contribution to the electron-hole interaction from the simple phonon exchange represented by Fig. 4 is calculated in Appendix A. Other diagrams contributing to $I(k, k', q)$ are (i) retardation diagrams, Fig. 7, where two phonon lines or a phonon line and a Coulomb line cross each other, and (ii) vertex corrections to all the above. We denote by $\tilde{I}_{\mathrm{ph}}$ the contribution of all diagrams of the type of Figs. 4 and 7.

In the BS equation (2.4) for the particle-hole $t$ matrix, the vertex[6] corrections occur in the combination $G_e \Lambda_e \tilde{I} \Lambda_h G_h$ for the important set of interactions. Here, $\tilde{I} = \tilde{I}_{\mathrm{ph}} + \tilde{I}_c$, $\Lambda_{e,h}$ refer to the vertices associated with the electron and the hole, respec-

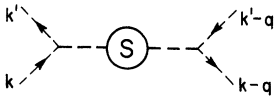


FIG. 3. Polarization corrections to the Coulomb interaction.

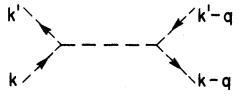


FIG. 2. Lowest-order Coulomb contribution to $I$, the irreducible particle-hole interaction.

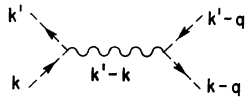


FIG. 4. Lowest-order phonon exchange contribution to $I$.

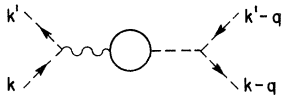


FIG. 5. Class of diagrams contributing to $I$ with both a Coulomb line and phonon exchange.

tively. The vertex $\Lambda_{e,h}$ is, in general, a function of $k$ and $k-k'=(\vec{t},\eta)$. The effect of including the vertex corrections is seen to be twofold: a modification of $\tilde{I}$ and an effective change in the single-particle propagators $G_{e,h}$. In general, these two effects cannot be separated unless $\Lambda(k,t)$ is a separable function of $k$ and $t$.

The vertex corrections due to Coulomb interactions are negligible[16] for $k^2/2m_{e,h} \ll \Delta$ and may be ignored for insulators with a large gap. Only the phonon contributions to $\Lambda_{e,h}$ are expected to be important. The lowest-order vertex corrections to $\Lambda_e$ is shown in Fig. 8, there being a similar contribution to $\Lambda_h$. The contribution to $\Lambda_e(k,t)$ from Fig. 8 is calculated in Appendix B. We utilize these results to discuss the phonon contributions to the vertex corrections in two limiting cases determined by $\omega_0/E_B'$ or equivalently $r_{ex}/r_{e,h}^*$. Here $E_B'$ is defined as the energy to separate an electron and a hole to infinity without varying the self-energies they had in the bound state. Thus $E_B' \neq E_B$. The Bohr radius corresponding to $E_B'$ is denoted by $r_{ex}$. We will show below, that in the two limits $\omega_0/E_B' \gg 1$ and $\omega_0/E_B' \ll 1$, the effect of $\Lambda(k,t)$ on the single-particle propagator is more important than on the interaction.

*Case I,* $\omega_0 \gg E_B'$

From Appendix B, we have for $\vec{t}=0$,

$$\Lambda_{e,c} = 1 + \tfrac{1}{2}\alpha_e - \tfrac{3}{4}\alpha_e \frac{E_B'}{\omega_0} + \frac{\frac{5}{4}\alpha_e |k|^2}{2\mu\omega_0(1-\frac{5}{2}E_B'/\omega_0)} + O\left(\frac{E_B'}{\omega_0}\right)^2, \quad (3.13)$$

$$\Lambda_{e,ph} = 1 + \tfrac{1}{2}\alpha_e - \tfrac{3}{4}\alpha_e\left(\tfrac{5}{3} - \tfrac{2}{3}\sqrt{2}\right)\frac{E_B'}{\omega_0} + \alpha_e \frac{21}{8}\frac{k^2}{2m_e\omega_0}\left(\frac{E_B'}{\omega_0}+1\right) + O\left(\frac{E_B'}{\omega_0}\right)^2. \quad (3.14)$$

The quasiparticle renormalization to the same order of approximation is given by[17,18]

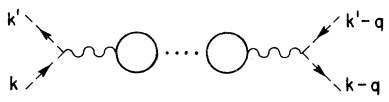


FIG. 6. Class of diagrams contributing to $I$ with both a Coulomb line and phonon exchange.

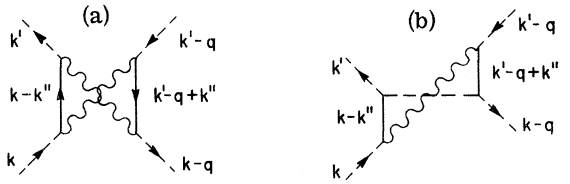


FIG. 7. (a) and (b) Retardation diagrams.

$$Z_e(\vec{k}) = 1 - \tfrac{1}{2}\alpha_e. \quad (3.15)$$

Thus in the limit $E_B' \to 0$ and $t \to 0$, the vertex correction and the quasiparticle renormalization cancel each other. In fact the cancellation in this limit is exact (not restricted to the second-order perturbation theory) as is seen from the Ward identity,[6]

$$\lim_{\substack{t\to 0\\ \eta\to 0}} \Lambda_e(k,t) = \Lambda_e^0(k) = 1 + \frac{\partial\Sigma_e(k)}{\partial\zeta}. \quad (3.16)$$

and

$$\Lambda_e^0(\vec{k}, E_e) = [Z_e(\vec{k})]^{-1}. \quad (3.17)$$

It is interesting to note that to order $E_B'/\omega_0$, the phonon vertex corrections to $\tilde{I}_{ph}$ and $\tilde{I}_c$ differ; this is so because the analytic properties of $\tilde{I}_{ph}$ and $\tilde{I}_c$ differ.

Now we examine how the vertex corrections alter the effective particle-hole interactions. We expand $\Lambda_e(k,t)$ in powers of $\vec{t}$, $t^2/2\mu^*\omega_0$ being in the present case a small parameter. From Appendix B we find the $t$ dependence of $\Lambda(k,t)$ to be

$$-\tfrac{3}{4}\alpha_e \frac{E_B'}{\omega_0}\frac{|\vec{t}|^2}{2\mu^* E_B'} + O\left(\frac{E_B'}{\omega_0}\right)^2. \quad (3.18)$$

On the other hand, if we expand $\tilde{I}(t)$, the Fourier transform of the $\vec{r}$-space potential given (in the local approximation) by Eq. (4.12) in terms of the parameter $E_B'/\omega_0$, we find that

$$I(t) \sim \frac{4\pi e^2}{\epsilon_0|\vec{t}|^2} + \frac{E_B'}{\omega_0}\frac{4\pi e^2}{\mu^*\omega_0}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right) + \frac{4\pi e^2}{3\mu^*\omega_0}\left(\frac{E_B'}{\omega_0}\right)^{3/2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\frac{|\vec{t}|^2}{2\mu^* E_B'}. \quad (3.19)$$

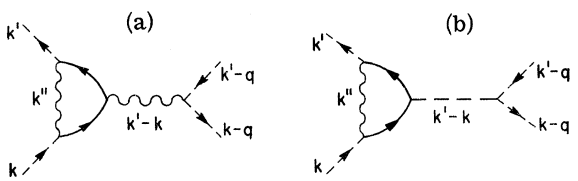


FIG. 8. (a) Phonon vertex correction to the phonon-exchange diagrams. Only the electron vertex is shown. (b) Phonon vertex correction to the Coulomb interaction between the electron and the hole.

If now we consider $\Lambda\tilde{I}\Lambda$ for its $\vec{t}$ dependence, we find that the vertex contributes additional terms to the effective interaction (i.e., $\vec{t}$-dependent terms[19]) which are at least of $O(E_B'/\omega_0)^{3/2}$. This is to be contrasted with the self-energy alterations due to $\Lambda$ which are of $O(E_B'/\omega_0)$. Thus in this limit we may regard the modification of the effective potential by the vertex to be relatively unimportant.

*Case II, $E_B' \gg \omega_0$*

In this limit, as discussed in Sec. IV, it is more appropriate to start from the bare electron and hole propagators (no polaron self-energies), and as a first correction consider the effect of including the vertex corrections on the potential and the self-energy. The self-energy and the potential alteration themselves are $O(\omega_0/E_B')$. The second-order phonon vertex correction to the Coulomb line [Fig. 8(b)] in the limit $(\omega_0/E_B') \ll 1$ is

$$\Lambda_{e,c}(k,t) \simeq 1 + \tfrac{1}{2}\alpha_e\left(\frac{\omega_0}{E_B'}\right)^{3/2} + \frac{5\alpha_e}{4}\frac{|\vec{k}|^2}{2\mu E_B'}\left(\frac{\omega_0}{E_B'}\right)^{3/2} - \frac{3\alpha_e}{4}\frac{|\vec{t}|^2}{2\mu E_B'}\left(\frac{\omega_0}{E_B'}\right)^{3/2}. \quad (3.20)$$

$\Lambda_{e,\mathrm{ph}}(k,t)$ has precisely the same $(\omega_0/E_B')$ dependence with different coefficients arising from the different analytic properties of $\tilde{I}_c$ and $\tilde{I}_{\mathrm{ph}}$. The above expansion is valid for small values of momentum transfer $\vec{t}$ only. In this limit the most important modification of the potential is a term independent of $\vec{t}$.[19] This comes from the product of the $\vec{t}^2$ term of the vertex and $1/\vec{t}^2$ term of the potential $\tilde{I}(t)$. This $\vec{t}$-independent term is $O(\omega_0/E_B')^{3/2}$, whereas the self-energy corrections are $O(\omega_0/E_B')$. The first $t$-dependent term goes as $(\omega_0/E_B')^{3/2}$. For large $\vec{t}$, the vertex falls off as $(\omega_0/E_B')(1/|\vec{t}|^2)$ and the modification of the potential is again expected to be small as the additional terms are $O(\omega_0/E_B')(1/|\vec{t}|^4)$. From the above argument we conclude that the modification of the potential $\tilde{I}(t)$ due to vertex corrections is less important than the self-energy corrections to the bare electron and hole propagators. It is to be noted that in this limit, we have here a Migdal-like theorem[20] where all the vertex corrections can be neglected.

The intermediate case where $\omega_0/E_B' \sim 1$ is quite difficult to handle in general. We shall utilize the results of the two limiting cases to develop a suitable interpolation procedure.

Before obtaining the form of the effective electron-hole potential, we examine the importance of retardation (nonladder) diagrams. These are shown in the Figs. 7(a) and 7(b). In Fig. 7(a) two phonon lines cross each other. The calculations are straightforward but tedious. In the small $\vec{t}$ limit, the lowest-order contribution is proportional to $\vec{t}$ in general but proportional to $|\vec{t}|^2$ when the electron and the hole masses are the same. These can be neglected compared to $1/|\vec{t}|^2$ contributions associated with the ladder diagrams. For large momentum transfers, their contribution to $\tilde{I}$ falls of as $1/|\vec{t}|^4$ and can therefore be neglected. The diagrams of type Fig. 7(b) are also found to be unimportant and so are the diagrams of type Fig. 9 as has been shown by Kohn.[21]

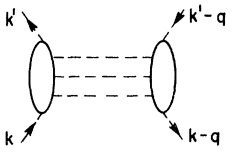


FIG. 9. Diagram contributing to the effective electron-hole interaction which are expected to be unimportant (see text).

## IV. WAVE EQUATION FOR EXCITONS

In this section, we utilize the single-particle Green's functions and the irreducible particle-hole interaction obtained in Sec. III to solve the homogeneous equation for the $t$ matrix (2.4). We start by considering the two limiting cases.

### A. Case 1, $r_{\mathrm{ex}} \gg r_{e,h}^* (E_B' \ll \omega_0)$

In this limit, the vertex corrections cancelled the quasiparticle renormalization factor, the corrections beyond this cancellation being $O(E_B'/\omega_0)$. We therefore omit both $Z_{e,h}$ and $\Lambda_{e,h}$ and use for $I(k,k')$ the following expression:

$$I(k,k') = \tilde{I}_c(\vec{k},\vec{k}') + \tilde{I}_{\mathrm{ph}}(k,k') = -\frac{4\pi e^2}{\epsilon_\infty |\vec{k}-\vec{k}'|^2} - \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\frac{2\pi e^2\omega_0}{|\vec{k}-\vec{k}'|^2} \times D(\vec{k}-\vec{k}';\zeta-\zeta'). \quad (4.1)$$

When $I(k,k')$ is energy dependent, the derivation of the effective-mass equation for the exciton is a little more difficult. The $t(k,k')$ matrix depends upon $\zeta$ and therefore the $\zeta''$ integration in Eq. (2.4) cannot be carried out in general. However, a pole approximation to the exciton Green's function (see Sham and Rice[7]) leads to an effective-mass equation (see Appendix A) for the exciton wave function $A(\vec{k}+\vec{Q},\vec{k})$ in the momentum space. The exciton wave function is given by

$$\Psi_{\vec{Q}}(\vec{r}_e,\vec{r}_h) = \sum_{\vec{k}} A(\vec{k}+\vec{Q};\vec{k})\, e^{+i(\vec{k}+\vec{Q})\cdot\vec{r}_e} e^{-i\vec{k}\cdot\vec{r}_h}. \quad (4.2)$$

The exciton wave function in momentum space $A(\vec{k}+\vec{Q};\vec{k})$ satisfies the integral equation[22]:

$$\left(\Delta-\omega-(\alpha_e+\alpha_h)\,\omega_0+\frac{\vec{k}^2}{2m_e^*}+\frac{(\vec{k}+\vec{Q})^2}{2m_h^*}\right)A(\vec{k}+\vec{Q};\vec{k})=\sum_{\vec{k}'}V_{\rm eff}(\vec{k},\vec{k}';\vec{Q}\omega)\,A(\vec{k}'+\vec{Q};\vec{k}')\,, \tag{4.3}$$

where

$$V_{\rm eff}(k,k';Q\omega)=-\frac{4\pi e^2}{|k-k'|^2}\left\{\frac{1}{\epsilon_\infty}-\frac{\omega_0}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\left[\left(\Delta-\omega-(\alpha_e+\alpha_h)\omega_0+\frac{\vec{k}'^2}{2m_e^*}+\frac{(\vec{k}+\vec{Q})^2}{2m_h^*}\right)^{-1}\right.\right.$$
$$\left.\left.+\left(\Delta-\omega-(\alpha_e+\alpha_h)\omega_0+\frac{\vec{k}^2}{2m_e^*}+\frac{(\vec{k}'+\vec{Q})^2}{2m_h^*}\right)^{-1}\right]\right\}. \tag{4.4}$$

For simplicity we shall put $\vec{Q}$, the total momentum of the exciton, equal to zero (this is justified when the electron-hole pair are created by optical absorption for a direct gap material). Recalling that the binding energy of the exciton $E_B$,

$$E_B=\Delta-\omega-(\alpha_e+\alpha_h)\omega_0\,, \tag{4.5}$$

$$(E_B+\vec{k}^2/2\mu^*)\,A(\vec{k})=\textstyle\sum_{\vec{k}'}V_{\rm eff}(\vec{k},\vec{k}';E_B)\,A(\vec{k}')\,, \tag{4.6}$$

where

$$V_{\rm eff}(\vec{k},\vec{k}';E_B)=-\frac{4\pi e^2}{|\vec{k}-\vec{k}'|^2}$$
$$\times\left\{\frac{1}{\epsilon_\infty}-\frac{\omega_0}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\left[\left(E_B+\frac{k^2}{2m_h^*}+\frac{k'^2}{2m_e^*}\right)^{-1}\right.\right.$$
$$\left.\left.+\left(E_B+\frac{\vec{k}'^2}{2m_h^*}+\frac{\vec{k}^2}{2m_e^*}\right)^{-1}\right]\right\}. \tag{4.7}$$

We now transform the wave equation (4.6) to coordinate space. The $\vec{r}$-space wave function $\Psi(\vec{r})$ is related to $A(\vec{k})$ by the relation

$$\Psi(\vec{r})=\int A(\vec{k})\,e^{i\vec{k}\cdot\vec{r}}\,\frac{d\vec{k}}{(2\pi)^3}\,, \tag{4.8}$$

$\vec{r}=\vec{r}_e-\vec{r}_h$ being the relative coordinate of the electron and the hole. $V_{\rm eff}(\vec{k},\vec{k}';E_B)$ depends separately on $\vec{k}$ and $\vec{k}'$. Thus, $V_{\rm eff}$ is nonlocal, and the wave equation for the exciton becomes

$$\left(E_B-\frac{\nabla^2}{2\mu^*}\right)\Psi(\vec{r})=\int V_{\rm eff}(\vec{r},\vec{r}')\,\Psi(\vec{r}')\,dr'\,, \tag{4.9}$$

where

$$V_{\rm eff}(\vec{r},\vec{r}')=-\frac{e^2}{\epsilon_\infty r}\,\delta(\vec{r}-\vec{r}')+\frac{1}{2}\,\frac{e^2\mu^*\omega_0}{|\vec{r}-\vec{r}'|}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)$$
$$\times\left[1\Big/\left|\frac{m_e^*}{M^*}\,\vec{r}'+\frac{m_h^*}{M^*}\,\vec{r}\right|+1\Big/\left|\frac{m_e^*}{M^*}\,\vec{r}+\frac{m_h^*}{M^*}\,\vec{r}'\right|\right]\exp\{-[2\mu^*(E_B+\omega_0)]^{1/2}\,|\vec{r}-\vec{r}'|\}\,. \tag{4.10}$$

### B. Case 2, $r_{\rm ex}\ll r^*_{e,h}(E'_B\gg\omega_0)$

In this limit, there is no simple way to estimate the contributions to $I$ from the electron and the hole vertices $\Lambda_e$ and $\Lambda_h$. As has been pointed out in Sec. III, the vertex corrections in this limit should be large enough to eliminate the self-energy clouds surrounding the interacting electron and hole polarons. We saw that if we start from a bare electron and a bare hole, then the vertex corrections are $O(\omega_0/E_B)$. For this case, therefore, it is more appropriate to start from the other extreme where the interactions with phonons are treated in second-order perturbation theory. The unperturbed states are the exciton states obtained in the potential $-1/\epsilon_\infty r$. In this analysis, it is seen that the change in $E_B$ of an exciton state due to phonons has two parts, both of order $\omega_0/E_B$. One of these terms can be interpreted as the change in electron and hole self-energy, and the other as a change in the interaction energy. A diagrammatic representation of the change in the interaction energy (up to second order) is provided by a single phonon exchange between the electron and the hole (not the multiple scattering as implied by treating the single phonon exchange as the irreducible particle-hole exchange) allowing only for the multiple scattering due to the Coulomb interaction.

To see the above more clearly, we consider the local potential introduced in Sec. IV C by Eq. (4.12). By a further approximation one obtains $V_{\rm app}(r)$ given by Eq. (4.13). If we expand $V_{\rm app}(r)$ in powers of $\omega_0/E'_B$, we see that in the limit $\omega_0/E'_B\to 0$,

$$V_{\rm app}(r)=-\frac{1}{\epsilon_\infty r}+\frac{1}{r}\,O\left(\frac{\omega_0}{E'_B}\right)\frac{1}{4}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\,. \tag{4.11}$$

Thus, the first correction to the potential is

$O(\omega_0/E_B')$. The above analysis shows that if in Eq. (4.9) one uses the potential $V_{app}(r)$ and self-energies (both the mass and the momentum-independent part) due to phonons obtained from a second-order perturbation theory, then the calculated binding energy is accurate up to $O(\omega_0/E_B')$. We expect this conclusion to be true for all $m_e/m_h$. We shall utilize this point along with our findings for the case of opposite extreme, $r_{ex} \gg r_{e,h}^*$, to obtain a suitable interpolation procedure for the intermediate case.

### C. Discussion of $V_{eff}(\vec{r},\vec{r}')$

We now discuss $V_{eff}(\vec{r},\vec{r}')$ given by (4.10) in detail. The first thing to note is that the range of nonlocality is $[2\mu^*(E_B+\omega_0)]^{-1}$. This is to be compared with the characteristic length in the problem, viz., $(2\mu^* E_B)^{-1}$. We conclude, what we noted in Sec. I, that nonlocality scales with the parameter $E_B/\omega_0$. To gain physical insight, we may handle the nonlocality in an average fashion by convoluting $V_{eff}(r,r')$ with a suitable wave function to obtain $V_{loc}(r)$:

$$V_{loc}(r)\Psi(\vec{r}) = \int V_{eff}(\vec{r},\vec{r}')\Psi(\vec{r}')\,d\vec{r}' \ . \qquad (4.12)$$

For simplicity we may use for $\Psi(\vec{r})$ the ground-state hydrogenic wave function of energy $-E_B$. We have not been able to perform the integral in (4.12) analytically. Numerical evaluation of $V_{loc}(r)$ has been done and will be discussed in Sec. V.

Since $V_{eff}(\vec{r},\vec{r}')$ contains the factor $e^{-\beta|\vec{r}-\vec{r}'|/|\vec{r}-\vec{r}'|}$ we can obtain an approximate local potential by putting $\vec{r}'=\vec{r}$ in the terms inside the large square brackets in (4.10). This approximation removes the explicit $m_e/m_h$ dependence of the potential. We can then perform the integral (4.12) analytically to obtain

$$V_{app}(r) = -\frac{e^2}{r}\left[\frac{1}{\epsilon_0}+\frac{2}{r}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\left(\frac{E_B}{\omega_0}\right)^{1/2}\frac{1}{(2\mu^*\omega_0)^{1/2}} \times\left(1-\exp\left\{\left((2\mu^*E_B)^{1/2}-[2\mu^*(E_B+\omega_0)]^{1/2}\right)r\right\}\right)\right] . \qquad (4.13)$$

Comparison with the numerical results shown that (4.13) is an excellent approximation to the actual potential for $E_B \gg \omega_0$. In (4.13) we have used $\mu^*$ which is the polaron reduced mass and is therefore appropriate for the case $E_B \ll \omega_0$. For the opposite limit $\mu^*$ should be replaced by $\mu$. In the case when either $m_h$ or $m_e \to \infty$, the donor or acceptor impurity limit, the integration in (4.12) can also be performed analytically. We obtain

$$V_{imp}(r) = -e^2\left\{\frac{1}{\epsilon_0 r}+\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\left(\frac{E_B}{\omega_0}\right)\left(\frac{1}{2\mu^*\omega_0}\right)^{1/2}\frac{1}{r^2} + \frac{1}{2r}\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon_\infty}\right)\left[1-2\left(\frac{E_B}{\omega_0}\right)^{1/2}\left(\frac{1}{2\mu^*\omega_0}\right)^{1/2}\frac{1}{r}\right] \times\exp\left\{\left((2\mu^*E_B)^{1/2}-[2\mu^*(E_B+\omega_0)]^{1/2}\right)r\right\}\right\}, \qquad (14)$$

where $\mu^* = m_e^*$ or $m_h^*$ as the case may be. For arbitrary $m_e/m_h$ numerical results are given in Sec. V.

Certain qualitative features of the potential $V_{app}$ will now be discussed. For large $r$, the exponential term falls off rapidly and can be ignored and the local potential has the form

$$V_{app}(r) \xrightarrow[\text{large } r]{} -e^2\left[\frac{1}{\epsilon_0 r}+2\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\left(\frac{E_B}{\omega_0}\right)^{1/2} \times\left(\frac{1}{2\mu^*\omega_0}\right)^{1/2}\frac{1}{r^2}\right] \ . \qquad (4.15)$$

The strength of the $r^{-2}$ term in the potential, given by (4.15), depends upon the product $(\alpha_e\alpha_h)^{1/2}$. The $r^{-2}$ contribution to the potential may be understood physically as the additional contribution to the electron-hole potential coming from the dynamic polarization of the lattice by the electron and the hole. Sham[8] has obtained a similar $r^{-2}$ potential in his study of the shallow impurity states in semiconductors. In that case, however, the dipoles are created by the static polarization of the lattice by the impurity ion.

The form of the potential $V_{app}(r)$ when $\Psi$ is $p$-like is given in the Appendix C.

### D. Intermediate Case ($r_{ex} \sim r_{e,h}^*$) and the Interpolation Scheme

We have seen that $V_{loc}(r)$ given by Eq. (4.12) behaves appropriately in the two limits. Furthermore, the effective potential is seen to be unaltered up to $O(\omega_0/E_B)$ in the large $E_B$ limit and up to $O(E_B/\omega_0)^{1/2}$ in the small $E_B$ limit if one includes the $t$-dependent part of the vertex corrections. We make the ansatz that the form of the potential remains the same even in the intermediate case. The important changes in the intermediate case takes place in the electron and hole propagators. When the electron and hole interact to form an exciton, they no longer behave either as free polarons or as bare particles. Let us denote the mass and the self-energy of the electron and the hole in this intermediate case as $m_{e,h}^{**}$, $\sigma_{e,h}^{**}$, respectively. In the limit $r_{ex} \gg r_e^*$, $m_e^{**}$ approaches $m_e^*$, the polaron mass, and $\sigma_e^{**}$ approaches the value $-\alpha_e\omega_0$. In the opposite limit, $m_e^{**}$ approaches $m_e$, the bare electron mass, and $\sigma_e^{**}$ approaches the value zero. A similar set of conditions hold for the hole, in this case $r_h^*$ and $r_{ex}$ being the relevant lengths to compare.

To obtain $E_B$, let us substitute the modified electron and hole energies

$$E_e(\vec{k}) = \Delta + |\vec{k}|^2/2m_e^{**} + \sigma_e^{**} \ , \qquad (4.16)$$

$$E_h(\vec{k}) = -|\vec{k}|^2/2m_h^{**} + \sigma_h^{**} \tag{4.17}$$

in Eq. (4.4). In the $\vec{Q}=0$ limit, the Schrödinger equation becomes

$$(E_B' + k^2/2\mu^{**}) A(\vec{k}) = \sum_{\vec{k}'} V_{\text{eff}}(\vec{k}, \vec{k}'; E_B') A(\vec{k}') , \tag{4.18}$$

where $V_{\text{eff}}(k, k'; E_B')$ is same as that given in Eq. (4.7) with $E_B$, $m_{e,h}^*$ replaced by $E_B'$, $m_{e,h}^{**}$. The local form of the potential also gets modified in the same way. The quantity $E_B'$ that enters in the Schrödinger equation (4.18) and the potential is given by

$$E_B' = \Delta - \omega + \sigma_e^{**} + \sigma_h^{**} . \tag{4.19}$$

Since $E_B$ is defined as the difference between the internal energy $\omega$ of an electron-hole pair and the energy of two free polarons, we have

$$E_B = E_B' + (\sigma_e^{**} - \sigma_e^*) + (\sigma_h^{**} - \sigma_h^*) . \tag{4.20}$$

$E_B'$ (which was qualitatively defined in Sec. III) can be physically interpreted as the energy required to separate an electron and hole apart without deforming their self-energy clouds, the self-energy clouds in this case being those of interacting electrons and holes rather than of free polarons. It is clear that the effective exciton radius $r_{\text{ex}}$ that we have been using to compare with $r_{e,h}^*$ should be related to $E_B'$ and not $E_B$. This is given by

$$r_{\text{ex}}^{-1} = (2\mu^{**} E_B')^{1/2} . \tag{4.21}$$

It is $E_B'$ and not $E_B$ that determines the radial extension of the exciton and hence the oscillator strength. For intermediate and strong coupling cases where $\alpha_{e,h}$ are quite large, one expects an appreciable difference between $E_B$ and $E_B'$. In order to obtain $E_B$ from $E_B'$ one needs to know $m_{e,h}^{**}$ and $\sigma_{e,h}^{**}$. We know their values in two limiting cases and also know on what basic parameters they should depend upon. An interpolation scheme between the two known limits may therefore be used. The interpolation scheme that we have used is consistent with the first corrections to the self-energy, and is

$$m_{e,h}^{**} = m_{e,h} \frac{r_{e,h}^{*2}}{r_{e,h}^{*2} + r_{\text{ex}}^2} + m_{e,h}^* \frac{r_{\text{ex}}^2}{r_{e,h}^{*2} + r_{\text{ex}}^2} , \tag{4.22}$$

$$\sigma_{e,h}^{**} = \sigma_{e,h} \frac{r_{\text{ex}}^2}{r_{e,h}^{*2} + r_{\text{ex}}^2} , \tag{4.23}$$

where $r_{\text{ex}}$ is defined in Eq. (4.21).

We have used other forms of the interpolation scheme and find that $E_B$ is not very sensitive to the choice, although the form of Eqs. (4.22) and (4.23) gives the best agreement with the experiment (see Sec. V). The relative insensitivity of $E_B$ to the interpolation scheme is due to the fact that the effects of $m_{e,h}^{**}$ and $\sigma_{e,h}^{**}$ on $E_B$ are in opposite directions.

## V. RESULTS AND DISCUSSION

### A. Discussion of the Potential

To find out how the local potential depends upon the parameters $\epsilon_0/\epsilon_\infty$, $m_e/m_h$, and $E_B'/\omega_0$, we have numerically evaluated $V_{\text{loc}}(r)$ using Eq. (4.12). For convenience we have plotted the quantity

$$-r\epsilon_\infty V(r)/e^2 = 1/\epsilon(r) , \tag{5.1}$$

which defines an effective $r$-dependent dielectric constant. For numerical calculation we have chosen $\hbar = \epsilon = 2\mu = \epsilon_\infty = 1$.

In Figs. 10(a) and 10(b) we have plotted $\epsilon_{\text{loc}}^{-1}(r)$ as a function of $r$ for several values of $m_e/m_h$ and $E_B'/\omega_0$. From these figures we can see that $V_{\text{loc}}(r)$ depends strongly on $E_B'/\omega_0$ whereas for a particular value of $E_B'/\omega_0$, the dependence on the mass ratio $m_e/m_h$ is rather weak. The potential approaches its asymptotic value for $r \to 0$ quicker, the larger the ratio $E_B'/\omega_0$. Conversely the asymptotic value at $r \to \infty$ is approached quicker the smaller the value of $E_B'/\omega_0$.

To find out how significantly the ratio $m_e/m_h$ affects the potential we have evaluated it in two limits: (a) $m_e/m_h = 0$, the impurity limit, $V_{\text{imp}}(r)$ and (b) $m_e/m_h = 1$. For comparison, in the same figures [11(a) and 11(b)] we also plot $V_{\text{app}}(r)$ which is, by virtue of the approximation made, independent of $m_e/m_h$. The following observations can be made: For $E_B'/\omega_0 \gg 1$, the difference in the three potentials is not significant. It is noteworthy that for $r=0$, the potential with $m_e/m_h = 1$ is significantly different from $m_e/m_h = 0$ (or $\infty$). For the impurity potential there is a correction for $r=0$ proportional to $\omega_0/E_B'$, as can be seen directly from Eq. (4.14). It is clear that for $m_e/m_h \to \infty$ and $E_B'/\omega_0 \to \infty$, the potential will depend on the order in which the two limits are taken.

$V_{\text{app}}(r)$ is an excellent approximation to $V_{\text{loc}}(r)$ which justifies our use of $V_{\text{app}}(r)$ in an earlier calculation.[2] However, there is some difference; $V_{\text{app}}(r)$ is less attractive than $V_{\text{loc}}(r)$ near the origin and more attractive for large $r$. In the present work we have calculated $E_B$ (actually $E_B'$) using $V_{\text{app}}(r)$ for computational reasons. This seems to be quite justified because for the cases of experimental interest, $E_B'/\omega_0 \gg 1$. We believe, however, that for large $m_e/m_h$ and small $E_B'/\omega_0$ one should use the potential $V_{\text{loc}}(r)$ instead of $V_{\text{app}}(r)$.

### B. Calculation and Comparison with Experiment

To obtain the exciton binding energy $E_B$, we have solved the Schrödinger equation (4.18) numerically to obtain $E_B'$ using $V_{\text{app}}(r)$ for the potential ex-

cept for the case of MgO which will be discussed below. Since the potential itself depends upon $E_B'$, we have used an iterative procedure whose convergence was found to be excellent.

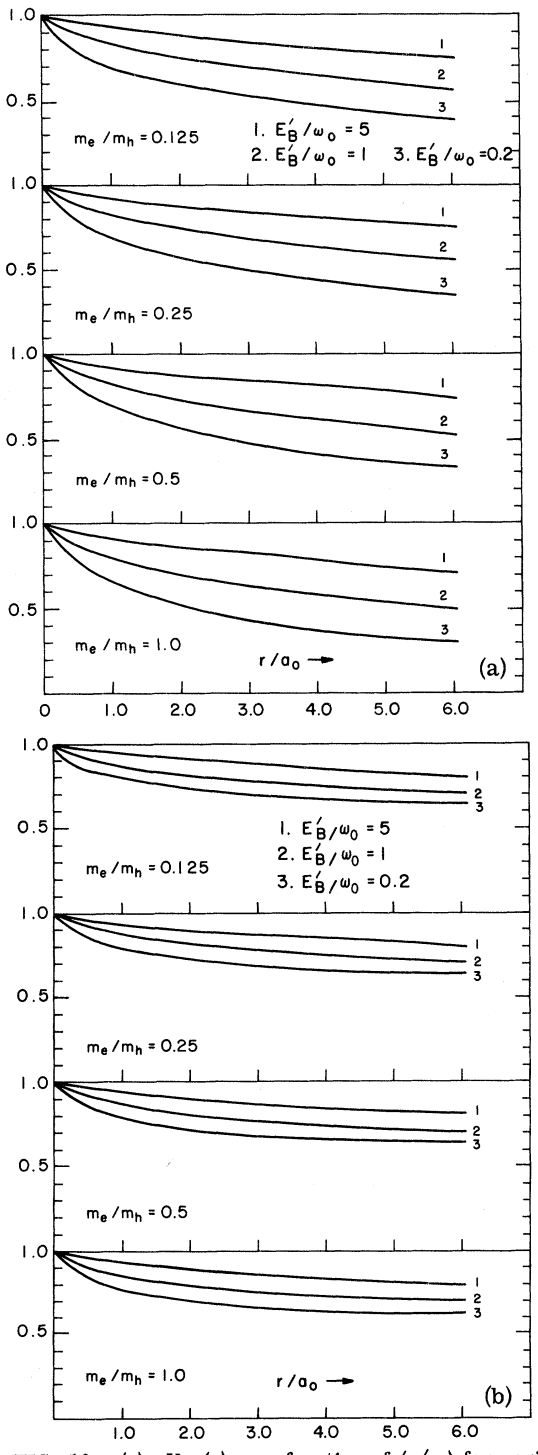


FIG. 10. (a) $rV_{loc}(r)$ as a function of $(r/a_0)$ for various values of $m_e/m_h$ and $E_B'/\omega_0$ and with $\epsilon_0/\epsilon_\infty = 7$. Reduced units are used such that $e = h/2\pi = 2\mu = \epsilon_\infty = a_0$ (Bohr radius) $= 1$. (b) $rV_{loc}(r)$ as a function of $(r/a_0)$ for various values of $m_e/m_h$ and $E_B'/\omega_0$ and with $\epsilon_0/\epsilon_\infty = 2$.

To calculate $E_B'$ and $E_B$, one needs to know the effective band mass of the electrons and holes. For the simplest case where both the conduction band minima and the valence band maxima are nondegenerate and the bands are isotropic, only two effective masses $m_e$ and $m_h$ appear in the calculation. The situation where the valence band maxima is degenerate or the valence band is anisotropic are more complicated. In such cases, we utilize a single effective hole mass in our numerical calculation.

Band structures parameters are known for many I-VII, II-VI, and III-V semiconductors. The effective masses near the conduction band minima are known accurately and the theoretical values are in reasonable agreement with experimental values derived from cyclotron resonance measurements. The corresponding situation for the hole masses is rather uncertain. This, together with the fact that the valence band is often degenerate (hole mass tensor is anisotropic), introduces some degree of uncertainty in the theoretical value of $E_B$. The relevant quantities $m_e$, $m_h$, $\alpha_e$, $\alpha_h$, $\hbar\omega_0$, etc., and the sources they were obtained from are given in Table I. From the entries in this table, we see that TlCl, TlBr, and MgO are examples of intermediate coupling systems $1 < \alpha_{e,h} < 6$, whereas the other compounds listed have their coupling constants $\alpha_{e,h} < 1$.

In Sec. IV, we had discussed the difference between $E_B'$, the energy which determines the exciton radius, and $E_B$, the actual binding energy that one gets from experiment. To obtain $E_B$ from $E_B'$

TABLE I. Values of various parameters used in the calculations.

| | $\hbar\omega_0$ | $\epsilon_0$ | $\epsilon_\infty$ | $m_e$ | $m_h$ | $\alpha_e$ | $\alpha_h$ |
|---|---|---|---|---|---|---|---|
| TlCl | 21.50 | 37.60 | 5.10 | 0.37[a] | 0.36[a] | 2.59 | 2.55 |
| TlBr | 14.30 | 35.10 | 5.40 | 0.18[b] | 0.38[b] | 2.16 | 3.31 |
| MgO | 90.00 | 9.80 | 2.97 | 0.25[c] | 3.20[c] | 1.44 | 5.16 |
| CdS | 37.83 | 8.90 | 5.20 | 0.18[d] | 0.57[d] | 0.79 | 1.41 |
| ZnS | 43.67 | 8.77 | 5.20 | 0.19[e] | 0.94[e] | 0.60 | 1.34 |
| CdTe | 21.34 | 10.90 | 7.20 | 0.11[d] | 0.35[d] | 0.35 | 0.63 |
| GeAs | 36.22 | 12.90 | 10.90 | 0.09[e] | 0.52[e] | 0.08 | 0.20 |

[a]S. Kurita and K. Kobayashi (Ref. 23). These values of $m_e$, $m_h$ for TlCl differ from those quoted by R. Z. Bachrach and F. C. Brown (Ref. 24), but are in good agreement with the theoretically calculated values of H. Overhof and J. Treusch (Ref. 25).

[b]R. Z. Bachrach and F. C. Brown (Ref. 24).

[c]C. Y. Fong (Ref. 26).

[d]B. Segall (Ref. 27). The electron (hole) polaron masses $m_e^*(m_h^*)$ obtained from the experiment are given. The band masses $m_e(m_h)$ are obtained by using the intermediate coupling polaron theory.

[e]J. P. Walter and M. L. Cohen (Ref. 28).

one needs to know the momentum-independent part of the self-energy $\sigma_{e,h}^{**}$ and the reduced mass $\mu^{**}$. These are obtained by making use of the interpolation equations (4.22) and (4.23). The quantities

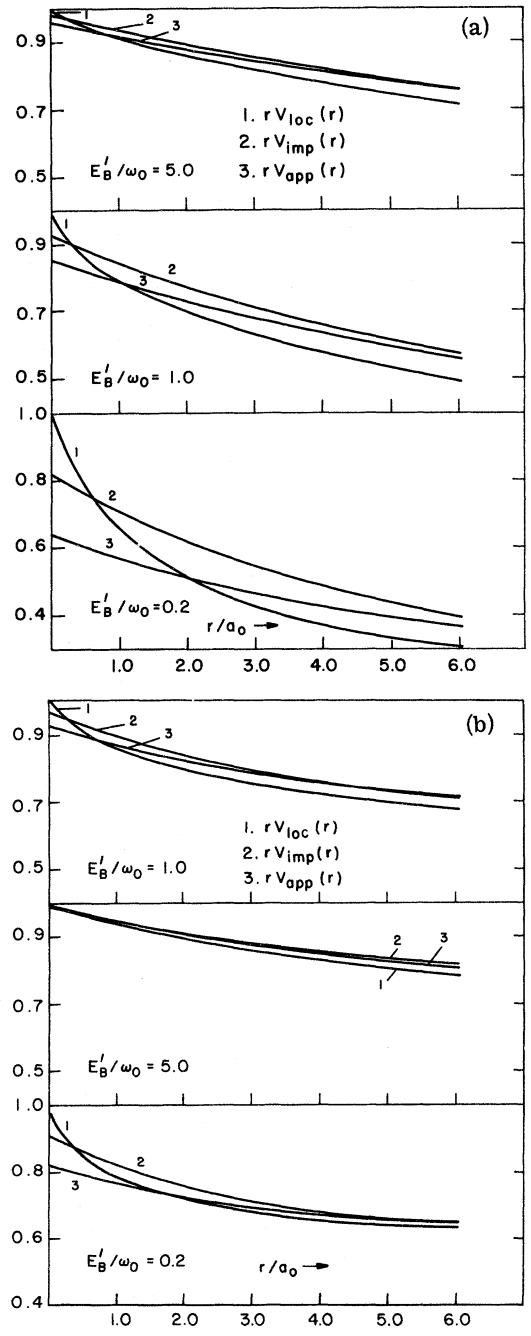


FIG. 11. (a) Comparison of the potentials derived in the text. $rV(r)$ is plotted as a function of $(r/a_0)$, where $V(r)$ is (1) $V_{loc}(r)$, with $m_e/m_h = 1$, (2) $V_{imp}(r)$, and (3) $V_{app}(r)$. For all cases $\epsilon_0/\epsilon_\infty = 7$. (b) Comparison of the potentials derived in the text. $rV(r)$ is plotted as a function of $(r/a_0)$, where $V(r)$ is (1) $V_{loc}(r)$, with $m_e/m_h = 1$, (2) $V_{imp}(r)$, and (3) $V_{app}(r)$. For all cases $\epsilon_0/\epsilon_\infty = 2$.

TABLE II. Theoretical and experimental values of exciton binding energies (BE) expressed in units of meV. $\mu^{**}$ is the interpolated reduced mass which goes to $\mu$(bare) and $\mu^*$(polaron) in two opposite limits. $E_B^H(\epsilon, \mu)$ is the hydrogenic BE using the dielectric constant $\epsilon$ and reduced mass $\mu$. $\sigma_{e,h}$ is the sum of electron and hole self-energies [Eq. (1.6) of the text]. $E_B^H(\epsilon_0, \mu^*)$ and $E_B^H(\epsilon_\infty, \mu)$ for TlCl as reported in Ref. 2 are different from that given here, as these were obtained by using $m_e, m_h$ values of Bachrach and Brown (Ref. 24). For all semiconductors except MgO, $E_B'$ was calculated with $V_{app}(r)$. For MgO, $V_{loc}$ was used.

| | $\mu^{**}$ | $E_B'$ | $\sigma_{e,h} - \sigma_{e,h}^{**}$ | $E_B$ | $E_B^H(\epsilon_0, \mu^*)$ | $E_B^H(\epsilon_\infty, \mu)$ | $E_B^{expt}$ |
|---|---|---|---|---|---|---|---|
| TlCl | 0.20 | 84.0 | −75.0 | 9.0 | 2.5 | 94.0 | $11 \pm 2$[a] |
| TlBr | 0.15 | 58.0 | −50.0 | 8.0 | 2.0 | 65.0 | $6 \pm 1$[a] |
| MgO | 0.24 | 257.0 | −159.0 | 98.0 | 42.0 | 358.0 | $85 \pm 10$[b] |
| CdS | 0.144 | 60.0 | −32.0 | 28.0 | 27.0 | 69.0 | $30 \pm 2$[c] |
| ZnS | 0.167 | 69.0 | −28.0 | 41.0 | 31.0 | 81.0 | $41 \pm 1$[d] |
| CdTe | 0.085 | 17.0 | −5.0 | 12.0 | 10.0 | 22.0 | $11 \pm 1$[e] |
| GaAs | 0.077 | 7.0 | −1.0 | 6.0 | 6.0 | 9.0 | 3.5[f] |

[a] R. Z. Bachrach and F. C. Brown (Ref. 24), also see S. Kurita and K. Kobayashi (Ref. 23).
[b] W. C. Walker, D. M. Roessler, and E. Loh (Ref. 29).
[c] D. G. Thomas (Ref. 30).
[d] C. Milloz and R. G. Wheeler (Ref. 31).
[e] D. G. Thomas, (Ref. 32).
[f] R. M. Sturge (Ref. 33).

$E_B'$, $\sigma_e^{**} + \sigma_h^{**}$, $\sigma_e + \sigma_h$, and $E_B$ are given in Table II for various polar semiconductors. The notable feature is the cancellation between $E_B'$ and $\sigma_{eh} - \sigma_{eh}^{**}$, where $\sigma_{eh} = \sigma_e + \sigma_h$. We observe that the change in the polaron self-energies when the electron and the hole bind to form an exciton reduces $E_B'$ appreciably. This leads to exciton binding energies $E_B$, which are in good agreement with experiment. As expected, the cancellation between $E_B'$ and $\sigma_{eh} - \sigma_{eh}^{**}$ is large for systems with large coupling constants. From Figs. 11(a) and 11(b), we see that for $E_B'/\omega_0 \gg 1$, $V_{loc}(r)$ is less attractive compared to $V_{app}(r)$ for a large range of $r$ values, although at the origin $V_{loc}(r)$ is more attractive. It is therefore likely that by using $V_{loc}(r)$ instead of $V_{app}(r)$, one might further improve the agreement between theory and experiment. We have tested this for the case of MgO; using $V_{app}(r)$, we find for MgO, $E_B' = 317.0$ meV, $\sigma_{eh} - \sigma_{eh}^* = -199.0$, giving $E_B = 118.0$ meV. A calculation with $V_{loc}(r)$ using the appropriate parameters for MgO yields the results given in Table II.

For comparison, we have tabulated the values of $E_B$ obtained by hydrogenic formula for the two limiting cases; one where the phonon effects are completely absent $(\epsilon_\infty, \mu)$ and the other when the phonon effects are very strong $(\epsilon_0, \mu)$. Both these limits fail to give agreement with experiment, the disagreement being severe for materials with large coupling constants.

The approximate exciton radius $r_{ex} = (2\mu^{**}E_B')^{-1/2}$

for TlCl and TlBr is seen to be smaller by a factor of 3.5 than one would have calculated from experimentally measured $E_B$. The radius $\langle r \rangle$ differs from $(2\mu^{**}E_B')^{-1/2}$ because the Schrödinger equation that gives $E_B'$ is not hydrogenic. However, we expect $\langle r \rangle$ not to differ appreciably from $r_{ex}$. For the weak coupling system, $r_{ex}$ does not differ much from the one obtained from the experimental $E_B$. The prediction made here concerning the exciton radius can be verified by measuring the diamagnetic shifts. As mentioned in Sec. I, these conclusions are applicable also to oscillator strengths.

### C. Best Hydrogenic Potential

The local electron-hole potential $V_{app}(r)$ of Eq. (4.13) can be interpreted as if the bare Coulomb potential $-e^2/r$ is screened by an $r$-dependent dielectric function $\epsilon_{eff}(r)$. As we have already discussed, $\epsilon_{eff}(r)$ approaches $\epsilon_\infty$ at small distances and $\epsilon_0$ at large distances. We can define an average dielectric function $\epsilon_{av}$ by

$$\frac{1}{\epsilon_{av}} = \int \frac{1}{\epsilon(r)} \, |\psi(\vec{r})|^2 \, d\vec{r} \Big/ \int |\psi(\vec{r})|^2 \, d\vec{r} \, . \tag{5.2}$$

Using the hydrogenic form for $\psi(\vec{r})$, we obtain

$$\frac{1}{\epsilon_{av}} = \frac{1}{\epsilon_0} + 4\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\left(\frac{E_B'}{\omega_0}\right) \ln\{\tfrac{1}{2}[1 + (1 + \omega_0/E_B')^{1/2}]\} \tag{5.3}$$

and the electron-hole potential in this approximation has the hydrogenic form

$$v_{hyd}(r) = -e^2/\epsilon_{av} r \, . \tag{5.4}$$

One can calculate $E_B'$ from Eqs. (5.2) and (5.3) and using Eqs. (4.20) and (4.23) obtain $E_B$. $E_B'$ is given by the equation

$$E_B' = [\mu(E_B')/\epsilon_{av}^2(E_B')] \text{ Ry} \, . \tag{5.5}$$

In principle, one can solve (5.4) self-consistently, allowing $\mu(E_B')$ and $\epsilon_{av}(E_B')$ to vary. For simplicity, we have used $\mu(E_B') = \mu$, the bare reduced mass, and $\mu(E_B') = \mu^{**}$, the interpolated reduced mass of Table II. The actual result should lie in between these two values if one carries out a self-consistent calculation. We have calculated $E_B'$ for TlCl, TlBr, and MgO. The two sets of $E_B'$ are, respectively, (80 and 90 meV), (56 and 61 meV), and (309 and 325 meV). Taking the mean of these pairs of values we have

$$E_B' = 85 \text{ meV for TlCl}$$
$$= 58 \text{ meV for TlBr}$$
$$= 317 \text{ meV for MgO} \, .$$

These values of $E_B'$ compare very well with those obtained from an actual numerical solution of the Schrödinger equation. This tells us that for the ground state, $\epsilon_{av}(E_B')$ with a hydrogenic model works beautifully. The values of exciton binding energies $E_B$ with the above values of $E_B'$ are practically the same as given in Table II.

For calculating the energy of other states, one could average (4.10) [or for a rough calculation (4.10) and (5.2)] with respect to the appropriate wave function. For the $2p$ state, the effective $V_{app}(r)$ is given in Appendix C.

### D. Comments on the Potential Derived by Haken

We would like to make some comments regarding the form of the effective electron-hole potential derived by Haken. Haken used a variational principle to obtain this effective form for the potential. His variational wave function was a linear combination of functions, which were products of electron and hole polaron wave functions $U_{\vec{p}}^{e(h)}(\vec{r}_{e,h}, b_{\vec{k}}^\dagger)$. However, in deriving the effective electron-hole potential he assumed $U_{\vec{p}}$ to be independent of the momentum $\vec{p}$. His form of the potential, which we denote by $V_H(r)$, is given by

$$V_H(r) = -\frac{e^2}{\epsilon_\infty r} + \frac{e^2}{r}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\left(1 - \frac{e^{-\kappa_e r} + e^{-\kappa_h r}}{2}\right) \, , \tag{5.6}$$

where $\kappa_{e,h}$ are the inverse of polaron radii, defined in Eq. (1.4). Bachrach and Brown[24] have used this potential to calculate the exciton binding energies of TlCl and TlBr. Using the known polaron masses ($\mu^*$), they find $E_B = 152$ meV for TlCl and $E_B = 75$ meV for TlBr. The experimental values given in Table II for these two are $(11 \pm 2)$ and $(6 \pm 1)$ meV, respectively. The theoretical values of $E_B$ are reduced if one uses the bare reduced mass $\mu$ instead of $\mu^*$. The agreement with the experiment is still poor.

The inadequacy of Haken potential is due to the nature of the variational wave function. By choosing it to be a product of two polaron wave functions, one does not allow the wave function to represent correlation effects, whereby when the electron and hole are close together, most of the polaron effects, are absent. In addition, the $\vec{p}$ dependence of $U_{\vec{p}}$ is expected to be quite important. Recently, Shindo[18] has also approached the problem of effective electron-hole interaction from a $t$-matrix point of view. As we have indicated in Sec. IV, the energy integration in the Bethe-Saltpeter equation for the $t$ matrix cannot be carried out when the irreducible particle-hole interaction is energy dependent. We have carried out the energy integration by making use of the spectral representation of the particle-hole $t$ matrix (equivalently the vertex function). On the other hand Shindo makes an approximation at this stage; he uses a form of the $t$ matrix that one would obtain in the *absence* of the phonon-mediated interaction $I_{ph}$. This form of

the $t$ matrix is not correct when $I_{ph}$ is included. In this sense, his electron-hole potential, as he points out, is correct for small $\alpha$ only. Shindo's results may be obtained for small $\alpha$ and small $E_B'/\omega_0$ in our formalism.

### E. Bound Polarons

The simpler problem of impurity levels may, of course, be handled in the formalism we have employed by letting one of the masses go to infinity. One has to use the potential $V_{imp}(r)$ of Eq. (4.14) in this case. However, the interpolation scheme we have developed on physical grounds is not directly applicable to this case. This is because there is no cancellation of polaron self-energies arising from the dynamic polarization around both the electron and the hole. On the other hand, one might interpolate just the electron (or hole) self-energy between its polaron value and zero using the parameter $E_B'/\omega_0$, where $E_B'$ is the binding energy obtained for the impurity potential $V_{imp}(r)$.

### F. Approximations Made

The major analytical approximation in this work is the ansatz that the effect of the vertex corrections plays an important role in altering the self-energies of the interacting electron and hole and does not affect their mutual interaction. We have shown that this is true in two limiting cases. The success of our ansatz (in that it predicts the binding energies very well) for the general case poses the theoretical question of its justification. This problem may be studied by looking at the spectral properties of the vertex functions.

In arriving a the conclusion that the leading corrections due to the vertex are smaller for the mutual interaction than for the self-energy, we have made two approximations: neglect of the incoherent part of the single-particle Green's function and the pole approximation to the exciton Green's function. We now justify these on heuristic grounds. For $E_B \ll \omega_0$, the incoherent part does not contribute because the continuum is separated by $\omega_0$ from the pole; for $E_B \gg \omega_0$, we expect that very little weight is left in the incoherent part. Thus, the first approximation would appear to be justified. The second approximation is related to the first; it amounts to assuming that an exciton is a combination of a quasiparticle and a quasihole. In the two limits, this would again seem to be justified; in one limit we have polarons, in the other, bare particles.

### ACKNOWLEDGMENTS

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### APPENDIX A: METHOD FOR PERFORMING ENERGY INTEGRATIONS

It was pointed out in the text that when the irreducible particle-hole interaction $I(k, k'')$ is energy dependent, the $t(k, k')$ matrix does not satisfy the simple Schrödinger equation (2.8). In this case the effective-mass equation (EME) for the exciton is obtained when one makes the pole approximation for the exciton Green's function (see Sham and Rice[7]). To obtain this EME, one has to integrate over the energy variables $\zeta$ and $\zeta'$ of $t(k, k')$. This is done by analyzing the analytic property of $I(\vec{k}\zeta, \vec{k}''\zeta'')$ as a function of both $\zeta$ and $\zeta''$. The general procedure for carrying out the energy integrations is to separate $I(k, k'')$ into four parts:

$$I(k, k'') = I_{++}(k, k'') + I_{+-}(k, k'') + I_{-+}(k, k'') + I_{--}(k, k''), \tag{A1}$$

where $I^{++}$ has poles in the lower-halves of both the $\zeta$ and $\zeta''$ plane, $I^{--}$ has poles in the upper-halves of the $\zeta$ and $\zeta''$ plane, $I^{+-}$ has poles in the lower-half of the $\zeta$ and the upper-half of the $\zeta''$ plane, and $I^{-+}$ has poles in the upper-half of the $\zeta$ and the lower-half of the $\zeta''$ plane. The $\zeta$ and $\zeta''$ contours are then closed such that one avoids the poles of $I(k, k'')$ and only the electron and hole poles contribute to the energy integration. Thus, after carrying out the $\zeta$ and $\zeta''$ integrations, one has

$$\begin{aligned} I(\vec{k}, \vec{k}''; \omega\vec{Q}) = {} & I_{++}(\omega, \omega + E_h(\vec{k} - \tfrac{1}{2}\vec{Q}), \omega + E_h(\vec{k}'' - \tfrac{1}{2}\vec{Q})) \\ & - I_{-+}(\omega, E_e(\vec{k} + \tfrac{1}{2}\vec{Q}), \omega + E_h(\vec{k}'' - \tfrac{1}{2}\vec{Q})) \\ & - I_{+-}(\omega, \omega + E_h(\vec{k} - \tfrac{1}{2}\vec{Q}), E_e(\vec{k}'' + \tfrac{1}{2}\vec{Q})) \\ & + I_{--}(\omega, E_e(\vec{k} + \tfrac{1}{2}\vec{Q}), E_e(\vec{k}'' + \tfrac{1}{2}\vec{Q})) . \end{aligned} \tag{A2}$$

In Eq. (A2), $\omega$ is the internal energy of the exciton, the second arguments of all the four parts of $I$ refer to the $\zeta$ variable, whereas the third arguments refer to the $\zeta''$ variable.

The contribution to $I(k,k'')$ from the single-phonon exchange is given by

$$\tilde{I}_{ph}(k, k'') = -\frac{4\pi e^2 \nu}{|\vec{k} - \vec{k}''|^2} \left( \frac{1}{\zeta'' - \zeta - \omega_0 + i\delta} - \frac{1}{\zeta'' - \zeta + \omega_0 + i\delta} \right) , \tag{A3}$$

where $\nu = \frac{1}{2}\omega_0(1/\epsilon_\infty - 1/\epsilon_0)$. The first term inside

the large parentheses of Eq. (A3) has poles in the upper-half of the $\zeta$ plane and the lower-half of the $\zeta''$ plane and is equivalent to $I_{-+}(k, k'')$. The second term has opposite analytic property and is equivalent to $I_{+-}(k, k'')$. After carrying out the $\zeta$ and $\zeta''$ integrations, one has

$$\tilde{I}_{\rm ph}(\vec{k}, \vec{k}''; \vec{Q}\omega) = \frac{4\pi e^2\nu}{|\vec{k}-\vec{k}''|^2}\left(\frac{1}{\omega + E_h(\vec{k}''-\vec{Q}) - E_e(\vec{k}+\frac{1}{2}\vec{Q}) - \omega_0} - \frac{1}{E_e(\vec{k}''+\frac{1}{2}\vec{Q}) - \omega - E_h(\vec{k}-\frac{1}{2}\vec{Q}) + \omega_0}\right) . \quad \text{(A4)}$$

## APPENDIX B: PHONON VERTEX CORRECTIONS TO (i) COULOMB AND (ii) PHONON EXCHANGE INTERACTIONS

While carrying out the $\zeta$ and $\zeta'$ intergrations one has to study the analytic behavior of $I(k, k')$ as a function of $\zeta$ and $\zeta'$. On inclusion of the phonon vertex corrections $\Lambda(\zeta, \zeta')$ it is the analytic properties of the $\Lambda\tilde{I}$ that are important. Although $\Lambda(\zeta, \zeta')$ is the same for both cases (i) and (ii), the analytic behavior of $\tilde{I}$ is different for these two cases. We therefore consider these cases separately.

(i) *Phonon correction to the Coulomb line.* Let us consider only the electron part, the hole part being exactly similar. The total contribution to $I$ is given by [see Figs. 8(a) and 8(b)]

$$\begin{aligned} I(k, k') &= \Lambda_e(k, k')\,\tilde{I}(k, k') \\ &= v(\vec{k}-\vec{k}')\int G_e(k-k'')\,G_e(k'-k'') \\ &\quad \times D(\vec{k}''\zeta'')\frac{4\pi e^2\nu}{|\vec{k}''|^2}\,\frac{d\vec{k}''}{(2\pi)^3}\,\frac{d\zeta''}{2\pi i}, \end{aligned} \quad \text{(B1)}$$

where $v(\vec{k}-\vec{k}')$ is the Coulomb interaction screened by the high-frequency dielectric constant $\epsilon_\infty$. We rewrite (B1) as

$$\begin{aligned} I(\omega, \zeta', \zeta) = v(\vec{k}-\vec{k}')\,4\pi e^2\nu \int \frac{d\vec{k}''}{(2\pi)^3}\,\frac{1}{|\vec{k}''|^2} \\ \times\left(\frac{1}{\zeta - \zeta'' - E_e(\vec{k}-\vec{k}'') + i\eta}\right. \\ \left.\times\frac{1}{\zeta' - \zeta'' - E_e(\vec{k}'-\vec{k}'') + i\eta}\right) \\ \times\left(\frac{1}{\zeta'' - \omega_0 + i\delta} - \frac{1}{\zeta'' + \omega_0 - i\delta}\right)\frac{d\zeta''}{2\pi i} . \end{aligned} \quad \text{(B2)}$$

The first term of the phonon propagator has a pole in the lower-half of the $\zeta''$ plane. For this term we close the contour in the upper-half plane, and both the electron poles contribute. The second term has poles in the upper-half of the $\zeta''$ plane; we close the contour in the lower-half, and there is no contribution from the electron poles. Therefore, the $\zeta''$ integration gives

$$\begin{aligned} I(\omega, \zeta', \zeta) = v(\vec{k}-\vec{k}')4\pi e^2\nu \int \frac{d\vec{k}''}{(2\pi)^3}\,\frac{1}{k''^2} \\ \times\left(\frac{1}{\zeta - \omega_0 - E_e(\vec{k}-\vec{k}'') + i\eta}\right. \\ \left.\times\frac{1}{\zeta' - \omega_0 - E_e(\vec{k}'-\vec{k}'') + i\eta}\right) . \end{aligned} \quad \text{(B3)}$$

Since the contribution to $I$ from $\tilde{I}$ is just $v(\vec{k}-\vec{k}')$, which is independent of $\zeta$ and $\zeta'$, the entire $\zeta$ and $\zeta'$ dependence is given by the term inside the large parentheses. As a function of both $\zeta$ and $\zeta'$ it has poles in the lower-half plane and is therefore equivalent to $I_{++}$. Therefore, the $\zeta$, $\zeta'$ integration gives

$$\begin{aligned} I(\vec{k}, \vec{k}'; \omega) &= v(\vec{k}-\vec{k}')4\pi e^2\nu \\ &\quad \times\int \frac{d\vec{k}''}{(2\pi)^3}\,\frac{1}{|k''|^2}\left(\frac{1}{\omega + E_h(\vec{k}) - \omega_0 - E_e(\vec{k}-\vec{k}'')}\right. \\ &\quad \left.\times\frac{1}{\omega + E_h(\vec{k}') - \omega_0 - E_e(\vec{k}'-\vec{k}'')}\right) \\ &\equiv v(\vec{k}-\vec{k}')\Lambda_{e,c}(\vec{k}, \vec{t}; \omega) . \end{aligned} \quad \text{(B4)}$$

We consider (B4) for small $\vec{t}$. The terms proportional to $\vec{t}\cdot\vec{k}''$ vanish when one carries out the $\vec{k}''$ angular integration. Also we look in the limit of small $\vec{k}$ to get

$$\Lambda_{e,c}(\vec{k}, t) \simeq \Lambda^c_{e,1} + \Lambda^c_{e,2} + \Lambda^c_{e,3} , \quad \text{(B5)}$$

where

$$\Lambda^c_{e,1} = 1 + \frac{\alpha_e}{2}\left(\frac{\omega_0}{\omega_0 + E'_B}\right)^{3/2} , \quad \text{(B6)}$$

$$\Lambda^c_{e,2} = -\frac{3\alpha_e}{4}\,\frac{t^2/2\mu}{E'_B}\,\frac{E'_B}{E'_B + \omega_0}\left(\frac{\omega_0}{E'_B + \omega_0}\right)^{3/2} , \quad \text{(B7)}$$

$$\Lambda^c_{e,3} = \frac{5\alpha_e}{4}\,\frac{|\vec{k}|^2}{2\mu}\left(\frac{\omega_0}{\omega_0 + E'_B}\right)^{3/2}\frac{1}{\omega_0 + E'_B} . \quad \text{(B8)}$$

(ii) *Phonon correction to the phonon line* [see Fig. 8(a)]. We have

$$\begin{aligned} \Lambda_{e,\rm ph}(k, t)\tilde{I}_{\rm ph} = (4\pi e^2\nu)^2 \int G_e(k-k')G_e(k'-k'')D(k'') \\ \times D(k'-k)\,\frac{1}{|\vec{k}''|^2}\,\frac{1}{|\vec{k}-\vec{k}'|^2}\,\frac{d\vec{k}''}{(2\pi)^3}\,\frac{d\zeta''}{2\pi i} , \end{aligned} \quad \text{(B9)}$$

which gives

$$\Lambda_{e,\mathrm{ph}}(k,t)\tilde{I}_{\mathrm{ph}}=\frac{(4\pi e^2\nu)^2}{|\vec{k}-\vec{k}'|^2}\int\frac{d\vec{k}''}{(2\pi)^3}\frac{1}{|\vec{k}''|^2}\left(\frac{1}{\zeta-\zeta''-E_e(\vec{k}-\vec{k}'')+i\eta}\ \frac{1}{\zeta'-\zeta''-E_e(\vec{k}'-\vec{k}'')+i\eta}\right)\frac{d\zeta''}{2\pi i}$$
$$\times\left(\frac{1}{\zeta''-\omega_0+i\delta}-\frac{1}{\zeta''+\omega_0-i\delta}\right)\left(\frac{1}{\zeta'-\zeta-\omega_0+i\delta}-\frac{1}{\zeta'-\zeta+\omega_0-i\delta}\right). \quad \text{(B10)}$$

The $\zeta''$ integration can be performed exactly in the manner as before, and one has

$$\Lambda_{e,\mathrm{ph}}\tilde{I}_{\mathrm{ph}}=\frac{(4\pi e^2\nu)^2}{|k-k'|^2}\int\frac{d\vec{k}''}{(2\pi)^3}\frac{1}{|\vec{k}''|^2}\left(\frac{1}{\zeta-\omega_0-E_e(\vec{k}-\vec{k}'')+i\eta}\ \frac{1}{\zeta'-\omega_0-E_e(\vec{k}'-\vec{k}'')+i\eta}\right)$$
$$\times\left(\frac{1}{\zeta'-\zeta-\omega_0+i\delta}-\frac{1}{\zeta'-\zeta+\omega_0-i\delta}\right). \quad \text{(B9')}$$

$\tilde{I}_{\mathrm{ph}}$, as distinct from the previous case, depends on $\zeta$ and $\zeta'$, and has poles in both upper- and lower-halves as functions of $\zeta$ and $\zeta'$. If we take the first phonon term, we see that the product $\Lambda_{e,\mathrm{ph}}\tilde{I}_{\mathrm{ph}}$ has poles in the lower-half of the $\zeta'$ plane, but has poles both in the upper- and lower-halves of the $\zeta$ plane. One has to separate this term such that these two poles in the $\zeta$ plane are separated. A similar situation arises for the second phonon term as a function of $\zeta'$. One has, therefore, four terms. After studying the analytic properties of these four terms and carrying out the $\zeta$, $\zeta'$ integrations, one has

$$\Lambda_{e,\mathrm{ph}}\tilde{I}_{\mathrm{ph}}=\frac{(4\pi e^2\nu)^2}{|\vec{k}-\vec{k}'|^2}\left(\frac{1}{\omega+E_h(\vec{k}')-E_e(\vec{k})-\omega_0}\,\bar{\Lambda}_{e,\mathrm{ph}}(\vec{k},t)\right.$$
$$\left.+\frac{1}{\omega+E_h(k)-E_e(k')-\omega_0}\,\bar{\Lambda}_{e,\mathrm{ph}}(\vec{k}',t)\right), \quad \text{(B11)}$$

where

$$\bar{\Lambda}_{e,\mathrm{ph}}=\int\frac{d\vec{k}''}{(2\pi)^3}\frac{1}{|\vec{k}''|^2}\left[\frac{1}{\omega+E_h(\vec{k}')-\omega_0-E_e(\vec{k}'-\vec{k}'')}\ \frac{1}{\omega+E_h(\vec{k}')-2\omega_0-E_e(\vec{k}-\vec{k}'')}\right.$$
$$\left.\times\left(1+\frac{\omega+E_h(\vec{k}')-\omega_0-E_e(\vec{k})}{\omega+E_h(\vec{k})-\omega_0-E_e(\vec{k}-\vec{k}'')}\right)\right]. \quad \text{(B11')}$$

Again, $\Lambda_{e,\mathrm{ph}}(\vec{k},t)$ can be expanded for small values of $\vec{t}$ and $\vec{k}$:

$$\Lambda_{e,\mathrm{ph}}=\Lambda_{e,1}^{\mathrm{ph}}+\Lambda_{e,2}^{\mathrm{ph}}+\Lambda_{e,3}^{\mathrm{ph}}, \quad \text{(B12)}$$

where

$$\Lambda_{e,1}^{\mathrm{ph}}=\frac{\alpha_e}{2}\left(\frac{\omega_0}{E_B+\omega_0}\right)^{1/2}-\alpha_e\frac{E_B}{\omega_0}\left[\left(\frac{\omega_0}{E_B+\omega_0}\right)^{1/2}-\left(\frac{\omega_0}{E_B+2\omega_0}\right)^{1/2}\right] \quad \text{(B13)}$$

and

$$\Lambda_{e,2}^{\mathrm{ph}}=-2\alpha_e t^2\ \omega_0^{3/2}\left[\frac{1}{2}\left(\frac{2}{3m_e}-\frac{1}{2\mu}\right)\left(\frac{1}{\omega_0^2}X-\frac{1}{2\omega_0(E_B+\omega_0)^{3/2}}\right)\right.$$
$$+\frac{1}{4}\frac{E_B+\omega_0}{2\mu}\left(\frac{2}{\omega_0^3}X-\frac{1}{\omega_0^2}\frac{1}{(E_B+\omega_0)^{3/2}}+\frac{3}{4\omega_0}\frac{1}{(E_B+\omega_0)^{5/2}}\right)$$
$$\left.-\frac{1}{9}\frac{(E_B+\omega_0)^2}{2m_e}\left(\frac{6}{\omega_0^4}X-\frac{3}{\omega_0^3(E_B+\omega_0)^{3/2}}+\frac{9}{4\omega_0^2}\frac{1}{(E_B+\omega_0)^{5/2}}-\frac{15}{8\omega_0(E_B+\omega_0)^{7/2}}\right)\right]$$
$$-\frac{t^2}{2\pi}(2m_e)^{1/2}\frac{E_B}{4m_h}\left(-\frac{2}{\omega_0^3}X+\frac{1}{2\omega_0^2(E_B+2\omega_0)^{3/2}}+\frac{1}{2\omega_0^2}\frac{1}{(E_B+\omega_0)^{3/2}}\right), \quad \text{(B14)}$$

where

$$X=\frac{1}{(E_B+\omega_0)^{1/2}}-\frac{1}{(E_B+2\omega_0)^{1/2}}$$

and

$$\Lambda_{e,3}^{\mathrm{ph}}=\alpha_e\frac{|\vec{k}|^2}{2m_e\omega_0}\left[\frac{1}{2}\left(\frac{1}{3}-\frac{m_e}{\mu}\right)Y-\frac{4m_e}{\mu}X\right.$$

$$-\frac{m_e}{2\mu}\left(1-\frac{4\mu}{2m_e}\right)\left(\frac{\omega_0}{E_B+\omega_0}\right)^{3/2} + \frac{m_e}{\mu}\frac{E_B+\omega_0}{\omega_0}Y\Bigg], \quad \text{(B15)}$$

where

$$Y=[\omega_0/(E_B+\omega_0)]^{3/2}-[\omega_0/(E_B+2\omega_0)]^{3/2}.$$

In (3.13), (3.14), and (3.20) the appropriate limits of the above expressions are taken for the case $m_e=m_h$.

## APPENDIX C: LOCAL POTENTIAL FOR THE $p$ STATE

We have the simplest form of the $p$-state wave function

$$\psi_p(\vec{r})=B_p r e^{-\alpha r}Y_{1m}(\hat{r}). \quad \text{(C1)}$$

While obtaining the local potential for the $s$ state, we had approximated $[(m_e^*/M^*)r+(m_h^*/M^*)r']\times(|\vec{r}-\vec{r}'|)^{-1}$ by $r/|\vec{r}-\vec{r}'|$. We make a similar approximation here. The potential for the $p$ state has the form (for simplicity we denote $\mu^{**}$ as $\mu$ and $E_B'$ as $E_B$; in the actual potential $\mu^{**}$ and $E_B'$ occur)

$$v_p(r)=-e^2[1/\epsilon_\infty r-v_{\rm ph}(r)], \quad \text{(C2)}$$

where

$$v_{\rm ph}(r)=\frac{1}{r}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)+\frac{A}{r^2}+\frac{B(r)}{r^3}+\frac{C(r)}{r^4}. \quad \text{(C3)}$$

In (C3), we have

$$A=4\left(\frac{E_B}{\omega_0}\right)^{1/2}\left(\frac{1}{2\mu\omega_0}\right)^{1/2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right),$$

$$B(r)=8\frac{E_B}{\omega_0}\frac{1}{2\mu\omega_0}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\Bigg[1-\left(\frac{E_B+\omega_0}{E_B}\right)^{1/2}\times\exp(-\{[2\mu(E_B+\omega_0)]^{1/2}-(2\mu E_B)^{1/2}\}r)\Bigg],$$

$$C(r)=8\left(\frac{E_B}{\omega_0}\right)^{1/2}\frac{1}{(2\mu\omega_0)^{3/2}}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\times\left(1-\exp\{-|[2\mu(E_B+\omega_0)]^{1/2}-(2\mu E_B)^{1/2}|r\}\right).$$

For large $r$, the leading contribution beyond the $-1/\epsilon_0 r$ potential is again $1/r^2$, and is proportional to $(E_B/\omega_0)^{1/2}$ as in the case of the $s$-state potential. The potential, however, is twice as large as that for the $s$ state and has to do with the angular charge distribution of the $p$ state. Although the potential has terms going as $1/r^3$ and $1/r^4$ they do not lead to any singularity at $r=0$. This is easily seen by expanding the exponentials occurring in $B(r)$ and $C(r)$ for small $r$. The first term of $C(r)$ goes as $r$ near the origin. Therefore, there is no $1/r^4$ contribution. The coefficient of the $1/r^3$ term also vanishes. The leading nonzero term is $O(1/r^2)$ and has no divergent contribution, as we are dealing with a $p$ state.

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# Effective Electron-Hole Interaction in Polar Semiconductors*

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The effective-mass equation for an exciton in a polar semiconductor is derived, including the corrections to the effective electron-hole interaction originating in electron (hole)–optical-phonon interaction. It is assumed that the electron (hole)–phonon coupling is weak (the Fröhlich constant $\alpha_{e,h} \ll 1$) and that the binding energy of the exciton is small [$\beta = (E_B/\hbar\omega_0)^{1/2} \ll 1$]. The electron and hole self-energies and the irreducible vertex part are calculated to include terms up to the order $\alpha\beta^4\hbar\omega_0$. The homogeneous Bethe-Salpeter equation is reduced to a hydrogenlike equation containing additional terms of the forms $p_{e,h}^4$ and $\delta(\vec{r})$. They are of the order $\alpha\beta^4\hbar\omega_0$ and correspond to the nonparabolicity of the dispersion laws and to the effect of the phonon-field fluctuations, respectively. Contrary to other theories, no term of the order $\alpha\beta^3\hbar\omega_0$ behaving asymptotically as $1/r^2$ is present in the effective Hamiltonian.

## I. INTRODUCTION

Two polarons, e.g., an electron and a hole in a polar semiconductor, interact to a good approximation via a Coulomb interaction which is screened by the static dielectric constant when their separation is large and by the optical constant at a small separation. The distance between the polarons is compared to the sum of the polaron radii[1]

$$\rho_{e,h} = (m_{e,h}^{(0)}\omega_0)^{-1/2}, \tag{1}$$

where $m_{e,h}^{(0)}$ are the effective masses of the electron and the hole assuming the ions are fixed and $\omega_0$ is the optical-phonon frequency. We put $\hbar = 1$. Haken[2] derived an interpolation formula for distances comparable to polaron radii on the basis of a variational principle. His formula predicts that the corrections to the Coulombic field at large distances decrease exponentially, reflecting the exponentially decreasing overlap between the clouds of the bound charges around the polarons.[3]

However, we can easily convince ourselves that there must exist corrections to the potential of other analytical forms. For instance, the interaction of the electron (hole) with the zero-point fluctuations of the phonon field (in other words the recoil effects caused by emission and reabsorption of virtual phonons) leads to an analog of the Zitterbewegung; thus a contact term [$\sim \delta(r)$] may be expected in the effective interaction.

The electron-hole system interacting with the phonon field is described by the Fröhlich[1] Hamiltonian

$$\sum_{\vec{k}} \frac{k^2}{2m_e} a_{\vec{k}}^\dagger a_{\vec{k}} + \sum_{\vec{k}} \frac{k^2}{2m_h} b_{\vec{k}}^\dagger b_{\vec{k}} - \frac{4\pi e^2}{\epsilon_\infty \Omega} \sum_{\vec{k}_1\vec{k}_2\vec{k}_3} \frac{1}{(\vec{k}_3 - \vec{k}_1)^2} b_{\vec{k}_4}^\dagger b_{\vec{k}_2} a_{\vec{k}_3}^\dagger a_{\vec{k}_1} + \sum_{\vec{q}} \omega_0 c_{\vec{q}}^\dagger c_{\vec{q}} + \frac{i}{\sqrt{\Omega}} \sum_{\vec{k},\vec{q}} V_{\vec{q}} (c_{-\vec{q}}^\dagger - c_{\vec{q}}) a_{\vec{k}+\vec{q}}^\dagger a_{\vec{k}}$$