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Comparison of Screened Exchange with the Slater Approximation for Silicon

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The exchange self-energy in silicon is calculated using the dynamic Penn dielectric function and pseudopotential wave functions. Comparison is made with Slater's $\rho^{1/3}$ approximation, and it is concluded that errors of the order of 0.5 to 2 eV result. The static dielectric function gives 15% errors in the average self-energy but only 2–3% errors in the exchange-gap enhancements.

I. INTRODUCTION AND CONCLUSIONS

The Hartree-Fock approximation has long been known to be highly unsatisfactory for calculating energy bands in solids.[1,2] Studies beyond the Hartree-Fock approximation have been made using many-body perturbation theory.[3] Most such calculations employ the random-phase approximation (RPA) which is equivalent to replacing the bare Coulomb interaction in the Hartree-Fock exchange terms by a dynamically screened interaction. It has been suggested that statically screened exchange would be sufficiently accurate for band calculations[1-3] because band gaps are small compared to the plasma frequency and we have found this to be the case.

Although calculations using screened exchange have recently been performed on the alkali halides,[4] the great majority of *a priori* band calculations have used Slater's "$\rho^{1/3}$" approximation to exchange.[5] Slater's method is a "local-density" approximation which uses the average exchange energy of the free-electron gas as a function of density as calculated in the Hartree-Fock approximation. The exchange energy is then assumed to follow the local density in the solid. Kohn and Sham[6] have justified the use of the "local-density" approach for calculations of the ground-state energy with slowly varying disturbances of small amplitude. They pointed out that the electron self-energy at the Fermi surface should be used rather than the average self-energy. This correction introduces a factor $\alpha = \frac{2}{3}$ in Slater's potential. Recently α has been used as an adjustable parameter which can be empirically determined to improve agreement between theory and experiment.[7]

Recent work on silicon using a completely empirical local valence-valence exchange potential suggested a fundamental incompatibility between experimental gaps and masses.[8] These quantities are connected by a $\vec{k}\cdot\vec{p}$ relation for a local potential. The incompatibilities amounted to 0.5 to 0.7 eV in band gaps or 15–20% in masses. These results do not strongly contradict Kohn and Sham's work, first because they refer to energy gaps rather than ground-state energies, and secondly because the energies are a small fraction of the total self-energy (−10 eV), whereas the atomic spacing is not really large compared to the Fermi wavelength.

In the present paper we compute the screened exchange interaction for silicon using RPA. We use the Penn model[9] to compute the dynamic dielectric function. We ignore "local-field effects"; i.e., we neglect those terms in the dielectric function which are nondiagonal in vectors of the reciprocal lattice.[10] (But we do *not* restrict momentum transfers to the first Brillouin zone as this would lead to an error of about a factor of 2.) We use pseudopotential wave functions as given by Brust's empirical pseudopotential.[11] We find that the static approximation to the dielectric function leads to errors of 15% in average exchange energies but to only 2–3% errors in the exchange contribution to the energy gaps.

We compare our screened-exchange results to Slater's $\alpha\rho^{1/3}$ method with $\alpha = 0.88$ which produces equal exchange energies at the top of the valence band, $\Gamma_{25'}$. We find some energy-band features agree closely in the two calculations while others differ by 0.5 to 2 eV. In general, we feel that Slater's method is not reliable in terms of present-day standards of accuracy and that more attention should be given to the problem of calculating screened exchange.

Our results here provide some support for our empirical observations concerning the inadequacies of local potentials.[8] However, we have not calculated masses with sufficient accuracy for quantitative support.

II. RPA SELF-ENERGY

A. Formalism

Hedin and Lundquist[3] give the following expressions for the electron self-energy operator $\hat{\Sigma}$ in the RPA approximation:

$$\hat{\Sigma}(\vec{r}_1, t_1; \vec{r}_2, t_2) = iW(\vec{r}_1, t_1; \vec{r}_2, t_2)\, G_0(\vec{r}_1, t_1; \vec{r}_2, t_2)\ , \tag{1}$$

$$W(\vec{r}_1, t_1; \vec{r}_2, t_2) = \int v(\vec{r}_1, \vec{r}_3)\ \kappa^{-1}(\vec{r}_3, t_1; \vec{r}_2, t_2)\, d\vec{r}_3\ , \tag{2}$$

$$G_0(\vec{r}_1, t_1; \vec{r}_2, t_2) = (1/2\pi) \int G_0(\vec{r}_1, \vec{r}_2, \omega) e^{-i\omega(t_1 - t_2)}\, d\omega, \tag{3}$$

$$G_0(\vec{r}_1, \vec{r}_2, \omega) = \sum_{n,\vec{k}} \frac{\Phi_{n\vec{k}}(\vec{r}_1)\ \Phi^*_{n\vec{k}}(\vec{r}_2) e^{i\delta\omega}}{\omega - \epsilon_{n\vec{k}} + i\delta\epsilon_{n\vec{k}}}\ . \tag{4}$$

In Eq. (4), δ is a positive infinitesimal. All energies are measured from the Fermi level, taken to be infinitesimally above the valence-band maximum.

In these equations $v(\vec{r}_1, \vec{r}_3)$ is the bare Coulomb potential $e^2/|\vec{r}_1 - \vec{r}_3|$ or in Fourier space

$$v(\vec{r}_1, \vec{r}_3) = (2\pi)^{-3} \int v_q e^{i\vec{q}\cdot(\vec{r}_1 - \vec{r}_3)}\, d\vec{q}\ , \qquad v_q = 4\pi/q^2\ . \tag{5}$$

κ is the propagating dielectric function,[12] and W is the dynamically screened potential. G_0 is the unperturbed propagator based on the Bloch eigenfunctions $\Phi_{n\vec{k}}(\vec{r})$ of the effective single-particle potential.

We assume that the dielectric function is diagonal in momentum space (i.e., we ignore local-field corrections).[10] Then following Schrieffer[12] and Adler,[10] we can write the dielectric function as

$$\kappa(q, \omega) = 1 + \frac{4\pi e^2 H_{\mathrm{ub}}}{q^2 V} \sum_{n_1, n_2, \vec{k}_1, \vec{k}_2} \frac{|\langle \Phi_{n_1\vec{k}_1} | e^{-i\vec{q}\cdot\vec{r}} | \Phi_{n_2\vec{k}_2} \rangle|^2\ [\theta(\epsilon_{n_1\vec{k}_1} - \epsilon_F) - \theta(\epsilon_{n_2\vec{k}_2} - \epsilon_F)]}{\hbar\omega + \epsilon_{n_1\vec{k}_1} - \epsilon_{n_2\vec{k}_2} + i\delta\hbar\omega}\ , \tag{6}$$

$$H_{\mathrm{ub}} = 1 - \frac{1}{2}\ \frac{q^2}{q^2 + k_F^2 + 2k_F/\pi a_0}\ ,$$

where $\theta(x)$ is the unit step function $\theta(+) = 1$, $\theta(-) = 0$. H_{ub} is the Hubbard correction factor for exchange as used by Heine and Abarenkov.[13] In some of the calculations we have set $H_{\mathrm{ub}} = 1$; a_0 is the Bohr radius. The matrix element requires

$$\vec{k}_1 = \vec{k}_2 - \vec{q} - \vec{K}\ , \tag{7}$$

where $\vec{K}$ is a vector of the reciprocal lattice. We do not limit $\vec{q}$ to the first Brillouin zone. We will find that outer zones make a significant contribution to $\hat{\Sigma}$.

We consider only the "diagonal" terms in the self-energy, namely

$$\hat{\Sigma}_{n,n} = \langle \Phi_{n\vec{k}}(\vec{r}_1) |\, \hat{\Sigma}(\vec{r}_1, \vec{r}_2, \omega)\, | \Phi_{n\vec{k}}(\vec{r}_2) \rangle\ , \tag{7a}$$

where the Fourier transform of $\hat{\Sigma}(\vec{r}_1, t_1; \vec{r}_2, t_2)$ in Eq. (1) has been introduced. In a completely first-principles calculation this approximation would require

$$|\hat{\Sigma}_{n,n'}(\vec{k})| \ll |\epsilon_{n\vec{k}} - \epsilon_{n'\vec{k}}| \quad . \tag{7b}$$

In our numerical work we use pseudopotential wave functions determined from an empirical pseudopotential. Therefore, to the extent that the limitations of the assumed form of the pseudopotential permit it, exchange has already been included in the wave functions and nondiagonal terms should *not* be further included. From this point of view, exchange is not a further correction to be added to the pseudopotential energies. Rather we seek to determine what fraction of the empirical energy is due to exchange. This cannot be accurately true because the three-parameter local effective potential is too limited in scope to represent a thorough empirical description of the energy bands but it should be a reasonable first approximation.

Using Eqs. (1), (2), and (6) in Eq. (7), we can write

$$\hat{\Sigma}_{n_1n_1}(\vec{k}_1, \omega) = \sum_{q, n_2, \vec{k}_2} v_q F_{n_1\vec{k}_1, n_2\vec{k}_2}(\vec{q}) S(q, \epsilon_{n_2\vec{k}_2}) \ , \tag{8}$$

$$F_{n_1\vec{k}_1, n_2\vec{k}_2}(\vec{q}) \equiv |\langle \Phi_{n_1\vec{k}_1}(\vec{r}) | e^{i\vec{q}\cdot\vec{r}} | \Phi_{n_2\vec{k}_2}(\vec{r}) \rangle|^2 \ , \tag{9}$$

$$S(q, \epsilon) \equiv \frac{i}{2\pi} \int_{-\infty}^{\infty} d\Omega \, \frac{1}{\kappa(q, \Omega)} \, \frac{e^{i\delta(\omega - \Omega)}}{(\omega - \Omega - \epsilon + i\delta\epsilon)} \ . \tag{10}$$

We divide S in Eq. (10) into three pieces using $\kappa^{-1} = (\kappa^{-1} - 1) + 1$, and deform the contour of integration for Ω from the real to the imaginary axis:

$$S = S_1 + S_2 + S_3 \ , \tag{11}$$

$$S_1 = -\theta(-\epsilon) \ , \tag{12}$$

$$S_2 = \left(\frac{1}{\kappa(q, \omega - \epsilon)} - 1\right) [\theta(\epsilon)\theta(\omega - \epsilon) - \theta(-\epsilon)\theta(\epsilon - \omega)] \ , \tag{13}$$

$$S_3 = -\frac{1}{2\pi} \int_{-\infty}^{\infty} dw \left(\frac{1}{\kappa(q, iw)} - 1\right) \frac{1}{(\omega - \epsilon - iw)} \ ; \tag{14}$$

S_2 comes from the poles of the G_0 factor in shifting the contour from the real to the imaginary axis.

Assuming inversion symmetry it is easily shown that $\kappa(q, -iw) = \kappa(q, iw)$. Using this relation and simplifying Eq. (13), we have

$$S_2 = \left(\frac{1}{\kappa(q, \omega - \epsilon)} - 1\right) [\theta(\epsilon) - \theta(\epsilon - \omega)] \ , \tag{15}$$

$$S_3 = \frac{-1}{\pi} \int_0^{\infty} dw \left(\frac{1}{\kappa(q, iw)} - 1\right) \frac{\omega - \epsilon}{(\omega - \epsilon)^2 + w^2} \ , \tag{16}$$

for $\omega - \epsilon$ such that $\kappa(q, i(\omega - \epsilon)) \simeq \kappa(q, 0)$, Eq. (16) becomes

$$S_3 = \frac{1}{2} \left(\frac{1}{\kappa(q, 0)} - 1\right) [\theta(\epsilon - \omega) - \theta(\omega - \epsilon)] \ , \quad |\epsilon - \omega| \text{ small.} \tag{17}$$

$\kappa(q, \omega)$ is sensitive to energies of the order of the energy gap in the Penn model[9] or the order of qk_F in the free-electron gas.[12] However, $(\kappa^{-1} - 1)$ is less sensitive and only varies appreciably for $|\epsilon - \omega| \sim \omega_p$ (ω_p is the plasma frequency). Hence, we need only require $|\epsilon - \omega| \ll \omega_p$ in Eq. (17).

Making the static approximation in Eq. (15) also, we can sum the three contributions and write Eq. (11) as

$$S = -\left(\frac{1 - \theta(\epsilon)}{\kappa(q, 0)}\right) + \frac{1}{2}\left(\frac{1}{\kappa(q, 0)} - 1\right) . \tag{18}$$

The first term in large parens on the right-hand side of Eq. (18) is a statically screened exchange (SX), while the second is the interaction of the electron with the induced charge it creates, the "Coulomb hole" (CH). These results have been previously obtained and interpreted by Hedin[14] and by Brinkman and Goodman.[2]

If we continue the static approximation in Eqs. (8) and (9), we find

$$\sum_{n_2, \vec{k}_2} F_{n_1\vec{k}_1, n_2\vec{k}_2}(\vec{q}) = 1 \ . \tag{19}$$

This result follows because $\Phi^*_{n_1\vec{k}_1}(\vec{r}) e^{i\vec{q}\cdot\vec{r}}$ is a state at wave vector $\vec{k}_2$, and the sum on n_2 in Eq. (8) is over a complete set of states at that wave vector. With this result the CH term in Eq. (18) simply lowers all bands by the same amount and has no effect on the band structure. This has been pointed out by Brinkman and Goodman.[2] Using Eqs. (18) and (19), Eq. (8) can be rewritten

$$\hat{\Sigma}_{n_1, n_1}(\vec{k}_1, \omega) = \hat{\Sigma}_{\text{CH}} + \hat{\Sigma}_{\text{SX}}(n_1, \vec{k}_1) \ , \tag{20}$$

$$\hat{\Sigma}_{\text{CH}} = \frac{1}{2} \sum_{\vec{q}} v_{\vec{q}} \left(\frac{1}{\kappa(\vec{q}, 0)} - 1\right) \ , \tag{21}$$

$$\hat{\Sigma}_{\text{SX}}(n_1, \vec{k}_1) = -\sum_{\vec{q}} \frac{v_q}{\kappa(\vec{q}, 0)} F_{n_1\vec{k}_1, \text{val}} \ , \tag{22}$$

$$F_{n_1\vec{k}_1, \text{val}} = \sum_{\text{occupied states}, n_2\vec{k}_2} |\langle \Phi_{n_1\vec{k}_1} | e^{i\vec{q}\cdot\vec{r}} | \Phi_{n_2\vec{k}_2} \rangle|^2 \ . \tag{23}$$

Since the sum in Eq. (23) is only over the states $n_2, \vec{k}_2$ which are occupied, $F_{n_1\vec{k}_1, \text{val}} \leq 1$. As $q \to 0$, $F_{n_1\vec{k}_1, \text{val}} \to 1$ for occupied states and $\to 0$ for empty states by the orthonormality of Bloch functions. This limit is extreme, of course, and is only approximately true for a small volume of q space. However, we expect that F will generally be larger for valence states than for conduction-band states. Detailed calculation shows this to be true for nearly all values of $\vec{q}$. Since F is larger for valence states, the effect is to increase the band gap, just as in the unscreened Hartree-Fock results, but by a lesser amount.

B. Numerical Calculation

The diagonal dielectric constant in Eq. (6) was calculated in the Penn model[9] fitted to a value $\kappa(0, 0) = 12$ with $k_F = 0.957 a_0^{-1}$ corresponding to a lattice constant $a = 10.263 a_0$. The exchange "overlap" integrals in Eq. (9) were calculated using pseudopotential wave functions based on Brust's coefficients $V(3) = -0.21$ Ry, $V(8) = 0.04$ Ry, and $V(11) = 0.08$ Ry.[11] Plane waves whose magnitude k^2 satisfied

$$k^2 \le (2\pi/a)^2 7 \qquad (24)$$

were included in the Hamiltonian, while plane waves satisfying

$$(2\pi/a)^2 7 < k^2 \le (2\pi/a)^2\, 19.5 \qquad (25)$$

were treated by Löwdin perturbation theory as described by Brust.[11] The Hamiltonian size varied from 15 to 23 depending on the point $\vec{k}$ of the zone. The Fourier coefficients obtained from diagonalizing the matrix were used in Eq. (9) without consideration of the states with $k^2 > (2\pi/a)^2 7$.

In the q sum of Eq. (8) a bcc mesh was determined in the form of a miniature Brillouin zone with lattice points $\frac{1}{4}\vec{K}_n$. The quantities F and S in Eq. (8) were evaluated at these lattice points while $1/q^2$ was integrated over a sphere centered at the lattice point with a volume equal to the volume per mesh point.

We write

$$\vec{q} = \vec{q}_0 + \vec{K}_n\,, \qquad (26)$$

where $\vec{q}_0$ is inside the first Brillouin zone and $\vec{K}_n$ is a principal lattice vector. We summed over the following $(a/2\pi)\vec{K}_n = (0, 0, 0)$, $(1, 1, 1)$, $(2, 0, 0)$, $(0, 2, 2)$, $(3, 1, 1)$, and $(2, 2, 2)$ for all $\vec{q}_0 = \frac{1}{4}\vec{K}_n$. The convergence of the self-energy is given in Table I where the cumulative self-energy is tabulated vs $\vec{K}_n$. In the first two rows of Table I the self-energy contribution from $\vec{q}$ in the first zone is compared for the two mesh sizes $\frac{1}{4}\vec{K}_n$ and $\frac{1}{8}\vec{K}_n$. The difference is about 2% so that we estimate no more than a 1% error in the total self-energy from mesh-size coarseness. The $\vec{q}$-space convergence appears good in Table I, but we can get a more accurate estimate by comparison with the free-electron-gas convergence in $\vec{q}$ which is more easily calculated. First we note that the average solid self-energy at the Γ point is only 2% different from the free-electron self-energy integrated over the same volume of $\vec{q}$ space. This indicates that the $\vec{q}$-space convergence in the solid should be nearly the same as in the free-electron gas. We further note that the free-electron self-energy for a $\vec{q}$-space volume equal to that of the Brillouin zones out to $\vec{K}_n = (2\pi/a)(2, 2, 2)$ inclusive is only 1.6% smaller than the total free-electron self-energy. (An expression based on a mesh in $1/q$ was used to sum over large q in the free-electron case.) Hence we conclude that the $\vec{q}$-space integration is accurate to a few percent both as to mesh size and total volume of integration.

In Table II the values of the exchange self-energy calculated with the dynamic Penn dielectric function are compared with the static approximation (values in parentheses). It is seen that the average values in the static limit are about 15% too low but the values of the energy gaps are only a few percent in error. Earlier work had suggested that the static approximation would be satisfactory.[1-3] This result is gratifying because it makes the calculations a great deal easier.

III. RESULTS AND DISCUSSION

The considerations in Sec. IIB suggest that computational inaccuracies and the use of the static approximation involve errors of only a few percent. The major unevaluated sources of error are the use

TABLE I. Self-energy at the Γ point vs volume of $\vec{q}$ integration. Sum is over complete zones. $\vec{Q}$ labels zone-center point of furthest zone included in sum. The dynamic Penn dielectric function was used, but no Hubbard correction was applied. Energies are in eV.

$(a/2\pi)Q$	$\Gamma_{25'}$	Γ_{15}	$\Gamma_{15}-\Gamma_{25'}$
000	−5.145	−4.291	0.855
000[a]	−5.194	−4.356	0.838
111	−8.255	−6.944	1.311
200	−9.708	−8.277	1.432
220	−10.39	−8.875	1.519
311	−10.89	−9.259	1.628
222	−11.02	−9.395	1.621

[a] Row computed with half the mesh spacing of all other entries. This value used in cumulative totals below.

TABLE II. Self-energies at the Γ, X, L points in eV. Bare numbers were calculated using the dynamic Penn dielectric function and no Hubbard correction. Numbers in parentheses were calculated using a static dielectric function and no Hubbard correction. Numbers in brackets are static with Hubbard correction.

$\Gamma_{25'}$	Γ_{15}	$\Gamma_{2'}$	$\Gamma_{15}-\Gamma_{25'}$	$\Gamma_{2'}-\Gamma_{25'}$
−11.02	−9.39	−10.04	1.62	0.978
(−12.55)	(−10.88)		(1.66)	
[−12.07]	[−10.31]	[−10.90]	[1.76]	[1.17]
$L_{3'}$	L_1		$L_1-L_{3'}$	
−11.06	−9.62		1.44	
(−12.62)	(−11.15)		(1.47)	
[−12.15]	[−10.62]		[1.53]	
X_4	X_1		X_1-X_4	
−10.95	−9.06		1.89	
(−12.61)	(−10.70)		(1.92)	
[−12.11]	[−10.11]		[2.00]	

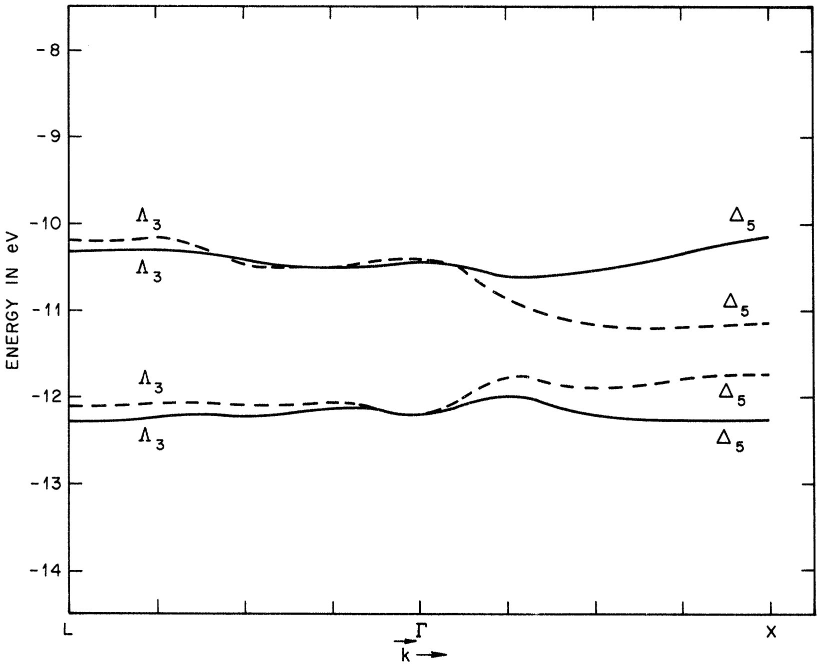

FIG. 1. Solid lines are the exchange self-energy for the Δ_5 and Λ_3 bands calculated using the static Penn dielectric function with a Hubbard correction factor. Dashed lines are Slater's $\rho^{1/3}$ approximation with $\alpha = 0.88$.

of pseudopotential wave functions, the neglect of "umklapp" nondiagonal terms in the dielectric function, and the use of the RPA approximation.

The static Penn dielectric function is a monotonically decreasing function of q whose value at small q is fixed by experiment. In view of the relative insensitivity of the exchange energy to the high-q dependence as evidenced by the results in Table II with and without the Hubbard correction, we do not think the dielectric function is a serious source of error apart from possible "umklapp" nondiagonality terms.

Although some results using the dynamic dielectric function are given in Table II, the more detailed calculations which we present in Figs. 1–3 were computed using the static dielectric function.

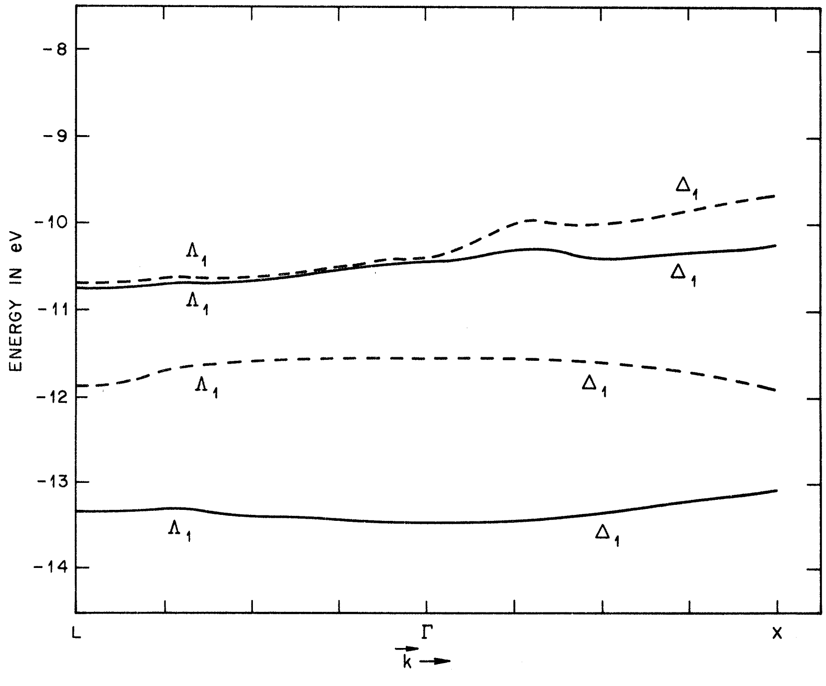

FIG. 2. Solid lines are the exchange self-energy for the Δ_1 and Λ_1 bands calculated using the static Penn dielectric function with a Hubbard correction factor. Dashed lines are Slater's $\rho^{1/3}$ approximation with $\alpha = 0.88$.

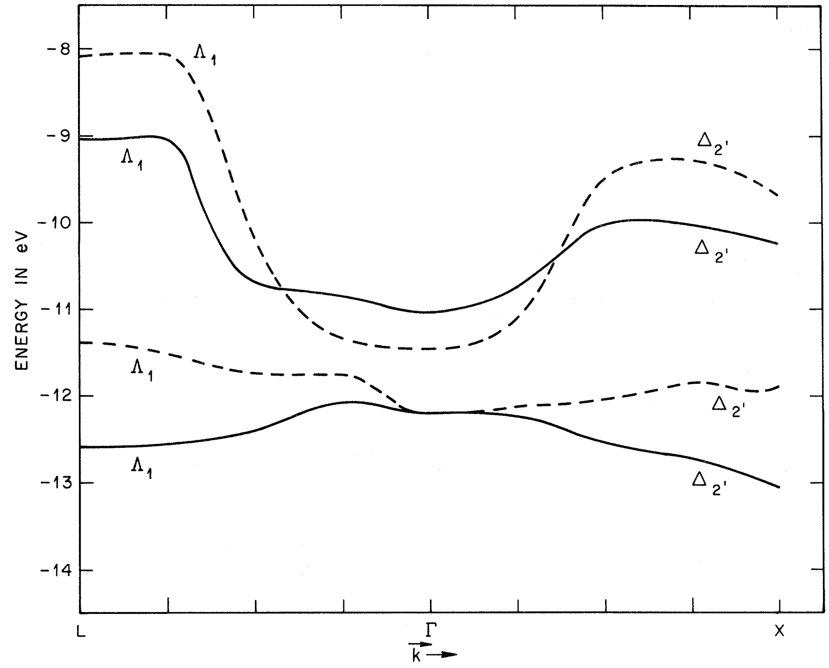

FIG. 3. Solid lines are the exchange self-energy for the $\Delta_{2'}$ and Λ_1 bands calculated using the static Penn dielectric function with a Hubbard correction factor. Dashed lines are Slater's $\rho^{1/3}$ approximation with $\alpha = 0.88$.

Points were computed at $\frac{1}{4}nX$ and $\frac{1}{4}nL$ and the bands sketched in by hand.

For comparison, we have also computed the same bands using the Slater approximation

$$V_{\rm Slater}(\vec{r}) = -\tfrac{3}{2}\,\alpha e^2[(3/\pi)\,\rho_{\rm val}(\vec{r})]^{1/3}\ . \qquad (27)$$

A value of $\alpha = 0.88$ was selected to give agreement for the $\Gamma_{25'}$ valence-band state. The values of $\rho_{\rm val}(\vec{r})$ were taken from Brinkman and Goodman[2] and the exchange self-energy defined by

$$\hat{\Sigma}_{\rm Slater} = \langle \Phi_{n\vec{k}}(\vec{r})\,|\,V_{\rm Slater}\,|\,\Phi_{n\vec{k}}(\vec{r})\rangle \qquad (28)$$

was computed using pseudopotential wave functions for $\Phi_{n\vec{k}}(\vec{r})$.[11]

Comparing the two results in Figs. 1–3, we see that some features agree surprisingly well while in other cases the agreement is quite poor. The $\Gamma_{25'} - \Gamma_{15}$ gap is quite accurate while the $\Gamma_{25'} - \Gamma_{2'}$ gap differs by 0.4 eV. The lowest Λ_1 and Λ_3 conduction bands and the Λ_3 valence band agree very well (see Figs. 1 and 2) while the Δ_5 bands disagree by 0.5 to 1 eV at the X point. The lowest valence band ($\Lambda_1 - \Delta_1$) disagrees by nearly 2 eV.

Strong structure such as that in the $\Lambda_1 - \Delta_{2'}$ conduction bands in Fig. 3 agrees qualitatively but is significantly less pronounced in the screened-exchange bands compared to the Slater bands.

There is a definite indication in the figures that the valence bands near $\Gamma_{25'}$ are flatter for screened exchange than for Slater exchange. The mesh size was not small enough to determine curvatures reliably. In a previous paper it was found impossible to fit both gaps and curvatures at Γ using a local potential. The differences found here are in the right direction to resolve this discrepancy but we cannot obtain accurate numbers for quantitative comparison.

We conclude that Slater's "$\rho^{1/3}$" approximation is not reliable enough for "first-principles" calculations even when α is treated as an adjustable parameter. It appears that more attention should be given to the problem of calculating screened exchange.

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Conductivity in Anisotropic Semiconductors: Application to Longitudinal Resistivity and Hall Effect in Saturation-Stressed Degenerately Doped n-Type Germanium†

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A variational iteration technique is developed for calculating the distribution function and electrical resistivity for semiconductors with anisotropic band structure. When only a single iteration is performed the result for the resistivity is identical to that obtained by an application of Kohler's principle with a relaxation-time approximation and the calculated distribution function includes anisotropic corrections to the zeroth-order energy-dependent relaxation time. The accuracy of the technique is demonstrated by comparing the results of a first-order calculation with the exact solution of the Boltzmann equation for the transverse resistivity and the distribution function for Brooks-Herring scattering by current carriers moving on an ellipsoidal constant-energy surface in the limit of infinite-mass anisotropy. The technique is applied to the calculation of the longitudinal resistivity and Hall r coefficient of saturation-stressed degenerately doped n-type Ge at $T=0$ °K. We find that r is within 5% of unity, thus justifying Katz's determination of the number of carriers from his Hall data but the theoretical upper bound to the resistivity is found to significantly underestimate the experimental results. However, when the calculation is approximately corrected for the known inaccuracies of the Born approximation together with contributions from multiple scattering and dressing effects, the theory is found to be in good agreement with experiment.

I. INTRODUCTION AND CONCLUSIONS

When stress is applied to germanium it is possible to lower the energy of one of the four conduction-band minima relative to that of the other three.[1] If the semiconductor is degenerately doped and saturation stress is applied, the conduction electrons will make a transition into the lowest conduction-band valley and only this valley will be occupied at $T=0$ °K. The cubic structure of unstressed Ge gives rise to an isotropic resistivity. However, since each conduction-band valley is highly anisotropic with an effective-mass ratio $m_{\parallel}/m_{\perp}\approx 19$, saturation-stressed degenerately doped Ge should exhibit anisotropy in the resistivity. This resistivity anisotropy has been directly observed[2] and has stimulated renewed interest in the transport properties of electrons moving on ellipsoidal constant-energy surfaces, a subject which is of signiicance not only for many semiconductors, but also for semimetals.

In an earlier work[3] (hereafter referred to as I) upper and lower bounds to the transverse resistivity predicted by Brooks-Herring scattering[4] were obtained. This was accomplished by exactly solving the Boltzmann equation for two other scattering functions which were either greater than (or equal to) or less than (or equal to) the scattering rate corresponding to the Brooks-Herring matrix element but were not significantly different from the latter. It is, however, not practical to use this method to calculate bounds on the longitudinal resistivity because to do so requires replacing $|k_x-k_x'|$ by either $|k_x|+|k_x'|$ or $|k_x|-|k_x'|$, which significantly changes the value of the scattering function and hence leads to results considerably different from an exact calculation. A second method employed in I was the use of Kohler's variational principle[5] with a simple trial solution for the change in the distribution function. This technique led to an upper bound for the resistivity that was at most approximately 20% higher than a lower bound previously derived and hence an accurate estimate of the resistivity was obtained for Brooks-Herring scattering without any isotropic-mass approximations.

In Sec. II we show that in the limit of infinite-mass anisotropy a simple application of the variational principle overestimates the exact transverse resistivity by less than 1%. Since the variational principle with a relaxation-time approximation is expected to improve with decreasing anisotropy, a similar claim can be made for the accuracy in the case of Ge, thus justifying a statement in I. Furthermore, by an iteration process we derive the distribution function for the infinitely aniso-