Self-energy correction for the energy bands of silicon by the full-potential linearized augmented-plane-wave method: Effect of the valence-band polarization

Noriaki Hamada,* Miaogy Hwang,† and A. J. Freeman
Department of Physics and Astronomy and Materials Research Center, Northwestern University, Evanston, Illinois 60208
(Received 31 July 1989)

A procedure is presented for calculating the electron self-energy within the dynamical GW approximation of Hedin (i.e., retaining the lowest term in the screened-Couloumb-interaction expansion) which utilizes eigenstates and eigenenergies generated by the full-potential linearized augmented-plane-wave method in the local-density approximation. For the dynamical dielectric matrix, we propose a new plasmon-pole model which has a suitable limit to the static dielectric matrix and has good behavior in a wide energy range. The self-energy is evaluated by using only the valence and conduction bands. Results of the numerical tests for silicon presented show that the Fourier representation for the dielectric matrix and the screened Coulomb interaction is useful for calculating the electron self-energy.

I. INTRODUCTION

Despite its great success for determining ground-state properties,[1] it is well established that conventional band-structure calculations in the Hohenberg-Kohn-Sham local-density approximation[2,3] (LDA) cannot yield the quasiparticle energy correctly. Thus, for example, the band gap in the LDA is typically half of the experimental value. This discrepancy is believed[4–8] to be due to the density-functional formalism which is a ground-state theory[2,3] rather than to the approximate formula of the exchange-correlation potential. Therefore, we have to go beyond the density-functional theory in order to calculate the quasiparticle energy.[9–12]

About a quarter of a century ago, Hedin[13] proposed a theory for calculating the self-energy in terms of the screened-Coulomb-interaction expansion. Recently, Hybertsen and Louie[11] have shown that the lowest term of this expansion—the GW approximation—is a good approximation to calculate the self-energy; they evaluate the self-energy within the framework of the first-principles pseudopotential method.[14] The major purpose of this paper is to propose an efficient calculational scheme to evaluate the quasiparticle energy by using the eigenstates and eigenenergies generated by the full-potential linearized augmented-plane-wave[15] (FLAPW) method in the LDA. Another is to show the efficiency of the plane-wave representation for the dielectric matrix also within the APW framework and to present a new plasmon-pole model which behaves well in a wide range of energy and which has the correct static limit. This model has poles away from the real axis, which supplies numerical stability in actual computations.

In Sec. II, a procedure for calculating the self-energy is presented and our plasmon-pole model for the dynamical dielectric matrix is studied in detail in Sec. III. In Sec. IV, the numerical results are presented for the self-energy in silicon. Finally, Sec. V is devoted to a brief discussion and concluding remarks.

II. FORMULATION

Hedin[13] gave an expression for the electron self-energy in terms of the perturbation expansion in the screened Coulomb interaction W:

$$\Sigma(1,2)=i\int d3\,d4\,G(1,3)\Gamma(3,2;4)W(4,1^+)\ , \tag{1}$$

where the numeral denotes a set of space, time, and spin coordinates, G is the electron Green function, and Γ is the vertex function.[16]

A. The GW approximation

We start with the GW approximation, in which we set $\Gamma(3,2;4)=\delta(3,4)\delta(2,4)$ in Eq. (1),

$$\Sigma(r,r';E)=i\int\frac{dE'}{4\pi}e^{-i\delta E'}G(r,r';E-E')W(r,r';E')\ , \tag{2}$$

and calculate the self-energy Σ with the eigenstates and eigenenergies generated by a FLAPW band-structure calculation. Denoting the eigenstate as

$$\phi_{nk}(r)=\langle r|nk\rangle\ , \tag{3}$$

and the eigenenergy as ε_{nk}, the Green function is expressed as

$$G(r,r';E)=\sum_{n,k}\frac{\phi_{nk}(r)\phi^*_{nk}(r')}{E-\varepsilon_{nk}+i\delta_{nk}}\ , \tag{4}$$

where $\delta_{nk}=0^-$ for $\varepsilon_{nk}<\mu$ and $\delta_{nk}=0^+$ for $\varepsilon_{nk}>\mu$. W is expanded in a Fourier series as

$$W(r,r';E)=\sum_{q,G,G'}e^{i(q+G)r}W_{GG'}(q,E)e^{-i(q+G')r'}\ . \tag{5}$$

Then we have

$$\langle nk|\Sigma(E)|n'k\rangle = i\int \frac{dE'}{4\pi} e^{-i\delta E'} \sum_{n_1,q,G,G'} \langle nk|e^{i(q+G)r}|n_1 k-q\rangle \times \langle n_1 k-q|e^{-i(q+G')r}|n'k\rangle \frac{W_{GG'}(q,E)}{E-E'-\varepsilon_{n_1,k-q}+i\delta_{n_1,k-q}} . \quad (6)$$

B. Screened Coulomb interaction

The screened Coulomb interaction is defined as

$$W_{GG'}(q,E) = \epsilon^{-1}_{GG'}(q,E')v(q+G) , \quad (7)$$

where $\epsilon^{-1}_{GG'}(q,E)$ is the inverse of the dielectric matrix, and $v(q+G)=4\pi/|q+G|^2$ is the bare Coulomb interaction. For numerical calculations, it is convenient to introduce a new quantity[17] for the dielectric matrix:

$$\tilde{\epsilon}^{-1}_{GG'}(q,E) = u^{-1}(q+G)\epsilon^{-1}_{GG'}(q,E)u(q+G') , \quad (8)$$

where $u(q+G)=[v(q+G)]^{1/2}=\sqrt{4\pi}/|q+G|$.

The dielectric matrix $\tilde{\epsilon}_{GG'}(q,E)$ is calculated by using the Bohm-Pines random-phase approximation (RPA) and a plasmon-pole model. The static dielectric matrix, $\tilde{\epsilon}_{GG'}(q)\equiv\tilde{\epsilon}_{GG'}(q,0)$, is calculated within the RPA by using the eigenstates and eigenenergies generated by the FLAPW band-structure calculation:

$$\tilde{\epsilon}_{GG'}(q) = \delta_{GG'} + u(q+G)4\sum_{v,c,k} \langle vk|e^{-i(q+G)r}|c,k+q\rangle \frac{\langle c,k+q|e^{iq(k+G')r}|vk\rangle}{\varepsilon_{c,k+q}-\varepsilon_{vk}} u(q+G') . \quad (9)$$

Now, $\tilde{\epsilon}_{GG'}(q)$ is a Hermitian matrix which is easily inverted by using the eigenvector $U_{Gi}(q)$ and eigenvalue $\varepsilon_i(q)$:

$$\sum_{G'} \tilde{\epsilon}_{GG'}(q)U_{G'i}(q) = U_{Gi}(q)\varepsilon_i(q) \quad (10)$$

or

$$\tilde{\epsilon}^{-1}_{GG'}(q) = \sum_i U_{Gi}(q)\frac{1}{\varepsilon_i(q)}U^{\dagger}_{iG'}(q) . \quad (11)$$

We propose a new plasmon-pole model to evaluate the dynamical dielectric matrix with a correct static limit. We assume that the dynamical dielectric matrix has the same form as Eq. (11) with the same matrix $U_{Gi}(q)$:

$$\tilde{\epsilon}^{-1}_{GG'}(q,E) = \sum_i U_{Gi}(q)\frac{1}{\varepsilon_i(q,E)}U^{\dagger}_{iG'}(q) . \quad (12)$$

Our plasmon-pole model has the following form,

$$\frac{1}{\varepsilon_i(q,E)} = 1 + \frac{C_i(q)}{|E|-\omega_i(q)} - \frac{C_i(q)}{|E|+\omega_i^*(q)} , \quad (13)$$

for the time-ordered dielectric function with a real-energy variable E. We replace $|E|$ by E for the retarded (physical) dielectric function. The choice of parameters, $C_i(q)$ and $\omega_i(q)$, is given in the next section.

C. Self-energies

Using Eqs. (8), (12), and (13) in Eq. (7), we obtain the final form for the self-energy from Eq. (6):

$$\langle nk|\Sigma(E)|n'k\rangle = \langle nk|\Sigma_{\rm SEX}(E)|n'k\rangle + \langle nk|\Sigma_{\rm COH}(E)|n'k\rangle , \quad (14)$$

where

$$\langle nk|\Sigma_{\rm SEX}(E)|n'k\rangle = -\sum_{n_1}^{\rm occ}\sum_{q,G,G'} \langle nk|e^{i(q+G)r}|n_1,k-q\rangle \langle n_1,k-q|e^{-i(q+G')r}|n'k\rangle u(q+G) \times \sum_i U_{Gi}(q)\left[1+\frac{C_i(q)}{|E-\varepsilon_{n_1,k-q}|-\omega_i(q)}-\frac{C_i(q)}{|E-\varepsilon_{n_1,k-q}|+\omega_i^*(q)}\right]U^{\dagger}_{iG'}(q)u(q+G') \quad (15)$$

for the real number of E, and

$$\langle nk|\Sigma_{\rm COH}(E)|n'k\rangle = \sum_{n_1}\sum_{q,G,G'} \langle nk|e^{i(q+G)r}|n_1,k-q\rangle \langle n_1,k-q|e^{-i(q+G')r}|n'k\rangle u(q+G) \times \sum_i U_{Gi}(q)\frac{C_i(q)}{E-\varepsilon_{n_1,k-q}-\omega_i(q)}U_{iG'}(q)u(q+G') . \quad (16)$$

D. The self-energy correction to the local-density approximation

We estimate the self-energy correction by the diagonal term of Eq. (14) with the quasiparticle energy E_{nk}:

$$\Delta\Sigma_{nk}(E_{nk})=\Sigma_{nk}(E_{nk})-V_{nk}^{xc} , \tag{17}$$

with

$$\Sigma_{nk}(E)\equiv\langle nk|\Sigma(E)|nk\rangle$$

and

$$V_{nk}^{xc}\equiv\langle nk|V^{xc}[\rho(r)]|nk\rangle ,$$

where $\rho(r)$ is the valence-electron density, and $V^{xc}(\rho)$ is the exchange-correlation potential in the local-density approximation. Hybertsen and Louie[11] have shown that the contribution of the off-diagonal term to the self-energy correction is small. In the numerical calculations which follow, we will give the correction up to the first derivative of the self-energy:

$$\Delta\Sigma_{nk}(E_{nk})\cong\Delta\Sigma_{nk}(\varepsilon_{nk})\left[1+\frac{\left[\frac{d\Sigma_{nk}}{dE}\right]_{E=\varepsilon_{nk}}}{1-\left[\frac{d\Sigma_{nk}}{dE}\right]_{E=\varepsilon_{nk}}}\right] . \tag{18}$$

III. PLASMON-POLE MODEL FOR THE DIELECTRIC FUNCTION

Our plasmon-pole model for the retarded dielectric function is given by Eqs. (10) and (12) and by

$$\frac{1}{\epsilon_i(q,E)}=1+C_i(q)\left[\frac{1}{E-\omega_i(q)}-\frac{1}{E+\omega_i^*(q)}\right] . \tag{19}$$

The parameter $C_i(q)$ in Eqs. (19) and (13) is taken as

$$C_i(q)=\frac{\omega_p^2}{2\,\mathrm{Re}\omega_i(q)} , \tag{20}$$

with the plasma frequency for the uniform valence-electron density n: $\omega_p^2=4\pi n$. This condition gives the suitable high-frequency limit:

$$\frac{1}{\epsilon_i(q,E)}\sim 1+\frac{\omega_p^2}{E^2}\quad\text{as } E\to\infty . \tag{21}$$

By using the unitarity of the matrix $U_{GG'}(q)$, we obtain

$$\tilde{\epsilon}_{GG'}^{-1}(q,E)\sim\left[1+\frac{\omega_p^2}{E^2}\right]\delta_{GG}\quad\text{as } E\to\infty . \tag{22}$$

Note that especially the macroscopic dielectric function has the correct limit:

$$\epsilon_{\mathrm{macro}}(q,E)=[\epsilon_{00}^{-1}(q,E)]^{-1}\sim 1-\frac{\omega_p^2}{E^2}\quad\text{as } E\to\infty . \tag{23}$$

The frequency sum rules are

$$\int_0^\infty dE\,E\,\mathrm{Im}\frac{1}{\epsilon_i(q,E)}=-\frac{\pi}{2}\omega_p^2 \tag{24}$$

and

$$\int_0^\infty dE\,E\,\mathrm{Im}\tilde{\epsilon}_{GG'}^{-1}(q,E)=-\frac{\pi}{2}\omega_p^2\delta_{GG'} \tag{25}$$

in our model. Since the correct f-sum rule[11] for the last equation should be

$$(-\pi/2)\omega_p^2\hat{\mathbf{e}}(q+G)\cdot\hat{\mathbf{e}}(q+G')\rho(G-G')/\rho(0) ,$$

where $\hat{\mathbf{e}}(q+G)$ is the directional vector for $q+G$ and $\rho(G)$ is the Fourier component of the valence charge density. Our model has the correct f-sum rule for diagonal elements, but not for off-diagonal elements. We can recover the correct f-sum rule, if we assume an appropriate energy dependence in $U_{Gi}(q)$ in Eq. (12). However, for calculating the self-energy, the lower-energy part ($E<\omega_p$) in the dielectric function is important, and is well described without the energy dependence of $U_{Gi}(q)$ because the limit of $E=0$ is assumed to be correct in Eq. (12). The exact f-sum rule is not a necessary ingredient for our purpose.

The $\omega_i(q)$ is determined so as to obtain the correct static limit: $\varepsilon_i(E,q)\to\varepsilon_i(q)$ for $E\to 0$, which gives

$$|\omega_i(q)|^2=\omega_p^2/[1-1/\varepsilon_i(q)] . \tag{26}$$

Now we allow $\omega_i(q)$ to be a complex number in the form of

$$\omega_i(q)=\omega_p\left[\frac{\varepsilon_i(q)}{\varepsilon_i(q)-1}\right]^{1/2}\frac{1-iy}{(1+y^2)^{1/2}} , \tag{27}$$

where a real nondimensional parameter y has been included for fitting the dielectric matrix to results of a complete (full-energy) calculation of the dielectric matrix including both frequency and wave-vector dependences. The value for y is typically taken as $y=0.2$ for semiconductors.

In the actual calculations, we use the RPA result for the static dielectric matrix, as mentioned in the preceding section. The RPA calculation is performed by using the eigenenergies and eigenstates generated by the FLAPW band-structure calculation within the local-density approximation.

We briefly mention the difference between our model and the generalized plasmon-pole model introduced by Hybertsen and Louie.[11] Their model has a plasmon pole, $\omega_{GG'}(q)$ for each set of q, G, and G', and requires the correct f-sum rule. However, we could not obtain a suitable solution of $\omega_{GG'}(q)$ for some sets of q, G, and G' due to the limitation of the simple form of the model function. On the other hand, our model has physically suitable plasmon poles, $\omega_i(q)$, for all i and q, which are always greater than ω_p. However, as mentioned above, our model does not satisfy the correct f-sum rule for off-diagonal elements.

Figures 1 and 2 show some elements of the dielectric matrix as functions of the energy for Si. The real parts of the dielectric matrix are shown in Figs. 1(a) and 1(b) for

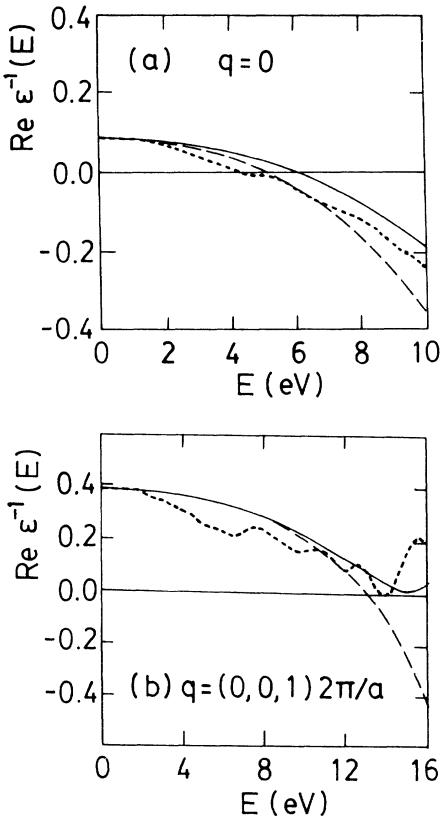

FIG. 1. Real part of ϵ^{-1} with $G=G'=0$ for Si. Solid line is the present model, dashed line the generalized plasmon-pole model of Hybertsen and Louie (Ref. 11), and dotted line the full-energy calculation by Walter and Cohen (also taken from Ref. 11). (a) For $\mathbf{q}=(0,0,0)$ and (b) for $\mathbf{q}=(1,0,0)2\pi/a$.

$q=0$ and $q=(0,0,1)2\pi/a$, respectively. Note that the results of our plasmon-pole model agree well with the results of the full RPA calculation done by Walter and Cohen[18] based on the pseudopotential band structure. The generalized plasmon-pole model proposed by Hybertsen and Louie is also shown in Fig. 1. The agreement among these curves is sufficient to calculate the electron self-energy, although the discrepancy might affect the result by about 0.1 eV at the most.

In Fig. 1(b), we see that our calculated results for $\mathrm{Re}\epsilon^{-1}(E)$ correctly changes from being a decreasing function to an increasing function at around 15 eV. This behavior is due to the imaginary part (the y parameter) in the plasmon frequency $\omega_i(q)$ in Eq. (27). The Walter-Cohen[18] result and the Hybertsen-Louie[11] result have zeros around $E=15$ eV, while our model does not have such a zero. We could have such a zero if we chose an appropriate y parameter slightly smaller than 0.2. However, the zero is not crucial for our purposes. The imaginary part of the dielectric matrix is shown in Fig. 2 for $q=0$. Our model reproduces well the result of Walter and Cohen as a whole, which is due to the use of the y parameter ($y=0.2$). The model of Hybertsen and Louie gives a δ function around $E=16$ eV, which causes the divergent behavior also in the real part.

For the purpose of calculating the real part of the electron self-energy, the y parameter is just a convenient tool to avoid the accidental error in the numerical calculation coming from the procedure of the n_1 summation in Eqs. (15) and (16). Actually, the choice of the y parameter of $y<0.25$ affects the results only on the order of 0.01 eV for the electron self-energy in Si. However, the y parameter will have a physical meaning when we attempt to determine the imaginary parts of the included quantities in a self-consistent way in the future.

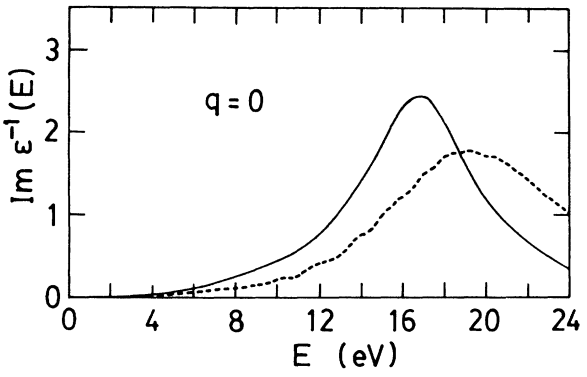

FIG. 2. Imaginary part of ϵ^{-1} with $\mathbf{q}=(0,0,0)$ and $\mathbf{G}=\mathbf{G}'=(0,0,0)$ for Si. Solid line is the present model; dotted the full-energy calculation by Walter and Cohen (Ref. 18).

IV. NUMERICAL RESULTS: SELF-ENERGY FOR SILICON

We assume the lattice constant of Si to be 10.263 a.u. We use the FLAPW method and the Vosko-Wilk-Nusair exchange correlation[19] within the LDA of density-functional theory. The parameters for the FLAPW calculation were taken as follows. Inside the muffin-tin sphere, the angular-momentum expansion was truncated at $l=6$ for the charge density and potential, and at $l=3$ for the wave functions. This $l=3$ value is rather small,

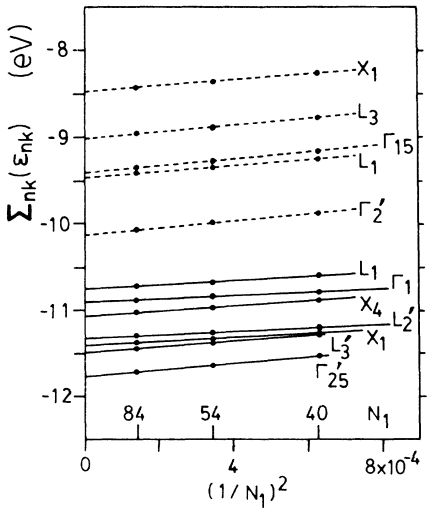

FIG. 3. Convergence of the self-energy for the n_1 sum in Eq. (16). Solid lines stand for the valence states; dotted for the conduction band.

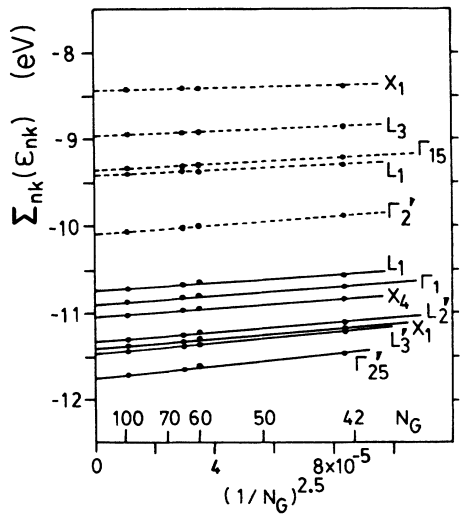

FIG. 4. Convergence of the self-energy for the G and G' sums in Eqs. (15) and (16). Solid lines denote valence states; dotted, conduction states.

TABLE I. Self-energies for several states (in eV).

	LDA	GW	Corrections
Γ_{1v}	−10.60	−11.16	−0.56
$\Gamma_{25'v}$	−11.41	−11.72	−0.31
Γ_{15c}	−10.19	−9.75	0.44
$\Gamma_{2'c}$	−11.25	−10.54	0.71
X_{1v}	−10.98	−11.59	−0.61
X_{4v}	−10.73	−11.23	−0.50
X_{1c}	−9.17	−8.99	0.18
$L_{2'v}$	−10.97	−11.58	−0.61
L_{1v}	−10.37	−11.01	−0.64
$L_{3'v}$	−11.18	−11.56	−0.38
L_{1c}	−10.30	−9.88	0.42
L_{3c}	−9.77	−9.35	0.42

which gives a larger gap compared with more accurate calculations with $l=7$, but the difference is only 0.03 eV. In the interstitial region, about 750 reciprocal-lattice vectors were considered in the Fourier representation of the charge density and potential. The LAPW functions with wave vectors $|\mathbf{k}+\mathbf{G}|<K_{\max}=2.7$ a.u. were used in the expansion of the eigenfunctions leading to about 90 basis functions. Nineteen inequivalent sampling k points and the linear tetrahedron scheme were used for the Brillouin-zone integration. We took the same parameter values for evaluating the matrix element in the self-energy calculation. We treated four upper occupied bands as the valence bands and took into account 85 conduction bands. These limited choices for parameters reduce the computing time without changing the result very much.

We tested the convergence for the n_1 sum and the G sum in Eqs. (15) and (16). With N_1 standing for the total number of the n_1 summation, the convergence can be expressed as $(1/N_1)^{\alpha}$. Figure 3 shows that this α value is 2, which is common for all states. Figure 4 shows the con-

TABLE II. Quasiparticle energies for several states in eV. E_g is the fundamental energy-band gap. Our "Hartree-Fock" result is only a first-order perturbation result described by the first term in the large parentheses of Eq. (15).

	LDA	Hartree-Fock approx.		GW approx.		Expt.[a]
		Present	(GB)[h]	Present	(HL)[i]	
Γ_{1v}	−11.95	−17.11		−12.21	(−12.04)	−12.5±0.6
$\Gamma_{25'v}$	0	0	(0)	0	(0)	0
Γ_{15c}	2.55	8.92	(9.27)	3.30	(3.35)	3.4
$\Gamma_{2'c}$	3.17	10.24	(11.04)	4.19	(4.08)	4.2
X_{1v}	−7.82	−11.13		−8.11		
X_{4v}	−2.84	−3.86	(−3.84)	−3.03	(−2.99)	−2.9[b], 3.3±0.2[c]
X_{1c}	0.65	6.48	(6.87)	1.14	(1.44)	1.3[d]
$L_{2'v}$	−9.63	−13.79		−9.92	(−9.79)	−9.3±0.4
L_{1v}	−6.98	−9.78		−7.31	(−7.18)	−6.7±0.2
$L_{3'v}$	−1.19	−1.61	(−1.48)	−1.26	(−1.27)	−1.2±0.2, 11.5[e]
L_{1c}	1.43	7.66	(8.13)	2.15	(2.27)	2.1[f], 2.4±0.15[g]
L_{3c}	3.35	9.90	(10.16)	4.08	(4.24)	4.15±0.1[g]
$L_{1c}-L_{3'v}$	2.62	9.27	(9.61)	3.41	(3.54)	3.45
E_g	0.52	6.35	(6.43)	1.01	(1.29)	1.17

[a]Reference 20, except where noted.
[b]Reference 21.
[c]Reference 22.
[d]Reference 11.
[e]Reference 23.
[f]Reference 24.
[g]Reference 25.
[h]Reference 26.
[i]Reference 11.

vergence of the G and G' sums: The convergence is like $(1/N_G)^{\beta}$ with $\beta=2.5$. Here N_G is the number of the G summation, and is also the dimension of the dielectric matrix of Eq. (9) which is inverted to obtain the inverse dielectric matrix of Eq. (12).

The values of $\alpha=2.0$ and $\beta=2.5$ are the optimum values in the range 40–90 of N_1 and N_G; however, the α and β parameters tend to have a larger value for larger N_1 and N_G values, i.e., the convergence is even better. Therefore, the self-energies calculated with the parameters $N_1=84$ and $N_G=95$ contain a numerical error of about 0.06 eV. The quasiparticle energies relative to the valence-band top have a typical error of 0.02 eV. The same order of errors comes from the q-space (the first-Brillouin-zone) integration. When the errors coming from the dielectric function are also considered, the typical error is inferred to be 0.2 eV for the self-energy and 0.1 eV for the relative quasiparticle energy to the valence-band top.

Figures 3 and 4 also show that since the tangents of the lines are almost independent of the states, we can expect to obtain fairly good results for the relative quasiparticle energy with even smaller numbers of N_1 and N_G, e.g., $N_1 \sim N_G \sim 50$.

Table I shows the self-energy corrections to the LDA result which are evaluated by Eq. (18). The correction has a negative sign for the valence band and a positive sign for the conduction band. Table II presents results for the quasiparticle energies compared to the experimental values[20–25] and other theoretical results. The agreement between our results and the results of Hybertsen and Louie[11] is remarkably good if we consider that these calculations are based on different calculational schemes: We used the LAPW wave functions, while Hybertsen and Louie used the pseudo-wave functions and we assumed a different plasmon-pole model. Table II also shows the "Hartree-Fock" results: In our case, it is only a first-order-perturbation result obtained by using LDA eigenstates, which is not an exact Hartree-Fock result. On the other hand, the calculation of Gygi and Baldereschi was performed self-consistently in the Hartree-Fock approximation. These two results show a reasonable agreement between them.

TABLE III. Fock and the SEX and COH terms [defined in Eqs. (15) and (16)] in the self-energy (in eV).

	Fock	SEX	COH
Γ_{1v}	−17.37	−4.44	−6.97
$\Gamma_{25'v}$	−13.02	−4.01	−7.80
Γ_{15c}	−5.43	−1.95	−7.68
$\Gamma_{2'c}$	−5.79	−1.90	−8.43
X_{1v}	−15.90	−4.56	−7.23
X_{4v}	−13.36	−3.89	−7.48
X_{1c}	−4.95	−1.85	−7.09
$L_{2'v}$	−16.76	−4.70	−7.11
L_{1v}	−14.78	−3.92	−7.29
$L_{3'v}$	−13.20	−4.02	−7.65
L_{1c}	−5.68	−2.08	−7.68
L_{3v}	−4.83	−1.81	−7.43

V. DISCUSSIONS AND CONCLUDING REMARKS

Table III shows the decomposition of the GW self-energy to the screened-exchange (SEX) term [Eq. (15)] and the Coulomb-hole (COH) term [Eq. (16)], together with the Fock term [the contribution from the first (unit) term in large parentheses of Eq. (15)]. We can observe a remarkable difference between the valence- and conduction-band contributions in the SEX term, while none is seen in the COH term. The same kind of difference is seen in the Fock term. This property comes from the vicinity of $q=0$ in the first-Brillouin-zone integration in Eq. (15). This means that a substantial part of the band gap comes from the long-range property of the Coulomb interaction through the SEX term.

We assumed four upper occupied bands as the valence bands in Si—a choice which is also reasonable for III-V compounds. However, for II-VI compounds, it is not easy to choose the valence band, because the d bands of the group-II element (Zn, Cd, etc.) appear in the energy region of the valence bands: considering the d bands as the valence bands together with the s and p bands requires a more careful treatment for the plasmon-pole model of the dynamical dielectric matrix. In this context, another problem shows up in Eq. (17), where we used the LDA exchange-correlation potential with the valence-electron density to estimate the LDA counterpart of the self-energy. This reference to the LDA potential works well in Si, but it is not generally guaranteed for other systems. Therefore, an all-electron treatment, including core electrons, is needed for a more consistent theory.

In conclusion, we have presented a procedure for calculating the self-energy correction by using the eigenstates and eigenvalues generated by a LDA-FLAPW method. A new plasmon-pole model is proposed, which appears to be a useful approximation with correct behavior in a number of limits. A test calculation for Si has shown that the procedure gives quasiparticle energies very similar to the pseudopotential calculation of Hybertsen and Louie. The self-energy decomposition into the SEX and COH terms implies that the long-range Coulomb interaction is responsible for the band-gap correction through the SEX term.

ACKNOWLEDGMENTS

We thank Jaejun Yu, Sandro Massidda, Jae Il Lee, and Hiroshi Ishida for helpful discussions. One of us (N.H.) thanks the NEC Corporation for financial support. This work was supported by the U.S. National Science Foundation (through the Northwestern University Materials Research Center, under Grant No. DMR-88-21571, and by a computing grant through its Division of Advanced Scientific Computing at the National Center for Supercomputer Applications, University of Illinois at Urbana-Champaign).

*Permanent address: NEC Fundamental Research Laboratories, NEC Corporation, 34 Miyukigaoka, Tsukuba 305, Japan.

†Present address: AT&T Bell Laboratories, Naperville, IL 60560.

[1]For example, *Theory of the Inhomogeneous Electron Gas,* edited by S. Lundqvist and N. H. March (Plenum, New York, 1983).

[2]P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).

[3]W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).

[4]S. B. Trickey, F. R. Green, Jr., and F. W. Averill, Phys. Rev. B **8**, 4822 (1973).

[5]J. P. Perdew and M. Levy, Phys. Rev. Lett. **51**, 1884 (1983).

[6]L. J. Sham and M. Schlüter, Phys. Rev. Lett. **51**, 1888 (1983); Phys. Rev. B **32**, 3883 (1985).

[7]L. J. Sham, Phys. Rev. B **32**, 3876 (1985).

[8]M. Lannoo, M. Schlüter, and L. H. Sham, Phys. Rev. B **32**, 3890 (1985).

[9]G. Strinati, H. J. Mattausch, and W. Hanke, Phys. Rev. Lett. **45**, 290 (1980); Phys. Rev. B **25**, 2867 (1982).

[10]S. C. Wang and W. E. Pickett, Phys. Rev. Lett. **51**, 597 (1983); Phys. Rev. B **30**, 4719 (1984).

[11]M. S. Hybertsen and S. G. Louie, Phys. Rev. Lett. **55**, 1418 (1985); Phys. Rev. B **32**, 7005 (1986); **34**, 5390 (1986).

[12]R. W. Godby, M. Schlüter, and L. J. Sham, Phys. Rev. Lett. **56**, 2415 (1986); Phys. Rev. B **35**, 4170 (1987); **36**, 6497 (1987); **37**, 10159 (1988).

[13]L. Hedin, Phys. Rev. **139**, A796 (1965).

[14]D. R. Hamann, M. Schlüter, and C. Chiang, Phys. Rev. Lett. **43**, 1494 (1979).

[15]E. Wimmer, H. Krakauer, M. Weinert, and A. J. Freeman, Phys. Rev. **24**, 864 (1981); H. J. F. Jansen and A. J. Freeman, *ibid.* **30**, 561 (1984).

[16]For example, J. C. Inkson, *Many-Body Theory of Solids* (Plenum, New York, 1984).

[17]A. Baldereschi and E. Tosatti, Phys. Rev. B **17**, 4710 (1978).

[18]J. P. Walter and M. L. Cohen, Phys. Rev. B **5**, 3101 (1972).

[19]S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1980).

[20]Landolt-Börnstein, *Zahlenwerte und Funktionen aus Naturwissenschaften und Technik,* edited by O. Madelung, M. Schulz, and H. Weiss (Springer, New York, 1982), Gp. 3, Vol. 17a.

[21]W. E. Spicer and R. C. Eden, in *Proceedings of the Ninth International Conference on the Physics of Semiconductors, Moscow, 1968* (Nauka, Leningrad, 1968), Vol. 1, p. 61.

[22]A. L. Wachs, T. Miller, T. C. Hsieh, A. P. Shapiro, and T.-C. Chiang, Phys. Rev. B **32**, 2326 (1985).

[23]F. J. Himpsel, P. Heimann, and D. E. Eastman, Phys. Rev. B **24**, 2003 (1981).

[24]R. Hulthen and N. G. Nilsson, Solid State Commun. **18**, 1341 (1976).

[25]D. Straub, L. Ley, and F. J. Himpsel, Phys. Rev. Lett. **54**, 142 (1985).

[26]F. Gygi and A. Baldereschi, Phys. Rev. B **34**, 4405 (1986).