Model study of the frequency-dependent dielectric properties of semiconductors

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We present calculations of the frequency-dependent dielectric properties of semiconductors using the Penn model in the random-phase approximation, including collision effects via a phenomenological relaxation time τ. Analytical expressions for $\epsilon_1(0,\omega)$ (with and without collision effects) and for $\epsilon_2(0,\omega)$ and $\mathrm{Re}\sigma(0)$ (including collision effects) have been obtained. The inclusion of collision effects leads to expressions which are valid in the entire energy range. However, they do not affect significantly the values of $\epsilon_1(0,\omega)$ and $\epsilon_2(0,\omega)$ except near the peak positions. Our calculations demonstrate that the peak heights in $\epsilon_1(0,\omega)$, $\epsilon_2(0,\omega)$, and $\mathrm{Im}[-\epsilon^{-1}(0,\omega)]$ are sensitive to the value of τ, while the peak positions are not.

INTRODUCTION

There exist a number of calculations of the complex dielectric function $\epsilon(\vec{q},\omega)$ in the limit $\vec{q}\to 0$ for semiconductors with the use of simple model band structures[1-7] or detailed band structures.[8-12] There have been a number of model calculations primarily because of their simplicity and in showing the explicit dependence of $\epsilon(0,\omega)$ on the band parameters. In our earlier papers[5,13] we reported the calculations of static dielectric function $\epsilon(\vec{q},0)$ for small $\vec{q}$ with the use of the Penn model.[14] We found that the results from our calculations were in good agreement with those obtained from detailed band-structure calculations. This seems to suggest that for $\epsilon(\vec{q},0)$ the finer details of the band structure are not important. In view of this we thought it is worthwhile to calculate $\epsilon(0,\omega)$ with the use of this model. Another reason for doing this is that $\epsilon(0,\omega)$, unlike $\epsilon(\vec{q},0)$, can be compared with the experimental data. Hence, we would be able to comment on the applicability of Penn model to $\epsilon(0,\omega)$. Breckenridge *et al.*[4] have evaluated $\epsilon(0,\omega)$ for semiconductors with the use of the Penn model. However, the calculated $\epsilon_1(0,\omega)$ [real part of $\epsilon(0,\omega)$] and $\epsilon_2(0,\omega)$ [imaginary part of $\epsilon(0,\omega)$] diverge in the vicinity of the energy equal to the energy gap (E_g). Also their $\epsilon_2(0,\omega)$ is not valid for the energies less than E_g and the energy-loss function $\mathrm{Im}[-\epsilon^{-1}(0,\omega)]$ is a sharply peaked function. Thus the calculations of Breckenridge *et al.* show a large discrepancy when compared with the experimental data. It is well known that sharp peaks can be broadened out by employing smoothing functions. It seems reasonable to expect the Penn model to give a good agreement with experimental data when collision effects are included in the random-phase-approximation (RPA) dielectric function via a phenomenological relaxation time τ.

In this article, with the use of the Penn model, we report calculations of $\epsilon_1(0,\omega)$ (with and without collision effects) and of dc conductivity $\mathrm{Re}\sigma(0)$ and $\epsilon_2(0,\omega)$ (including collision effects). For the collision case the calculations are performed in two ways: (i) not conserving electron number[15,16] and (ii) conserving electron number.[17,18] Our calculations give good agreement with the experimental data. To draw from our results we find that (i) the peak heights in $\epsilon_1(0,\omega)$, $\epsilon_2(0,\omega)$, and $\mathrm{Im}[-\epsilon^{-1}(0,\omega)]$ are sensitive to τ while the peak positions are not, and (ii) the corrections introduced by enforcing number conservation are relatively small except near the peak positions. Our calculations show that $\hbar/\tau \ll E_g$ in contrast to the conclusions of Philipp and Ehrenreich[15] who obtained $\hbar/\tau \sim E_g$. Our calculations differ from the model calculations of Milchev[3] and Sturm[6] in that they are consistent and are valid for the entire energy range. The plan of our paper is as follows. In Sec. II, we report analytic expressions for $\mathrm{Re}\sigma(0)$, $\epsilon_1(0,\omega)$, and $\epsilon_2(0,\omega)$. The results obtained are discussed in Sec. III. We summarize our conclusions in Sec. IV.

II. CALCULATION WITH THE USE OF THE PENN MODEL

In order to evaluate the dielectric function, we need energy eigenvalues and wave functions. These have been reported in our earlier papers.[13]

A. Expressions for $\epsilon_1(0,\omega)$ without collision effects

The usual RPA expression for the dielectric function does not include collision effects and has been given by various workers.[19–21] In order to evaluate $\epsilon_1(0,\omega)$, we need the values of matrix element squared $|M|^2$ and the energy difference ΔE between the valence and conduction bands in the limit $\vec{q}\to 0$. Substituting the values of $|M|^2$ and ΔE from our earlier work,[13] we obtain

$$\epsilon_1(0,\omega)=\epsilon_0+\frac{E_P^2}{E_g^2}\left[\frac{(1-\Delta^2)}{3\delta^2}t_0(\delta^2 t_0^2-3\Delta^2)+\frac{\Delta^4}{\delta^4}(1+\delta^2-\Delta^2)I_1 - \frac{2\Delta^4}{\delta^2}\left[I_2-\frac{1}{\Delta}+t_0\right]-\left[t_0+\frac{2\Delta}{3}-\frac{\Delta^4 t_0^3}{3}\right]\right] . \tag{1}$$

Here,

$$I_1=\begin{cases}\dfrac{\delta}{(\Delta^2-\delta^2)^{1/2}}\tan^{-1}\left[\dfrac{t_0\delta}{(\Delta^2-\delta^2)^{1/2}}\right] & \text{when } \hbar\omega<E_g \\ \dfrac{\delta}{2(\delta^2-\Delta^2)^{1/2}}\ln\left[\dfrac{t_0\delta-(\delta^2-\Delta^2)^{1/2}}{t_0\delta+(\delta^2-\Delta^2)^{1/2}}\right] & \text{when } \hbar\omega>E_g\end{cases}$$

and

$$I_2=\frac{1}{2\delta}\ln\frac{(1-t_0\delta)(\Delta+\delta)}{(1+t_0\delta)(\Delta-\delta)} ,$$

where $t_0=1/(1+\Delta^2)^{1/2}$, $\Delta=E_g/4E_F$, $\delta=\hbar\omega/4E_F$, E_P is the free-electron plasmon energy, and E_F is the Fermi energy. Breckenridge *et al.* did not report any analytic expression for $\epsilon_1(0,\omega)$. We have shown here that the integrals can be evaluated analytically.

B. Expressions for $\epsilon(0,\omega)$ with collision effects

The collision effects can be included qualitatively with the use of the isotropic relaxation-time approximation. The assumption of isotropic scattering time preserves the equality of longitudinal and transverse dielectric functions in the limit $\vec{q}\to 0$. With the use of a standard relaxation-time approximation (in a time interval dt the probability to suffer a collision by an electron is dt/τ), an expression for $\epsilon(0,\omega)$ within the RPA has been given by[15,16]

$$\epsilon(0,\omega)=1-\lim_{\vec{q}\to 0}\frac{4\pi e^2}{q^2\Omega}\sum_{\vec{k},l,l'}\frac{f_0(E_{\vec{k}+\vec{q},l'})-f_0(E_{\vec{k},l})}{E_{\vec{k}+\vec{q},l'}-E_{\vec{k},l}-\hbar(\omega+i/\tau)}|\langle\vec{k}+\vec{q},l'|e^{i\vec{q}\cdot\vec{r}}|\vec{k},l\rangle|^2 \tag{2}$$

We note here that the τ is an intrinsic property of the system while the infinitesimal α [which appeared in the expression for $\epsilon(0,\omega)$ without collision effects] is related to the external perturbation. However, the relaxation-time approximation used to derive Eq. (1) fails to conserve the local electron number. Mermin[17] pointed out that this defect can be overcome using a relaxation-time approximation in which the collisions relax to a local equilibrium density matrix and not to a uniform equilibrium density matrix. This gives the local chemical potential which supplies the additional degree of freedom to obtain number conservation. Mermin has derived expressions for the dielectric function for a free electron. Garik and Ashcroft[18] (GA) have extended Mermin's approach for an electron moving in the periodic crystal potential. However, the expression of $\epsilon(0,\omega)$ does not differ from that of Mermin. The dielectric function within the RPA in the limit $\vec{q}\to 0$ is given by[17,18]

$$\tilde{\epsilon}(0,\omega)=1+\frac{(1+i/\omega\tau)[\epsilon(0,\omega+i/\tau)-1]}{1+(i/\omega\tau)[\epsilon(0,\omega+i/\tau)-1]/[\epsilon(0,0)-1]} . \tag{3}$$

Here $\epsilon(0,\omega+i/\tau)$ is equivalent to $\epsilon(0,\omega)$ defined by Eq. (2). It is interesting to note that the $\mathrm{Re}\sigma(0)$ for interband transitions vanishes in the case where electron number is not conserved. However, Eq. (3) yields a nonzero value of $\mathrm{Re}\sigma(0)$.

Evaluation of the real and imaginary parts of Eq. (2) and of $\mathrm{Re}\sigma$ with the use of the Penn model yields

$$\epsilon_1(0,\omega)=1+\frac{E_P^2\Delta^2}{16E_F^2}\left\{\left[\frac{A(2\Delta t_0-1)}{\alpha\Delta^2}+\frac{A(A-\rho^2)-B}{2\alpha\rho^3\cos\varphi}\tan^{-1}\left[\frac{2(1-\Delta t_0)(\Delta+t_0\rho^2)\rho\cos\varphi}{4\rho^2 t_0\Delta\cos^2\varphi+(1-\rho^2t_0^2)(\Delta^2-\rho^2)}\right]\right]\right.$$
$$+\frac{(1-\Delta^2)[A\gamma-\lambda^2(2A\beta+\Delta^2-A)+\lambda^2A-A+\Delta^2}{4\lambda^3\alpha\Delta^2\cos\psi}$$
$$\times\left[\tan^{-1}\left[\frac{t_0^2-\lambda^2}{2\lambda t_0\cos\psi}\right]+\frac{\pi}{2}\right]+\frac{A(A+\rho^2)-B}{4\alpha\rho^3\sin\varphi}$$
$$\times\ln\frac{(1+\rho^2t_0^2+2\rho t_0\sin\varphi)(\Delta^2+\rho^2-2\Delta\rho\sin\varphi)}{(1+\rho^2t_0^2-2\rho t_0\sin\varphi)(\Delta^2+\rho^2+2\Delta\rho\sin\varphi)}$$
$$\left.+\frac{(1-\Delta^2)[A\gamma+\lambda^2(2A\beta+\Delta^2-A)-\lambda^2A-A+\Delta^2]}{8\alpha\Delta^2\lambda^3\sin\psi}\ln\frac{t_0^2+\lambda^2+2\lambda t_0\sin\psi}{t_0^2+\lambda^2-2\lambda t_0\sin\psi}\right\} \tag{4}$$

and

$$\epsilon_2(0,\omega)=\frac{E_P^2}{128E_F^4}\frac{\hbar^2\omega}{\tau}\left\{\frac{(1-2\Delta t_0)}{\alpha\Delta^2t_0}+\frac{(1-\lambda^2)+(1-\Delta^2)(2\lambda^2\beta-\lambda^2-r)}{4\lambda^3\alpha\Delta^2\cos\psi}\left[\tan^{-1}\left[\frac{t_0^2-\lambda^2}{2\lambda t_0\cos\psi}\right]+\frac{\pi}{2}\right]\right.$$
$$+\frac{(1+\lambda^2)-(1-\Delta^2)(2\beta\lambda^2-\lambda^2+\gamma)}{8\lambda^3\alpha\Delta^2\sin\psi}\ln\frac{t_0^2+\lambda^2+2\lambda t_0\sin\psi}{t_0^2+\lambda^2-2\lambda t_0\sin\psi}$$
$$-\frac{(2A-\rho^2)}{2\alpha\rho^3\cos\varphi}\tan^{-1}\left[\frac{2(1-\Delta t_0)(\Delta+t_0\rho^2)\rho\cos\varphi}{4\rho^2t_0\cos\varphi+(1-\rho^2t_0^2)(\Delta^2-\rho^2)}\right]$$
$$\left.-\frac{(2A-\rho^2)}{4\alpha\rho^3\sin\varphi}\ln\frac{(1+\rho^2t_0^2+2\rho t_0\sin\varphi)(\Delta^2+\rho^2-2\Delta\rho\sin\varphi)}{(1+\rho^2t_0^2-2\rho t_0\sin\varphi)(\Delta^2+\rho^2+2\Delta\rho\sin\varphi)}\right\}, \tag{5}$$

where

$$A=\hbar^2\left[\omega^2-\frac{1}{\tau^2}\right]\Big/16E_F^2,\quad B=\hbar^4\omega^2/64E_F^2\tau^2,\quad \alpha=A^2+B,\quad \beta=1-\frac{A\Delta^2}{\alpha},$$
$$\gamma=1-\frac{(2A-\Delta^2)\Delta^2}{\alpha},\quad \rho=\alpha^{1/4},\quad \cos(2\varphi)=-A/\rho^2,\quad \lambda=\gamma^{1/4},$$

and

$$\cos(2\psi)=-\beta/\lambda^2 .$$

Equation (5) is valid for $\hbar\omega\gtrless E_g$. For the energy values not close to E_g the values of $\epsilon_1(0,\omega)$ and $\epsilon_2(0,\omega)$ from Eqs. (4) and (5) are not very different from the collisionless values of Eqs. (1) and (2.15) of Ref. 4. With the use of Eqs. (3) and (4) it is easy to show that $\mathrm{Re}\sigma(0)$ is given by

$$\mathrm{Re}(0)=\frac{E_P^2}{4\pi\tau E_g^2}\left[\frac{\Delta^2(1-\Delta^2)t_0}{a'^2}-\frac{(1-a'^2-\Delta^2)\Delta^4}{2a'^3(a'^2+\Delta^2)^{1/2}}\ln\left[\frac{(a'^2+\Delta^2)^{1/2}+t_0a'}{(a'^2+\Delta^2)^{1/2}-t_0a'}\right]\right.$$
$$\left.-\frac{2(1-\Delta t_0)\Delta^3}{a'^2}+\frac{2\Delta^4}{a'^3}\tan^{-1}\left[a'\frac{(1-\Delta t_0)}{(\Delta+t_0a'^2)}\right]\right], \tag{6}$$

where $a'=\hbar/(4E_F\tau)$.

III. RESULTS AND DISCUSSION

In this section, we report calculations of $\epsilon_2(0,\omega)$, $\tilde{\epsilon}_2(0,\omega)$, $\mathrm{Im}[-\epsilon^{-1}(0,\omega)]$, $\mathrm{Im}[-\tilde{\epsilon}^{-1}(0,\omega)]$, and $\mathrm{Re}\sigma(0)$ for various semiconductors. However, a detailed discussion has been given only for Si. Our calculations have two adjustable parameters, E_g and τ. E_g has been determined in our earlier work.[5] A

rough value of the lower limit of cutoff scattering time τ_c may be determined with the use of the arguments of Garik and Ashcroft (GA).[18] For this we plot $h\,\mathrm{Re}\sigma(0)$ as a function of $\log_{10}\tau$ for Si in Fig. 1. (h is Planck's constant.) We find that $\mathrm{Re}\sigma(0)$ tends to zero in the limits $\tau\rightarrow\infty$ and $\tau\rightarrow 0$. This is similar to the case of Al reported by GA. Thus, following the arguments of GA for the electrons contributing to dielectric function, we have

$$v_F\tau > a \ , \tag{7}$$

where v_F and a are the Fermi velocity and lattice parameters, respectively. τ is obtained so as to get agreement between our calculated $\epsilon_1(0,\omega)$ and $\epsilon_2(0,\omega)$ and those from the first-principles calculations.[10,22] (To perform the first-principles calculations pseudopotential form factors have been fitted from experimental data, thus these already include collision effects in some sense.) Our $\hbar/\tau$ is much less than that determined by Philipp and Ehrenreich obtained by matching the free-electron and experimental value of $\epsilon_1(0,\omega)$ and $\epsilon_2(0,\omega)$ somewhere in the range with $\hbar\omega > E_g$. They had found $\hbar/\tau$ to be in range 3—5 eV for a number of semiconductors. This indicates that $\hbar/\tau \sim E_g$. It also gives $v_F\tau < a$, which is contrary to the arguments of GA and hence unphysical. As a word of caution, we would like to emphasize that τ is just a parameter and has nothing to do with real scattering.

Using the τ determined above, we calculate $\epsilon_1(0,\omega)$, $\tilde{\epsilon}_1(0,\omega)$, $\epsilon_2(0,\omega)$, $\tilde{\epsilon}_2(0,\omega)$, $\mathrm{Im}[-\epsilon^{-1}(0,\omega)]$, and $\mathrm{Im}[-\tilde{\epsilon}^{-1}(0,\omega)]$. We plot, for Si, $\epsilon_2(0,\omega)$ and $\tilde{\epsilon}_2(0,\omega)$ in Fig. 2, and $\mathrm{Im}[-\epsilon^{-1}(0,\omega)]$ and $\mathrm{Im}[-\tilde{\epsilon}^{-1}(0,\omega)]$ in Fig. 3 along with the experimental data.[23] We note that two curves from our work do not differ significantly from each other except around the peak positions. Our calculations give good agreement with the experimental data for the entire energy range. However, agreement with experimental data may be improved further by including the local-field effects[8,12] and excitonic effects.[9] We have also calculated the real and imaginary parts

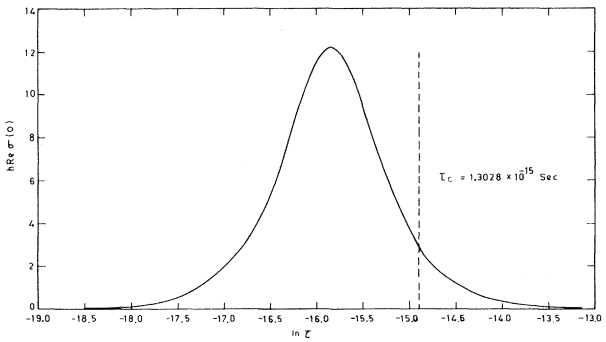

FIG. 1. $h\,\mathrm{Re}\sigma(0)$ has been plotted as a function of $\log_{10}\tau$.

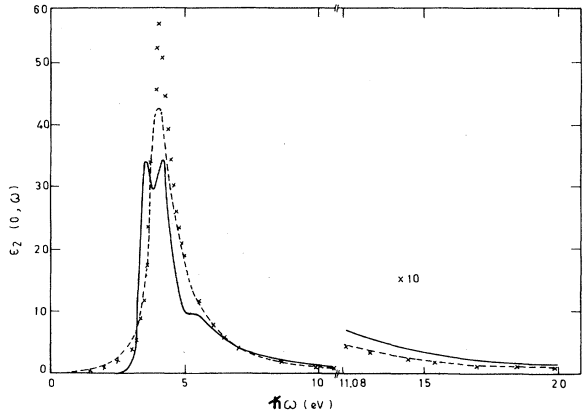

FIG. 2. Plot of the imaginary part of the dielectric function as a function of ω. $\times\times\times\times$ from Eq. (2), ----- from Eq. (3), and —— experimental data from Ref. 23.

of the dielectric function and the energy loss function from Eqs. (2) and (3) at various τ values. We find that peak heights are sensitive to τ while peak positions are not.

Encouraged by the above agreement for Si we have performed similar calculations for other semiconductors. The position of maxima, maxima height, and full width at half maxima of

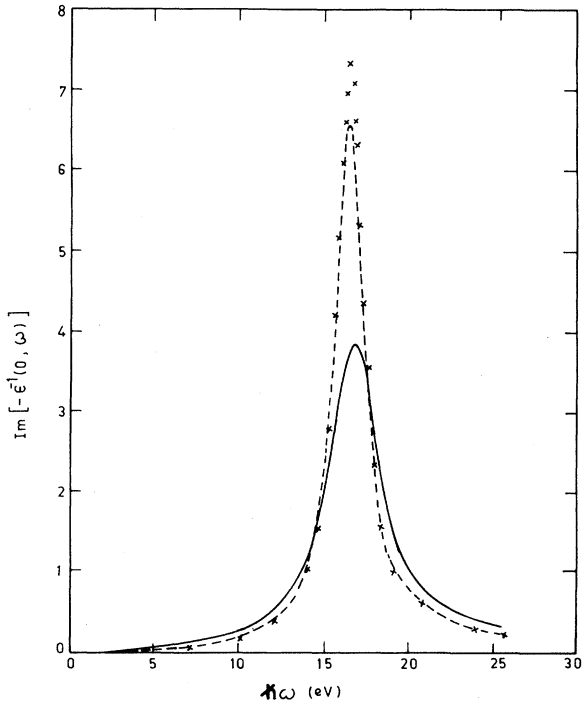

FIG. 3. Plot of the energy-loss function as a function of ω. $\times\times\times\times$ from Eq. (2), ---- from Eq. (3), and —— experimental data from Ref. 23.

TABLE I. Plasma energy, plasma peak, and plasma linewidth.

		From this work			Experimental data			From Ref. 6		
Semiconductor	$\hbar/\tau$ (eV)	$\hbar\omega_P$ (eV)	$\mathrm{Im}(-\tilde{\epsilon}^{-1})_{\max}$	$\Delta_{1/2}$ (eV)	$\hbar\omega_P$	$\mathrm{Im}[-\epsilon^{-1}]_{\max}$	$\Delta_{1/2}$ (eV)	$\hbar\omega_P$	$\mathrm{Im}(-\epsilon^{-1})_{\max}$	$\Delta_{1/2}$ (eV)
Si	0.25	16.52	6.55	2.26	16.45[a] 16.9[b] 16.64[c]	6.3[a] 5.3[b] 3.9[c]	3.6[a] 3.2[b] 3.8[c]	17.3	7.6	2.2
Ge	0.28	15.46	6.42	1.90	15.95[a] 16.2[b] 15.5[d]	5.4[a] 5.2[b] 3.6[d]	3.4[a] 3.1[b] 3.6[d]	16.5	7.4	2.1
GaAs	0.28	15.6	5.0	2.24	15.7[e]	3.6[e]	4.1[e]	16.8	6.8	2.3
GaP	0.26	16.66	4.93	2.64	16.5[e]	3.5[e]	3.5[e]	16.9	6.3	2.7
GaSb	0.34	13.74	5.07	1.88	13.3[e]	3.7[e]	2.8[e]	14.9	6.6	2.1
InSb	0.39	12.52	4.58	1.76	12.8[e]	3.1[e]	3.1[e]	14.0	6.7	1.9
InAs	0.33	13.78	4.39	1.96	13.8[e]	2.7[e]	3.7[e]	15.4	6.3	2.2

[a]Reference 24.
[b]Reference 25.
[c]Reference 23.
[d]Reference 26.
[e]Reference 27.

$\mathrm{Im}[-\epsilon^{-1}(0,\omega)]$ termed as plasma energy ($\hbar\omega P$), plasma peak [$\mathrm{Im}(-1/\epsilon)_{\max}$], and plasma linewidth ($\Delta_{1/2}$) from our work along with those obtained from experimented data[24–27] as well as other calculations[6] are reported in Table I. The table demonstrates that our calculations for compound semiconductors also give good agreement with the experimental data[27] as well as recent model calculations of Sturm and Oleveira.[6] We note here that for Ge and compound semiconductors d-core corrections have been taken into account by using an empirical method.[15,28]

IV. CONCLUSIONS

We have reported analytic expressions for the real and imaginary parts of ω-dependent dielectric functions and $\mathrm{Re}\sigma(0)$ with the use of the Penn model. Our calculations show that the Penn model gives reasonably good agreement with experimental data in the optical regime when collision effects introduced via a phenomenological relaxation time τ have been included in the RPA dielectric function.

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