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Model dielectric function for semiconductors

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We present a model for the dielectric function of semiconductors. It has been tested successfully for Si, Ge, GaAs, and ZnSe. In conjunction with the single plasmon-pole approximation it yields plasmon-energy dispersions in fair agreement with experiments. It allows one, moreover, to deduce an analytical expression for the Coulomb-hole part of the static self-energy operator.

In the last decade a new interest has grown for the modeling of the dielectric response of semiconductors. In fact, in first-principles calculations of the electronic excitation spectrum, the knowledge of the screening function of the material is needed.[1,2] This is in general a very demanding task from the computational point of view and can be performed systematically for simple structures only. Hence the study of models for the dielectric response of semiconductors has become fundamental in order to reduce the computational effort associated with the calculations of quasiparticle energies and band gaps in complex structures.[3–6]

In the present paper we propose a model static dielectric function for systems with an energy gap in their electronic excitation spectrum. Here we focus on the random-phase-approximation (RPA) dielectric function, because it is the one that is normally used in self-energy calculations.[1,2] Our model is obtained by introducing a fitting parameter in an older model, developed by Bechstedt and Enderlein,[7] and reproduces with high accuracy the calculated RPA dielectric function of Walter and Cohen.[8] This is a relevant point in quasiparticle energy calculations;[1,2] the previous models fulfill this particular point with less accuracy than the present one does.[7–11] The value of the fitting parameter entering in our model turns out to be practically constant for all the materials considered (Si, Ge, GaAs, and ZnSe). The model dielectric function is extended to nonzero frequencies according to the single plasmon-pole approximation, yielding plasmon-energy dispersions in fair agreement with experiments[12,13] and more complete calculations.[13] The present model allows one, moreover, to derive a simple analytical form for the static Coulomb-hole part of the self-energy operator of semiconductors. This constitutes an important step toward finding simple analytical expressions for the quantities involved in self-energy calculations, in order to reduce the computational effort.

We introduce a dielectric function of the form

$$\epsilon(q)=1+\{[\epsilon(0)-1]^{-1}+\alpha(q/q_{\mathrm{TF}})^2 + \hbar^2 q^4/(4m^2\omega_p^2)\}^{-1}, \quad (1)$$

where the Thomas-Fermi wave vector q_{TF} and the plasma frequency ω_p depend on the electron density ρ. We neglect for the moment local-field effects; therefore, ρ must be intended here as the average electron density. An expression similar to (1), but with $\alpha=1$, has been introduced by Bechstedt and Enderlein in 1979.[7] Expression (1) can be understood in the following way, for $\alpha=1$: the second term in the curly brackets, proportional to q^2, results from the Thomas-Fermi treatment of the screening for the homogeneous electron gas. The first term is added in order to account for the $q=0$ finite value $\epsilon(0)$, and the third one to describe the free-electron-gas behavior $1+\hbar^2\omega_p^2/(\hbar^2q^2/2m)^2$ at large q. However, to simply add the Thomas-Fermi-like and $q=0$ terms is questionable; therefore, we introduce the parameter α, which increases the flexibility and hence the accuracy of the model. This fitting parameter is sufficient to obtain curves in excellent agreement with those of Ref. 8.

We find for each material a particular value α_0 which gives the best fit of Eq. (1) to the RPA dielectric function of Walter and Cohen.[8] To be precise, we are fitting our dielectric function to the arithmetic average of the results of Walter and Cohen for the $\mathbf{q}=(1,0,0)$ and (1,1,1) directions for Si, Ge, GaAs, and ZnSe, respectively. We then calculate the root-mean-square error $\lambda=\lambda(\alpha)$ between the resulting curve and the one obtained from (1), and its minimum as a function of $\alpha,\lambda(\alpha_0)$. In the second and third columns of Table I, are reported the α_0 and $\lambda(\alpha_0)$ values, respectively, for Si, Ge, GaAs, and ZnSe. Since the α_0 values are very close to each other (within 3%), we use in (1) their average, $\langle\alpha\rangle=1.563$. It can be seen that the errors $\lambda(\langle\alpha\rangle)$, reported in the fourth column of Table I, are only slightly larger than the $\lambda(\alpha_0)$'s. This means that it is a very good approximation to use $\langle\alpha\rangle$ (a

TABLE I. Parameters used to reproduce with the model given in Eq. (1), the RPA dielectric function of Ref. 8, and corresponding root-mean-square errors (RMSE's). In the first column are the dielectric constants from Ref. 8 [$\epsilon(0)$], in the second are the values of the fitting parameters that minimize the RMSE's for each material (α_0). In the third and fourth columns are the RMSE's corresponding to α_0 and to the average value $\langle\alpha\rangle=1.563$. In the fifth column are the RMSE's obtained for the Levine-Louie dielectric function (Ref. 11).

Element	$\epsilon^{\mathrm{RPA}}(0)$	α_0	$\lambda(\alpha_0)$	$\lambda(\langle\alpha\rangle)$	λ_{LL}
Si	11.3	1.537	0.075	0.0736	0.2506
Ge	14.0	1.604	0.1604	0.1660	0.2425
GaAs	8.9	1.584	0.0623	0.0638	0.1940
ZnSe	4.8	1.527	0.0572	0.0586	0.1460

constant not dependent on the material) to reproduce the RPA dielectric function of different semiconductors starting from (1). Hence the suitable factor that multiplies the second-order term in q in (1) turns out to be *universal*. It allows one to obtain very good fits in the intermediate-q region.

In Figs. 1–4 are reported the curves obtained from Eq. (1) for Si, Ge, GaAs, and ZnSe, with the values of $\epsilon(0)$ taken from Walter and Cohen[8] (first column of Table I) and $\alpha=\langle\alpha\rangle$. In the figures are also reported the curves obtained with the Levine-Louie dielectric function (Ref. 11) using the same values of $\epsilon(0)$. The Levine-Louie dielectric function models semiconductor screening starting from Lindhard's formula for the electron gas, which is modified to account for the finite value of $\epsilon(0)$ in semiconductors.[11] It is clear from those curves that a good agreement results between the Levine-Louie function and the dielectric function (1) in the region $q\rightarrow 0$ due to the same choice of $\epsilon(0)$. But in the intermediate region $q\simeq 2\pi/a$ (where a is the lattice constant), the Levine-Louie dielectric function results are always larger than the one of Walter and Cohen, and as a consequence are larger than the one determined by us from (1). A quantitative measure of such deviation is given by calculating the root-mean-square error between the Levine-Louie and the Walter-Cohen dielectric functions, reported in the fifth column of Table I. They are larger than those reported in the third and fourth columns, which refer to the curves obtained from (1). The behavior of the Levine-Louie dielectric function in the intermediate-q region determines a slight overestimate of the semiconductor screening in that region with respect to the RPA one. This might be the reason for the 0.10–0.15-eV underestimate of the band gaps of semiconductors, found in Ref. 5 using the Levine-Louie dielectric function, with respect to those based on *ab initio* calculated dielectric functions. The use of the Penn or other models, instead of that of Levine and Louie, further worsens the agreement with the calculated RPA dielectric function.[10,11]

In the figures are also reported the available data from more-recent RPA calculations (for Si and Ge from Ref. 14, for GaAs and ZnSe from Ref. 15). The $\epsilon(0)$ values after Refs. 14 and 15 for GaAs and Ge are larger than those of Ref. 8; for ZnSe and Si the values are, respectively, smaller, and coincident with those calculated by Walter and Cohen. We decided to fit, starting from Eq. (1), the RPA dielectric function of Walter and Cohen and not the more-recent calculations because a continuous set of values is given instead of the very few points of Refs. 14 and 15.

From our model dielectric function, a simple analytical expression for the Coulomb-hole part of the self-energy operator for semiconductors can be determined. The static Coulomb-hole contribution to the self-energy operator can be written as[1,2]

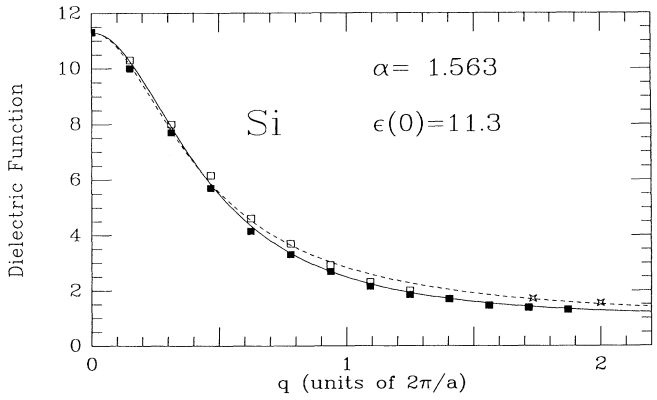

FIG. 1. Dielectric functions for Si. Closed boxes [along the $\mathbf{q}=(1,1,1)$ direction] and open boxes [along the $\mathbf{q}=(1,0,0)$ direction] are from the RPA calculations of Walter and Cohen (Ref. 8). The solid line is from Eq. (1) with $\epsilon(0)=\epsilon_0^{\mathrm{RPA}}=11.3$ from the calculations of Ref. 8 and $\alpha=\langle\alpha\rangle=1.563$. Dashed line: Levine-Louie model (Ref. 11). Stars are from Ref. 14.

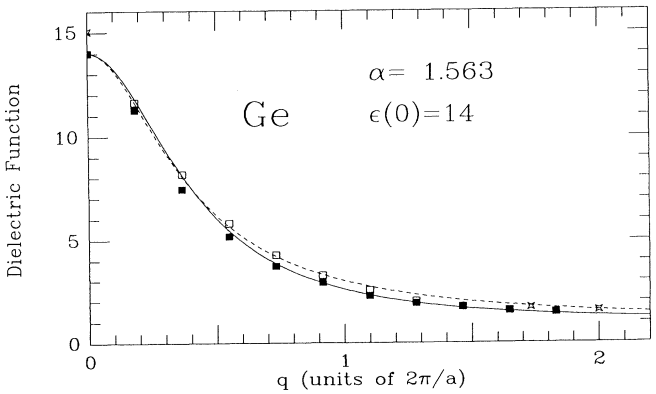

FIG. 2. As in Fig. 1 but referred to Ge with $\epsilon(0)=\epsilon_0^{\mathrm{RPA}}=14$. Stars are from Ref. 14.

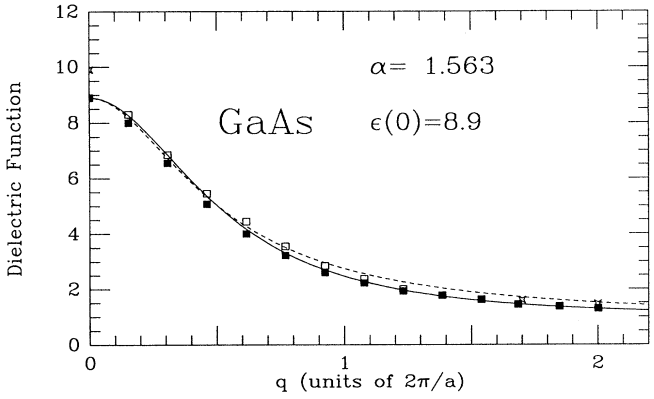

FIG. 3. As in Fig. 1 but referred to GaAs with $\epsilon(0)=\epsilon_0^{\mathrm{RPA}}=8.9$. Stars are from Ref. 15.

$$\Sigma_{\mathrm{COH}}^{\mathrm{st}}(\mathbf{r},\mathbf{r}')=\tfrac{1}{2}\delta(\mathbf{r}-\mathbf{r}')[w(\mathbf{r},\mathbf{r}';0)-v(\mathbf{r}-\mathbf{r}')] \ . \quad (2)$$

In (2) $w(\mathbf{r},\mathbf{r}';E=0)$ and $v(\mathbf{r}-\mathbf{r}')$ are the statically screened and bare Coulomb potentials, respectively. In order to account for local-field (LF) effects, we consider the local-density-like ansatz for the screened Coulomb potential proposed in Ref. 5,

$$w(\mathbf{r},\mathbf{r}';0)=\tfrac{1}{2}[w^h(\mathbf{r}-\mathbf{r}',\rho(\mathbf{r}))+w^h(\mathbf{r}-\mathbf{r}',\rho(\mathbf{r}'))] \quad (3)$$

(w^h is the screened Coulomb interaction calculated neglecting LF effects), which has been tested with good results in the case of several semiconductors.[5,6,16] In this way from (2) and (3) we find for the static Coulomb-hole term the expression

$$\Sigma_{\mathrm{COH}}^{\mathrm{st}}(\mathbf{r},\mathbf{r}')=\tfrac{1}{2}\delta(\mathbf{r}-\mathbf{r}')\frac{1}{(2\pi)^3} \times\int d^3\mathbf{q}\frac{4\pi e^2}{q^2}\left[\frac{1}{\epsilon(q,\rho(\mathbf{r}))}-1\right] . \quad (4)$$

From (1) and (4) we obtain, after straightforward algebra,

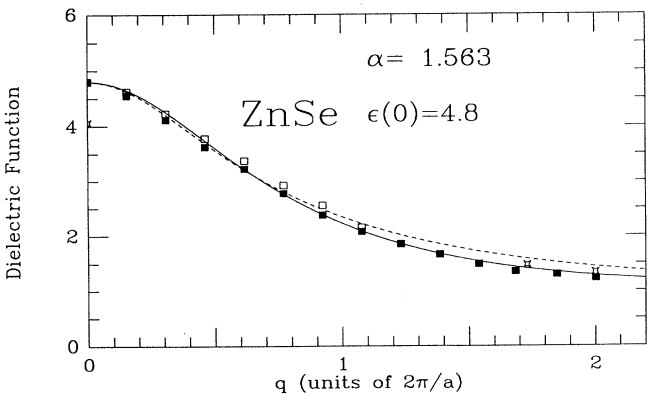

FIG. 4. As in Fig. 1 but referred to ZnSe with $\epsilon(0)=\epsilon_0^{\mathrm{RPA}}=4.8$. Stars are from Ref. 15.

$$\Sigma_{\mathrm{COH}}^{\mathrm{st}}(\mathbf{r},\mathbf{r}')=-\delta(\mathbf{r}-\mathbf{r}')\frac{e^2}{2}\left[1-\frac{1}{\epsilon(0)}\right]^{1/2}\frac{q_{\mathrm{TF}}[\rho(\mathbf{r})]}{\alpha^{1/2}} \times\left[1+\frac{q_{\mathrm{TF}}[\rho(\mathbf{r})]}{\alpha k_F[\rho(\mathbf{r})]}\left[\frac{3\epsilon(0)}{\epsilon(0)-1}\right]^{1/2}\right]^{-1/2} , \quad (5)$$

where the Fermi wave vector $k_F[\rho(\mathbf{r})]$ and $q_{\mathrm{TF}}[\rho(\mathbf{r})]$ are computed for the local density $\rho(\mathbf{r})$. We see from (5) that the Coulomb-hole term is expressed in a simple analytical form, which, by way of contrast, cannot be obtained from the expression of Levine and Louie.[11] It is desirable to find analytical forms for the exchange-correlation self-energy in semiconductors, which lead to well-founded simple methods reducing the computational effort in these materials. Equation (5) for the Coulomb-hole part of the static self-energy operator represents progress in that direction.

The model of the static dielectric function (1) can be generalized to nonzero frequencies using the single plasmon-pole approximation.[1] One obtains

$$\epsilon(q,\omega)=1+\{[\epsilon(0)-1]^{-1}+\alpha(q/q_{\mathrm{TF}})^2 +\hbar^2q^4/(4m^2\omega_p^2)-\omega^2/\omega_p^2\}^{-1} , \quad (6)$$

where, neglecting LF effects, q_{TF} and ω_p are calculated for the average electron density. The plasmon energy $\Omega_p(q)$ is easily obtained, for small q, in the form

$$\Omega_p(q)=\omega_p\{\epsilon(0)/[\epsilon(0)-1]\}^{1/2}+\alpha_D\hbar q^2/m \ , \quad (7)$$

with

$$\alpha_D=(\alpha/2)(m/\hbar)\{\epsilon(0)/[\epsilon(0)-1]\}^{1/2}\omega_p/q_{\mathrm{TF}}^2 . \quad (8)$$

We calculate $\alpha_D=0.38$ for Si, and $\alpha_D=0.34$ for GaAs. For these materials calculations and/or measurements are available:[12,13] experiments yield $\alpha_D=0.37$ for Si (Ref. 13, average between the Λ and Δ lines), and $\alpha_D=0.42$ for polycrystalline GaAs.[12] Calculations for Si yield values ranging from 0.38 to 0.55,[13] depending on the ingredients and accuracy of the calculations. An analysis of the subtleties of the dielectric-function calculations (the treatment of exchange and correlation, LDA versus empirical pseudopotential calculations, the inclusion or not of local-field effects) is beyond the scope of the present paper. Nevertheless, we see that our calculated α_D values are in fair agreement with experiments and more-complete calculations. If $\alpha=1$ was used in (6) we would get $\alpha_D=0.24$ and 0.22 for Si and GaAs, respectively, about a factor of 2 smaller than the experimental or theoretical values quoted in Refs. 12 and 13.

On the other hand, the plasmon dispersion can also be calculated from the model of Levine and Louie. One finds, without using the single plasmon-pole approximation,

$$\alpha_D^{\mathrm{LL}}=\tfrac{9}{10}(m/\hbar)\{\epsilon/[\epsilon(0)-1]\}^{1/2}\omega_p/q_{\mathrm{TF}}^2 . \quad (9)$$

Our factor $\alpha/2$ is here replaced by the well-known RPA factor ($\frac{9}{10}$); this fact supports our conjecture of a universal value of $\alpha=\langle\alpha\rangle=1.563$, and also sheds some light on

the reason for this particular value: it approaches 1.8, which would reproduce the Levine-Louie result (9). Equation (9) yields $\alpha_D^{LL}=0.44$ and 0.39 for Si and GaAs, respectively. These values are similar to those obtained from (8), and agree equally well with experiments and the more-refined calculations.

In conclusion, we propose a model dielectric function that reproduces with high accuracy the RPA dielectric function of Walter and Cohen. Apart from the dielectric constant $\epsilon(0)$, we use just one fitting parameter α, which turns out to be practically constant for such different materials as Si, Ge, GaAs, and ZnSe. The model permits one, moreover, to calculate a simple analytical expression for the static Coulomb-hole term of the self-energy operator for semiconductors. When the model is used in conjunction with the single plasmon-pole approximation in order to mimic the frequency dependence of the dielectric function, the dispersion of the plasmon energy can be obtained. The results compare fairly well with more-complete calculations and experiments. Such agreement is lost if the older model of Bechstedt and Enderlein,[7] with $\alpha=1$, is used.

It is worth comparing our model with that proposed by Levine and Louie.[11] Our model yields a slightly better description of the static dielectric function, thanks to the fitting parameter α. Both models yield a fairly good description of the plasmon dispersion. We believe that the main advantage of the Levine-Louie model is its exact description of the homogeneous electron-gas behavior, obtained for $\epsilon(0)$ going to infinity. By way of contrast, in this case our model presents noticeable differences with respect to the Lindhard function.[17] On the other hand, the main advantages of our model are the simplicity, which allows analytical calculations to be carried out, and the flexibility, which might allow it to describe other kinds of dielectric functions, such as, for instance, the macroscopic dielectric function accounting for local-field effects, by simply changing the values of $\epsilon(0)$ and α. Moreover, simplified GW calculations carried out using the present model are in agreement with full GW ones that rely on *ab initio* calculated dielectric functions.[16,17]

[1]M. S. Hybertsen and S. G. Louie, Phys. Rev. B **34**, 5390 (1986).
[2]R. W. Godby, M. Schlüter, and L. J. Sham, Phys. Rev. B **37**, 10 159 (1988).
[3]F. Gygi and A. Baldereschi, Phys. Rev. Lett. **62**, 2169 (1989).
[4]F. Bechstedt and R. Del Sole, Phys. Rev. B **38**, 7710 (1988).
[5]M. S. Hybertsen and S. G. Louie, Phys. Rev. B **37**, 2733 (1988).
[6]X. Zhu and S. G. Louie, Phys. Rev. B **43**, 14 142 (1991).
[7]F. Bechstedt and R. Enderlein, Phys. Status Solidi B **94**, 239 (1979); **95**, 185 (1979).
[8]J. P. Walter and M. L. Cohen, Phys. Rev. B **2**, 1831 (1970).
[9]D. R. Penn, Phys. Rev. **128**, 2093 (1962).
[10]R. Resta, Phys. Rev. B **16**, 2717 (1977).
[11]Z. H. Levine and S. G. Louie, Phys. Rev. B **25**, 6310 (1982).
[12]R. Manzke, J. Phys. C **13**, 911 (1980).
[13]R. Daling and W. van Haeringen, Phys. Rev. B **45**, 8970 (1992), and references cited therein.
[14]A. Baldereschi and E. Tosatti, Phys. Rev. B **17**, 4710 (1978).
[15]R. Resta and A. Baldereschi, Phys. Rev. B **23**, 6615 (1981).
[16]F. Bechstedt, R. Del Sole, G. Cappellini, and Lucia Reining, Solid State Commun. **84**, 765 (1992).
[17]G. Cappellini, Ph.D. thesis, University of Rome "La Sapienza," 1992.