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Phenomenological approximations to the self-energy operator by a generalized $X\alpha$ method

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The generalized $X\alpha$ method, based on a local, energy-independent operator derived from the exchange-correlation potential of the local-density approximation by changing the weight of the exchange term, is revisited with the aim of building an optimized starting point for band-structure calculations within the GW method. We find that the optimal choice coincides with the unmodified local-density approximation potential, i.e., with $\alpha=2/3$. Moreover, we show that the use of an $X\alpha$ method to mimic the self-energy effects in the calculation of absorption spectra leads to worse results than the simpler ''scissors operator'' approach.

I. INTRODUCTION

Ab initio calculations based on the density-functional theory in the local-density approximation[1] (DFT-LDA), and the subsequent corrections accounting for self-energy effects computed in the GW approximation within the many-body quantum field theory, are now considered as a standard way to describe the electronic structure of condensed-matter systems. The method can be summarized as follows: The first step is the solution of the DFT-LDA (Kohn-Sham) equations, a set of single-particle equations to be solved self-consistently. It is well known that the results obtained in this way yield directly only the ground-state properties, such as lattice parameters, elastic constants, etc. In fact, density-functional theory, as initially formulated, is a ground-state theory; excited states are not directly accessible. Nevertheless, the calculated Kohn-Sham eigenvalues, which have no direct physical meaning, are often interpreted as single-particle excitation energies, and found in quite a good agreement with experimental quasiparticle energies (e.g., photoemission spectra). This implies, however, some drawbacks, the most important one being an evident underestimate of the band gaps in semiconductors and insulators. For this reason excited-state properties like optical-absorption spectra are often not well described in DFT.

A proper description of excited-state properties is provided by the many-body quantum field theory (MBQFT), or Green's-function method, where a central role is played by the self-energy $\Sigma(\mathbf{r},\mathbf{r}',\omega)$, a nonlocal, energy-dependent operator. The central equations of the theory, known as the Hedin equations,[2] form a complex system of five integro-differential equations to be solved self-consistently. The so-called GW approximation, in which $\Sigma=GW$, i.e., the self-energy is written as a convolution of the one-particle Green's function G with the screened Coulomb interaction W, is obtained from Hedin's equations by neglecting vertex diagrams beyond the bare vertex. The work of Godby, Schlüter, and Sham[3] and Hybertsen and Louie[4] demonstrated the usefulness of the GW scheme in practical calculations for real semiconductors. They start from the Kohn-Sham (KS) DFT-LDA electronic structure, and evaluate perturbatively self-energy corrections to KS eigenvalues by computing the expectation values of $(G^{\mathrm{LDA}}W^{\mathrm{RPA}}-V_{\mathrm{xc}}^{\mathrm{LDA}})$, where $V_{\mathrm{xc}}^{\mathrm{LDA}}$ is the exchange-correlation potential. This is based on the fact that the Kohn-Sham equations

$$[H_0+V_{\mathrm{xc}}^{\mathrm{LDA}}(\mathbf{r})]\phi_i(\mathbf{r})=\epsilon_i\phi_i(\mathbf{r}) \tag{1}$$

have the same structure of the quasiparticle equations of the MBQFT,

$$H_0\phi_i(\mathbf{r})+\int d^3r'\,\Sigma(\mathbf{r},\mathbf{r}',\epsilon_i)\,\phi_i(\mathbf{r}')=\epsilon_i\phi_i(\mathbf{r}) \tag{2}$$

and that the difference between the expectation values of the self-energy and of the exchange-correlation potential is of the order of 5% or 10%. The results obtained in this way are usually in excellent agreement with experimental data.[3,4] Moreover, it was found that in bulk semiconductors the KS eigenvectors reproduce extremely well the true quasiparticle wave functions.[4] This justifies *a posteriori* the use of first-order perturbation theory.

Perturbative GW proved to give good results in many cases, but reveals very heavy for complex systems like surfaces or clusters, due to the large computational effort needed in the evaluation of the self-energy matrix elements. For large and complex systems, the possibility to mimic the self-energy operator with a local, energy-independent potential closer to Σ than $V_{\mathrm{xc}}^{\mathrm{LDA}}$ is clearly an interesting issue. Moreover, the solution of KS equations containing such a modified potential could be used as a better starting point in a subsequent evaluation of self-energy corrections within the GW scheme.[5] A possible form for this local and energy-independent potential, following the maximum simplicity criterion, may be obtained within the generalized $X\alpha$ approach, i.e., by modifying the weight α of the exchange term in the LDA exchange-correlation potential. This method is clearly inspired by the original formulation of Slater,[6] where a ''local exchange'' potential was introduced in an approximate Hartree-Fock scheme. After the development of DFT, it became clear that Slater's local exchange potential overestimated by a factor of 3/2 the DFT-LDA exchange potential. However, when applied to solids, Slater's exchange, at variance with the DFT-LDA exchange, generally yields energy gaps in good agreement with experiments.

In this paper we explore the possibility of reproducing *GW* eigenvalues in semiconductors by treating the weight (α) of the exchange potential as an adjustable parameter. Differently from Slater's original approach, we keep the correlation potential as calculated within the LDA. We take bulk GaAs as a test case.

The problem to solve is how to determine α. If one is interested in obtaining good gaps (that is, in agreement with *GW* calculations and experiments), the natural way is to choose α by fitting the energy gaps at some high-symmetry points in the Brillouin zone. This has been our first approach. We found α of the order of 1.1, where $\alpha=1$ is Slater's, and $\alpha=2/3$ is DFT-LDA. However, the gaps do not increase equally, as happens going from LDA to *GW*. A further shortcoming of the approach is that the absorption spectrum calculated using the adjusted α value has a reduced intensity with respect to the LDA and experimental spectra. This point, related to the *f*-sum rule, is discussed in Sec. III.

If, on the other hand, one hopes to produce a better starting point than DFT-LDA for self-energy calculations, as proposed by Del Sole, Reining, and Godby,[5] the quantities to be reproduced are not the gaps, but rather the expectation values of the exchange-correlation self-energy. This approach is described in Sec. IV. Quite surprisingly, the best results are obtained for α close to 2/3, that is using the LDA exchange-correlation potential.

II. THEORY

The bare exchange energy per particle of the homogeneous electron gas at density n is

$$\epsilon_{\mathrm{x}}^{\mathrm{HEG}}(n)=-\frac{3}{4\pi}(3\pi^2 n)^{1/3}. \tag{3}$$

In the LDA approximation, the exchange potential (appearing in the Kohn-Sham equations) is hence

$$\begin{aligned} V_{\mathrm{x}}^{\mathrm{KS}}(n(\mathbf{r}))&=\frac{\delta}{\delta n}\int d^3r\, n(\mathbf{r})\epsilon_x^{\mathrm{HEG}}(n(\mathbf{r}))\\ &=\epsilon_x^{\mathrm{HEG}}(n(\mathbf{r}))+n(\mathbf{r})\frac{\partial}{\partial n}\epsilon_x^{\mathrm{HEG}}(n(\mathbf{r}))\\ &=-\frac{1}{\pi}(3\pi^2 n(\mathbf{r}))^{1/3}. \end{aligned} \tag{4}$$

So the KS exchange is exactly 2/3 of the Slater local exchange[6]

$$\overline{V}_{\mathrm{x}}[n]=-\frac{3}{2\pi}(3\pi^2 n)^{1/3}. \tag{5}$$

In the spirit of a phenomenological $X\alpha$ method, we are then lead to consider a generalized "exchange potential," taking α times the Slater exchange

$$V_x^{X\alpha}(n(\mathbf{r}))=-\alpha\frac{3}{2\pi}(3\pi^2 n(\mathbf{r}))^{1/3}. \tag{6}$$

In this expression, α must be considered an adjustable parameter. Physically, the exchange interaction lowers the filled bands with respect to the empty ones, because it is larger where the density is larger. Therefore, choosing α larger than 2/3 (the DFT-LDA value) yields larger energy gaps, correcting the well-known LDA underestimation of the experimental band gap. Hence, one can hope that a generalized $X\alpha$ could be used to obtain a band structure closer to the *GW* results than the standard LDA one. We stress the fact that we are interested only in the band structure, and not in ground-state properties (as total energies and lattice constants) which might be given incorrectly by a self-consistent $X\alpha$ calculation.

As addressed in the Introduction, two strategies can be followed in the choice of α: in the first, its value is chosen by simply minimizing the difference between the resulting LDA and *GW* gaps. In the second, one can choose the α value which minimizes the differences between the diagonal matrix elements of the $X\alpha$ exchange-correlation potential and those of the *GW* self-energy operator, i.e., minimizing the perturbative corrections to the $X\alpha$ electronic structure.

GW corrections to the $X\alpha$ electronic structure can be computed along the same line of Refs. 3 and 4. Considering the $X\alpha$ modified Kohn-Sham equation,

$$[H_0+V_{\mathrm{xc}}^{X\alpha}(\mathbf{r})]\phi_i^{X\alpha}(\mathbf{r})=\epsilon_i^{X\alpha}\phi_i^{X\alpha}(\mathbf{r}), \tag{7}$$

and comparing it to the true quasiparticle equation (2), first-order corrected quasiparticle energies can be written as

$$\epsilon_i=\epsilon_i^{X\alpha}+\frac{\langle\phi_i^{X\alpha}|\Sigma(\epsilon_i^{X\alpha})-V_{\mathrm{xc}}^{X\alpha}|\phi_i^{X\alpha}\rangle}{Z_i}, \tag{8}$$

with

$$Z_i=1-\langle\phi_i^{X\alpha}|\frac{d\Sigma}{d\epsilon}\bigg|_{\epsilon_i^{X\alpha}}|\phi_i^{X\alpha}\rangle, \tag{9}$$

where the perturbative part of the Hamiltonian, $(\Sigma-V_{\mathrm{xc}}^{X\alpha})$, is considered to be small.

The self-energy operator in the *GW* approximation is

$$\Sigma(\mathbf{r},\mathbf{r}',\omega)=\frac{i}{4\pi}\int_{-\infty}^{\infty}d\omega' e^{i\omega'\delta}W(\mathbf{r},\mathbf{r}',\omega')G(\mathbf{r},\mathbf{r}',\omega+\omega') \tag{10}$$

(δ is a positive infinitesimal).

To construct Σ, the free Green's function G can be computed using the eigenvalues and eigenfunctions of the LDA, or those from an $X\alpha$ calculation:

$$G^{X\alpha}(\mathbf{r},\mathbf{r}',\omega)=2\sum_i\frac{\phi_i^{X\alpha}(\mathbf{r})\phi_i^{X\alpha}(\mathbf{r}')}{\omega-\epsilon_i^{X\alpha}\pm i\delta}. \tag{11}$$

Similarly, the screened Coulomb interaction,

$$W=\varepsilon^{-1}V_{\mathrm{C}}, \tag{12}$$

obtained from the random-phase approximation (RPA) dielectric function $\varepsilon=1-V_C\chi^{(0)}$, requires the calculation of the independent-particles polarizability $\chi^{(0)}$:

$$\chi^{(0)}(\mathbf{r},\mathbf{r}',\omega)=2\sum_{i,j}(f_i-f_j)\times\frac{\phi_i^{X\alpha}(\mathbf{r})\phi_j^{*X\alpha}(\mathbf{r})\phi_i^{*X\alpha}(\mathbf{r}')\phi_j^{X\alpha}(\mathbf{r}')}{\epsilon_i^{X\alpha}-\epsilon_j^{X\alpha}-\omega-i\delta}, \tag{13}$$

which can be computed in the same way starting from the LDA or from the $X\alpha$ electronic structure. In both cases, as in Ref. 3, every matrix element of $W'_{\mathbf{GG}}(\omega)$ is explicitly calculated at two imaginary energies, then its energy dependence is fitted to a plasmon-pole model along the imaginary axis.

We calculate the DFT electronic structure of bulk GaAs using a dynamical minimization approach (the Car-Parrinello method), *ab initio* norm-conserving pseudopotentials, and a plane-wave basis set. The pseudopotentials used are of the Bachelet-Hamann-Schlüter type[7] in a fully separable Kleinman-Bylander representation.[8] The parametrization and cutoff radii are the default ones of Ref. 9, tailored to avoid ghost-states problems.[10] We use the Ceperley and Alder[11] LDA exchange-correlation energy functional, as parametrized by Perdew and Zunger;[12] in the $X\alpha$ calculation, we simply allow the coefficient α of the exchange term to take values different from 2/3 (the LDA one). We keep the standard, LDA pseudopotentials throughout all the calculation. This is justified by the fact that the modified exchange term has the limited scope of mimicking the GW corrections to the band structure of the solid, with no concerns about total energy. Moreover, the ''wave-function stability'' discussed below suggests that using an $X\alpha$–generated pseudopotential would have only a small effect. The kinetic energy cutoff is 18 Ry (corresponding to about 300 plane waves at a general point in the Brillouin-zone), and the Brillouin-zone integration is done using ten special points of the Monkhorst and Pack type[13] in the irreducible Brillouin zone (IBZ). All the calculations are performed at the LDA theoretical lattice constant (10.51 a.u.).

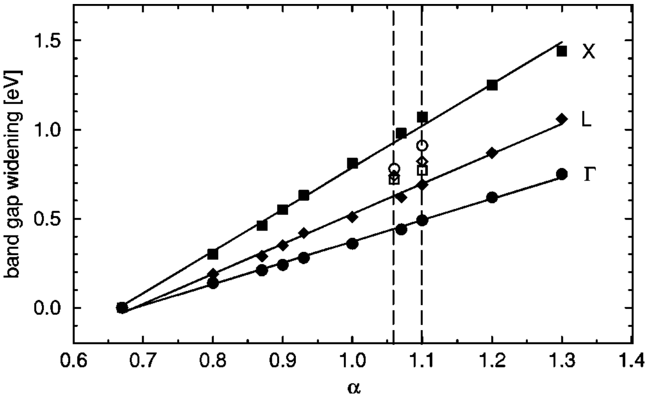

FIG. 1. Band-gap widening with respect to the LDA ($\alpha=2/3$) value in bulk GaAs. Filled circles: Γ point; filled squares: X point; filled diamonds: L point. The empty symbols correspond to the GW widening, and are located on vertical dashed lines at the α values which better reproduce the GW results (left dashed line: present work; right dashed line: Ref. 3).

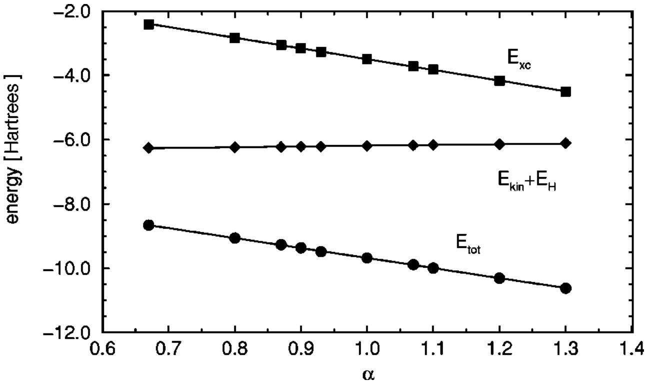

FIG. 2. Different components of the total energy per GaAs unit cell versus α (atomic units). Circles: total energy; squares: exchange-correlation energy; diamonds: kinetic plus electrostatic energy.

III. RESULTS: GAP OPTIMIZATION

In this section, we adjust the parameter α with the aim of obtaining energy gaps as close as possible to the GW gaps. Figure 1 shows the influence of α on the direct band gaps at k points Γ, X, L. Taking as a reference the gaps obtained with $\alpha=2/3$, we find a widening which increases linearly with α, the slope being different for the different k points. Hence, the effect is different with respect to the GW method, where the conduction bands are almost rigidly upshifted by a constant value (the so-called scissors operator). The almost perfect linearity of the effect suggests that the wave functions are not significantly changed by a change of α. This is confirmed by the behavior of the exchange-correlation contribution to the total energy of the system, as shown in Fig. 2. The total energy changes linearly with α, driven by the exchange-correlation term, while the kinetic plus electrostatic term remains constant.

In order to check this ''wave-function stability,'' we evaluated explicitly two different energy functionals (i.e., using $\alpha=2/3$ and $\alpha=1$) over two different sets of wave functions: the first one obtained self-consistently from the KS equations with $\alpha=2/3$, the second obtained using $\alpha=1$ (Slater exchange). Table I shows the values of the total and

TABLE I. Exchange correlation and total energies of bulk GaAs, obtained using the Kohn-Sham exchange ($\alpha=2/3$, KS) and the Slater exchange ($\alpha=1$, SL), evaluated both on the set of wave functions that minimizes the Kohn-Sham functional ($\phi_{\alpha=2/3}$) and on the set of wave functions that minimizes the modified-exchange functional ($\phi_{\alpha=1}$). Energies are in eV/unit cell.

	$\phi_{\alpha=2/3}$	$\phi_{\alpha=1}$
$E_{\mathrm{xc}}^{\mathrm{KS}}$	-2.41	-2.45
$E_{\mathrm{xc}}^{\mathrm{SL}}$	-3.42	-3.49
$E_{\mathrm{tot}}^{\mathrm{KS}}$	-8.66	-8.65
$E_{\mathrm{tot}}^{\mathrm{SL}}$	-9.67	-9.68

the exchange-correlation energies, obtained in the four cases. Clearly, the values are almost independent on the wave functions used. In order to check if also the conduction bands are ''stable'' with respect to α, we computed explicitly the superposition between KS and Slater wave functions for the first ten bands (four valence and six conduction). We found that the two wave function sets coincide within 0.1%. The situation is similar to that reported about the comparison between LDA and *GW* wave functions in bulk semiconductors (Ref. 4).

As shown in Fig. 1, the true *GW* electronic structure cannot be exactly reproduced by any value of α. It is, however, possible to consider the α value which minimizes the mean square deviation between the $X\alpha$ and the *GW* band structure at the high-symmetry k points Γ, X, and L. Considering the *GW* corrections calculated in the present work, we obtain $\alpha = 1.06$, slightly over the Slater value ($\alpha = 1$). A similar value, $\alpha = 1.10$, is obtained if we consider the *GW* corrections as calculated in Ref. 3.

Since the absorption spectrum embodies both wave functions and energies, in order to check the reliability of the $X\alpha$ method it is interesting to compare the results for the dielectric function obtained from it with the DFT-LDA results. Within the dipole approximation and neglecting the effects of the nonlocal part of the pseudopotential, the electronic transition induced by a radiation field are described in terms of the matrix elements of the momentum operator **p**. Hence, the imaginary part of the dielectric function $\varepsilon(\omega)$ is

$$\varepsilon_2(\omega) = \frac{8\pi^2 e^2}{\omega^2 m^2 V} \sum_{v,c} \sum_{\mathbf{k}} |\langle v,\mathbf{k}|\mathbf{p}|c,\mathbf{k}\rangle|^2 \delta \times [E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega], \tag{14}$$

where v and c label valence and conduction states of energy $E_v(\mathbf{k})$ and $E_c(\mathbf{k})$, and V is the crystal volume; the sum over $\mathbf{k}$ is restricted to the first Brillouin zone. In order to achieve a full convergence of the spectra, this sum is performed on a mesh of 825 special **k** points in the irreducible wedge of the Brillouin zone, and six conduction bands are considered in the sum. The results are shown in Fig. 3, where we report the imaginary part of the $X\alpha$ and LDA dielectric functions calculated according to Eq. (14). We also report the dielectric function resulting from the DFT-LDA electronic structure by applying a ''naif scissors operator'' of 0.75 eV, i.e., a rigid shift of all the conduction levels (dashed line). The experimental points are taken from Ref. 14. In the $X\alpha$ calculation, the main features of the GaAs dielectric function (the E_1 and E_2 peaks) are shifted toward higher energies of about the same amount as in the scissors operator approach. Their heights, due to the energy denominator in Eq. (14), are quite strongly reduced in both cases. Minor differences appear between the $X\alpha$ and naif scissors operator spectra.

The main drawback of the naif scissors operator, due to the neglect of the proper renormalization of the momentum matrix elements in the presence of a nonlocal self-energy, is the large underestimation of peak heights.[15] As shown in the figure, our $X\alpha$ approach displays a similar effect. The correct scissors operator approach, which instead embodies such renormalization, coincides with the LDA spectrum rigidly shifted by 0.75 eV to higher frequencies.[16]

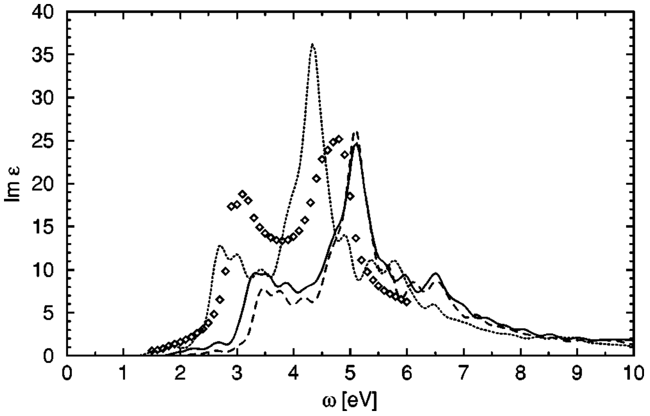

FIG. 3. Imaginary part of the dielectric function of GaAs. Solid line: using the $X\alpha$ electronic structure; dotted line: using ordinary DFT-LDA electronic structure; dashed line: using DFT-LDA electronic structure plus a ''naif scissors operator'' shift of 0.75 eV; diamonds: experimental data from Ref. 14. A broadening of 0.1 eV has been superimposed to all theoretical spectra.

In Fig. 4 we compare the $X\alpha$ dielectric function with the dielectric function obtained through Eq. (14) using a mixed electronic structure, i.e., the $X\alpha$ energy levels and the LDA wave functions. Differences between the two curves are small, confirming that the DFT-LDA and $X\alpha$ wave functions are very similar.

In conclusion, we face a strange situation: the $X\alpha$ method yields wave functions and energies very close to the corresponding *GW* quantities, but a different optical spectrum, strongly reduced in intensity with respect to the LDA, *GW*, or experimental spectra. This happens because the matrix elements of **p** in Eq. (14) are different from those needed within the *GW* method, which contain a contribution of the nonlocal self-energy. It is also worth noticing that the $X\alpha$ method satisfies the *f*-sum rule, while the *GW* method does not, because it embodies a nonlocal self-energy. These differences must occur between the *GW* method and *any* approach mimicking the self-energy with a local potential.

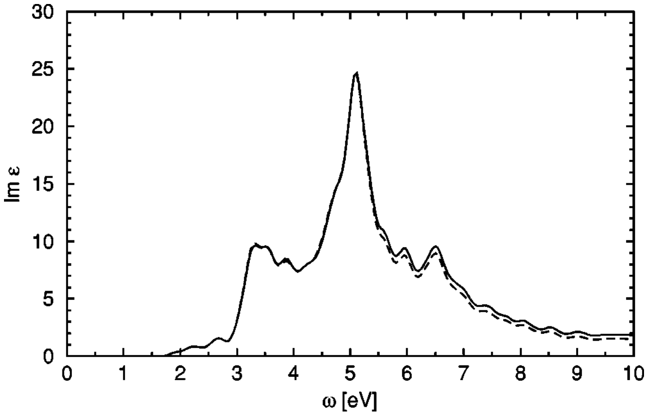

FIG. 4. Solid line: Imaginary part of the dielectric function of GaAs obtained within $X\alpha$; dashed line: results obtained with a mixed electronic structure ($X\alpha$ energy levels, and DFT-LDA wave functions).

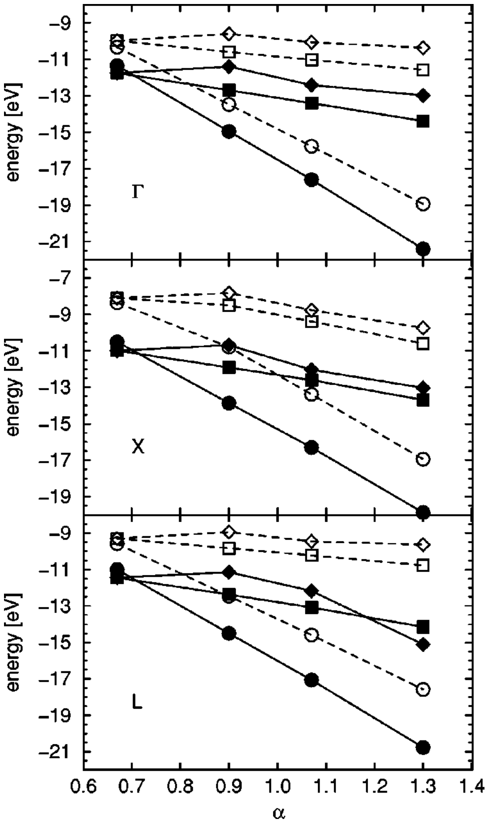

FIG. 5. Mean values of operators $V_{\mathrm{xc}}^{X\alpha}$ (circles), $\Sigma^{X\alpha}$ (squares), and Σ^{KS} (diamonds), evaluated on the $X\alpha$ states at k points Γ (top panel), X (middle panel), and L (bottom panel), for the lowest empty state (empty symbols) and for the highest occupied state (filled symbols).

IV. THE $X\alpha$ POTENTIAL AS AN APPROXIMATION FOR THE SELF-ENERGY

In this section we adopt the second strategy devised above to determine α. Starting from the $X\alpha$ electronic structure, we are now interested in the GW corrections to the $X\alpha$ levels. In this case we are looking for the α value which minimizes the difference between the exchange-correlation potential $V_{\mathrm{xc}}^{X\alpha}$ and the self-energy operator, in such a way that $(\Sigma - V_{\mathrm{xc}}^{X\alpha})$ is small, and perturbation theory can be applied safely. We consider for Σ two possible expressions:

$$\Sigma^{X\alpha} = G^{X\alpha} W^{X\alpha}, \tag{15}$$

and

$$\Sigma^{\mathrm{KS}} = G^{\mathrm{DFT\text{-}LDA}} W^{\mathrm{DFT\text{-}LDA}}. \tag{16}$$

Then we compare the mean values of the two operators evaluated on the following $X\alpha$ states: Γ_{15v}, Γ_{1c}, X_{5v}, X_{1c}, L_{3v}, and L_{1c}. The expectation values of $V_{\mathrm{xc}}^{X\alpha}$ are evaluated on the same states.

Our results are shown in Fig. 5, where we considered four different values for α. Empty points refer to mean values of the operators evaluated on conduction states, while filled points refer to occupied states. Circles are used for $\langle V_{\mathrm{xc}}^{X\alpha} \rangle$, squares and diamonds are used for the two expressions of the self-energy operator, respectively $\langle \Sigma^{X\alpha} \rangle$ and $\langle \Sigma^{\mathrm{KS}} \rangle$. It is clear that the mean values of $V_{\mathrm{xc}}^{X\alpha}$ and Σ keep near each other only for α around 2/3. At that point the GW corrections act in such a way that the gaps are increased, negative corrections occurring to valence states and positive corrections to conduction states. Such corrections, however, look rather small on the energy scale of the figure. Going to higher α's, the operators $V_{\mathrm{xc}}^{X\alpha}$ and Σ tend to be far away. Although the $X\alpha$ gaps are close to the GW gaps for α close to 1.06, the expectation values of the $X\alpha$ exchange-correlation potential on individual states are strongly different from those of the GW self-energy. In this sense, the exchange-correlation $X\alpha$ potential $V_{\mathrm{xc}}^{X\alpha}$ that better approximates the self-energy operator is that one corresponding to the value $\alpha = 2/3$, i.e., the exchange-correlation potential of the ordinary DFT-LDA.

V. CONCLUSIONS

We have explored the possibility of using the $X\alpha$ method in band-structure calculations, with the aim of mimicking the self-energy effects, or, alternatively, in order to obtain an optimized starting point for GW calculations. With respect to the scissors operator, the $X\alpha$ has the advantage that it does not introduce nonlocal terms, so that sum rules are obeyed by the $X\alpha$ dielectric function. In order to reproduce at best the GW gaps, we have to choose $\alpha = 1.06$, to be compared with the LDA value of 2/3. $X\alpha$ wave functions are within 0.1% from the LDA and the GW quasiparticle wave functions, while GW energies are reproduced within 0.1–0.2 eV. However, the intensity of the absorption spectrum is reduced, as in the ''naif scissors operator'' approach.

Moreover, although the GW gaps are well reproduced, the expectation values of the α-dependent exchange-correlation potential over individual states largely overestimate (in absolute value) the GW self-energy. This is due to the overestimation (for $\alpha > 2/3$) of the local exchange potential. Such an overestimation, which depends on the local density, has negligible effects in nearly-free-electron-like semiconductors as bulk GaAs, but might lead to the wrong results in the case of surfaces, clusters, etc. It turns out that self-energy expectation values on individual states can be best reproduced at the DFT-LDA level, that is for $\alpha = 2/3$.

It is our opinion that phenomenological approximations to the self-energy operator better than the LDA exchange-correlation potential, cannot be searched among local operators like the $X\alpha$ exchange-correlation potential studied here, even if more adjustable parameters are introduced. Considering the optical spectra indeed, the satisfaction of the f-sum rule by local operators implies that a local operator that improves the position of the peaks, toward high energies with respect to the LDA spectrum, gives necessarily a reduction of the global intensity of the spectrum, resulting in a worsening of the agreement with the experimental data.

In conclusion, the $X\alpha$ exchange-correlation potential studied here cannot simultaneously (i.e., for the same α value) describe at best self-energy effects on individual states and on gaps. Hence we do not recommend its usage in band-structure calculations.

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