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Self-consistent GW for a quasi-one-dimensional semiconductor

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We present self-consistent GW calculations for a quasi-one-dimensional model semiconductor, using multipole representations for W , the screened interaction, and G , the electron Green function. In the case of G , we distinguish between the quasiparticle contribution and the so-called incoherent contribution. We consider various strengths of the external potential. For two different starting points of the self-consistency cycle, local-density approximation and Hartree-Fock, the band gaps converge to the same values. The self-consistent GW band gaps differ very little from the Hartree-Fock band gaps. There is considerable disagreement with quantum Monte Carlo calculations for the same model, indicating the importance of vertex corrections.

I. INTRODUCTION

The GW approach, proposed in 1965 by Hedin,¹ has proven to be a useful and accurate tool for the calculation of the electronic structure of a large group of crystalline materials. The approach owes its name to the crucial approximation made in it; the restriction in the infinite series of Feynman diagrams, for the self-energy operator M to a set of diagrams, which can be represented by a Fock-like diagram in which the bare Coulomb interaction is replaced by a dynamically screened interaction W . We will symbolically write this approximation as $M = GW$. Since the screened interaction W is in some sense weaker than the bare Coulomb interaction v , higher-order diagrams in W are expected to be small.

The full Green function G , the bare Green function G^H , which is the Green function of the electrons moving in the external potential plus the Hartree potential, and the self-energy M are related to each other through the Dyson equation, symbolically written as $G^{-1} = G^H{}^{-1} - M$. It is immediately clear that one faces a self-consistency problem, since in order to determine G , M has to be known, but M itself depends on G .

An analogous self-consistency problem is linked to the determination of the screened interaction. This screened interaction W , the bare Coulomb interaction v , and the polarizability P are related to each other through $W^{-1} = v^{-1} - P$. Equivalently to the GW approximation of M , one can approximate the polarizability by its lowest- (zeroth-) order contribution in W , the random phase approximation (RPA), or bubble approximation, symbolically written as $P = GG$. Hence, in order to determine W , one has to know P , which depends on G , which depends on M , which depends on W , etc. To obtain full self-consistency within the GW approximation $M = GW$ and the RPA approximation $P = GG$, one repeatedly has to go through the “ GW cycle” until the results stabilize.

Up to now, practical GW calculations (e.g., Refs. 2–4)

have been performed by starting from a one-electron Hamiltonian, usually obtained within the framework of density functional theory in the local-density approximation (LDA), and going through the GW cycle only once. The results for a wide class of semiconductors turn out to be quite good: experimentally obtained energy gap values are reproduced within typically 0.1 eV. However, no one has yet succeeded in performing any really self-consistent GW calculation.

The purpose of this paper is to study the effects of self-consistency in the GW framework for a quasi-one-dimensional semiconductor, which is the same model that has recently been investigated by Knorr and Godby (KG).⁵ They have performed quantum Monte Carlo (QMC) calculations within this model for small systems of $N = 8$ and $N = 12$ electrons. From the obtained ground state density, these authors calculate the exchange-correlation potential leading to the same ground state density when inserted into the Kohn-Sham equations, hence constructing an “exact” density functional theory (DFT) for this system. These authors also calculate the band gap of this system by performing QMC calculations for $N - 1$ and $N + 1$ electrons, and extrapolating their results to infinite systems. We shall compare our results to these QMC results.

Extensive diagrammatic calculations on the present model have been performed by Farid.⁶ By considering Feynman diagrams contributing to the density to first order in a “residual interaction” (the bare Coulomb interaction or the screened interaction minus the exchange-correlation potential), he constructs an exchange-correlation potential in a self-consistent way. We will also compare with his results.

In the next section we describe the model. In Sec. III, we discuss the pole representations that we have used for G and W . We demonstrate that a calculation of the self-consistent G and W is possible with arbitrary precision. In Sec. IV we present results of self-consistency cycles starting from LDA or Hartree-Fock zeroth-order Green functions and discuss these results.

II. QUASI-ONE-DIMENSIONAL MODEL

We adopt the same quasi-one-dimensional model that has recently been investigated by Knorr and Godby,⁵ and by Farid.⁶ Similar models have been studied by Lannoo *et al.*,⁷ by Toet,⁸ and by Engel *et al.*⁹ We consider a quasi-one-dimensional crystal, consisting of a chain of atoms along the z direction with lattice constant a . We have chosen $a = 5$ a.u. We use Hartree atomic units throughout this paper. The electrons are confined to a line by the transverse potential

$$V(x, y) = \frac{1}{2}\gamma^4(x^2 + y^2). \quad (1)$$

Here γ is the strength of the potential, for which we choose $2(2\pi/a)$. In the transverse directions, we assume the wave functions to be in their energetically lowest eigenstate, $\chi(x, y) = \frac{\gamma}{\sqrt{\pi}} \exp[\frac{1}{2}\gamma^2(x^2 + y^2)]$. In the longitudinal z direction, the electrons move in a periodic potential. Their band structure is one dimensional. We consider the spin-compensated¹⁰ case. We have two electrons per unit cell, which means that we have one completely filled valence band.

An effective one-dimensional Coulomb interaction $v(z)$ can be derived from the three-dimensional Coulomb interaction $v(x, y, z)$ using⁵

$$\begin{aligned} v(z - z') &= \int dx dx' dy dy' |\chi(x, y)|^2 |\chi(x', y')|^2 \\ &\quad \times V(x - x', y - y', z - z') \\ &= \sqrt{\frac{\pi}{2}} \gamma \exp\left(\frac{\gamma^2(z - z')^2}{2}\right) \operatorname{erfc}\left(\frac{\gamma(z - z')}{\sqrt{2}}\right), \end{aligned} \quad (2)$$

where erfc is the complementary error function. The one-dimensional Fourier transform of Eq. (2) is

$$\begin{aligned} v(k + K) &= \frac{1}{a} \int_0^a dz e^{-i(k+K)z} v(z) \\ &= \exp\left[\frac{1}{2} \left(\frac{k + K}{\gamma}\right)^2\right] E_1\left[\frac{1}{2} \left(\frac{k + K}{\gamma}\right)^2\right], \end{aligned} \quad (3)$$

E_1 being the exponential integral and K a reciprocal lattice vector.

A zeroth-order Green function G^0 used as a starting point for our self-consistency procedure can quite generally be written as

$$G_{K,K'}^0(k, \epsilon) = \sum_l \frac{d_{l,K}^0(k) d_{l,K'}^0(k)}{\epsilon - \epsilon_l^0(k) + i\eta \operatorname{sgn}[\epsilon_l^0(k) - \mu]}, \quad (4)$$

where K and K' are reciprocal lattice vectors and ϵ is the energy. The sum is over the energy bands l , and the chemical potential μ is chosen somewhere in the energy gap of the semiconductor. The quantity η is infinitesimally small and positive. The poles in Eq. (4) can be associated with either electrons in a conduction band or

holes in a valence band, depending on $\operatorname{sgn}[\epsilon_l^0(k) - \mu]$ being negative or positive. The $d_{l,K}^0(k)$'s and the $\epsilon_l^0(k)$'s are the normalized eigenvector coefficients and eigenvalues, respectively, following from the band structure equation

$$\begin{aligned} \left[\frac{1}{2}(k + K)^2 - \epsilon_l^0(k)\right] d_{l,K}^0(k) + \sum_{K'} \left(V_{K,K'}^{\text{ext}} + V_{K,K'}^H \right. \\ \left. + \left[\begin{array}{l} (1) V_{K,K'}^{\text{xc}} \\ (2) V_{K,K'}^F(k) \end{array} \right] \right) d_{l,K'}^0(k) = 0, \end{aligned} \quad (5)$$

in which we consider either a density functional approximation (1) or the Hartree-Fock approximation (2). V^{ext} is the external potential, which is taken to be $V^{\text{ext}}(z) = A \cos(2\pi z/a)$. Hence, the band gap in a model with non-interacting electrons is approximately equal to A . V^H is the Hartree potential, with matrix elements

$$V_{K,K'}^H = V_{K-K'}^H = n_{K-K'}^0 v(K - K'). \quad (6)$$

The Fourier components of the electron density are given by

$$n_K^0 = 2 \int_0^{2\pi/a} \frac{dk}{2\pi} \sum_{K'} d_{l_v,K}^0(k) d_{l_v,K'+K}^0(k), \quad (7)$$

where l_v is the valence band index, and where the factor 2 is due to spin summation. We choose the Brillouin zone between 0 and $2\pi/a$. As usual, we approximate the exchange-correlation potential V^{xc} , arising in density functional theory, by the local-density approximation,¹¹ for which we use the Perdew-Zunger¹² interpolation form of the data of Ceperley and Alder.¹³

The matrix elements $V_{K,K'}^{\text{xc}}$ are obtained by first calculating $V^{\text{xc}}(n)$ in direct space, using

$$n(x, y, z) = \sum_K n_K e^{iKz} |\chi(x, y)|^2, \quad (8)$$

integrating $V^{\text{xc}}[n(x, y, z)] |\chi(x, y)|^2$ over x and y and finally Fourier transforming back to k space. The matrix elements of the nonlocal Fock potential, symbolically written as $V^F = Gv$, representing the exchange interaction between electrons, can be expressed as

$$\begin{aligned} V_{K,K'}^F(k) &= - \int_0^{2\pi/a} \frac{dk'}{2\pi} \sum_G d_{l_v,G}^0(k') d_{l_v,G+K'-K}^{0*}(k') \\ &\quad \times v(k - k' + K - G). \end{aligned} \quad (9)$$

The effective one-dimensional Coulomb interaction $v(k)$ diverges logarithmically for $k \rightarrow 0$. However, the divergence is integrable. To handle this divergence numerically, we subtract the term $d_{l_v,G}^0(k) d_{l_v,G+K'-K}^{0*}(k) \ln[(k - k' + K - G)/2\gamma^2]$ from the integrand. This term can be integrated analytically, and the remaining integral can be carried out numerically. We note that both LDA and Hartree-Fock ask for a self-consistent treatment. The required self-consistency is easily obtained in our model. (This self-consistency should not be confused with the self-consistency within *GW*.)

By increasing A , the strength of the external potential, we create systems ranging from semiconductors to insulators. We consider four different values for the strength of the external potential: $A = 0.10, 0.15, 0.25$, and 1.0 .

Having determined a self-energy M , the full Green function can be obtained from the Dyson equation, or, equivalently, from

$$G_{K,K'}(k, \epsilon) = \sum_l \frac{d_{l,K}(k, \epsilon) d_{l,K'}(k, \epsilon)}{\epsilon - E_l(k, \epsilon)}, \quad (10)$$

in which the normalized coefficients $d_{l,K}(k, \epsilon)$ and the energies $E_l(k, \epsilon)$ obey the equation

$$\begin{aligned} & \left[\frac{1}{2}(k + K)^2 - E_l(k, \epsilon) \right] d_{l,K}(k, \epsilon) \\ & + \sum_{K'} [V_{K,K'}^{\text{ext}} + V_{K,K'}^H + M_{K,K'}(k, \epsilon)] d_{l,K'}(k, \epsilon) = 0. \end{aligned} \quad (11)$$

In general, M is an energy dependent and non-Hermitian matrix, giving rise to energy dependent and complex eigenvalues $E_l(k, \epsilon)$.

III. POLE REPRESENTATIONS OF G AND W

In Ref. 9, a representation of the screened interaction W in terms of simple poles has been put forward. The positions of these poles are fixed beforehand and the weights are chosen to fit the exact W . This representation resembles a plasmon pole model, but the poles are not connected to physical plasmons. The purpose merely is to give a good numerical description of the screened interaction. We will apply this representation to W , but also to the electron Green function G . In the latter case we will first subtract the quasiparticle contribution.

The idea in Ref. 9 is to approximate a function $f(z)$, which is analytic except on a branch cut, by a pole representation $g(z)$

$$g(z) = \sum_j \frac{w_j}{z - \xi_j}. \quad (12)$$

The difference

$$I = \int_{-\infty}^{\infty} d\epsilon \left| \sum_j \frac{w_j}{\epsilon - \xi_j} - f(\epsilon) \right|, \quad (13)$$

between the real function $f(z)$ and the fitting function $g(z)$ on the real energy axis is minimized with respect to the weights w_j . Fixing the positions of the poles ξ_j , this leads to the following set of equations for the weights w_j :

$$\sum_j \frac{1}{\xi_i^* - \xi_j} w_j = f(\xi_i^*). \quad (14)$$

This means that we have to calculate f at the complex conjugates of the pole positions.

According to the prescription in Ref. 9, the positions

of the poles are chosen along a contour in the complex energy plane, described by

$$\begin{aligned} \xi_j &= y_j \pm i \frac{\sqrt{(y_j - \alpha)(\beta - y_j)}}{\beta - \alpha} \\ &\times (y_{N/2+1} - y_{N/2}), \quad j = 1, 2, \dots, N. \end{aligned} \quad (15)$$

In this expression, the y_j are the zeros of the Chebyshev polynomial of order N (N even), rescaled to the interval $[\alpha, \beta]$. The use of Chebyshev polynomials is not essential, but they guarantee that the distance of the poles to the real energy axis is approximately equal to the distance between two successive poles. This is necessary for the description of analytic functions, which are smooth on the real energy axis. The signs of the imaginary parts of the poles ξ_j depend on the position of the branch cut of the function f . The poles are chosen to lie on the same side of the real energy axis as this branch cut. The choice of α and β is determined by the boundaries of the branch cut. In principle, the branch cut extends from α to infinity, but because in practice one can only take into account a finite number of bands, effectively an energy cut off β is introduced. We postpone the discussion of the details of the particular choice of α and β in our model to the end of this section.

The positions of the contours are prescribed by the analytical structure of G and W (see Fig. 1). Because W and G both have two branch cuts, we apply the procedure described above twice. The advantage of having a pole representation for both G and W is that all energy integrals that arise in the self-consistent GW scheme can be performed analytically by means of contour integration.

We will now discuss the details of the expressions for W and G . The expression for the screening part $\tilde{W} = W - v$ of the screened interaction W is

$$\tilde{W}_{K,K'}(k, \epsilon) = \sum_m w_{K,K'}^m \left(\frac{1}{\epsilon - \omega_m(k)} - \frac{1}{\epsilon + \omega_m(k)} \right), \quad (16)$$

where $w_{K,K'}^m$ denote the amplitudes and ω_m the poles on the contour Eq. (15). Writing $\tilde{W}$ in the form Eq. (16) guarantees that W obeys the symmetry relation

$$W_{K,K'}(k, \epsilon) = W_{K,K'}(k, -\epsilon). \quad (17)$$

In our self-consistency procedure, we also need a pole

FIG. 1. The positions of the branch cuts in the complex energy plane of the screened interaction W and the electron propagator G . The wiggly lines denote the branch cuts of W and G , just above or below the real energy axis.

representation for G . For G we adopt a different strategy. The reason is that the quasiparticle poles are very close, or even on, the real energy axis, which prohibits a direct representation of G of the form Eq. (12). Therefore, it is necessary to treat the quasiparticle contribution to G separately. First, we accurately determine the quasiparticle energies and weights. To this end we solve Eq. (11) for a few real valued ϵ near the expected solution of the quasiparticle equation $\epsilon_l(k) = E_l(k, \epsilon_l(k))$. We fit a second-order polynomial $P_2(\epsilon)$ through the eigenvalues $E_l(k, \epsilon)$ and then solve the equation $P_2(\epsilon) = \epsilon$ for complex ϵ . The weights of the quasiparticle poles are equal to the products of the eigenvector coefficients $d_{l,K}(k, \epsilon)$ and the wave function renormalization factor, defined by

$$Z_l(k) = \left(1 - \frac{dE_l(k, \epsilon)}{d\epsilon} \Big|_{\epsilon=\epsilon_l(k)} \right)^{-1}. \quad (18)$$

Next, we subtract the quasiparticle part, denoted by G^{qp} , from the full Green function G . The quasiparticle part G^{qp} can be written as

$$G_{K,K'}^{\text{qp}}(k, \epsilon) = \sum_l Z_l(k) \frac{d_{l,K}(k, \epsilon_l(k)) d_{l,K'}(k, \epsilon_l(k))}{\epsilon - E_l(k, \epsilon_l(k))}. \quad (19)$$

The remainder is the so-called incoherent part of G : $G^{\text{ip}} = G - G^{\text{qp}}$. Finally, we apply the fitting method we discussed above to describe the incoherent part of G in terms of simple poles. The general expression for G is now

$$G_{K,K'}(k, \epsilon) = \sum_{i \in v} \frac{h_{i,K,K'}(k)}{\epsilon - \epsilon_i(k)} + \sum_{i \in c} \frac{h_{i,K,K'}(k)}{\epsilon - \epsilon_i(k)}, \quad (20)$$

where the first sum is over the quasiparticle poles and the additional poles in the valence energy region, and the second sum is over the quasiparticle poles and the additional poles in the conductance energy region.

In Ref. 9, the approximation Eq. (12) for the screened interaction W was investigated. It was found that this approximation works well, taking only ten poles. We can confirm this result for W . For the incoherent part of the electron Green function G , the approximation Eq. (12) works well with ten poles in the valence energy region and ten poles in the conductance energy region.

Using the pole representation for G , Eq. (20), the expression for the polarizability in the RPA is

$$P_{K,K'}(k, \epsilon) = \int_0^{2\pi/\alpha} \frac{dk'}{2\pi} \sum_{G,G'} \sum_{i \in v, i' \in c} \left[\frac{h_{i,G,G'}(q) h_{i',G'-K',G-K}(k' - k)}{\epsilon_i(k') - \epsilon - \epsilon_{i'}(k' - k)} - \frac{h_{i',G,G'}(q) h_{i,G'-K',G-K}(k' - k)}{\epsilon_{i'}(k') - \epsilon - \epsilon_i(k' - k)} \right]. \quad (21)$$

Having calculated the polarizability $P_{K,K'}(k, \epsilon)$ at energies $\omega_m^*(k)$, we can find the screened interaction W by $W^{-1} = v^{-1} - P$ and determine its pole representation by Eq. (14). From W we can calculate the self-energy matrix $M = GW = Gv + G\tilde{W} = Gv + \tilde{M}$, with $\tilde{M}$ given by

$$\tilde{M}_{K,K'}(k, \epsilon) = \int_0^{2\pi/\alpha} \frac{dk'}{2\pi} \sum_{G,G'} \sum_{i,m} \frac{h_{i,G,G'}(k') w_{m,G-K,G'-K'}(k - k')}{\epsilon - \epsilon_i(k') - \omega_m(k' - k) \text{sgn}[\text{Re}(\epsilon_i(k')) - \mu]}. \quad (22)$$

In the *GW* self-consistency scheme, we also have to update the Hartree and the Fock potentials after each cycle. The Hartree potential depends on the density, Eq. (7), which now becomes

$$n_K = 2 \int_0^{2\pi/\alpha} \frac{dk'}{2\pi} \sum_{G,i \in v} h_{i,G,K+G}(k'). \quad (23)$$

The updated Fock term (Gv) is

$$V_{K,K'}^F(k) = - \int_0^{2\pi/\alpha} \frac{dk'}{2\pi} \sum_{G,i \in v} h_{i,G,G+K'-K}(k') \times v(k - k' + K - G). \quad (24)$$

With the updated Hartree term, Fock term, and $\tilde{M}$ obtained after each cycle, we can solve Eq. (11) to find new eigenvectors $d_{l,K}(k, \epsilon)$ and new eigenvalues $E_l(k, \epsilon)$. Then we apply the fitting procedure described above to construct an updated G and W and the whole process can be repeated.

We will now discuss the particular choice of the contour parameters α and β used in the representations of W and the incoherent part of G . For the representation of W , our choice of α and β is inspired by Eq. (21):

$$\alpha^{(W)}(k) = \min_{k', l \in v, l' \in c} \text{Re}[\epsilon_{l'}(k') - \epsilon_l(k' - k)], \quad (25)$$

$$\beta^{(W)}(k) = \max_{k', l \in v, l' \in c} \text{Re}[\epsilon_{l'}(k') - \epsilon_l(k' - k)], \quad (26)$$

where the indices l and l' run over valence bands and conductance bands, respectively. The choice of the contour parameters Eqs. (25) and (26) is such that most of the structure of W on the real energy axis appears within the intervals bounded by these parameters on the positive and negative energy axis. Equivalently, the choice of the parameters α and β of the contours used in the representation of G^{ip} is inspired by the expression for the self-energy Eq. (22). In the valence energy region, we choose

$$\alpha^{(G,v)}(k) = \min_{l \in v, m, k'} \text{Re}[\epsilon_l(k') - \omega_m(k' - k)], \quad (27)$$

$$\beta^{(G,v)}(k) = \max_{l \in v, m, k'} \text{Re}[\epsilon_l(k') - \omega_m(k' - k)]. \quad (28)$$

This contour is placed above the real energy axis [by taking the minus sign in Eq. (15)]. The parameters of the contour in the conductance energy region we choose as

$$\alpha^{(G,c)}(k) = \min_{l \in c, m, k'} \text{Re}[\epsilon_l(k') \omega_m(k' - k)], \quad (29)$$

$$\beta^{(G,c)}(k) = \max_{l \in c, m, k'} \text{Re}[\epsilon_l(k') + \omega_m(k' - k)]. \quad (30)$$

This contour is placed below the real axis. In the choices of α and β , Eqs. (25)–(30), we restrict ourselves to the quasiparticle poles of G , and do not consider the extra poles describing the incoherent part of G . If we would take into account all poles of G in the choices of α and β , then in the GW self-consistency cycle the intervals $[\alpha, \beta]$ would increase indefinitely. The choices Eqs. (25)–(30) are justified *a posteriori* by the fact that the total electronic charge is almost conserved in all GW iteration steps in all our calculations. In the next section we will return to this issue.

IV. RESULTS AND DISCUSSION

In this section we present the results of our self-consistent GW calculations, where we have used two different starting points for G^0 to initiate the self-consistency cycle. We concentrate on the two starting points [see Eq. (5)]:

- (i) $V^{\text{ext}} + V^H + V^{\text{xc}}$, the external potential plus the LDA potential;
- (ii) $V^{\text{ext}} + V^H + V^F$, the external potential plus the Hartree-Fock potential.

We could have started the self-consistency cycle with a Hartree or even a noninteracting Green function, i.e., only including the external potential in Eq. (5). For instance, for $A = 0.25$, we have done self-consistent calculations and both the Hartree and the noninteracting G^0 converge to the same self-consistent G as the LDA or the Hartree-Fock G^0 .

We have calculated the band gaps of our quasi-one-dimensional crystal for a number of values of A , changing the system from a semiconductor to an insulator. In all calculations we used a regular grid of 64 k points in the Brillouin zone integrations. We have taken into account four energy bands, one valence band and three conduction bands, and, accordingly, we used four plane waves, with $K = 0, \pm 2\pi/a, -4\pi/a$.

Our LDA results agree with those of KG (Ref. 5) and those of Farid;⁶ our Hartree results also agree with those of Farid. The DFT_z results of Farid, in which the Feynman diagrams to first order in the bare Coulomb interaction minus the exchange-correlation potential are considered (this is in some sense a local equivalent of Hartree-Fock), are very different from our Hartree-Fock results. The reason for this is the essential nonlocal character of the Fock interaction in this model, manifesting itself in a strong k dependence of the Fock matrix.

For the various G^0 's, we observe the same trends that occur in real three-dimensional semiconductors. If we compare our results to those of von der Linden *et al.*¹⁴ for silicon (Table I), we see that the band gap from a Hartree

TABLE I. Comparison of the gaps (in Hartree atomic units) in our quasi-one-dimensional system for $A = 0.15$ with the direct gap of silicon at the Γ point for different approximate one-particle potentials.

	Present model	Silicon
Only external pot.	0.1497	0.1168 ^a
Hartree	0.0277	0.0478 ^b
LDA	0.0400	0.0845 ^b
Hartree-Fock	0.3369	0.2940 ^b

^aPseudopotential calculation.

^bSee Ref. 14.

calculation (without exchange or correlation) is much smaller than the LDA band gap, whereas the Hartree-Fock band gap is much larger than the LDA band gap. Both in our model and in silicon, the value of the gap for noninteracting electrons (only external potential) lies in between the Hartree-Fock result and the LDA result. For silicon, we have calculated this gap with the *ab initio* pseudopotential of Bachelet *et al.*¹⁵

In Table II and in Fig. 2 we present the self-consistent GW results for the band gaps. We have performed ten GW iterations starting with a LDA and with a Hartree-Fock G^0 . We observe that for both starting points the gap converges to the same value, for all values of the external potential A . Also, the Fourier components of the charge density converge to the same values, as can be seen in Table III and Fig. 3.

We see that the self-consistent GW band gap is slightly larger than the Hartree-Fock band gap for $A = 0.10$ and $A = 0.15$. For these values of A , we checked that for the static screened interaction there are regions for z and z' where $W(z, z'; \epsilon = 0)$ is larger than the bare Coulomb interaction. Apparently these regions with antiscreening

TABLE II. The gap (in Hartree atomic units) after 0, 1, and 10 GW iterations, using LDA or Hartree-Fock as a starting point, for different values of A .

$A = 0.10$	0	1	10
LDA	0.0246	0.0467	0.3528
Hartree-Fock	0.2762	0.2458	0.3533
$A = 0.15$	0	1	10
LDA	0.0400	0.0884	0.3898
Hartree-Fock	0.3369	0.3194	0.3895
Knorr and Godby ^a		0.128 $\pm$ 0.05	
Farid ^b		0.048 83	
$A = 0.25$	0	1	10
LDA	0.0750	0.1836	0.4454
Hartree-Fock	0.4663	0.4460	0.4411
Knorr and Godby ^a		0.311 $\pm$ 0.05	
$A = 1.0$	0	1	10
LDA	0.4704	1.0387	1.1342
Hartree-Fock	1.1424	1.1361	1.1342

^aQMC results of Ref. 5.

^bDFT_{sz} results of Ref. 6.

FIG. 2. The band gap as a function of the number of *GW* iterations for different strengths of the external potential: $A = 0.10$, $A = 0.15$, $A = 0.25$, and $A = 1.0$. The two different symbols denote the starting points that have been used to calculate G^0 , triangles, LDA: squares, Hartree-Fock.

dominate the regions with screening in the evaluation of the self-energy M . Hence, the self-consistent *GW* gap is larger than the Hartree-Fock gap. For $A = 0.25$ and $A = 1.0$, the bare Coulomb interaction is slightly screened and the self-consistent *GW* gap lies a little below the Hartree-Fock gap. We remark that for large distances (large $|z - z'|$) the screening is absent in this one-dimensional model. Consequently, the macroscopic dielectric constant equals unity.

It can generally be proven, using symmetry relations for G and W , that the total electronic charge of the system should be conserved after each *GW* cycle. Numerically, we have found that the total charge remains conserved in all *GW* iterations up to a few percent. For a number of cases we have checked that the charge conservation improved by increasing the number of poles describing the incoherent part of G . However, the influence on the gap was negligible. For this reason, and because of

TABLE III. The first two Fourier components (in Hartree atomic units) of the charge density after 0, 1, and 10 *GW* iterations, using LDA or Hartree-Fock as a starting point, for $A = 0.15$.

$A = 0.15$	0	1	10
First Fourier components			
LDA	-0.0438	-0.0789	-0.0958
Hartree-Fock	-0.0797	-0.0835	-0.0960
Second Fourier components			
LDA	0.0006	-0.0001	-0.0070
Hartree-Fock	0.0007	-0.0064	-0.0069

FIG. 3. The first and second Fourier components of the density as a function of the number of *GW* iterations for $A = 0.15$. The different symbols denote the starting points that have been used to calculate G^0 , triangles, LDA: squares, Hartree-Fock.

reasons of computer time we reported the results of calculations with ten poles for W and ten additional poles both for the valence and conductance part of G .

In the exact theory, in which vertex correction diagrams are taken into account, it has been proven that the head element of the polarizability $P_{0,0}(k, \epsilon)$ quadratically goes to zero as $k \rightarrow 0$ for all energies.¹⁶ Due to the energy dependence of the self-energy, the RPA expression for $P_{0,0}(k, \epsilon)$, which contains no vertex corrections, only vanishes quadratically for $k \rightarrow 0$ when $\epsilon = 0$. This can be proven using the biorthonormal representation for G .¹⁷ For $\epsilon \neq 0$, the RPA expression for $P_{0,0}(k, \epsilon)$ goes to a finite value for $k \rightarrow 0$. We could enforce the correct behavior of the polarizability by subtracting this value. Numerically, however, we have found that this value is negligibly small (in the order of one part in a thousand of typical values of the matrix elements of the polarizability P for $k \neq 0$).

If we compare our self-consistent *GW* gap values with the QMC results of KG (Ref. 5) (see Table II) we note that our gap values are considerably higher. If we consider the gap values of KG as the exact gap values, the conclusion should be that the reason for the disagreement is the neglect of vertex corrections in the RPA *GW*. We also note that the non-self-consistent band gap after one *GW* cycle starting from LDA is in agreement with the gap reported by KG for $A = 0.15$ (our value lies just within the error bar) whereas for $A = 0.25$ the non-self-consistent *GW* gap is considerably lower than the KG value. This is in contrast to the situation for realistic three-dimensional materials, where the non-self-consistent *GW* band gaps starting from LDA are almost always in excellent agreement with the exact, experimental, values. The reason for this disagreement in the present one-dimensional model could be the importance of the incoherent part of the Green function. In Table IV, we give the percentage of the contribution of the incoherent part to the total electronic charge after one and ten *GW* iterations starting from LDA or Hartree-Fock.

TABLE IV. The percentage of the contribution of the incoherent part to the total electronic charge, after 1 and 10 GW iterations, starting from LDA or Hartree-Fock, for different values of A .

$A = 0.10$	1	10
LDA	70.6	13.9
Hartree-Fock	18.5	13.9
$A = 0.15$	1	10
LDA	68.9	12.6
Hartree-Fock	16.6	12.6
$A = 0.25$	1	10
LDA	66.0	10.9
Hartree-Fock	12.5	11.2
$A = 1.0$	1	10
LDA	25.6	3.4
Hartree-Fock	2.6	3.3

Starting from LDA, for the cases $A = 0.10, 0.15$, and 0.25 , approximately 70% of the total charge is accounted for by the incoherent part after one GW iteration. This is in sharp contrast to the situation in, for instance, silicon, where the wave function renormalization factor [Eq. (18)] is about 0.7,² and consequently the contribution of the incoherent part to the total electronic charge is only about 30%. The reason why in our model the incoherent part is so important in a first iteration starting from LDA is that the plasmon resonance energy is of the order of the band gap, in contrast to the situation for, e.g., silicon. In Fig. 4, we plot the density of states in our model for $A = 0.15$, after one and ten GW iterations, starting from LDA. Again, the large contribution of the incoherent part can clearly be observed for the case of one GW iteration.

Comparing with the approximations to DFT put forward by Farid,⁶ we note that our self-consistent GW gap values are much larger than his so-called DFT_{sz} gaps. Farid's DFT_{sz} results have been obtained by considering the Feynman diagrams contributing to the density to first order in the screened interaction minus the exchange-correlation potential. Farid claims that this is the best approximation to exact DFT among the various approximations he considers. He also claims that the DFT_{sz} gap should be equal to the self-consistent GW band gap. Our results do not substantiate the latter claim.

The goal of the present study was to explore the pos-

FIG. 4. The density of states after one and ten GW iterations starting from LDA.

sibilities for performing self-consistent GW calculations. We have shown that by using pole representations for G and W , self-consistent GW calculations in the quasi-one-dimensional model we studied are possible. However, the gap values we obtained are far too large. Of course one should be very cautious to extrapolate the conclusions of this paper to realistic three-dimensional systems. There is a lot of controversy about the importance of vertex corrections, either to the polarizability or to the self-energy. In a calculation by two of the present authors, the vertex correction contribution of the self-energy to the direct gap of silicon was found to be small.¹⁸ Del Sole *et al.*, included vertex corrections to the polarizability and the self-energy in their so-called $G\Gamma$ approach, and found both corrections to be small.¹⁹ However, these conclusions were criticized by Farid.⁶ In a recent paper by Verdozzi *et al.*,²⁰ in which several GW approximations for the self-energy of a Hubbard cluster were compared to the exact self-energy, it was concluded that improving G and W without including vertex corrections does not lead to a major improvement of the self-energy. In future work we will investigate the effect of inclusion of vertex corrections in the present model.

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