Quasiparticle self-consistent GW method: a short summary

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Abstract

We have developed a quasiparticle self-consistent GW method (QSGW), which is a new self-consistent method to calculate the electronic structure within the GW approximation. The method is formulated based on the idea of a self-consistent perturbation; the non-interacting Green function G^0, which is the starting point for GWA to obtain G, is determined self-consistently so as to minimize the perturbative correction generated by GWA. After self-consistency is attained, we have G^0, W (the screened Coulomb interaction) and G self-consistently. This G^0 can be interpreted as the optimum non-interacting propagator for the quasiparticles.

We will summarize some theoretical discussions to justify QSGW. Then we will survey results which have been obtained up to now: e.g., band gaps for normal semiconductors are predicted to a precision of 0.1–0.3 eV; the self-consistency including the off-diagonal part is required for NiO and MnO; and so on. There are still some remaining disagreements with experiments; however, they are very systematic, and can be explained from the neglect of excitonic effects.

1. Introduction

Nowadays, it is increasingly required to have an accurate simulator for the electronic structure of materials. The experimental techniques to measure materials at the atomic level continue to advance. However, the information from them is somehow limited and complex: the data obtained can often be hard to understand without simulations. With the help of simulation, we can resolve what the experimental data means. Also, the electronic structure calculational techniques can themselves be used as tools to design materials from the atomic level. Such a new direction is replacing the old-fashioned way of mere trial and error to find new materials. We need to know what factors control the required properties of materials. Then we can make a

new strategy to develop better materials efficiently. We expect such a simulator to treat a wide range of materials in a unified method, because materials are complex; e.g., some possible spintronics materials contain magnetic atoms embedded in semiconductors.

The standard method to calculate the electronic structure from first principles is the local density approximation (LDA) to density functional theory (DFT) [1, 2]. Though it has been highly successful, it is still limited. It can fail in many cases, especially when electrons are localized, as are d and f electrons, or very sparse (then the charge fluctuation is large). The mirror potential near a metal surface and the van der Waals interactions are also not well described. In addition, the eigenvalues obtained by DFT are not simply taken as the quasiparticle energy (QPE) from the beginning; DFT–LDA underestimates band gaps. This often makes the interpretation of its results very problematic. Transition metal compounds, diatomic molecules such as F_2, and so on, are not described well [3].

To overcome these difficulties, kinds of method 'to go beyond LDA' have been proposed. Popular ones are the GW approximation (GWA) and LDA $+ U$.

The standard procedure of the GWA [4] in an *ab initio* method is a perturbation treatment to calculate QPEs starting from the Kohn–Sham eigenfunctions and eigenvalues given by DFT–LDA [5]. We refer to this as '1shotGW'. This has been applied to various kinds of cases, resulting in much improvement over DFT–LDA. However, as we showed in [6], 1shotGW is less satisfactory than was generally believed, because many calculations were done within a pseudopotential framework. In our full-potential based GWA, the band gaps given by 1shotGW are systematically smaller than experimental values [6, 7]. Further, 1shotGW is worse in cases when the DFT–LDA is poor as a starting point. Too-small band gaps in DFT–LDA overestimate screening, which is not so suitable for executing GWA. One example is InN: as shown in [6, 7], the band gap ∼0.0 eV given by 1shotGW is too small in comparison with the recent experimental value of 0.7 eV [8]. (However, note that even 1shotGW is still useful. In fact, figure 1 in [7] contained a prediction that the old experimental value ∼1.9 eV was wrong; the figure showed too large 'GW error' for InN: only InN violated the trend seen in other semiconductors. We had no explanation, but finally it turned out that experimental value was wrong at that time.) So we somehow need a better starting point than DFT–LDA to cover a wide range of materials.

A possible choice is to make GWA somehow self-consistent. The effects of the eigenvalue-only self-consistency (keeping the eigenfunctions as given in LDA), was discussed by Surh *et al* [9]. Recently, Luo *et al* [10] applied it to ZnS and ZnSe, where they showed that the band gaps of 1shotGW 3.19 and 2.32 eV for ZnS and ZnSe are increased to 3.64 and 2.41 eV by the eigenvalue-only self-consistency. The differences suggest the importance of this self-consistency. Furthermore, for ZnSe, the value 2.41 eV changes to 2.69 eV when they use eigenfunctions given by generalized gradient approximation (GGA). This difference suggests that we may need to look for a means to determine optimum eigenfunctions for GWA. Aryasetiawan and Gunnarsson applied another kind of self-consistent scheme to NiO [11]. They introduced a parameter for the non-local potential which affects the unoccupied e_g level, and made it self-consistent. They showed that the band gap of 1shotGW is ∼1 eV, and that it is improved to ∼5.5 eV by the self-consistency. Our newly developed 'quasiparticle self-consistent GW' (QSGW) method [12–17] is such a kind of self-consistent method.

On the other hand, the GWA starting from the optimized effective potential (OEP) method with exact exchange (EXX) has been performed recently, e.g. in [18, 19]. However, it is not clearly justified from the logical point of view and also in practice. The EXX-only (or with LDA level of correlation) OEP method does not necessarily give the true Kohn–Sham eigenvalues. As shown in [20], the RPA correlation cancels out a large portion of the band gap enhancement in EXX, especially for d electron systems. This finding was recently confirmed

by others in semiconductors [21]. The larger band gap (better agreement with experiments) given by EXX is somehow accidental. Furthermore, from the beginning, there is no strong reason to calculate QPEs in GWA starting from even the true Kohn–Sham eigenfunctions. The discussion below about the G^0W^0 approximation (Z cancellation) suggests that G^0 should be made not of the Kohn–Sham eigenfunctions, but the QPE and QP eigenfunctions. In practice, EXX-only overestimates the magnetic moments in transition metals such as Fe and Ni, and EXX + RPA corrects the poorness of EXX-only, as shown in [20].

The LDA + U method [22] is widely used to correct the difficulty in the LDA. It succeeded in giving some reasonable explanation of the electronic structure for systems such as transition metal compounds, which are poorly treated within the LDA. The success is because it includes a screened exchange term for d electrons (or f electrons) in it; the term pushes down only the occupied states and enhances the splitting between d electrons. However, it contains difficulties:

 (i) Its formulation is somehow ambiguous. It adds the U term for d electrons to the total energy, then subtracts the double-counting (dc) term from the LDA exchange–correlation potential. The definition of the dc term is not so convincing. The centre of d bands relative to, for example, the oxygen 2p band cannot be changed relative to the LDA; however, there is no reason why this must be so.

 (ii) The determination of U is not so simple; it cannot be easily determined within the method. Further, it is not so clear whether the assumption of fixed J and J' (obtained from atomic calculations) is valid.

(iii) The special treatment for d electrons is problematic when the hybridization between sp electrons is important; it can cause an artificial imbalance in the electron occupation. Further, the definition of d orbitals can be ambiguous.

Thus it is reasonable to identify LDA + U as a method falling between a model and a first-principles method. A problem is that the important features such as dielectric response and transport are mainly dominated by sp electrons even in such systems; LDA + U gives no improvement for sp electrons [23]. Methods that build on LDA + U, but enhance it, such as LDA + DMFT, cannot improve these problems.

As we will show, QSGW includes the advantages of GWA and also of LDA + U. QSGW is completely parameter-free in principle. From the perspective of LDA + U, it may be taken as an extension in which U is internally determined self-consistently; yet it is more than that: QSGW is free from the difficulties explained above. From the perspective of the GWA, not only the eigenvalue but also the eigenfunction are made self-consistent; thus it is satisfactory as regards the Z factor cancellation as discussed below, and from the perspective of self-consistent perturbation [17]. In section 2, we present some theoretical discussion. In section 3, we survey our results so far.

2. Theoretical discussion: why QSGW?

We summarize the considerations of why we are using QSGW [17]. First, we explain the Z factor cancellation, which justifies the so-called G^0W^0 approximation (here G^0 means the QP part included in G). Then we show that the total energy minimization cannot be a way to determine G; but the total energy can be used to determine QPE. Finally, we present a minimum explanation for the fundamental equation of QSGW.

2.1. Justification of G^0W^0 approximation from $\Sigma[G]$—Z factor cancellation

Here we will explain the 'Z factor cancellation'. This justifies the so-called G^0W^0 approximation.

The Luttinger–Ward (LW) functional (a version of LW functional) $E[G]$ [24] can be derived from the functional Legendre transformation and the adiabatic connection (the coupling constant is λe^2, where λ changes from zero to one) in a straightforward manner [20, 25, 26] as

$$E[G] = -\mathrm{i}\,\mathrm{tr}\left[\ln G + \mathrm{i}\frac{\partial G}{\partial t}\right] + E_{\mathrm{k}}[G] + E_{\mathrm{ext}}[G] + E_{\mathrm{H}}[G] + E_{\mathrm{xc}}[G], \qquad (1)$$

where the second–fifth terms on the right-hand side are the kinetic, external, Hartree, and exchange–correlation terms, which are functionals of G. For definition of the first term, some regularization procedure is assumed to remove constant infinity. Along the path of the adiabatic connection (for any λ between 0 and 1), we keep G fixed by the non-local time-dependent potential $V_\lambda^{\mathrm{eff}}(\mathbf{r}, \mathbf{r}', \omega)$. G for the given external potential is determined by

$$0 = \frac{1}{-\mathrm{i}}\frac{\delta E[G]}{\delta G} = G^{-1} - \omega + \left(\frac{-\nabla^2}{2m} + V^{\mathrm{ext}} + V^{\mathrm{H}} + \Sigma\right). \qquad (2)$$

$-G^{-1} + \omega$ comes from the derivative of the first term in equation (1). The self-energy is given by $\Sigma[G] = \frac{1}{-\mathrm{i}}\frac{\delta E^{\mathrm{xc}}[G]}{\delta G}$. As is well known, this $\Sigma[G]$ is symbolically written as $\Sigma = GW\Gamma$. We use symbolical notations in the following. Note that this kind of formalism is sometimes useful as the basis for formal discussion, e.g. conservation laws (symmetry of $E[G]$ on G), dynamics of G (effective action formalism), and so on [25].

G can be written as

$$G = ZG^0 + \bar{G}, \qquad (3)$$

where G^0 is the QP part of G, Z is the renormalization factor, and the $\bar{G}$ is the incoherent part. Let us consider how the contributions from G^0 are included in $\Sigma[G] = GW[G]\Gamma[G]$. With equation (3), $\Sigma[G]$ is written as $\Sigma = (ZG^0 + \bar{G})W[ZG^0 + \bar{G}]\Gamma[ZG^0 + \bar{G}]$. Z looks explicitly included; however, we will show that the contributions from the Z factors essentially cancel out. The arguments are summarized in (a) and (b) below.

(a) In the integration of $GW\Gamma$ for given G, W, and Γ, $W(\mathbf{q} \to 0, \omega \to 0)$ is the dominant part. In this limit

$$\Gamma \to 1 - \frac{\partial \Sigma}{\partial \omega} = 1/Z. \qquad (4)$$

from a Ward identity. Here we need to assume the insulator case. Then there is a cancellation between Z from ZG^0 and $1/Z$ from Γ. In the case of a metal, there is an additional term in the right-hand side of (4) due to the existence of the Fermi surface; then we expect $\Gamma > 1/Z$, see e.g. [27]; point (b) below should be interpreted in the same manner. In any case, we can claim the poorness of fully self-consistent GW which neglect Γ, as discussed in the following.

(b) Given the proper polarization function Π, $W = v(1 - v\Pi)^{-1}$. $\Pi(1, 4) = \bar{\Pi}(1, 1; 4, 4)$, which is written as

$$\bar{\Pi}(1, 2; 3, 4) = G_2 + G_2 I G_2 + G_2 I G_2 I G_2 + \cdots, \qquad (5)$$

where $G_2(1, 2; 1'2') = G(1, 2)G(2', 1')$. This formula is in matrix notation, e.g. $G_2 I$ means $\sum_{2,2'} G_2(1, 1'; 2, 2')I(2, 2'; 3, 3')$. G_2 contains an electron–hole pair excitation with weight Z^2 because G_2 contains $ZG^0 \times ZG^0$. Let us consider how much the pair excitation is included in the proper polarization $\bar{\Pi}$ as its intermediate states. To do so, consider how $\bar{\Pi}(1, 2; 3, 4)$ changes when the pair excitation is added (or removed); this means taking the derivative. As we can show $\frac{\delta \Pi(1,4)}{\delta G_2(2,2';3,3')} = \Gamma(1, 2, 2')\Gamma(4, 3', 3)$, we can see that the pair excitation is included

in $\bar{\Pi}$ with Z factor weights $\frac{1}{Z} \times Z^2 \times \frac{1}{Z} = 1$ for $\mathbf{q} \rightarrow 0, \omega \rightarrow 0$, because of (4) ($\frac{1}{Z}$ is from a Γ). Bechstedt *et al* demonstrated this cancellation in practice in the lowest level of approximation [28]. This suggests that $\Pi(1,2) \approx -iG^0 \times G^0$ is a reasonable approximation because it contains the electron–hole pair weights in its intermediate states with unit weight, as expected.

This analysis has assumed that the GWA is dominated by the long-range part of W; thus we may expect that such Z cancellation can be less effective if W is short-range. The above discussion explains why a method that constructs Σ through the so-called fully self-consistent GW approximation [29–33] is poor; because of the omission of the vertex function, Z in $G = ZG^0 + \bar{G}$ is not cancelled. In principle, $\Sigma = \frac{\delta E_{xc}[G]}{\delta G}$ must be formally exact; however, this series of expansion should be very inefficient: it contains large cancellations between terms so as to cancel out the effect of Z as seen in (a) and (b).

On the other hand, the G^0W^0 approximation looks reasonable, because it includes the contributions from QPs with correct weights. From the beginning, this is what we expect from the Landau–Silin quasiparticle picture. This Z factor cancellation is generally important. For example, the Bethe–Salpeter equation (BSE) can be described as the sum of the ladder diagram; if one uses G instead of G^0 in the sum, it should give a poor result.

To conclude, it looks promising to calculate $\Sigma[G]$ through the quasiparticle part of G^0 contained in G. This requires the mapping $G \rightarrow G^0 \rightarrow \Sigma$, where we can use the G^0W^0 approximation for $G^0 \rightarrow \Sigma$. From this Σ, we can calculate the new G; this suggest a self-consistency cycle like $G \rightarrow G^0 \rightarrow G \rightarrow G^0 \ldots$. The problem is how to extract G^0 from G; the QSGW method gives a prescription.

2.2. G is not determined by total energy minimization

We now assume that there is some non-interacting Green function $G^0 = 1/(\omega - H^0)$ which well reproduces the QP propagator G^0 in G in the previous section. The important contribution is low-energy part: high-energy parts are irrelevant (or not necessarily so accurate) for determining W and the ground state. With some non-local static Hermitian potential $V^{\text{eff}}(\mathbf{r}, \mathbf{r}')$, H^0 is written as

$$H^0 = \frac{-\nabla^2}{2m} + V^{\text{eff}}(\mathbf{r}, \mathbf{r}'). \tag{6}$$

We can construct the RPA total energy E^{RPA} with the adiabatic connection [17] as a functional of G^0 (thus of V^{eff}). It consists of the Hartree–Fock (HF) part of the energy plus the RPA correlation energy $E^{\text{c,RPA}}$. Note that the HF part of the total energy does not include QPEs (eigenvalues of H^0), but $E^{\text{c,RPA}}$ includes them.

Contrary to the local potential case as in the Kohn–Sham construction of DFT, it is meaningless to minimize E^{RPA} with respect to $V^{\text{eff}}(\mathbf{r}, \mathbf{r}')$. As $V^{\text{eff}}(\mathbf{r}, \mathbf{r}')$ contains degrees of freedom that can shift the QPE while keeping the eigenfunctions as they are, it is possible to change only $E^{\text{c,RPA}}$ through the change of QPE caused by a change of $V^{\text{eff}}(\mathbf{r}, \mathbf{r}')$. Thus $E^{\text{c,RPA}}$ can become negative infinite (no lower bound) when all QPEs are moved to the Fermi energy.

On the other hand, it is possible to determine QPEs from the total energy E^{RPA}; the functional derivative of E^{RPA} with respect to the occupancy of the states Ψ_i gives the QPE as $\varepsilon_i = \frac{\partial E^{\text{RPA}}}{\partial n_i}$ [34]. This is in agreement with QPEs calculated by the GWA starting from H^0. Thus, under the constraint of fixed QP eigenfunctions, we can determine the QPE self-consistently; we use these ε_i in the expression of E^{RPA} and take its derivative to determine next ε_i: this is repeated until convergence. This is nothing but the eigenvalue-only self-consistent scheme. QPEs are not determined by the total energy minimization, but this self-consistency condition is meaningful.

In contrast to QPEs, QP eigenfunctions might be determined by the minimization of E^{RPA}. However, such a formalism looks too complicated. Further, only the occupied QP eigenfunctions are included in the HF part of it; thus, continuity (smoothness) from the occupied eigenfunctions to unoccupied eigenfunctions will be lost. Thus we take another possibility to determine not only QPEs but also QP eigenfunctions in a self-consistent manner in the following.

2.3. QSGW formalism

In QSGW, we consider how to make a self-consistent cycle $G^0 \rightarrow G \rightarrow G^0 \rightarrow \ldots$ to determine G^0. Here G^0 is reproduced from some H^0 (or V^{eff}) as in (6). We use the GWA for the mapping $G^0 \rightarrow G$. As for the mapping $G \rightarrow G^0$, we gave a discussion from a perspective of self-consistent perturbation theory so as make the difference between G and G^0 as small as possible in some sense (we must define how to measure the difference) [17]. A good choice is

$$V^{\text{xc}} = \frac{1}{2} \sum_{ij} |\psi_i\rangle \left\{ \text{Re}[\Sigma(\varepsilon_i)]_{ij} + \text{Re}[\Sigma(\varepsilon_j)]_{ij} \right\} \langle\psi_j| \tag{7}$$

for the mapping $G \rightarrow G^0$; the time-dependent $\Sigma(\omega)$ in G is replaced with the static V^{xc}.

This is consistent with the conclusions drawn about self-consistency in the previous sections. In fact, we can say that G^0 here represents the QP part of G (because $V^{\text{xc}}_{ii} = \text{Re}\,\Sigma(\varepsilon_i)_{ii}$ in (7); the QPE in G is in agreement with those in G^0 if we neglect off-diagonal terms).

3. Summary of QSGW results

We have applied QSGW to wide range of materials and to some topics [12–17]. QSGW can give satisfactory results in comparison with experiments. We still observed some discrepancies from experiments, but they are quite systematic. Here we will summarize what we have done so far.

For semiconductors and insulators [14, 15, 17], QSGW gives rather satisfactory results. For example, for GaAs [14], the QSGW fundamental gap and conduction-band effective mass are $E_g = 1.93$ eV (compare with $E_g^{\text{expt+correction}} = 1.52 + 0.17$ eV, where 0.17 eV is the correction due to spin–orbit (SO) coupling and zero point motion), and $m_c^* = 0.077\,m_0$ ($m_c^{*,\text{expt}} = 0.065\,m_0$). The QS$GW$ optical dielectric constant is $\epsilon_\infty = 8.4$ ($\epsilon_\infty^{\text{expt}} = 10.8$). For comparison, 1shot$GW$ underestimates gaps and masses: $E_g^{G^{\text{LDA}}W^{\text{LDA}}} = 1.29$ eV and $m_c^{*,G^{\text{LDA}}W^{\text{LDA}}} \approx 0.059\,m_0$, while $E_g^{\text{LDA}} = 0.21$ eV and $m_c^{*,\text{LDA}} = 0.020\,m_0$. (See also the discussion when we use $Z = 1$ [6].) This case is a typical case; in a wide range of semiconductors and insulators, we have seen generally that band gaps are predicted to be a little too large (typically, ∼0.1–0.3 eV), and the effective masses are well improved (these are also a little high). Further, the remaining differences from experiments are rather systematic [14, 17].

Neglecting the off-diagonal part in equation (7), that is, the eigenvalue-only self-consistency, while keeping the eigenfunctions as given in the LDA (e-only), is not so bad an approximation for the usual semiconductors. We can see the effects of the off-diagonal part from the difference of the e-only result and the QSGW results [17]. Even for ZnO, the band gap given by e-only $E_g^{\text{e-only}} = 3.64$ eV is not so far from the results including the off-diagonal part: $E_g^{\text{QS}GW} = 3.87$ eV (LDA: 0.71 eV, 1shotGW: 2.46 eV, expt + correction: 3.44+0.164 eV). However, in the cuprate Cu_2O, the difference is larger: $E_g^{\text{e-only}} = 1.98$ eV and
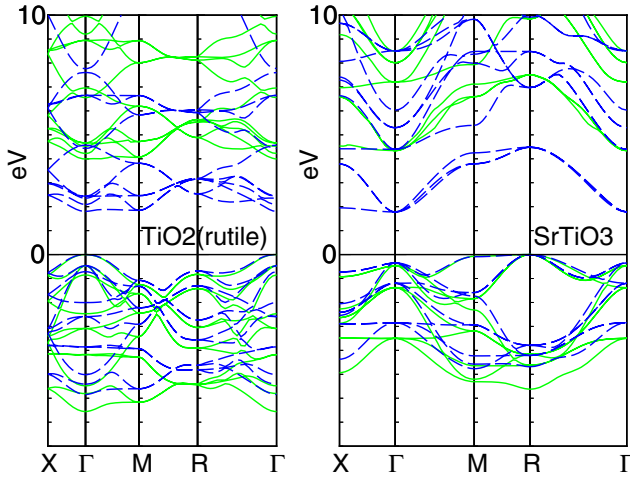
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Figure 1. Energy bands for TiO$_2$ (rutile) and SrTiO3 LDA: broken line (blue). QSGW: solid line (light green).

(This figure is in colour only in the electronic version)

$E_g^{\text{QS}GW} = 2.36$ eV; (LDA: 0.53 eV, 1shotGW: 1.88 eV, experiment: $2.17 + 0.33$ eV). In NiO and MnO, the e-only self-consistency shows very poor results as seen in figure 9 in [17]. From the beginning, e-only does not improve the magnetic moments. For NiO, QSGW improved the magnetic moment well (QSGW gives 1.72 μ_{B}; 1.9 μ_{B} in experiment and 1.28 μ_{B} in the LDA).

In NiO and MnO (where the gap is between d bands), QSGW predicts ~1–2 eV larger band gaps than found in experiments (see [17] for details). We think that this is reasonable: in these systems the excitonic effects are larger compared with the ordinary semiconductors. This will generate larger errors. As a next step, it will be necessary to include excitonic effects and make it self-consistent in the same manner as QSGW with (7).

We found an interesting fact that, even for these oxides, the error of the dielectric constant is almost ~20%, as we will explain in detail elsewhere. ϵ_{∞} values are 3.9 (QSGW) and 4.95 (experiment) in MnO; and 4.4 (QSGW) and 5.43 (experiment) in NiO (see table 6 in [17]). This is similar to the ratio of the GaAs case, with 8.4 (QSGW) versus 10.8 (experiment).

Recently, we have implemented a method to calculate the spin susceptibility based on QSGW. It assumes a scaler Stoner I, which is determined by the spin wave condition as $\omega_{\text{sw}} \to 0$ at $\mathbf{q} \to 0$. Our preliminary results for the spin wave dispersion are in good agreement with experiment for MnO (we will report this elsewhere). Furthermore, for ferromagnetic MnAs (in NiAs-type and in zinc blende phase) we found that the spin wave spectrum shows that the ferromagnetism for the ground state is stable, though the calculation based on the LDA shows that it is unstable.

The energy bands of the Ti compounds rutile TiO$_2$ and SrTiO$_3$ are shown in figure 1. The band gap occurs between O(2p) and Ti(3d). In these cases, the band gaps are enhanced compared with the LDA. Further, the oxygen valence bands widen; the density of states of this oxygen valence bands for SrTiO$_3$ is in excellent agreement with XPS data [13]. The (optical) experimental band gaps are ~3.0 eV (TiO$_2$) [35] and 3.25 eV (SrTiO$_3$) [36]; QSGW values are ~1 eV higher. This is consistent with other cases.

In [15], we have applied QSGW to evaluate spin splittings for semiconductors for various of III–V and II–VI semiconductors. This is an important quantity for spintronics applications: it is a factor needed to determine the spin-relaxation life time, among other things. In spite of its importance related to the spintronics recently, no first-principles methods were available. We evaluated the effect of the SO coupling on the self-consistent QSGW results without SO coupling. We found reasonable agreements with experiments, and we gave some predictions.

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This success is thanks to the fact that QSGW gives a satisfactory description of the band gap, effective mass, and also eigenfunctions.

In summary, we have developed a new self-consistent GW method which seems rather satisfactory from a theoretical viewpoint. We have applied it to various kinds of materials: semiconductors, transition metal oxides, and so on. We generally obtain very good agreement with experiments; the remaining errors are systematic and are interpreted as being due to what is not yet included in QSGW. Thus it will be possible to include them.

Acknowledgments

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