Electronic phase transitions of bismuth under strain from relativistic self-consistent $GW$ calculations

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We present quasiparticle self-consistent $GW$ (QSGW) calculations of semimetallic bulk Bi. We go beyond the conventional QSGW method by including the spin-orbit coupling throughout the self-consistency cycle. This approach improves the description of the electron and the hole pockets considerably with respect to standard density functional theory (DFT), leading to excellent agreement with experiment. We employ this relativistic QSGW approach to conduct a study of the semimetal-to-semiconductor and the trivial-to-topological transitions that Bi experiences under strain. DFT predicts that an unphysically large strain is needed for such transitions. We show, by means of the relativistic QSGW description of the electronic structure, that an in-plane tensile strain of only 0.3% and a compressive strain of 0.4% are sufficient to cause the semimetal-to-semiconductor and the trivial-to-topological phase transitions, respectively. Thus, the required strain moves into a regime that is likely to be realizable in experiment, which opens up the possibility to explore bulklike topological behavior of pure Bi.

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Bismuth exhibits a series of peculiarities that has made it the subject of experimental and theoretical interest for decades. The very low density of carriers with high carrier mobility and a very long mean free path make bismuth very interesting for electronic transport studies. With the recent introduction of the classification of solids according to topology classes of the electronic structure, Bi has again moved into the limelight of current discussions. With a lattice structure that bears similarities to graphene and a very large spin-orbit interaction, it has all the potential to be a topological semimetal or semiconductor. From the theoretical point of view, the large spin-orbit coupling (SOC), the semimetallic character, and the very small local direct band gap at the L point of the Brillouin zone make ab initio calculations of the electronic structure of Bi very challenging.

As for its topological classification, some important aspects are not yet fully understood. It is widely accepted that bulk Bi is topologically trivial in contrast to Sb. This is in agreement with angle-resolved photoemission spectroscopy (ARPES) measurements of Bi$_2$Se$_3$ and Bi$_{1-x}$Sbx alloys as well as transport studies, in which a semimetal-to-semiconductor (SMSC) and a topological transition are observed as the Sb concentration is varied from the topologically trivial Bi to the topological semimetal Sb, resulting in three-dimensional (3D) topological insulators for some of the alloys. However, controversies concerning the topological properties of bismuth persist. For example, it has recently been claimed on the basis of ARPES measurements that bulk bismuth is topologically nontrivial, a claim that is in conflict with most previous findings including ab initio calculations based on density functional theory (DFT). The authors of Ref. 12 attributed these discrepancies to the systematic underestimation of the band gaps obtained in the local-density (LDA) or generalized gradient (GGA) approximations of DFT. Given the very small experimental value (11–15 meV) for the direct band gap at the L point ($E_g$), whose “sign” (order of the states) controls the topological nature of Bi, it is very conceivable that DFT might incorrectly predict the sign of the band gap, and not just its magnitude. Our parity analysis within LDA is in agreement with results in the literature (see, e.g., Refs. 16–18) and confirms the trivial character of Bi. But surprisingly, LDA presents an unusual overestimation of the band gap at L (86 meV; see Table I), which is an effect usually characteristic of inverted gaps, as with those in topological insulators. The gap at L is indeed inverted, as can be seen by varying the SOC strength from zero to 100%: the two states at L exchange order for a certain SOC strength. But the gap at T is inverted as well. There is, hence, an even number of inverted gaps, which rise to a topologically trivial value of the $Z_2$ invariant.

The cause of the band-gap problem of DFT is well known. Strictly, the single-particle energies cannot be interpreted as quasiparticle energies of the interacting electron system. The $GW$ approximation for the electronic self-energy, applied as a one-shot correction to DFT or, more rarely, in the quasiparticle self-consistent $GW$ (QSGW) approach, remedies the aforementioned problem and is often used to correct the band gaps obtained from LDA or GGA. In most cases it increases the band gap leading to a much better agreement with experiments. However, we show here (cf. Table I) that
in the case of bismuth, the GW quasiparticle correction is negative, i.e., it correctly reduces the band gap to 32 meV in one-shot GW (which corresponds to the first iteration of QSGW) and to 13 meV within the self-consistent QSGW scheme. The latter value lies in the range of experimental values. For these calculations, we have devised and implemented a method that combines the SOC with the many-body renormalization in a consistent way (see below). The sign of the band gap is not changed by the quasiparticle correction, i.e., bismuth remains trivial, in accordance with the vast majority of experimental and theoretical studies. However, the phase boundary at which bismuth becomes topologically nontrivial is considerably closer in QSGW than in LDA. We will show that only a relatively modest in-plane tensile strain of 0.3% and compressive strain of 0.4% are sufficient to cause the SMSC and TT phase transition, respectively, which opens up the possibility to explore the 3D topological properties of pure Bi.

Bulk bismuth crystallizes in the A7 rhombohedral structure with R3m space group and two atoms per unit cell. The cell and the atomic positions are determined by the internal parameter \( u \), the rhombohedral lattice parameter \( a_{\text{rho}} \), and the rhombohedral angle \( \alpha_{\text{rho}} \) [see Fig. 1(a)]. The layered structure consists of Bi bilayers separated by a van der Waals gap. For the undistorted reference lattice, we employ experimental parameters from Ref. 31: \( a_{\text{rho}}=4.7458 \ \text{Å}, \ \alpha_{\text{rho}}=57.23^\circ, \ u=0.23389 \). Equivalently, the structure can be described as hexagonal with in-plane and out-of-plane lattice constants \( a_0=4.5460 \ \text{Å} \) and \( c_0=11.862 \ \text{Å} \) (\( c_0/a_0=2.6093 \)). These lattice parameters were measured at 298 K. The gray vertical areas in Fig. 1 show the range of experimental values of \( c/a \) for temperatures between 4 and 298 K. All of our calculations are carried out with the DFT code FLEUR and the GW code SPEX realizations in the all-electron full-potential linearized augmented-plane-wave (FLAPW) formalism. The convergence parameters of the DFT, GW, and QSGW calculations are given in the Appendix. To include relativistic effects in the DFT calculations, we employ the scalar-relativistic approximation inside the muffin-tin spheres, and the SOC is included in a self-consistent manner.

Most of the one-shot GW calculations that include SOC and all of the QSGW ones published so far, employ the SOC as an \textit{a posteriori} correction after the quasi-particle correction to DFT has been carried out without SOC. This is, of course, an approximation. For example, many-body renormalization effects of spin-orbit split bands are then not taken into account (see Ref. 37 for a detailed discussion). In our relativistic calculations, the SOC is already incorporated in the noninteracting system that serves as the starting point for the quasiparticle calculation. The one-shot GW self-energy thus acquires terms that couple the two spin channels, enabling a many-body renormalization of the SOC itself. In this work, we propose to extend this principle to the self-consistent QSGW calculations, so that the self-energy contains spin off-diagonal blocks that it inherits from the SOC throughout the whole self-consistent process. (In analogy to the notation \( G^{\text{SOC}}W^{\text{SOC}} \) of Ref. 36, one could denote this approach by \( \text{QSGW}^{\text{SOC}}W^{\text{SOC}} \), but for simplicity we will simply write GW and QSGW in the following.) Our results show that this treatment is crucial for Bi. The \textit{a posteriori} correction mentioned above, on the other hand, leads to unphysical results for Bi (see Appendix), which then appears as a topological insulator with large band gaps (83 and 259 meV in one-shot GW and QSGW, respectively) instead of a trivial semimetal.

In addition to the value of the band gap at the \( L \) point, the properties of Bi are also determined by the states at the symmetry point \( T \). In particular, the semimetallic character of bismuth is caused by the overlap between the highest valence band at \( T \) and the lowest conduction band at \( L \) [see Fig. 1(a)]. This creates three very small electron pockets (at the three \( L \) points in the Brillouin zone) and one hole pocket at \( T \). Several attempts to describe these pockets theoretically have been published in recent years. For a review and comparison of them see, e.g., Table II in Ref. 17. The approaches used include LDA and GGA,30,31,32 tight-binding models,32 and empirical pseudopotential calculations,36 but no GW results

| TABLE I. Values of the direct band gap at \( L \) (\( E_g \)) and the indirect band gap (\( E_\text{II} \)) [see Fig. 2(b)] for bulk bismuth (in meV) calculated within LDA, GGA, GW, and QSGW, compared with experimental results. |
|---|---|---|---|---|
| LDA | GGA | GW | QSGW | Expt. |
| direct gap at \( L \) (\( E_g \)) | 86 | 74 | 32 | 13 | 11–15 |
| indirect gap \( T-L \) (\( E_\text{II} \)) | -105 | -72 | -66 | -33 | -32 | -39 |

a 11.0 [13], 13.6 [13], 15.0 [13] and 13.0 [12]  
b -32.0 [24], -36.0 [15], -38.0 [27], -38.2 [15], -38.5 [12]
have been published so far. The results from the models
and DFT calculations have not been satisfactory: the abso-
olute value of the overlap, or in other words the indirect
band gap $E_0$, came out too large in general compared to
experiment.

Our values of $E_0$ are shown in Table I. Both the LDA
and GGA overestimate indeed this indirect band gap,
in line with previous publications. While the one-shot
$GW$ approach does correct $E_0$ in the right direction, it
uses LDA as a starting point and, thus, inherits some of
this overestimation. The self-consistent procedure of
$QSGW$, on the other hand, makes the result independent
of the starting point and moves $E_0$ inside the range of
experimental values.

Figure 2 shows the band structure of bulk bismuth
obtained with LDA, $GW$, and $QSGW$ along the path
connecting the high-symmetry $k$ points represented in
Fig. (1b). Whereas the overall shape of the band structure
remains basically unaffected by the many-body correc-
tions, there are important changes in the details. In
particular, while in most parts the valence and conduc-
tion bands are shifted apart by the many-body corrections
as commonly seen in $GW$ calculations, the changes of the
dispersion in the vicinity of the Fermi energy are such that
the absolute values of $E_g$ and $E_0$ get smaller and reach values of 13 and $-33$ meV, respectively. As has already been discussed before,\textsuperscript{19,20,36,37} this is the result of a delicate interplay between the SOC and the many-body renormalization described by the $GW$ approxima-
tion. We conclude that the present relativistic $QSGW$

Bi and its topological character as well as the TT and
SMSC transitions that Bi experiences under strain.

A TT transition was indeed recently observed experi-
mentally for strained Bi(111) ultrathin films\textsuperscript{23} and a
similar transition was found for strained Bi nanowires
elongated about 2%\textsuperscript{24}. In the case of thin films, a strain
can be introduced naturally by a lattice mismatch be-
tween film and substrate. To simulate the strain in our
calculations, we apply a volume-conserving distortion of
the structure by varying the $c/a$ ratio, and keeping the
internal parameter $u$ constant. A compression in the $c$
direction is accompanied by a corresponding increase
of $a$, and vice versa. This is equivalent to varying the
rhombohedral angle $\alpha_{rbo}$, see Fig. (1a). As the $c/a$
ratio increases, the nearest-neighbor distance reduces and
the van der Waals gap expands. Both effects lead to
a strengthening of the in-plane interactions, while the
interbilayer coupling weakens. The altered crystal field
reduces the band gap at L until it reaches a zero value at
a critical $c/a$ ratio and becomes negative. This undoes
the band inversion and causes a sign change in the cal-
culation of the $Z_2$ topological invariants\textsuperscript{21,22} which, for
systems with inversion symmetry, derive from the pari-
ties of the occupied states at the time-reversal invariant
momenta. The parity of a wave function remains un-
changed upon applying the $GW$ quasiparticle correction.
The $Z_2$ topological invariants can, thus, only change if
there is an interchange of valence and conduction states
with respect to LDA. A topological-to-trivial transition
in the topological insulator Bi$_2$Se$_3$ as a result of strain
has also been discussed in the literature. It has been argued\textsuperscript{21,22} that tensile out-of-plane strain reduces the
spin-orbit strength leading to a trivial phase. We do not
find such an effect for bulk Bi: no substantial increase
or decrease in the spin-orbit strength is observed upon
application of strain.

Figure 3a) shows the direct band gap as a function of the
$c/a$ ratio with the range of equilibrium experimental
values of bulk Bi represented as gray shaded areas. Posi-
tive values of the gap denote a trivial phase, whereas nega-
tive values correspond to a topologically nontrivial case.
In addition to the semimetallic state (solid symbols) in
Fig. 3a), we also observe a transition to a semiconduct-
ing state (open symbols) for tensile in-plane strain. This
SMSC transition can also be seen in Fig. 3c) showing
the variation of the indirect band gap, which changes
sign and becomes positive at the point of transition.

At the SMSC transition, the $GW$ and $QSGW$ curves
exhibit abnormal behavior; there is a jump (dashed lines)
where we expect the curve to be continuous. An ana-
gous steplike behavior can be seen in the $QSGW$ curve
at the TT transition. As shown in the Appendix, these
anomalies are an artifact of the $k$-point convergence:
The steps get systematically smaller when one improves
the $k$-point sampling, and convergence is achieved much
more readily in the trivial semimetallic phase than in the
other two phases, so that we can take the points be-
tween the transitions in Fig. 3 as converged, and the
of in-plane strain. The range of experimental values of the indirect gap at L, $E_{\text{ind}}$, as a function of the ratio $c/a$ are due to the use of a reduced $k$-point set; see Appendix.

In conclusion, we propose a QSGW scheme in which the SOC is included throughout the whole self-consistent process. Our results show that such relativistic QSGW calculations are the right $ab$ initio approach to determine the electronic structure and the topological classification of bismuth. They predict its two most significant and delicate electronic properties in quantitative agreement with experiments: The direct gap at L, which determines whether Bi is topological or trivial, and the indirect gap between L and T, which describes the overlap between the electron and hole pockets and thus determines the semimetallic character of Bi. In response to a recent controversy, we conclude the following from our calculations: bulk Bi is a trivial semimetal.

We showed that Bi can undergo electronic phase transitions under rather small lattice strain: a trivial SMSC transition under 0.3% in-plane tensile strain and a TT...
semimetal transition under 0.4% compressive strain. In contrast to LDA and GGA, the critical strains predicted by QSGW are attainable by experiments. The presented results motivate additional experimental efforts to prepare Bi as a topological insulator, by opening band gaps in slightly strained Bi. For example, the small strain needed to cause the TT transition concluded by this work, together with the SMSC transition driven by quantum-size effects in relatively thick films, reveals the potential to observe a topological insulating behavior in bulk-like films of pure Bi. In fact, first experimental evidences of 3D-like topological thin films of Bi are currently under discussion.

The present results demonstrate that LDA and GGA lack the quantitative accuracy to predict the critical strain for which the electronic phase transitions occur. We speculate that standard DFT also yields wrong predictions for the critical concentration at which Bi experiences a TT transition upon alloying with other elements (such as in Bi1−xSbx alloys, or for the critical thickness at which a SMSC transition caused by quantum-size effects takes place). Bi is one example, but we believe it is much more general. Other examples could include the very large strains necessary to induce topological phase transitions in Bi2Se3, Bi2Te3, and in TlBiS2 and TISbS2. It would thus be desirable to reinvestigate the critical points for these transitions within the relativistic QSGW method proposed in this work.

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APPENDIX

The calculations are carried out with the DFT code FLEUR and the GW code SPEX, which are based on the all-electron FLAPW formalism. For the valence electrons, space is partitioned into spherical regions around the atoms (muffin-tin spheres) and interstitial region between the spheres. We use an angular momentum cutoff \( l_{\text{max}} = 10 \) in the muffin-tin spheres and a plane-wave cutoff of 4.5 bohr\(^{-1} \) in the interstitial region. For the DFT calculations, we employ either the Perdew-Zunger parametrization of the LDA exchange-correlation functional or the Perdew-Burke-Ernzerhof parametrization of the GGA. The one-shot GW calculations are always performed using the LDA mean-field system as a starting point.

Due to the very small band gap of bulk Bi (11 to 15 meV for the direct one\(^ {11,13,15} \) and \(-32 \) to \(-39 \) for the indirect one\(^ {13,15,29-30} \)), all computational parameters entering the GW and QSGW calculations are chosen after a systematic study in order to obtain thoroughly converged results. An angular momentum cutoff of \( l = 5 \) and a linear momentum cutoff of 2.9 bohr\(^{-1} \) are employed to construct the mixed product basis\(^ {33-34} \) used to represent the dielectric matrix and the screened interaction.

The one-shot GW and self-consistent QSGW results for the undistorted structure are obtained with a 6×6×6 k-point mesh sampling the Brillouin zone (Table I and Fig. 2). Fortunately, we found that the QSGW results converge faster with respect to the number of k points than the results of one-shot GW so that we could afford to reduce the k-point mesh to 4×4×4 for the QSGW calculations of bismuth under strain. For more details about the k-point convergence, see below.

To compute the Green function and the polarization function, 500 bands are used. This corresponds to approximately 130 eV above the Fermi energy. The complete fifth shell of Bi is treated as valence states by the use of local orbitals. In this way, the contribution of the 5s5p5d states to the Green function and the electronic screening is fully taken into account. Despite their low energetic position, inclusion of the 5s and 5p states affects a change of 5 meV in the band gap at L. To describe high-lying states accurately and to avoid linearization errors, we complement the basis for the valence electrons for each atom by two local orbitals per angular momentum up to \( l = 3 \) with energy parameters far up in the unoccupied states. For the interpolation of the band structures in Fig. 2 maximally localized Wannier functions obtained by the wannier90 library\(^ {33} \) and a 6×6×6 k-point mesh were employed.

We employ the Dirac equation for the core electrons (up to and including the fourth shell) so that relativistic effects are fully accounted for. The core states are thus represented by four-component spinors. This representation is retained for the evaluation of the core-valence contribution to the exchange self-energy. (Using averaged core states that are represented in terms of non-relativistic \( l m \) spherical harmonics instead of the \( j m_j \) spinors introduces an error of 4 and 7 meV in the direct band calculated with one-shot GW and QSGW, respectively.)

As a semimetal, bismuth exhibits metallic screening, which is described technically by the so-called Drude term in the screened interaction \( W \). This term stems from virtual intraband transitions across the Fermi surface. It can be formulated in a functional form being proportional to the square of the plasma frequency, which in turn is evaluated by an integration over the Fermi surface. The Drude term can be treated analytically\(^ {36} \) and, as long as the Fermi surface is sufficiently big, it normally does not pose any numerical problem. How-
however, bismuth has a very small Fermi surface due to the tiny electron and hole pockets, which eventually leads to a very sharp “Drude peak” in the GW self-energy, impeding a straightforward numerical solution of the non-linear quasiparticle equation. One could also say that, while the Drude term is actually treated correctly, it gets too much weight because of the finite \( k \)-point mesh. Therefore, we neglect the Drude term in our calculations and, instead, simply scale the head element of \( W(k, \omega) \) in the limit \( k \to 0 \) to enforce metallic screening. This hardly changes \( W \), and we have found that it leads to a very favorable \( k \)-point convergence; see below. (In the limit of dense \( k \)-point sets, the treatment of the Drude term, which affects only a single \( k \) point, i.e., the \( \Gamma \) point, becomes immaterial.)

In Fig. 4 we show the direct band gap at the L point for each iteration in the QS GW self-consistency procedure, in particular, we distinguish between calculations (i) without SOC, (ii) with spin-orbit coupling added \( a \) \textit{posteriori} to a result obtained without SOC (QS GW+SOC), which is a correction scheme used in most GW calculations so far, and (iii) the relativistic approach used in the present work in which spin-orbit coupling is included in the calculation of both \( G \) and \( W \) throughout the whole self-consistent procedure. (In an earlier publication \textsuperscript{36} we have used the notation \( G^{\text{SOC}} W^{\text{SOC}} \) for the corresponding one-shot calculation. By analogy, one could use the notation QS GW\textsuperscript{SOC} W\textsuperscript{SOC} for the present self-consistent approach.) The \( a \) \textit{posteriori} SOC correction leads to unphysical results for Bi, which appears as a topological insulator instead of a trivial semimetal. We attribute the lack of published GW results of bulk Bi to the crucial and delicate treatment of SOC, but also to the difficulties encountered with the semimetallicity of the system exhibiting very tiny electron and hole pockets (leading to a very sharp Drude peak in the self-energy, as discussed above) and to the smallness of the gaps requiring the calculations to be converged to within a few meV.

We have also performed relativistic QSGW\textsubscript{0} calculations, i.e., we keep the \( W \) at the LDA level while \( G \) is updated self-consistently. The converged QSGW\textsubscript{0} result for the band gap at L differs only by 0.3 meV from the QSGW one. This indicates that the screening obtained with LDA is a good approximation and that self-consistency induces changes mainly in \( G \). Finally, to quantify the effects of dynamics, we have also performed self-consistent calculations within the static Coulomb-hole screened-exchange (COHSEX)\textsuperscript{26} approximation to the GW self-energy (including SOC). In this approximation, the changes are more pronounced. With respect to QSGW, the direct gap at L is reduced by 12 meV, nearly making the system topological, and the indirect band gap shrinks to -4 meV, nearly making the system semiconducting.

To explain the discontinuities in Figs. 3(a) and 3(c) and to prove their origin as a \( k \)-point convergence issue, we have performed GW and QSGW calculations with increasing number of \( k \) points (Fig. 5). To allow for these calculations, we had to reduce some of the parameters in the calculation such as the plane-wave cutoff in the interstitial region for the LDA calculations (now 4.0 bohr\(^{-1}\)), and both the angular momentum cutoff (\( l = 4 \)) and the linear momentum cutoff (2.6 bohr\(^{-1}\)) to construct the mixed product basis for the GW calculations. We also reduced the number of bands for the GW calculations to 100 and only 5\( d \) local orbitals were used in the calculations. This obviously reduces the accuracy of the band gaps obtained—and therefore they differ from those of the main text—but it is not our intention in this appendix to analyze the quantitative results, only the qualitative behavior due to the \( k \)-point convergence.

From Fig. 5 we can conclude the following about the \( k \)-point convergence of one-shot and self-consistent GW results: (1) The calculations of the trivial semimetallic phases can be considered converged with a 6\( \times \)6\( \times \)6 \( k \)-point set for the one-shot GW calculations and 4\( \times \)4\( \times \)4 for the QSGW ones. (2) The semiconducting and topological phases require much larger \( k \)-point meshes, but (3) the corresponding results converge systematically towards an extrapolated quadratic (linear) fit to the converged trivial semimetallic phases for the direct (indirect) band gap. We note that in the case of one-shot GW calculations, the discontinuity in the curves due to the \( k \)-point convergence of the topological phases does not appear at the TT transition of GW but at that of LDA, because of the use of the LDA mean-field system as the starting point for the one-shot GW quasiparticle correction.
FIG. 5. (Color online) LDA, GW, and QSGW values of the direct and indirect band gaps of bulk Bi as a function of the ratio $c/a$ for different k-point sets, but for a set of reduced convergence parameters, see text.

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