Report on Workshop "Challenges and solutions for GW calculations in complex systems"

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REPORT

The Workshop "Challenges and solutions in GW calculations for complex systems" was meant to be an opportunity to (1) bring all the major players in the GW method up to date in the most recent developments in the field, (2) review the available software implementations, (3) define standardization criteria to render the comparison between GW calculations from different codes meaningful, and (4) identify future major challenges in the area of quasiparticle calculations.

We had two talks describing quasiparticle calculations of defect energies in semiconductors and oxides (Louie, Bruneval). We had four talks on the use of GW calculations for metal/molecule contacts and for quantum transport calculations: Hybertsen (reporting also on new static approximations to the self-energy), Neaton (interfacial energy-level alignment and effect of off-diagonal matrix elements of the self-energy), Ferretti (off-diagonal corrections to the GW self-energy in quantum transport), Thygesen (fully self-consistent GW calculations for metal/molecule interfaces on localized Wannier basis). Three talks focused on the use of self-consistent GW: Van Schilfegaarde (review of the formalism and application to magnetic systems), Rinke (all-electron self-consistent GW), Thygesen (GW calculations for quantum transport). Two talks focussed specifically on the use of GW techniques for correlated electron system (Miyake, Gatti), and three talks reported on total energy calculations based on the GW method (Godby, Rinke, Ismail-Beigi). We had five talks on GW calculations without empty states (Louie, Galli, Huebener, Umari, Berger). These talks stimulated an intense discussion as described in the following section. All-electron GW calculations were reported by Ambrosch-Draxl, who performed a very systematic comparison between all-electron and pseudopotential calculations. We also had reports on the use of Coulomb truncation techniques (Martin-Samos), the use of GW for spin-dependent transport (Bluegel), X-ray spectroscopy (Rehr), the accuracy limit of GW calculations set by zero-point vibrations of the lattice (Marini), an update on the recent controversy about the electronic structure of ZnO (Rignanese), self-consistent solutions of the Dyson and Kadanoff-Baym equations (Stan), and applications to graphitic systems (Lebegue).

There has been an ongoing discussion throughout the workshop about the need of removing unoccupied states from the calculations of the screened Coulomb interaction. Several speakers proposed interesting strategies: approximations of the Kohn-Sham states at high energy using symmetrized planewaves and diffuse orbitals (Louie), use of an effective energy technique (Berger), use of a small number of dielectric eigenvalues obtained by iterative diagonalization (Galli), the use of the self-consistent Sternheimer method (Huebener), and the use of the Lanczos recursion method (Umari). There is a consensus on the need of eliminating empty states in order to bring GW calculations on systems with hundreds of atoms. Another interesting discussion took place around the accuracy of localized basis sets for calculating the GW self-energy. Several speakers reported on the use of localized basis sets (Rinke, Thygesen, Umari, Bluegel, Huebener), although no systematic tests on the convergence

with basis sets were reported. An important point of the workshop has been to try and establish the accuracy of GW quasiparticle calculations.
On the optimistic end we heard of accuracies around 0.2-0.3 eV (most speakers), but for instance in the case of ZnO the results appear rather sensitive to the convergence with empty states and to the method used for carrying out frequency integrations (Rignanese). Also it was pointed out that claiming an accuracy below 0.2-0.3 eV may not be meaningful if we consider that lattice vibrations may lead to zero-point effects which may go up to 0.6 eV (Marini, Giustino).

This workshop has been extremely successful insofar the main groups active in the area of GW calculations (both development and application) were represented, and also the discussions were lively and motivating. The workshop highlighted a recent trend across all groups to make a substantial effort in order to render their software and calculations reproducible. As anticipated in the workshop proposal, there is a growing need to standardize the technical details of GW calculations and the corresponding software implementations. It is likely that this workshop will lead to define quality control strategies in the near future, and in this sense maybe a follow-up workshop in 2013 focussing entirely on validation and standardization would be in order. We point out that our unusual workshop format, comprising of 25 min talks followed by 20 min discussions, proved very successful. Indeed all participants appreciated the opportunity for in-depth discussions following each talk, and the workshop resembled more of an intense round-table discussion than a showcase for the results of individual groups.
In addition, this workshop has been so successful that the Editors of the European Physical Journal B have offered us the opportunity to edit a Special Issue of their journal reporting on the key advances in the area of GW calculations as presented within this workshop.

PROGRAMME

Day 1 – Tuesday June 7, 2011

14:00 to 14:10 – Welcome

Session I : Introduction

- 14:10 to 14:55 - **Steven G. Louie**
  GW method for defects, nanostructures, and molecular systems: recent progress and challenges

- 14:55 to 15:40 - **Mark Hybertsen**
  New static approximations in the GW approach

15:40 to 16:05 - Coffee Break

Session II: Total energy

- 16:05 to 16:50 - **Takashi Miyake**
  Constrained RPA method for correlated electron systems

- 16:50 to 17:35 - **Sohrab Ismail-Beigi**
  The GW-RPA correlation energy and Luttinger-Ward theory: exact rewriting, systematic approximations and fundamental challenges

- 17:35 to 18:20 - **Patrick Rinke**
  All-electron GW ground and excited state calculations in a localized basis

Day 2 – Wednesday June 8, 2011

Session III: Unoccupied states A

- 9:00 to 9:45 - **Giulia Galli**
  GW and BSE calculations without explicit calculations of empty electronic orbitals

- 9:45 to 10:30 - **Hannes Hübener**
  Progress on Sternheimer-GW using local orbitals basis sets

10:30 to 11:00 - Coffee Break

Session IV: Methodological advances A

- 11:00 to 11:45 - **Rex Godby**
  Algorithmic and physics options for improving GW-type calculations

- 11:45 to 12:30 - **Adrian Stan**
  Algorithms for self-consistent solutions of the Dyson and Kadanoff-Baym equations.

Equilibrium and the time-dependent properties of inhomogeneous systems.

12:30 to 14:00 - Lunch

Session V: Methodological advances B

- 14:00 to 14:45 - **Mark van Schilfgaarde**
  Reduced Hamiltonians from the quasiparticle self-consistent GW approximation and applications

- 14:45 to 15:30 - **Matteo Gatti**
  Metal-insulator transitions in the GW approximation: beyond a quasi-particle description

- 15:30 to 16:15 - **Fabien Bruneval**
  The GW approximation when the number of particles changes for real

16:15 to 16:45 - Coffee Break

Session VI: Poster presentations

- 16:45 to 19:00 - Poster presentation

Day 3 – Thursday June 9, 2011

Session VII: All-electrons methods

- 9:00 to 9:45 - **Stefan Blügel**
  The GW approximation in the FLAPW method: towards magnetic systems

- 9:45 to 10:30 - **Claudia Ambrosch-Draxl**
  The impact of widely used approximations to the G_0W_0 method: an all-electron perspective

10:30 to 11:00 - Coffee Break

Session: VIII: Unoccupied states B

- 11:00 to 11:45 – **Paolo Umari**
  The GWL method: GW calculations without empty states

- 11:45 to 12:30 - **Berger Arjan**
  The effective-energy technique: GW calculations without summing over empty states.

12:30 to 14:00 - Lunch

Session IX: Transport

- 14:00 to 14:45 - **Jeff Neaton**
  Electronic energy-level alignment at metal-organic interfaces with GW approaches

- 14:45 to 15:30 - **Andrea Ferretti**
  Hybrid functional and GW corrections to quantum transport calculations

- 15:30 to 16:15 - **Kristian Thygesen**
  Fully self-consistent GW calculations for metal-molecule interfaces: level alignment and electron transport

16:15 to 16:45 - Coffee Break

Session X: Spectroscopy

- 16:45 to 17:30 - **John Rehr**
  Many-pole models of inelastic losses and satellites in x-ray spectra

- 17:30 to 18:15 - **Andrea Marini**
  Giant zero-point-motion effects in carbon-based nanostructures

20:00 – Dinner

Day 4 – Friday June 10, 2011

Session XI: Applications

- 9:00 to 9:45 - **Gian-Marco Rignanese**
  What is the G_0W_0 band gap of ZnO ?

- 9:45 to 10:30 - **Michael Rohlfing**
  Excited electronic states from a perturbative LDA+GdW approach

10:30 to 11:00 - Coffee Break

- 11:00 to 11:45 - **Layla Martin-Samos**
  Wigner-Seitz cell cutoff to handle Coulomb divergences in anisotropic systems

- 11:45 to 12:30 - **Sebastien Lebegue**
  Advanced computational methods for the study of functionalized graphene and graphite

12:30 to 12:45 - **Closing word**

ABSTRACTS OF PRESENTED PAPERS

GW method for defects, nanostructures, and molecular systems: recent progress and challenges

Steven G. Louie
University of California at Berkeley, USA

In this talk, we present some recent progress and challenges in employing and extending the GW approach to defects in solids, nanostructures, and molecules. Results from some selected systems and several conceptual and methodological issues are discussed. We discuss some of the subtleties in using a supercell GW method to compute charge transition levels of defects in solids and present results on oxygen vacancies in hafnia. We show that, for quantitatively accurate results, several important effects must be accounted for and that the oxygen vacancies are not negative U centers as reported in most previous studies. A bottleneck in conventional GW method is the extensive summation over unoccupied states. This difficulty is further exasperated in molecular systems by the need to include thousands of empty states in the continuum and the need to include hundreds of off-diagonal elements of the self-energy operator for resonant states. We present a simplified and fast scheme for including these effects without sacrificing accuracy. Finally, despite the multitude of important systems with degenerate ground states, ranging from open-shell atoms and molecules to magnetic defects in solids, the GW approach thus far has been applied basically to closed-shell systems. We address some of the issues associated with degenerate systems (such as spin contamination, the multiplet problem, the proper definition of the Green function in open-shell systems, etc.) and present advances that we have made on this front for open-shell molecules.

New static approximations in the GW approach

Mark Hybertsen
Brookhaven National Laboratory, USA

One of the key technical factors limiting broad applicability of the GW approach has been the problematic convergence with respect to the sum over empty states at the heart of the usual implementations. While recent developments that avoid such explicit sums look very promising, system size scaling will still be a limitation. There are also significant technical advantages for applications if a static approximation can have sufficient accuracy. Hedin's original COHSEX approximation results in a relatively easy static approximation to apply. However, it is known to substantially overestimate energy band gaps. I will present an analysis of the errors in the COHSEX approximation. This analysis motivates a wave-vector dependent correction factor that can be easily incorporated into the COH term. Tests for diverse materials give surprisingly accurate results for the energy band gap. In combination with models for the dielectric screening, this provides a new route to approximate GW calculations for more complex materials.

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Constrained RPA method for correlated electron systems

Takashi Miyake
Nanosystem Research Institute AIST, Tsukuba, Japan

We present a procedure for constructing low-energy models from first-principles using the GW-RPA and Wannier function technique [1,2]. The procedure starts with dividing the Hilbert space into two subspaces: the low-energy part (d space) and the rest of the space (r space). The low-energy model is constructed for the d space by eliminating the degrees of freedom of the r space. The effective electron interaction of the model is expressed by a partially screened Coulomb interaction which is calculated in the constrained random-phase-approximation (cRPA), where screening channels within the d space are subtracted. As an illustration, the procedure is applied to iron-based superconductors. It is found that strength of electron correlation is strongly material dependent [3]. The LDA+DMFT calculations using the obtained effective parameters indicate that LaFeAsO is moderately-correlated [4], whereas FeSe is an orbital-selective non-Fermi liquid [5].

[1] *T. Miyake, F. Aryasetiawan, Phys. Rev. B 77, 085122 (2008).*
[2] *T. Miyake, F. Aryasetiawan, M. Imada, Phys. Rev. B 80, 155134 (2009).*
[3] *T. Miyake et al., J. Phys. Soc. Jpn. 79, 044705 (2010).*
[4] *M. Aichhorn et al., Phys. Rev. B 80, 085101 (2009).*
[5] *M. Aichhorn et al., Phys. Rev. B 82, 064504 (2010).*

The GW-RPA correlation energy and Luttinger-Ward theory: exact rewriting, systematic approximations and fundamental challenges

Sohrab Ismail- Beigi
Yale University, USA

A very attractive feature of the Luttinger-Ward approach, compared to Density Functional Theory (DFT), is that it provides an *ab initio* energy functional of trial one-particle Green's functions that at its extremum yields both the exact total energy and Green's function (e.g., exact quasi-particle energies and wave functions). However, aside from the familiar problem of choosing an exchange-correlation functional, one also faces the challenges of (a) much larger computational costs compared to DFT, and (b) choosing an appropriate set of trial Green's functions. We will discuss our recent results on both fronts [1], focusing primarily on the standard workhorse functional: the random phase approximation (RPA) correlation functional which yields the GW self-energy. (a) We present an exact rewriting of the GW-RPA correlation energy that has significant computational advantages over the standard expression for the functional. Time permitting, we show that this exact rewriting is also convenient for computing quasiparticle energies. Next, we discuss approximate forms for the correlation energy that create a ladder of approximations for the self-energy operator. (b) We discuss how blind extremization of the total energy functional over the usual and simplest choice of Green's functions (i.e. non-interacting Green's functions) yields unphysical results. This signals the absolute necessity of imposing physical constraints on the Green's functions, but understanding the relative merits of various constraints is an open question.

[1] *S. Ismail-Beigi, Phys. Rev. B 81, 195126 (2010).*

All-electron GW ground and excited state calculations in a localized basis

Patrick Rinke

Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany

The GW approach has become the method of choice for the description of quasi-particle band structures of solids as measured in direct and inverse photoemission. For photoelectron spectra of molecules and clusters GW has only recently gained popularity and an assessment of its performance is emerging. Concomitantly, the exploration of advanced DFT functionals like the random-phase-approximation (RPA), which is closely related to the {GW} formalism, is in full stride. Due to their numerical cost, RPA and GW calculations are mostly performed perturbatively following a Hartree-Fock or density-functional theory calculation (denoted G_0W_0@HF/DFT). This introduces an undesired starting point dependence. Moreover, the commonly applied pseudopotential approximation to remove core states for the benefit of computational speed-up is questionable for RPA and GW [1]. In this talk I will present an all-electron implementation of {G_0W_0} and fully self-consistent GW (sc-GW) in the numeric atom-centered basis function code FHI-aims [2]. The sc-GW implementation is based on the iterative solution of Dyson's equation on the imaginary frequency axis. GW total energies are calculated by means of the Galiskij-Migdal formalism. We calculated the spectral function of a set of 30 molecules at self-consistency. The ionization energies, extracted from the spectral function, are in excellent agreement with experiment, with an average deviation of ~2.9% for sc-GW and ~1.5% for sc-GW_0 (with the screening fixed at the RPA level), whereas the deviation for G_0W_0@LDA amounts to ~6%. sc-GW total energies close to the complete basis-set limit for small test systems agree well with full configuration interaction (CI) reference data and with previous work [3]. Based on our results, we conclude that sc-GW provides a systematic improvement in the description of both ionization energies and total energies of finite systems with respect to conventional perturbative G_0W_0@DFT-LDA/GGA calculations.

[1] *R. Gomez-Abal it et al., Phys. Rev. Lett. f 101, 106404 (2008).*
[2] *V. Blum it et al., Comp. Phys. Comm. f 180, 2175 (2009).*
[3] *A. Stan it et al, J. Chem. Phys. f 130, 114105 (2009).*

GW and BSE calculations without explicit calculations of empty electronic orbitals

Giulia Galli

University of California, Davis, USA

We will discuss an approach [1] recently developed to compute optical absorption spectra of molecules and solids, which is suitable for the study of large systems and gives access to spectra within a wide energy range. The quantum Liouville equation is solved iteratively within first order perturbation theory [2], with a Hamiltonian containing a static self-energy operator. Explicit calculations of single particle excited states and inversion and storage of dielectric matrices [3] are avoided using techniques based on Density Functional Perturbation Theory. Applications to clusters, solids and nanowires [4] will be presented.

[1] *D.Rocca, D. Lu, G. Galli, J. Chem. Phys. 133, 164109 (2010).*
[2] *D.Rocca, R.Gebauer, Y.Saad, S.Baroni, J. Chem. Phys. 128, 154105 (2008).*
[3] *H. Wilson, F. Gygi, G. Galli, Phys. Rev. B. 78,113303 (2008); H. Wilson, D. Lu, F. Gygi and G. Galli, Phys. Rev. B. 79, 245106 (2009).*
[4] *Y.Ping, D.Rocca, D.Lu, G.Galli, 2011 (preprint).*

Progress on Sternheimer-GW using local orbitals basis sets

Hannes Hübener

University of Oxford, United Kingdom

We present a scheme to perform GW quasi-particle calculations without performing expansions over unoccupied states and using a local orbital basis. In order to avoid the expansion of the screened Coulomb interaction and the non-interacting Green's function over empty states we solve self-consistently linear-

response Sternheimer equations [1]. In the solution of the Sternheimer equations the bare Coulomb potential is used as the initial perturbation and the screened Coulomb potential is obtained at the RPA level. While the original proposal of this method was based on a plane waves basis representation, we here present a formalism that further improves the scaling properties of this scheme by using localized pseudo atomic-orbitals [2]. The Hamiltonian, the overlap matrix, and the projector on the occupied state manifold appearing in the Sternheimer equation are sparse matrices in the local orbital basis, thereby allowing for a solution of the linear system with O(N) scaling. To avoid issues with the incompleteness of the atomic orbital basis the screened Coulomb interaction W and the Green's function are represented on a real space grid. This combination of sparse matrices in the Sternheimer equation and a real space representation for G and W yields in principle an asymptotic $O(N^3)$ scaling. This favourable scaling, however, does not take into account the inadequacy of the atomic orbital basis for the description of excited states. We discuss possible strategies to overcome this difficulty using augmented basis sets.
** Work done in collaboration with M. Perez, P. Ordejon, and F. Giustino*

[1] *F. Giustino, M.L. Cohen, S.G. Louie, Phys. Rev. B 81, 115105 (2010).*
[2] *J.M. Soler, E. Artacho, J.D. Gale, A. Garcia, J. Junquera, P. Ordejon, D. Sanchez-Portal, J. Phys.: Condens. Matter 14, 2745 (2002).*

Algorithmic and physics options for improving GW-type calculations

Rex Godby
University of York, United Kingdom

The GW approximation is the first-order term in an expansion of the electronic self-energy operator Sigma in powers of the dynamically screened electron-electron interaction, W. From Sigma, the one-particle Green's function G may be calculated, from which various spectral and ground-state properties of electrons in matter are available. For transport properties (as well as certain other excited-state properties), the two-electron Green's function is required, which may also be formulated at the same level of approximation as GW. In applying GW to the ground-state total energy [1], the choice of whether G and/or W are required to be consistent with the Green’s function that arises from Sigma is important. I shall present results for finite and infinite systems at the relevant levels of self-consistency. These include results resulting from the incorporation of self-consistency and GW total-energy techniques into our GWST “space-time” supercell code [2]. I shall also address options for approximating the vertex function [3], in order to go beyond the GW level of approximation, and the interplay with self-consistency and total energy.

[1] *P. García-González, R.W. Godby, Phys. Rev. Lett. 88 056406 (2002).*
[2] *H.N. Rojas, R.W. Godby, R.J. Needs, Phys. Rev. Lett. 74 1827 (1995).*
[3] *A. J. Morris, M. Stankovski, K. T. Delaney, P.Rinke, P. García-González, R.W. Godby, Phys. Rev. B 76 155106 (2007); M. Stankovski et al., to be published.*

Algorithms for self-consistent solutions of the Dyson and Kadanoff-Baym equations. equilibrium and the time-dependent properties of inhomogeneous systems.

Adrian Stan
University of Jyvaskyla, Finland

Green function methods have been used with great success to calculate a wide variety of properties of electronic systems, ranging from atoms and molecules to solids. The interactions of an electronic system, i.e., the effects of exchange and correlation, are incorporated into the so-called self-energy operator Σ which depends on the one particle Green function G. When integrated on the Keldysh contour, the equation of motion for the one particle Green function yields the Kadanoff- Baym equations [1]. Regarding the self-energy, there are different possible approximations which completely determine the properties of the system, with the GW approximation being one of the most successful and used [2]. In this approximation, the self-energy is the product of the Green function G that describes the propagation of particles and holes in the system, and the dynamically screened interaction W which describes how the bare interaction between electrons is altered in the presence of the other electrons. In recent years the GW calculations started to be carried out in a true self-consistent manner [1, 3]. Firstly I will discuss some ground state properties of finite inhomogeneous systems and the effect of self-consistency of the Dyson equation, within the GW approximation of the self-energy. The different levels of self-consistency are shown to be, in fact, simplified GW schemes, characterized by different constrains in self-consistency and propose a new partially self-consistent GW scheme GW_{fc}, in which the correlation part of the self-energy is kept fixed throughout the self-consistency cycle [4]. The second objective of this talk is to discuss a time-propagation scheme for the Kadanoff-Baym equations for general interacting and inhomogeneous systems in the presence of time dependent external fields. The external fields are treated nonperturbatively whereas the many body interactions are incorporated perturbatively using Φ-derivable self-energy approximations. Here I will address the question of converging the Kadanoff-Baym equations for every time-step. The discussion will consider correlated systems, both finite and coupled to infinite leads in a quantum transport setup, and examine the ultrafast electron dynamics and the role of electron correlation in e.g., bistability, and processes far from steady state, e.g., electron pumping, within TDGW and other conserving approximations [5, 6].

[1] *A. Stan, N.E. Dahlen, R. van Leeuwen, J. Chem. Phys. 130, 224101 (2009).*
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[6] *E. Khosravi, A.M.Uimonen, A. Stan, G. Stefanucci, S. Kurth, R. van Leeuwen, E.K.U. Gross, (in preparation).*

Reduced Hamiltonians from the quasi-particle self-consistent GW approximation, and applications

Mark van Schilfgaarde
Arizona State University, Tempe, USA

This talk focuses on developing strategies to map potentials generated by the quasi-particle self-consistent GW (QSGW) approximation (QSGW) onto reduced Hamiltonians. A primary motivation for developing reduced Hamiltonians is to build as a framework for many-body Hamiltonians, such as dynamical mean field theory. The letter can be used to study many- body effects outside perturbation theory. Also, errors in the quasi-particle self-consistent GW (QSGW) approximation are analyzed, and found to be systematic. Even at the one-particle level there is need for improvement in the QSGW one-body potential, in particular where shallow core-like levels are present. Inclusions of interactions should make it possible to describe many-body effects in a parameter-free manner, and at the same time one- body potential generated by QSGW. A second motivation is to describe large systems beyond the range of QSGW at present. We take a very simple approach, which makes heuristic adjustments the LDA potential to match some property of QSGW eigenvalues and eigenfunctions. The enhanced potential is used to evaluate defects in semiconductors, and magnetic exchange interactions in the dilute magnetic semiconductor $Mn_xGa_{1-x}As$ for a wide range of x. The magnetic exchange interactions can deviate significantly from the LDA description, and we analyze the source of the discrepancy.

Metal-insulator transitions in the GW approximation: beyond a quasiparticle description

Matteo Gatti
Nano-Bio Spectroscopy Group, University of the Basque Country, San Sebastian, Spain

The GW approximation is the method of choice for the calculation of band structures in sp semiconductors and metals. Instead, its use in correlated-electron materials (e.g. transition-metal oxides) has been questioned for long time. Here I will discuss our recent efforts in pushing the limits of the GW approximation towards correlated materials, with an emphasis on understanding metal-insulator transitions and signatures of electronic correlations beyond a quasi-particle description.

The GW approximation when the number of particles changes for real

Fabien Bruneval
CEA-Saclay, France

A stringent test for an exchange-correlation approximation in electronic structure calculations is the equality between the ionization energy of the neutral system and the affinity of the singly positively charged system. All of the commonly used approximations (local, semi-local, hybrid) for the exchange-correlation within density functional theory fail badly with this test. This is related to the non-straight-line behavior for fractional electron numbers. It has been shown that it can be related to a localization or delocalization error, resulting in a HOMO-LUMO gap over- or under-estimation [1]. We show here that the GW approximation also suffers from the localization error to some extent, even though it is the best framework available in our study [2]. The small remaining error can be further reduced by devising a ΔSCF-like method within the GW approximation. The proposed approach is necessary as soon as localized states are involved: we apply it for molecules and defect states in crystals [3].

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[2] *F. Bruneval, Phys. Rev. Lett. 103, 176403 (2009).*
[3] *F. Bruneval and G. Roma, Phys. Rev. B 83, 144116 (2011).*

The GW approximation in the FLAPW method: towards magnetic systems

Stefan Blügel, Ersoy Sasioglu and Christoph Friedrich
Jülich Research Centre, Germany

Modern spintronics and quantum information explores a large spectrum of materials with interesting magnetic and spin properties. Low energy excitations play an important role. The GW approximation for the electronic self-energy yields quasi-particle band structures in very good agreement with experiment. Most implementations so far are based on the pseudopotential approach, which limits their range of practicable applicability. We have developed an implementation (SPEX, http://www.flapw.de/spex/) [1] within the full-potential linearized augmented-plane-wave (FLAPW) method, which treats core and valence electrons on an equal footing. Within this method a large variety of materials can be treated, including d- and f-electron systems, oxides and magnetic systems. Our implementation employs a mixed product basis for the representation of basis-function products in the interstitial and muffin-tin regions. The self-energy can be evaluated either by an analytic continuation from the imaginary frequency axis or directly by a contour integration. A basis transformation to the eigenfunctions of the Coulomb potential allows a reduction of the basis-set size, thus leading to a considerable speed up in computation time. The code can also deal with spinor wave functions that result from a spin-orbit coupling term in the Hamiltonian. First results for mercury chalcogenide compounds show a considerable quantitative improvement of the inverted band structures, in particular for the negative band gap, but also for the spin-orbit splitting. Furthermore, Stoner and collective spin excitations, including life-time effects, can be calculated by solving the Bethe-Salpeter equation, in which the four-point T matrix is represented in a basis of maximally localized Wannier functions [2]. It has been realized early on that GW calculations converge badly with respect to the number of unoccupied states - ZnO is a prominent example [3,4]. A similar problem is found in optimized-effective potential (OEP) calculations. Recently, we have implemented a "finite-basis correction" [5] for the OEP approach, which is based on the solution of radial Sternheimer equations in the muffin-tin spheres. These solutions incorporate, to a certain extent, the infinite spectrum of one-particle states. In fact, this approach reduces the number of unoccupied states needed to converge the response function considerably. It is expected that a similar approach is also beneficial for GW calculations. We present illustrative results of GW and spin wave calculations.

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[5] *M. Betzinger, C. Friedrich, S. Blügel, in preparation.*

The impact of widely used approximations to the G_0W_0 method: an all-electron perspective

Claudia Ambrosch-Draxl[1] Xin Zheng Li[2] Ricardo Gomez-Abal[3], Hong Jiang[3], Matthias Scheffler[3]
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Using the fundamental band gaps in Si, diamond, BN, LiF, AlP, NaCl, CaSe, and GaAs, and the semicore d-state binding energies in ZnS, ZnSe, ZnTe, CdS, CdSe, CdTe, and GaN, we analyze discrepancies between the pseudopotential (PP) and all-electron (AE) G_0W_0 results. Approximations underlying PP-G_0W_0, i.e., the frozen-core, the core-valence partitioning, and the use of pseudo-wavefunctions, are separately addressed. The largest differences, of the order of theeV, appear in the exchange part of the self-energy and the exchange-correlation (xc) potential due to the core-valence partitioning. These differences cancel each other and, in doing so, make the final core-valence partitioning effect on the band gaps controllable when the semicore states are treated as valence states. This cancellation, however, is incomplete for semicore d-state binding energies, due to the strong interaction between these semicore states and the deeper core. The remaining error can be reduced by treating the outermost two shells as valence shells. However, reliably describing these many-body interactions at the G_0W_0 level and providing benchmark results requires an all-electron approach.

The GWL method: GW calculations without empty states

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In this talk we will illustrate a recently introduced method [1,2], which allows for the calculation of quasi-particle spectra in the GW approximation in large systems, yet avoiding any explicit reference to empty one-electron states. First, an optimal basis set for the polarizability operator is constructed, which permits to considerably reduce the size of this operator, while maintaining the accuracy of well-converged calculations performed in a plane-waves basis set. Then, the matrix elements of the irreducible-polarizability and self-energy operators are expressed through a set of linear-response equations, which are efficiently solved using a Lanczos-chain algorithm for imaginary frequencies. After validating the approach with a case study of the isolated benzene molecule and bulk silicon, we will illustrate its capabilities with some realistic and challenging examples, including:
i) the calculation of the photoemission spectra of some porphyrin derivatives and their comparison with experimental data from synchrotron-radiation photoemission; ii) the calculation of the electronic densities of states of some disordered materials, such as silica and amorphous silicon nitride; iii) the electronic properties of some metallo-porphyrins, and iv) the quasi-particle density of states of large models of single-strand DNA molecules, comprising up to 500 atoms and 1600 electrons.

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The effective-energy technique: GW calculations without summing over empty states.

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I will present a recently developed GW method which uses occupied states only [1]. All the empty states are accounted for by a single effective energy, which is obtained from first principles. In this way we keep the simplicity and precision of the standard sum-over-states approach while speeding up calculations by more than an order of magnitude. I will demonstrate the power of this effective-energy technique (EET) by applying it to the GW method because a huge summation over empty states appears twice (screening and self-energy). I will show the precision of the EET for GW calculations of bulk silicon and argon. I will then use it to determine the band structure and optical spectrum of the technologically important oxide SnO_2.

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Electronic energy-level alignment at metal-organic interfaces with GW approaches

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Understanding and predicting orbital energies at metal-organic interfaces are important for a range of applications in charge transport and energy conversion. However, the Kohn−Sham orbital energies are well known to be too close to the metal Fermi level within standard approximations to DFT, a misalignment of energy levels that arises from many-electron self-energy effects, and that has the same physical origin as that of the well-known DFT “band gap” problem in semiconductors. Here, using DFT and many-body perturbation theory within the GW approximation and a plane-wave basis, we report the orbital energies of a well-studied molecule, benzene diamine, physisorbed and chemisorbed to Al and Au surfaces, taking particular care to assess convergence, semi-core states, and dynamical screening. For physisorbed BDA on flat Au(111), we find that a G_0W_0 calculation including off-diagonal corrections results in a highest occupied molecular orbital energy of -1.5 eV, which compares well with experiment [1] and a physically-motived, GW-inspired model self-energy correction

(-1.6 eV) derived from prior calculations on a related system, benzene on graphite [2]. For chemisorbed BDA at undercoordinated adatom sites on Al and Au surfaces, our G_0W_0 are smaller than in the physisorbed case, and significantly different from that obtained from hybrid functionals. We compare and thoroughly discuss our G_0W_0 results for physisorbed and chemisorbed monolayers in the context of a model self-energy approach [2,3], which can be applied to larger systems at greatly reduced computational cost; existing spectroscopy and conductance experiments; and, where possible, higher-level quantum chemistry calculations.

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Hybrid functional and GW corrections to quantum transport calculations

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The unprecedented technological development in the microelectronics industry eventually arrives at its ultimate limit when individual electronic devices reach the nanoscale. The design of these systems will rely on a accurate quantum-mechanical ab-initio modeling of electronic transport through them. The non-resonant tunneling regime for charge transfer across nano-junctions is critically dependent on the so-called beta parameter, governing the exponential decay of the current versus the length of the junction. For periodic materials, this parameter can be theoretically evaluated by computing the complex band structure (CBS) --or evanescent states - of the material forming the tunneling junction. In this work we present the calculation of CBS for organic polymers using a variety of computational schemes, including standard local/semilocal DFT and hybrid DFT functional. We validate the computed electronic structure with respect to state-of-the-art G_0W_0 calculations. We compare the description of localization and beta parameters among the adopted methods and with experiments. We show that LDA/GGA DFT systematically underestimates the beta parameter, while hybrid schemes go in the direction of correcting this drawback, resulting in a much better agreement with experiments. The case of GW corrections is discussed together with the use of Wannier functions to interpolate its electronic band structure.

Fully self-consistent GW calculations for metal-molecule interfaces: level alignment and electron transport

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Electron transport across a metal-molecule interface is of fundamental importance to a number of applications including nano- and organic electronics, organic photovoltaics, and photochemistry. The theoretical description of quantum transport in molecular junctions has been a long-standing challenge which has so far been addressed using a combination of non-equilibrium Green functions (NEGF) and density functional theory (DFT). The DFT approach is known to suffer from several problems related to its effective single-particle description of exchange-correlation effects which lead to incorrect predictions of energy gaps. This problem is significant already for isolated molecules [1], but becomes even more pronounced in the vicinity of a metal surface where the dynamical screening is enhanced [2,3], and under non-equilibrium conditions [4]. I will discuss a recent implementation of the fully self-consistent, non-equilibrium GW approximation within a real space (localized atomic orbital basis) Projector Augmented Wave method. Results will be presented for the energy levels of isolated molecules, molecules adsorbed on metallic and semiconducting substrates, as well as for the quantum conductance of metal-molecule-metal junctions. Particular focus will be put on the role of self-consistency in the GW self-energy, the effect of substrate induced dynamical screening (image charge and dynamical charge transfer), and the effect of a finite bias voltage. The GW approximation is shown to significantly improve the DFT results both for the level alignment and the electrical conductance of gold/thiolate and gold/amine linked molecular junctions yielding good agreement with experimental data [5]. Finally, some consequences of substrate-induced screening for the optical properties of adsorbed molecules will be discussed [6].

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Many-pole models of inelastic losses and satellites in x-ray spectra

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Calculations of inelastic losses in x-ray absorption spectra (XAS) and other core-spectroscopies typically employ semi-empirical or simplified models, such as the plasmon-pole self-energy and the quasi-particle approximation. Here we review an efficient approach for calculating inelastic losses due to intrinsic and extrinsic inelastic losses and the interference between them using a many-pole representation and a quasi-boson model [1]. This approach includes both quasi-particle effects and the satellite structure in the spectral function. This method is based on first principles calculations of the dielectric function in the long-wavelength limit and an approximate excitation dispersion relation, which is then fit to a pole model with about 100 poles. This method is compared with an alternative, more precise approach based on a Lanczos algorithm for the inverse of the dielectric matrix [2]. Both approaches yield approximations for the complex GW self-energies and for the satellite terms in the spectral function. The approaches are illustrated with applications to XAS spectra.

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Giant zero-point-motion effects in carbon-based nanostructures

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The Ab-Initio methods represent one of the most accurate, parameter-free and up-to-date description of the electronic properties of bulk and nano-sized materials. These techniques benefit of the predictivity and accuracy of Density-Functional Theory merged with Many-Body Perturbation Theory. The goal of the ab-Initio methods is to describe and predict in a quantitative manner, the opto-electronic properties of any electronic system, starting from its atomic configuration. The result is a wealth of techniques like the GW method that has been successfully applied to a large number of different systems, among which carbon-based nano-structures. In the GW approach, as well as in other applications of the ab-Initio methods, a standard approximation is to assume the atoms frozen in their equilibrium positions. Many years ago, however, the pioneering works of Heine, Allen and Cardona (HAC) pointed to the fact that, even when the temperature vanishes, the zero-point-motion effect (ZPME) can induce large corrections to the electronic levels, making purely electronic theories (like the GW method) inadequate. The ZPME can be understood by using simple arguments. At finite temperature the atoms oscillate around their equilibrium positions. These oscillations can be mapped in a system of non-interacting harmonic oscillators. As a consequence of the quantistic nature of the atoms, when the temperature goes to zero the atoms collapse in a ground state with a finite energy. This is the zero-point energy that induces quantum fluctuations of the atoms. In this talk we show that the ZPME induces giant dynamical effects on the opto-electronic properties of Diamond and trans-polyacetylene, a paradigmatic nano-structure. The sub-gap peaks appearing in the experimental absorption spectrum of Diamond are interpreted in terms of polaronic states, composed of entangled electron-phonon pairs, that cannot be described by the HAC theory. When the reduced dimensionality of the system enhances the amplitude of the atomic vibrations, the ZPME even fragments the electrons in a continuum of polaronic states. This is the case of trans-polyacetylene, where the single particle band-structure is replaced by a jelly-like polaronic distribution and the wave-functions of electrons and atoms are modified by the ZPME. This is the break-down of the band-theory. By disclosing the physical motivations of the ZPME, we discuss how the present results lead to potentially ground-breaking consequences on our understanding of the opto-electronic properties of carbon-based nano-structures.

What is the G_0W_0 band gap of ZnO ?

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Recently, ZnO has drawn considerable attention as a candidate material for low-cost transparent conducting oxides. Even in its natural wurtzite bulk phase, it is numerically difficult to evaluate the GW_0 quasi-particle (QP) corrections for ZnO. Therefore, there have been a wide range of theoretical QP gaps quoted in the literature (from ~1.6 eV to ~3.6 eV to be compared with 3.44 eV experimentally). Typically, many approximations are used extit{en route}. Trying to find the correct theoretical gap, we perform calculations of unprecedented accuracy. First, we study the GW0 band gap using different ground-state DFT starting point approximations (LDA and GGA) and we consider the effect of including scalar-relativistic corrections. Second, we compare norm-conserving pseudopotentials with all-electron techniques (both PAW and FP-LAPW). Four different plasmon-pole models are compared with the more accurate contour-deformation approach. Finally, the effect of a Hubbard U parameter for the 3d-states of Zn is shown to depend on the exact details of application. This work shows that the band-gap of ZnO is indeed underestimated in the G_0W_0 approach.

Excited electronic states from a perturbative LDA+GdW approach

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We discuss an efficient approach to excited electronic states within ab-initio many-body perturbation theory (MBPT). Quasi-particle corrections to density-functional theory result from the difference between metallic and non-metallic dielectric screening. They are evaluated as a small perturbation to the DFT-LDA band structure, rather than fully calculating the self-energy and evaluating its difference from the exchange-correlation potential. The dielectric screening is described by a model, which applies to bulk crystals, as well as, to systems of reduced dimension, like molecules, surfaces, interfaces, and more. We will discuss results for several typical systems.

Wigner-Seitz cell cutoff to handle Coulomb divergences in anisotropic systems

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The integrable Coulomb potential singularity and the speed-up of Brilouin zone sums in periodic conditions has been the subject of many studies since the former work of Ewald [1]. Recently, the booming of GW calculations and of functionals containing Fock-like terms, together with the increased interest in strongly anisotropic systems has pointed out the need of finding a general formalism able to treat Fock like Brillouin zone sums efficiently. Here we present an alternative proposal to "random integration technique" [2] based on a Wigner-Seitz cutoff. Our approach is stable with respect to G sums in any anisotropic supercell, reducing subsequently the number of unnecessary k-points to be included in a converged calculation. Moreover, within a controllable approximation, WS cutoff is also compatible with the use/implementation of Martyna-Tuckerman [3] method that accelerate convergence with respect to the vacuum in molecules. As an application of our method we will show the electronic band structure of two prototype polymers Poly-Acetylene and PPV, and the optical absorption spectra of some substituted corannulene molecules.

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Advanced computational methods for the study of functionalized graphene and graphite

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Using the GW approximation, we have studied the electronic structure of the recently synthesized hydrogenated graphene, named graphane. For both conformations, the minimum band gap is found to be direct at the Gamma point, and with a value of 5.4 eV in the stable chair conformation [1,2].In the metastable boat conformation the energy gap is 4.9 eV. Then the electronic structure of graphane was modified by introducing either a hydroxyl group or an H vacancy. In this last case, an impurity state appears at about 2 eV above the valence-band maximum. With the same method, we have also studied graphene derivatives involving Group IA or Group VIIA elements, forming what we refer to as graphXene [3]. In several cases, large band gaps can be found to open up whereas in other cases, a semimetallic behavior is found. In particular, the band gap obtained for a fully-fluorinated graphene sheet (also known as fluorographene) is found to be as large as 7.4 eV. The results presented allow us to propose that by careful tuning of the relative concentration of the adsorbed atoms, it should be possible to tune the band gap of graphXene to take any value between 0 and 6.4 eV. The second part of the talk will be devoted to the structural properties of graphite, such as the interlayer equilibrium distance, the elastic constant, and the net layer binding energy, as obtained using the adiabatic-connection fluctuation-dissipation theorem in the random phase approximation [4]. Excellent agreement is found with the available experimental data; however, our computed binding energy of 48 meV per atom is somewhat smaller than the one obtained by quantum Monte Carlo methods. The asymptotic behavior of the interlayer dispersion interaction, previously derived from analytic approximations, is explicitly demonstrated to follow a d^{-3} behavior at very large distances.

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