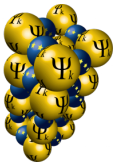
GW goes large-scale

08-10 June 2020

Abstract Book



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Monday

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Large-Scale GW calculations : an embedded all-electron space-time approach

Xavier Blase[1], Ivan Duchemin[2]

[1] *CNRS, Institut Néel, Grenoble, France*
[2] *CEA, MEM, L_Sim, Grenoble, France*

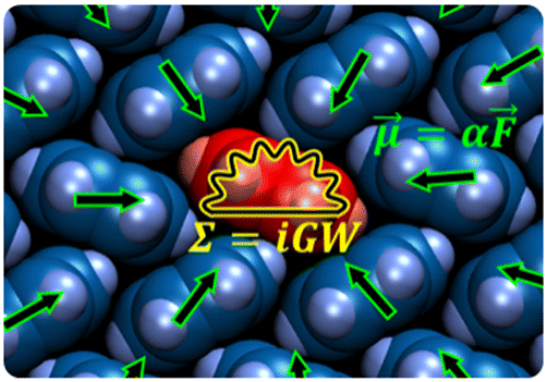

Figure 1: Symbolic representation of an embedded QM/MM GW calculations (from Ref. [3]).

Applying GW calculations to large complex systems may be achieved following several complementary directions. On one hand, we will present an approach that adapts the standard space-time approach to all-electron calculations, leading to cubic scaling calculations with small prefactors [1,2]. Further, the development of multiscale, or embedding, strategies, where the electrostatic and dielectric environmental effects are treated at a "degraded" level in a QM/MM fashion, represents another path towards the study of large complex systems where the partitioning between an "active" subspace and a reactive environment is relevant. We will show that the language of Green's functions and screened Coulomb potential allows a straightforward implementation of such strategies at the GW and Bethe-Salpeter level [3,5], allowing further to bypass fundamental difficulties encountered by embedded DFT or TD-DFT approaches [6].

[1] I. Duchemin, X. Blase, "Separable Resolution-of-the-Identity with All-Electron Gaussian Bases: Application to Cubic-scaling RPA", J. Chem. Phys. 150, 174120 (2019).

[2] I. Duchemin, X. Blase, "Robust analytic continuation approach to many-body GW calculations", J. Chem. Theory Comput 2020 (in press; arXiv:1912.06459).

[3] Jing Li, Gabriele DÁvino, Ivan Duchemin, David Beljonne, Xavier Blase, "Combining the Many-Body GW Formalism with Classical Polarizable Models: Insights on the Electronic Structure of Molecular Solids", J. Phys. Chem. Lett. 7, 14, 2814 (2016).

[4] I. Duchemin, D. Jacquemin and X. Blase, "Combining the GW formalism with the polarizable continuum model: A state-specific non-equilibrium approach", J. Chem. Phys. 144, 164106 (2016).

[5] J. Li, G. DÁvino, I. Duchemin, D. Beljonne, X. Blase, "Accurate description of charged excitations in molecular solids from embedded many-body perturbation theory", Phys. Rev. B 97, 035108 (2018).

[6] I. Duchemin, C. A. Guido, D. Jacquemin and X. Blase, "The Bethe-Salpeter Formalism with Polarisable Continuum Embedding: Reconciling Linear-Response and State-Specific Features", Chem. Sci., 9, 4430 (2018).

Low-scaling GW calculations for molecules with benchmark accuracy

Jan Wilhelm[1],

[1] *Institute of Theoretical Physics, University of Regensburg, D-93053 Regensburg, Germany*

In traditional GW implementations, the computational cost is growing as O(N^4) in the system size N, which prohibits their application to many systems of interest. I present a GW algorithm in a Gaussian-type basis, whose computational cost scales with N^2 to N^3. It will be shown that large minimax grids and resolution of the identity with the truncated Coulomb metric improve the accuracy of the low-scaling GW algorithm to $<$ 0.01 eV for the GW100 test set. Large-scale applications of low-scaling GW will be discussed.

[1] J. Wilhelm, D. Golze, L. Talirz, J. Hutter, and C. A. Pignedoli, "Toward GW Calculations on Thousands of Atoms", J. Phys. Chem. Lett. 9, 306-312 (2018)

Large-Scale GW calculations: all-electron space-time approach

Ivan Duchemin[1], Xavier Blase[2]

[1] *L_Sim, MEM, CEA. France*
[2] *Institut Neel, CNRS, France*

Targeting GW calculations on large complex systems, we will present an approach that adapts the standard space-time approach to all-electron calculations, leading to cubic scaling calculations with small prefactors [1,2]. The talk will focus on two key element of the present formalism: i) analytical continuation on W instead of Sigma and ii) a separable all electrons resolution of the identity.

[1] I. Duchemin, X. Blase, J. Chem. Phys. 150, 174120 (2019).
[2] I. Duchemin, X. Blase, J. Chem. Theory Comput. 2020 (arXiv:1912.06459).

Stochastic techniques for the many-body perturbation theory

Vojtech Vlcek[1],

[1] *Department of Chemistry and Biochemistry, University of California, Santa Barbara*

I will present the principles of the stochastic approach to the many-body perturbation theory, which allows reducing the computational cost of such calculations significantly. The technique accelerates the calculations by employing a randomized sampling of wavefunctions and operators combined with stochastic compression techniques. Computation of quasiparticle energies and gaps for systems containing more than 10,000 electrons is thus feasible with only small statistical fluctuation (± 0.05 eV) and consumes a modest amount of CPU time. I will further present new stochastic approaches that go beyond the popular G_0W_0 approximation and include non-local vertex corrections in the screened Coulomb interaction ($G_0W_0^{tc}$) as well as in the self-energy ($G_0W_0^{tc}\Gamma_x$). I will discuss a stochastic implementation in real-time and space, which scales linearly with the number of electrons. I will exemplify the stochastic many-body calculations on various molecules and periodic systems, e.g., bilayer semiconductors.

[1] V Vlček, E Rabani, D Neuhauser, R Baer- Stochastic GW calculations for molecules - Journal of chemical theory and computation 13 (10), 4997-5003 (2017)

[2] V Vlček, E Rabani, D Neuhauser - Quasiparticle spectra from molecules to bulk, Physical Review Materials 2 (3), 030801 (2018)

[3] V Vlček, R Baer, E Rabani, D Neuhauser - Simple eigenvalue-self-consistent $\bar{\Delta}GW\_0$, The Journal of chemical physics 149 (17), 174107 (2018)

[4] V Vlček, W Li, R Baer, E Rabani, D Neuhauser - Swift G0W0 beyond 10,000 electrons using sparse stochastic compression, Physical Review B 98 (7), 075107 (2018)

[5] V Vlček - Stochastic vertex corrections: linear scaling methods for accurate quasiparticle energies, Journal of chemical theory and computation 15 (11), 6254-6266 (2019)

[6] J Brooks, G Weng, S Taylor, V Vlček- Stochastic many-body perturbation theory for Moiré states in twisted bilayer phosphorene, Journal of Physics: Condensed Matter (2020)

Tuesday

11:00 - 11:45	**Xinguo Ren** All-electron periodic G_0W_0 with numerical atomic orbital basis functions: algorithm and benchmarks
11:45 - 12:00	Break
12:00 - 12:20	**Patrick Seewald** Low-scaling GW calculations based on sparse tensor contractions
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16:20 - 16:40	**Volker Blum** Scalable Eigenvalue and Density Matrix Solutions with the ELSI Infrastructure
16:40 - 17:00	Break
17:00 - 17:45	**Diana Qiu** Scaling up Ab Initio MBPT Calculations for Nanostructured Systems: Applications to Defects and Core-Level Excitations
17:45 - 18:00	Break
18:00 - 18:45	**Mauro Del Ben** Achieving Performance Portability on Hybrid GPU-CPU Architectures for Large Scale GW Applications

All-electron periodic G_0W_0 with numerical atomic orbital basis functions: algorithm and benchmarks

Xinguo Ren[1],

[1] *Institute of Physics, Chinese Academy of Sciences, Beijing*

We present an all-electron, periodic G_0W_0 implementation within the numerical atomic orbital (NAO) basis framework. A localized variant of the resolution of identity (RI) approximation is employed to reduce the otherwise intractable computational cost of evaluating and storing the two-electron Coulomb repulsion integrals. We demonstrate that the error arising from localized RI approximation can be reduced to an insignificant level by enhancing the set of auxiliary basis functions, used to expand the products of two single-particle NAOs. An efficient algorithm has been developed to deal with the Coulomb singularity in the Brillouin zone sampling that is suitable for the NAO framework. We perform systematic convergence tests and identify a set of computational parameters, with which reliable G_0W_0 results can be obtained. Benchmark calculations are carried out for a set of prototypical semiconductors and insulators, and compared to highly accurate reference values obtained from an independent G_0W_0 implementation based on the linearized augmented plane waves and high-energy localized orbitals (LAPW+HLOs) basis set. With a moderate (FHI-aims tier 2) NAO basis set, our G_0W_0 calculations produce fairly accurate band gaps for the tested materials. The algorithms and techniques developed in this work pave the way for efficient implementations of correlated methods in general within the NAO framework.

Low-scaling GW calculations based on sparse tensor contractions

Patrick Seewald[1],

[1] *Department of Chemistry, University of Zurich, Switzerland*

Low-scaling implementations of RPA & GW are an interesting alternative to canonical implementations scaling as $O(N^4)$ with respect to system size N. Lower-scaling algorithm potentially allow to treat much larger system than what is feasible within a canonical implementation.

The CP2K electronic structure software package implements a low-scaling RPA/GW algorithm [1,2] (scaling between $O(N^2)$ and $O(N^3)$) based on sparse data by use of localized atomic basis sets. Whereas canonical implementations are mostly based on dense linear algebra and can therefore employ well-established linear algebra libraries, our low-scaling approach is based on irregular sparse data, hence posing the challenge of implementing and optimizing a general sparse linear algebra library. The challenge is two-fold:

1) matrix multiplication for sparse data at high performance 2) generalization to tensors of rank 2 to 3 and tall-and-skinny matrices

In this talk/poster, I will present the DBCSR (Distributed Block Compressed Sparse Row) library [3] that was specifically developed to address these requirements. Newest developments in DBCSR have demonstrated performance improvements with respect to the published results [1,2] by nearly one order of magnitude.

The low-scaling GW method implemented in CP2K will already be presented by invited speaker Dr. Jan Wilhelm. This talk/poster will complement Dr. Wilhelm's talk by presenting the DBCSR library and more technical aspects of the method, focusing on performance and implementation of sparse tensor contractions.

[1] Toward GW Calculations on Thousands of Atoms Jan Wilhelm, Dorothea Golze, Leopold Talirz, Jürg Hutter, and Carlo A. Pignedoli The Journal of Physical Chemistry Letters 2018 9 (2), 306-312 DOI: 10.1021/acs.jpclett.7b02740

[2] Large-Scale Cubic-Scaling Random Phase Approximation Correlation Energy Calculations Using a Gaussian Basis Jan Wilhelm, Patrick Seewald, Mauro Del Ben, and Jürg Hutter Journal of Chemical Theory and Computation 2016 12 (12), 5851-5859 DOI: 10.1021/acs.jctc.6b00840

[3] https://github.com/cp2k/dbcsr

Quadratic scaling evaluation of the KS density response function for large-scale GW calculations

Arno Förster[1], Lucas Visscher[1]

[1] *Theoretical Chemistry, Vrije Universiteit, De Boelelaan 1083, NL-1081 HV, Amsterdam, The Netherlands*

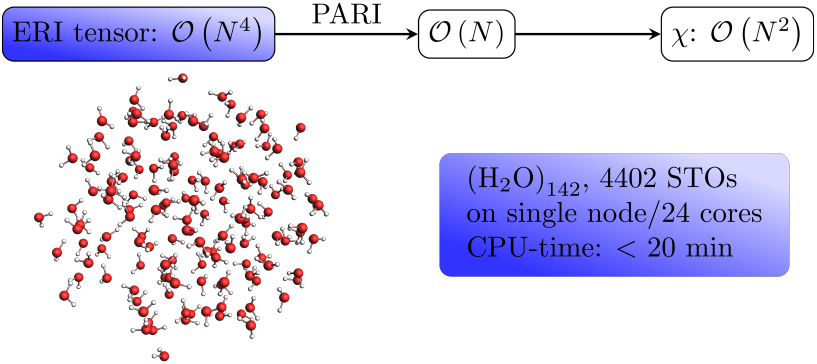

Figure 1: CPU-time required to calculate the KS density-response function for a cluster of42 Water molecules using PARI

The computational bottleneck of GW calculations in molecular systems is the evaluation of the KS density response function, $\chi = -iGG$, scaling as N^4 with system when canonical orbitals are used. All other steps are of order-N^3 at most[1]. Based on the imaginary time Green's functions and using the pair atomic resolution of the identity approximation[2] to exploit sparsity in the AO-basis, we have recently implemented a quadratic scaling SOS-MP2 algorithm with a very low prefactor in the Slater-type orbital (STO) based ADF code and demonstrated the robustness and accuracy of the approach[3,4].

In this talk, I will demonstrate that the previously presented algorithm is a specific application of a more general approach to evaluate the KS density response function in a local, atom-centred basis. The procedure will be outlined and it will be shown how it can be used to obtain G_0W_0 as well as self-consistent GW quasi-particle spectra of large molecules in a routine fashion[5].

[1] Wilhelm, J.; Golze D.; Talirz L.; Hutter, J.; Pignedoli C.A., Toward GW Calculations on Thousands of Atoms, J. Phys. Chem. Lett. 2018, 9, 306−312

[2] Merlot, P.; Kjærgaard, T.; Helgaker, T.; Lindh, R.; Aquilante, F.; Reine, S.; Pedersen, T. B., Attractive electron-electron interactions within robust local fitting approximations, J. Comput. Chem. 2013, 34, 1486−1496

[3] Förster, A.; Franchini, M.; van Lenthe, E.; Visscher, L., A Quadratic Pair Atomic Resolution of the Identity Based SOS-AO-MP2 Algorithm Using Slater Type Orbitals, J. Chem. Theory Comput., 2020, 16, 875-891

[4] Förster, A.; Visscher, L., Submitted

[5] Förster, A.; van Lenthe, E.; Visscher, L., In Preparation

Optimal finite temperature grids for large scale RPA and GW calculations

Georg Kresse[1], Merzuk Kaltak[2]

[1] *University of Vienna, Faculty of Physics, Sensengasse 8, 1090 Wien*
[2] *VASP Software GmbH, Sensegasse 8, 1090 Wien*

The random phase approximation to the correlation energy and the GW approximation for the self-energy are widely used methods to go beyond the semi-local density functional theory approximation. Here, I will briefly describe how we achieve cubic system size scaling for both the total correlation energy as well as the self-energy. The core feature of our implementation is that is relies on optimal time and frequency grids to represent the polarizability and Green's functions either in the imaginary time or imaginary frequency. Furthermore, first derivatives of the RPA with respect to external perturbations will be briefly discussed.

The main thrust of the talk is, however, on the development of optimal time and frequency grids for dealing with metallic systems. In the past, we have used optimal time and frequency grids designed for insulating systems. A simple and straightforward generalization to metallic systems turned out to be more difficult than initially anticipated. For instance, in metals, we have previously used uncontrolled approximations to obtain (seemingly well behaved) total correlation energies. However, derivatives of the RPA correlation energy were unpractical to calculate for metals using that approximation. Hence, we went back to the blackboard and designed optimal time and frequency grids for both perturbational RPA calculations, as well as self-consistent GW calculations. This now allows us to evaluate consistently and without further approximations the correlation energy in the RPA at finite temperature, as well as the GW energy in selfconsistent calculations from the Luttinger-Ward or Galitskii-Migdal equations. The number of time and frequency points can be as small as 16 for RPA calculations on top of DFT calculations, and 24 for selfconsistent GW calculations. This means that we can avoid the expensive finite temperature Matsubara grids commonly used, reducing the compute cost by many orders of magnitude.

Plane wave basis set correction methods for GW self-energies

Stefan Riemelmoser[1], Merzuk Kaltak[2], Georg Kresse[1]

[1] *Faculty of Physics and Center for Computational Materials Science, University of Vienna, Austria*
[2] *VASP Software GmbH, Vienna, Austria*

GW self-energies converge slowly with respect to the plane wave basis set size. This is related to the cusp condition, and is analog to the slow convergence of RPA correlation energies [1,2]. Recently, we have introduced two new methods to handle the plane wave basis set incompleteness error for the latter [3]. One method adapts the framework of range-separated DFT, the other uses an optimized long-range potential. Both methods become exact in the limit of large cutoff energies. We will present the underlying theory and discuss how the methods can be applied to GW self-energies.

[1] J. Klimeš, M. Kaltak, and G. Kresse, Phys. Rev. B 90, 075125 (2014)
[2] A. Gulans, The Journal of Chemical Physics 141, 164127 (2014)
[3] S. Riemelmoser, M. Kaltak, and G. Kresse, arXiv preprint arXiv:2001.08124 (2020)

Ab initio many-body perturbation theory towards the exascale: Yambo on GPUs

Andrea Ferretti[1, 5], Ivan Marri[1, 2], Daniele Varsano[1, 5], Nicola Spallanzani[1], Pietro Bonfà[3], Davide Sangalli[4, 5], Andrea Marini[4, 5]

[1] *Centro S3, Istituto Nanoscienze—Consiglio Nazionale delle Ricerche (CNR-NANO), Modena, Italy*
[2] *Dipartimento di Scienze e Metodi dellÍngegneria, Universitad i Modena e Reggio Emilia, Modena, Italy*
[3] *Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Universitad i Parma, Parma, Italy*
[4] *Istituto di Struttura della Materia—Consiglio Nazionale delle Ricerche (CNR-ISM), Division of Ultrafast Processes in Materials (FLASHit), Monterotondo Stazione, Italy*
[5] *European Theoretical Spectroscopy Facility (ETSF)*

Ab initio Many-body perturbation theory (ai-MBPT) methods such as the GW scheme or the Bethe Salpeter Equation (BSE) are emerging state-of-the-art approaches in the field of electronic structure simulations. Implemented since the 80s, nowadays they have become a tool of choice for many computational works and are among the methods that can best benefit from the exascale race in HPC because of their workload.

Here we focus on a modern ai-MBPT tool, Yambo [1,2], to discuss and validate a porting strategy for GW and BSE methods on GPU accelerated system. Our approach is based on CUDA Fortran, with extensive use of CUF kernel directives to automatically generate GPU code and CUDA libraries (FFT and BLAS). This strategy allows us to keep the software base as close as possible to the CPU version of the code, while fully exploiting the GPU accelerators. Full porting of the GW and BSE workflows has been achieved and numerical benchmarks have shown a speedup of 5-10x comparing the timing of a full socket CPU vs GPU.

[1] http://www.yambo-code.org

[2] D. Sangalli et al, Many-body perturbation theory calculations using the yambo code, J. Phys.: Condens. Matter 31, 325902 (2019).

Scalable Eigenvalue and Density Matrix Solutions with the ELSI Infrastructure

Volker Blum[1],

[1] *Department of Mechanical Engineering and Material Science, Duke University, United States*

This talk describes our work in the open-source infrastructure "ELSI" (https:// wordpress.elsi-interchange.org/ and Ref. [1,2]), which provides simple access to state-of-the art solutions to the Kohn-Sham and other eigenvalue problems for different codes and solvers using a single uniform interface. ELSI provides solutions ranging from simple serial to large-scale massively parallel execution, with efficient matrix conversion between dense and sparse matrix formats. Supported solvers include ELPA (massively parallel $O(N^3)$ eigenproblem solutions), PEXSI ($O(N^2)$ density-matrix based solutions including for metallic systems), NTPoly (O(N) density matrix purification), and several further, specialized solvers. ELSI is a cross-code development, now used in production versions of FHI-aims, Siesta, DFTB+, and DGDFT; additionally, ELSI is part of the broader "Electronic Structure Library" Bundle of open-source libraries for electronic structure theory. Different solvers have different use scenarios in terms of system size, system type and parallelism, assessed in a comprehensive set of benchmarks in this talk. For the ELPA eigensolver, we show a new, cross-node scalable GPU version of its most scalable "two-stage" variant [3]. Finally, we outline a new reverse communication interface (RCI) enabling the facile, efficient implementation of different iterative solver strategies aimed at plane wave basis sets, led by ELSI project members Yingzhou Li and Jianfeng Lu (Duke University).

[1] V. W.-z. Yu et al., Comput. Phys. Commun. 222, 267 (2018).
[2] V. W.-z. Yu et al., arXiv:1912.13403 (2019).
[3] V. W.-z. Yu et al., arXiv:2002.10991 (2020).

Scaling up Ab Initio MBPT Calculations for Nanostructured Systems: Applications to Defects and Core-Level Excitations

Diana Qiu[1],

[1] *Department of Mechanical Engineering and Materials Science, Yale University, USA*

Ab initio many-body perturbation theory methods, like GW and GW-BSE, are well-established and highly-accurate techniques for calculating the quasiparticle and optical properties of moderate-sized systems. There remain, however, a number of challenges when it comes to scaling up these techniques to address systems with a large number of heterogeneous atoms, various forms of aperiodicity, and large energy scales well-outside the optical regime. In this talk, I will discuss our approaches to GW-BSE calculations on low-dimensional and amorphous systems that exemplify these challenges. Specifically, we apply GW-BSE to study the optical response of defects in quasi-two-dimensional (quasi-2D) materials–which require both a large number of atoms and fine resolution of the highly spatially-inhomogeneous screening–and the effect of electron-hole interactions on core-level spectra of quasi-2D materials and amorphous water, including dynamic effects due to scattering to the electron-hole continuum. The calculations are made possible through a combination of physically motivated approximations and algorithms, including non-uniform spatial sampling, low-rank approximations, and subspace partitioning and matrix downfolding techniques. We find that electron-hole interactions allow defects to modify optical selection rules for bulk states and also play an essential role in the scattering of core-level excitations with excitations from the valence band.

Achieving Performance Portability on Hybrid GPU-CPU Architectures for Large Scale GW Applications

Mauro Del Ben[1],

[1] *Computational Research Division, Lawrence Berkeley National Laboratory*

Large-scale GW calculations are state-of-the-art to accurately describe excited state phenomena in materials, which is critical for the design of novel new devices based on complex materials with applications in many fields. Application of the GW method to complex systems is often perceived as being limited due to high computational cost. In this respect, the continuous growth of the computational power combined with the developments of novel methods, algorithms and optimal implementations on modern HPC systems, offers the possibility to study complex materials at scale and accuracy not even thinkable only a few years ago. On the other hand, performance portability of a large scale code on new architectures, particularly to exploit accelerators on heterogeneous systems, is a non-trivial task and faces several challenges. This talk will showcase the various techniques used to accelerate the Material Science code BerkeleyGW on hybrid GPU-CPU systems, targeting large scale simulations with thousands of atoms. The techniques explored in our performance portability strategy includes the efficient use of available accelerated libraries, careful memory handling and data structure refactorization, host/device asynchronous operations for both computation and memory transfer, batched operations, shared memory, and the overlapping of MPI communication on host and computation on device. The porting of BerkeleyGW on hybrid architectures allowed us to achieve good strong- and weak-scaling on thousands of GPUs, high fraction of peak performance and a 16x or more improvement on FLOPs/Watt efficiency compared to the CPU-only implementation. We show in this way that the application of the GW method to systems made of thousands of atoms can be achieved with excellent time to solutions of the order of minutes when running at scale on available hybrid architectures.

Wednesday

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16:00 - 16:20	**Gianni Marchetti** Small and Large Momentum Transfer Forms of the Effective Coulomb Interaction in the Random Phase Approximation for Condensed Matter Systems
16:20 - 16:40	**Georg Siegmund Michelitsch** Dynamical vertex corrections beyond GW from time-dependent density-functional theory
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17:20 - 17:40	**Paolo Umari** Easy-GW an highly parallelisable G_0W_0 approach with no empty states and with exact evaluation of W_0
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Real-time approach to nonlinear optics

Myrta Grüning[1], Claudio Attaccalite[2]

[1] *Queens University Belfast, Northern Ireland*
[2] *CINaM Marseille, France*

In the past decades, many-body approaches based on the GW approximation and the Bethe-Salpeter equation have become state-of-the-art for calculating optical absorption in solids and nanostructures. In this talk, I'll first present a real-time approach derived from the non-equilibrium Green's function, that allows extending the GW+BSE approach beyond the linear regime.[1,2] Using this approach, I'll address the importance of many-body effects and in particular of excitonic effects for nonlinear optical properties.[3] For example, I'll look at the case of single-layer monochalcogenide whose strong Second Harmonic Generation cannot be reproduced within the independent-particle approximation.[4]

[1] Attaccalite, C., Grüning, M. & Marini, A., (2011) Physical Review B 84, 24, 245110 [
[2] Attaccalite, C. & Grüning, M., (2013) Physical Review B 88, 235113
[3] Grüning, M. & Attaccalite, C., (2014) Physical Review B 89,081102
[4] Claudio Attaccalite, Maurizia Palummo, Elena Cannuccia, Myrta Grüning, (2019) Phys Rev Mat 3, 074003

Small and Large Momentum Transfer Forms of the Effective Coulomb Interaction in the Random Phase Approximation for Condensed Matter Systems

Gionni Marchetti[1],

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In the Hartree and Hartree-Fock theories, the electron lifetime in doped semiconductors and impure metals is infinite. More generally, the quantum observables can be beset by infinities assuming that the interaction is a long-range bare Coulomb potential. In this regard, the random phase approximation (RPA) remains one of the most successful many-body technique to include screening effects of the Coulomb interaction in condensed matter systems. It is also an important starting strategy for including other quantum (correlation and exchange) effects beyond the RPA in material science and chemistry. In its self-consistent dieletric formulation (Lindhard screening) one can recover a linearized Thomas-Fermi potential for small momentum transfer (or long wavelength limit). In this talk we shall present a study of of the RPA for large momentum transfer which contains quantum effects neglected by its semiclassical counterpart. To our best knowledge, there are no studies about it. We shall discuss the consistencies of these two RPA potentials for a given model semiconductor in the more possible general context. To this end, we used Calogero's variable phase method, a the nonrelativistic phase shift formalism which allow us to solve Schroedinger equation from first principles. As application of this problem we have computed the single-particle relaxation time within the RPA and the first Born approximation. Finally, we briefly address the above problem of choosing the suitable RPA potential for the problem at hand within a general Bayesian approach (Ockham's razor principle).

Dynamical vertex corrections beyond GW from time-dependent density-functional theory

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Strong many-body effects in solid state materials are the reason for features such as satellites in electronic excitation spectra. Many-body perturbation theory approaches based on the Green's function formalism are the state-of-the-art in their understanding, commonly applied in terms of the GW approximation to the self-energy, which neglects the so-called vertex correction in Hedin's equations. Although successful for some observables such as band gaps, this approximation cannot sufficiently well describe satellite peaks observed in experiment. Vertex corrections beyond GW can be taken into account thanks to time-dependent density-functional theory[1]. However, only adiabatic approximations have been considered so far. Here we make use of a non-adiabatic approximation[2] to investigate dynamical vertex corrections within a model self-energy. We compare our results to calculations where a static vertex is included and report first successes in terms of a correction to the satellites in the spectral function of sodium.

[1] R. Del Sole et al. Phys. Rev. B, 49(12), 8024 (1994)
[2] M. Panholzer et al. Phys. Rev. Lett., 120, 166402 (2018)

Acene and Acene-like Derivatives as Intermolecular Singlet Fission Candidates

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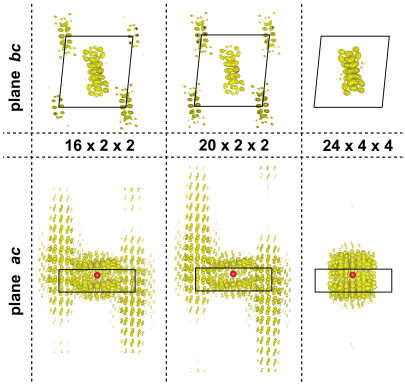

Figure 1: Visualization of the singlet state EWFs of TBHA with different supercell sizes. The EWF is viewed in the bc and ac planes. The hole position is indicated by a red dot the electron charge distribution is shown in yellow. All EWFs were plotted with an isosurface value of$8 \times 10{-}6$ a.u. after normalization. The central unit cell is indicated by a black box. Atoms are not shown for clarity. For unconverged supercells of $16 \times 2 \times 2$ and $20 \times 2 \times 2$, significant electron density is observed close to the supercell edges. For a converged supercell of $24 \times 4 \times 4$, the EWF is contained in the central region.

Singlet fission (SF) is the conversion of a singlet exciton into two triplet excitons. SF could increase the efficiency of organic solar cells by harvesting two carriers from one photon. Polyacene crystals, such as tetracene and pentacene, have shown outstanding SF performance. However, their instability prevents them from being utilized in SF-based photovoltaic devices. In search of practical SF chromophores, we use many-body perturbation theory with the GW approximation and Bethe-Salpeter equation to study the excitonic properties of pyrene-stabilized acenes. We propose a criterion to determine the convergence of exciton wave-functions (EWFs) with respect to the fine k-point grid used in the BerkeleyGW code. An open-source Python code is presented to perform exciton wave-function convergence checks and streamline the double-Bader analysis of exciton character. We find that the singlet excitons in pyrene-stabilized acenes have a higher degree of charge transfer character than in the corresponding acenes. The pyrene-fused tetracene and pentacene derivatives exhibit comparable excitation energies to their corresponding acenes, making them potential SF candidates. The pyrene-stabilized anthracene derivative is considered as a possible candidate for triplet-triplet annihilation (TTA).

[1] Xingyu Liu, Rithwik Tom, Xiaopeng Wang, Cameron Cook, Bohdan Schatschneider, and Noa Marom. Pyrene-stabilized acenes as intermolecular singlet fission candidates: importance of exciton wave-function convergence, J. Phys.: Condens. Matter. 32, 184001, 2020.

Easy-GW an highly parallelisable G_0W_0 approach with no empty states and with exact evaluation of W_0

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I will illustrate how the G_0W_0 approach can be implemented calculating separately the response of G_0 and W_0 at individual points in real space. This permits to avoid any explicit sum over empty orbitals and any explicit representation of the screened Coulomb interaction. In turn, this allows, on one side, to fast and approximate evaluations of the self-energy, which we then use for testing purposes only. On the other side, this allows for fully converged calculations. As each GW evaluation of the self-energy concerns separate and independent calculations for a number of points in real space, our method is highly and trivially parallelisable. We have implemented this scheme within the Quantum Espresso package which is based on the plane-waves pseudopotentials paradigm and we follow the analytic continuation scheme for achieving the self-energy on the real energy from its previous evaluation on the imaginary one.

Large-scale many-body perturbation theory calculations

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Many-body perturbation theory (MBPT) has been shown to provide an accurate description of excited state properties for the simulation of spectroscopic signatures of weakly correlated materials and molecules. We will discuss methodological advances implemented in the WEST code [http://west-code.org] to expand the applicability of MBPT methods to systems with thousands of valence electrons. We will present new functionalities enabled by the concurrent use of WEST and the Qbox code [http://qboxcode.org] for both GW and BSE, with focus on interoperability paradigms. We will present strategies based on quantum embedding to describe highly correlated electronic states, focusing on the calculation of spectroscopic properties of insulators and semiconductors hosting optically addressable spin-defects.

Posters

Miguel A. Caro
Predicting core-electron binding energies from multi-scale machine learning models trained from GW and DFT data

Pablo Aguado-Puente
GW study of Pressure-induced topological insulator transition in group IV-tellurides

Merzuk Kaltak
Minimax Isometry Method: A compressive sensing approach for Matsubara summation

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Relativistic correction to core level excitations from GW

Dario Alejandro Leon Valido
Frequency dependence of W made simple using a multi-pole approximation. The case of the Gr/Co/Ir interface

Nicolino Lo Gullo
A Scalable Numerical Approach to the Solution of the Dyson Equation for the Non Equilibrium Single Particle Green's Function

Vladimir Rybkin
Density Functional Embedding Theory Formulation Suitable for Periodic All-electron Calculations with Gaussian Basis Functions

Lorenzo Sponza
Modelling changes of environmental screening on the gap of 2D materials

Predicting core-electron binding energies from multi-scale machine learning models trained from GW and DFT data

Miguel A. Caro[1, 2], Markus Hirvensalo[2], Dorothea Golze[2]

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[2] *Department of Applied Physics, Aalto University, Finland*

Machine learning (ML) techniques have emerged in recent years as a powerful tool to inexpensively predict the properties of atomic systems, *provided that enough data is available*. Unfortunately, the cost of generating accurate reference data can be prohibitively expensive in some cases. For instance, computing core-level binding energies, used to predict XPS spectra, using GW is a very CPU-intensive task [1]. On the other hand, different approaches based on DFT do not offer satisfactory accuracy. In this study, we generated two databases of core-electron binding energies for C/H/O-containing systems (materials and molecules). One large database was generated relatively inexpensively at the DFT level of theory, while a smaller database was generated at the GW level of theory. By using kernel-based ML interpolation, in combination with a state-of-the-art many-body atomic kernel developed by us [2], we are able to predict the correction to the DFT estimate, bringing it close to GW accuracy, at a small fraction of the CPU cost. We can also estimate, less accurately, the core-electron binding energy with a pure ML model (i.e., one that does not rely on a DFT calculation) at negligible CPU cost.

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[2] M.A. Caro. Phys. Rev. B 100, 024112 (2019)

GW study of Pressure-induced topological insulator transition in group IV-tellurides

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We calculate the electronic structure of the narrow gap semiconductors PbTe, SnTe and GeTe in the cubic phase using density functional theory (DFT) and the G_0W_0 method. Within DFT, we show that the band ordering obtained with a conventional semilocal exchange-correlation approximation is correct for SnTe and GeTe but wrong for PbTe. The correct band ordering at the high-symmetry point L is recovered adding G_0W_0 quasiparticle corrections. However, one-shot G_0W_0 produces artifacts in the band structure due to the wrong orbital character of the DFT single-particle states at the band edges close to L. We show that to correct these artifacts it is enough to consider the off-diagonal elements of the G_0W_0 self-energy corresponding to these states. We also investigate the pressure dependence of the band gap for these materials and the possibility of a transition from a trivial to a non-trivial topology of the band structure. For PbTe, we predict the band crossover and topological transition to occur at around 4.8 GPa. For GeTe, we estimate the topological transition to occur at 1.9 GPa in the constrained cubic phase. The latter pressure is lower than the pressures to crystallize in the cubic structure. SnTe is a crystalline topological insulator at ambient pressure, and the transition into a trivial topology would take place under a volume expansion of approximately 10%.

Minimax Isometry Method: A compressive sensing approach for Matsubara summation

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We present a compressive sensing approach for the long standing problem of Matsubara summation in many-body perturbation theory. By constructing low-dimensional, almost isometric subspaces of the Hilbert space we obtain optimum imaginary time and frequency grids that allow for extreme data compression of fermionic and bosonic functions in a broad temperature regime. The method is applied to the random phase and self-consistent GW approximation of the grand potential and integration and transformation errors are investigated for Si and $SrVO_3$.

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Relativistic correction to core level excitations from GW

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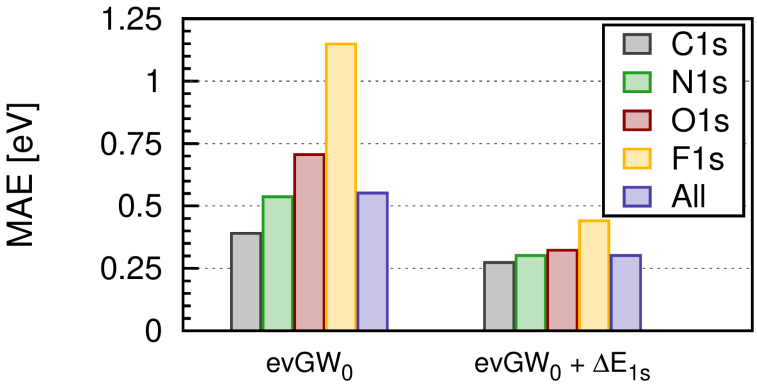

Figure 1: Mean absolute error (MAE) of evGW_0 core excitation by atomic species without (left) and with (right) relativistic correction.

We present a simple relativistic correction to improve the accuracy of GW 1s core-level energies. GW has become the method of choice for the calculation of addition and removal energies for valence electrons [1], and recently it has been shown to also provide good accuracy for core states [2,4]. However, even for light (2nd period) elements, relativistic effects begin to dominate the error in core state quasiparticle energies, leading to a species dependence in the magnitude of the overall error. We solve the radial Kohn-Sham (KS) and 4-component Dirac-Kohn-Sham equations self consistently for a free neutral atom on a fully numeric real-space grid, and evaluate the difference ΔE_{1s} between their 1s eigenvalues [3]. We examine the dependence of ΔE_{1s} on molecular environment and on the amount of exact exchange in the exchange correlation functional, and find it to be within the range of experimental error ($\leq$ 0.05 eV). We investigate the effect of shifting the KS eigenvalues prior to an eigenvalue-self-consistent GW calculation (evGW_0) by this corrective term for a benchmark set of 65 2nd period core excitations [4]. We similarly consider the effect of applying this correction to the quasiparticle energies subsequent to an evGW_0 calculation. The mean absolute error (MAE) in quasiparticle energies is calculated as the mean absolute difference between the negative of the ionization potential and the 1s quasiparticle energy extrapolated to the basis set limit. The MAE is reduced by either corrective procedure from 0.55 to 0.30 eV, and the species dependence of the MAE is eliminated.

[1] D Golze, M Dvorak, and P Rinke, "The GW Compendium", Frontiers in Chemistry 7:377 (2019)

[2] D Golze et al, "Core-Level Binding Energies from GW: An Efficient Full-Frequency Approach within a Localized Basis" JCTC 14:9, pp. 4856–4869 (2018)

[3] O Čertı k, JE Pask, and J Vackář, "DFTATOM: A robust and general Schrödinger and Dirac solver for atomic structure calculations", CPC 184:7, pp. 1777-1791 (2013)

[4] D Golze, L Keller, and P Rinke, "Accurate absolute and relative core-level binding energies from GW", JPCL 11:5 (2020) 1840-1847

Frequency dependence of W made simple using a multi-pole approximation. The case of the Gr/Co/Ir interface

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In the GW approximation, the screened interaction W is a dynamic property represented by a frequency dependence in the Fourier space, that makes the calculation of quasiparticles computationally time-consuming. A full description of the frequency dependence in a large energy range is in many cases prohibitive. For this reason, it is a common practice/strategy to approximate the dependence by a plasmon pole (PP) model. Unfortunately PP may fails for in-homogeneous systems, such as interfaces and defects, and also for some bulk materials, including e.g. metals. Several strategies and approximations to overcome this problem have been proposed to get reasonable results in the self-energy. In this work we explore a multi-pole (MP) model for getting a simple and effective representation of W.

We aim at applying the MP approximation to technologically relevant complex interfaces composed by a graphene monolayer grown on transition metal substrates. In particular we are interested in Gr on Co and Co/Ir systems, where previous attempts to compute W with the PP model fail, and a full frequency calculation is extremely expensive in terms of computational resources.

A Scalable Numerical Approach to the Solution of the Dyson Equation for the Non Equilibrium Single Particle Green's Function

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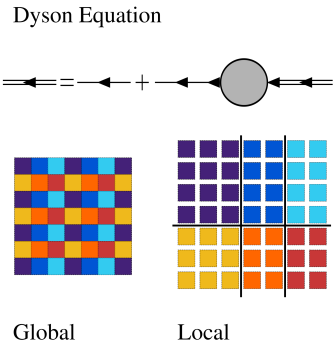

Figure 1: Top: Diagrammatic representation of the Dyson Equation; Bottom: Schematics of the distribution of a global matrix into local ones on the different processes

Within the framework of the non-equilibrium Green's functions I will present a scalable approach to solve the Dyson equation both in the two-time plane and in the frequency domain. Special emphasis will be put on the methods employed to compute the Second Born and GW self-energies which is one of the two bottlenecks the other being the inversion of the kernel of the Dyson equation. I will also discuss some applications of this method to different physical problems.

[1] W.N. Talarico, S. Maniscalco and N. Lo Gullo, A Scalable Numerical Approach to the Solution of the Dyson Equation for the Non Equilibrium Single Particle Greenś Function, Phys. Status Solidi B 1800501, (2019)

Density Functional Embedding Theory Formulation Suitable for Periodic All-electron Calculations with Gaussian Basis Functions

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Density functional embedding theory (DFET) [1] is a promising tool for performing accurate calculations of large systems at a reduced computational cost by combining DFT with many-body correlated methods. The embedding potential added to the higher-level Hamiltonian as a one-electron term is obtained at the DFT by maximising the Wu-Yang functional. Representing the potential on the plane-wave grid provides smooth convergence of optimisation and is natural for periodic systems. However, such representation is not favourable for all-electron calculations and transfer of the potential on the grid to non-periodic quantum-chemistry solvers is problematic. On the other hand, representation of the potential as a linear combination of local basis functions is not flexible and results in poorly converged potentials. Expansion of the potential in the product space of Gaussian basis functions [2] removes this problem, providing good convergence while keeping the embedding potential in a compact matrix form. This formalism requires computation of four-centre overlap integrals, which can be efficiently performed analytically with the resolution of identity approximation. Analytical evaluation of integrals allows to apply the scheme for periodic pseudopotential and all-electron calculations of periodic systems with Gaussian-and-plane-waves [3] and Gaussian-and-augmented-plane-waves formalisms [4], respectively. The approach is implemented within the developer version of the CP2K program and the performance is illustrated.

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Modelling changes of environmental screening on the gap of 2D materials

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Nano-objects, and more specifically ultra-thin films with a thickness of a few atomic layers, are extremely sensitive to variations of the surroundings. Although the change of the environmental screening is not the only cause, in many cases is seems to be the dominant one [1,2,3,4]. This is particularly true for optical properties such as absorption or emission.

From the theoretical point of view, absorption onsets and emission thresholds can be computed accurately within many body perturbation theory by subtracting the excitonic binding energy from the quasiparticle gap. Unfortunately these calculations are extremely heavy and often unaffordable even for few-layer free-standing films. The inclusion of environmental effects (substrate/solvant) is an even more challenging task.

Despite these difficulties, simple models of the electron-hole pair based on the Wannier-Mott exciton can be adapted to the specific problem of ultra-thin films in contact with an environment [5,6,7]. However they only give access to (a reasonable approximation of) the exciton binding energy. In this poster I will present a recent work [8] focusing on how we have been able to adapt these models to the case of mono-, bi- and trilayer balck phosphorus and how we aim at extending them.

[1] L. V. Keldysh, Coulomb interaction in thin semiconductor and semimetal films, JETP Lett., 29, 658, 1979

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