yambo: An ab initio tool for excited state calculations

Andrea Marini\textsuperscript{a,e,*}, Conor Hogan\textsuperscript{b,e}, Myrta Grünig\textsuperscript{c,e}, Daniele Varsano\textsuperscript{d,e}

\textsuperscript{a} Dipartimento di Fisica, CNISM, and SMC Institute for Statistical Mechanics and Complexity, Università di Roma "Tor Vergata", Via della Ricerca Scientifica 1, I-00133 Roma, Italy
\textsuperscript{b} Dipartimento di Fisica and INFM-CNR, Università di Roma "Tor Vergata", Via della Ricerca Scientifica 1, I-00133 Roma, Italy
\textsuperscript{c} Unité PCPM, Université Catholique de Louvain, 1348 Louvain-la-Neuve, Belgium
\textsuperscript{d} National Center on nanoStructures and Biosystems at Surfaces (S3) of INFM-CNR, I-41100 Modena, Italy
\textsuperscript{e} European Theoretical Spectroscopy Facility (ETSF)

**Abstract**

\textit{yambo} is an \textit{ab initio} code for calculating quasiparticle energies and optical properties of electronic systems within the framework of many-body perturbation theory and time-dependent density functional theory. Quasiparticle energies are calculated within the \textit{GW} approximation for the self-energy. Optical properties are evaluated either by solving the Bethe–Salpeter equation or by using the adiabatic local density approximation. \textit{yambo} is a plane-wave code that, although particularly suited for calculations of periodic bulk systems, has been applied to a large variety of physical systems. \textit{yambo} relies on efficient numerical techniques devised to treat systems with reduced dimensionality, or with a large number of degrees of freedom. The code has a user-friendly command-line based interface, flexible I/O procedures and is interfaced to several publicly available density functional ground-state codes.

**Program summary**

Program title: \textit{yambo}
Catalogue identifier: AEDH\_v1\_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEDH\_v1\_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: GNU General Public Licence v2.0
No. of lines in distributed program, including test data, etc.: 149265
No. of bytes in distributed program, including test data, etc.: 2848169
Distribution format: tar.gz
Programming language: Fortran 95, C
Computer: any computer architecture, running any flavor of UNIX
Operating system: GNU/Linux, AIX, Irix, OS/X
Has the code been vectorised or parallelized?: Yes
RAM: 10–1000 Mbytes
Classification: 7.3, 4.4, 7.2
External routines:
\begin{itemize}
  \item BLAS (http://www.netlib.org/blas/)
  \item LAPACK (http://www.netlib.org/lapack/)
  \item MPI (http://www-unix.mcs.anl.gov/mpi/) is optional.
  \item BLACS (http://www.netlib.org/scalapack/) is optional.
  \item SCALAPACK (http://www.netlib.org/scalapack/) is optional.
  \item FFTW (http://www.fftw.org/) is optional.
  \item netCDF (http://www.unidata.ucar.edu/software/netcdf/) is optional.
\end{itemize}

Nature of problem: Calculation of excited state properties (quasiparticles, excitons, plasmons) from first principles.

\* This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).
* Corresponding author at: Dipartimento di Fisica, CNISM, and SMC Institute for Statistical Mechanics and Complexity, Università di Roma “Tor Vergata”, Via della Ricerca Scientifica 1, I-00133 Roma, Italy.
E-mail address: andrea.marini@roma2.infn.it (A. Marini).

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1. Introduction

Ab initio calculations in the framework of density functional theory (DFT) [1] have yielded high-quality results for a large variety of systems, ranging from periodic solids to molecules and nanostructures [1]. These results are however mostly limited to quantities related to the electronic ground state, whereas additional phenomena that occur in the excited state are not correctly described [2].

It was recognized at an early stage [3] that in extended systems the standard approximations for DFT – the local density (LDA) or generalized gradient (GGA) approximations – fail to describe, among other effects, the band gap of insulators and semiconductors [2]. In contrast, many-body perturbation theory (MBPT) [4] provides, by means of the quasiparticle (QP) concept, a more adequate and accurate approach that yields band gaps (and band structures, in general) in good agreement with the experimental values [2].

While the first successful QP calculations were performed in the mid 80s [5], it was only in the late 90s that many-body effects have been included in the ab initio calculation of optical properties of real materials [6]. It is now well known that a quantitative description of the optical response of an interacting electron system must account for electron–hole interactions (excitonic effects) [2]. This is achieved by solving the Bethe–Salpeter (BS) equation for the electron–hole Green’s function, within the MBPT framework. Nowadays, solving the BS equation is the state-of-the-art approach for calculating optical properties in extended systems. The importance of including excitonic effects is clear on comparison with the experimental absorption spectra of semiconductors and insulators. In particular, for wide-gap insulators there is hardly any resemblance between the spectrum calculated within a noninteracting theory and the experiment.

An alternative approach to the study of correlation in many-body systems is given by time dependent DFT (TDDFT) [7]. Similar to the paradigm of DFT for ground-state properties, TDDFT has emerged as a very powerful tool for the description of excited states. In principle TDDFT is an exact theory for neutral excited state properties. Nevertheless, in practice it has a number of commonly cited failings related to the approximation of the exchange-correlation (xc) kernel. One example is the difficulty encountered when studying the optical properties of extended systems; another is the severe underestimation of high-lying excitation energies in molecules. On the other hand, the combination of TDDFT with simple approximations for the xc kernel (based on the homogeneous electron gas) has been successfully applied to the study of the optical response of molecules and nanostructures.

Quasiparticles, excitons and plasmons are the excitations that can be calculated using the yambo code. These excitations are ubiquitous in the ab initio description of the electronic and optical properties of any physical system. The yambo code uses as input the result of standard DFT calculations obtained by means of publicly available codes [8,9]. The theoretical tools implemented in yambo are TDDFT and the BS equations for the response function and the Dyson equation in the GW approximation for the QPs.

The paper is structured as follows. In Section 2 we introduce the most important theoretical concepts as they are utilized in yambo, before describing some of the most important numerical algorithms implemented in the code in Section 3. Section 4 outlines the structure and capabilities of yambo. A more detailed description of how the code is actually utilized is presented in Section 5, before some brief notes regarding installation in Section 6. Finally, an illustrative example of a typical yambo calculation is outlined in Section 7.

2. Theoretical background

2.1. Quasiparticles: the plasmon-pole approximation

MBPT is a rigorous approach based on the Green’s function method, and provides a proper framework for accurately computing excited state properties. For details of the Green’s function formalism and many-body techniques applied to condensed matter, we refer the reader to several comprehensive papers in the literature [4,10]. Here we shall just present some of the main equations used for the quasiparticle and optical spectra calculations.

The basic component of a many-body perturbative expansion is the reference noninteracting system, that in yambo is represented by the solution of the DFT Kohn–Sham (KS) equations. In the following we will label these single particle levels as |nk⟩, n being the band index and k the generic vector of the grid used to sample the Brillouin Zone (BZ). In this basis the noninteracting Green’s function G0 takes the form

\[
G_{nk}^0(\omega) = \frac{f_{nk}}{\omega - \varepsilon_{nk} - i\Omega^+} + \frac{1 - f_{nk}}{\omega - \varepsilon_{nk} + i\Omega^+},
\]

where \(f_{nk}\) is the occupation factor and \(\varepsilon_{nk}\) the KS energies. The basic relation between \(G_0\) and the exact Green’s function is given by the Dyson equation

\[
G_{nk}(\omega) = \left(\left[G_{nk}^0(\omega)\right]^{-1} - \Sigma_{nk}(\omega) + V^{xc}_{nk}\right]^{-1},
\]

where the contribution due to the DFT exchange-correlation potential \(V^{xc}\) is removed from the single-particle energies appearing in \(G_{nk}^0(\omega)\) in order to prevent double counting of correlation effects induced by the self-energy \(\Sigma\). Since the basic physical process that distinguishes a bare particle from a quasiparticle is the screening of the particle by means of the polarization of the surrounding medium, yambo uses the GW approximation for the electronic self-energy \(\Sigma\) [11] which is diagrammatically depicted in Fig. 1. In this approximation the self-energy is a function of \(G^0\) and of the inverse dynamical dielectric function \(\varepsilon^{-1}(\mathbf{r}_1, \mathbf{r}_2; \omega)\), and it is composed of an exchange (x) and of a correlation (c) part:

\[
\Sigma_{nk}(\omega) = \Sigma^x_{nk} + \Sigma^c_{nk}(\omega).
\]
The exchange part is simply the Fock term of the Hartree–Fock self-energy, and it can be rewritten as

\[ \Sigma_{\text{int}}^{\text{X}}(\omega) = (n|\Sigma^{\text{X}}(r_1, r_2)|n) \]

\[ = - \sum_{m} \int_{BZ} \frac{dq}{(2\pi)^3} \sum_{G} v(q + G) |\rho_{\text{int}}(k, q, G)|^2 f_{m (k - q)}. \]  

where \( \rho_{\text{int}}(k, q, G) = (n|e^{i(q-G)\cdot r}|m - q), \) \( G \) are the reciprocal lattice vectors, and \( v(q + G) \equiv 4\pi/(q + G)^2 \). The correlation part of the self-energy is given by

\[ \Sigma_{\text{int}}^{\text{C}}(\omega) = (n|\Sigma^{\text{C}}(r_1, r_2; \omega)|n) \]

\[ = i \sum_{m} \int_{BZ} \frac{dq}{(2\pi)^3} \sum_{G} \frac{4\pi}{q + G} |g_{\text{int}}(k, q, G)|^2 \rho_{\text{int}}(k, q, G) \]

\[ \times \int d\omega' G_{n - q}^0(\omega' - \omega)\epsilon_{-G}^1(q, \omega'). \]

The energy integral entering Eq. (5) can be solved once the inverse dielectric function is known. The equation of motion for \( \epsilon^{-1} \) follows from that of the reducible response function \( \chi \) [10] as

\[ \epsilon_{\text{GC}}^{-1}(q, \omega) = \delta_{\text{GC}} + v(q + G)\chi_{\text{GC}}(q, \omega). \]  

(6)

The GW approximation for the self-energy is obtained when \( \chi \) is calculated within the random phase approximation (RPA) [10]

\[ \chi_{\text{GC}}(q, \omega) = \left[ \delta_{\text{GC}} - v(q + G')\chi_{\text{GC}}^0(q, \omega) \right]^{-1} \chi_{\text{GC}}^0(q, \omega). \]  

(7)

The noninteracting response function is easily calculated in terms of the bare Green’s function \( G_0 \):

\[ \chi_{\text{GC}}^0(q, \omega) = \sum_{n} \int_{BZ} \frac{dk}{(2\pi)^3} \rho_{\text{int}}^n(q, G) \rho_{\text{int}}^n(q, G') f_{nk}(1 - f_{nk}) \]

\[ \times \left[ \frac{1}{\omega + \epsilon_{nk - q} - \epsilon_{nk} + i0^+} - \frac{1}{\omega + \epsilon_{nk - q} - \epsilon_{nk} - i0^+} \right]. \]  

(8)

As the numerical integration of \( \epsilon^{-1} \) in Eq. (5) would require the inversion of Eq. (7) for many frequency points, \( \text{yambo} \) adopts the plasmon-pole approximation (PPA) for the GW self-energy [11]. In the PPA the \( \epsilon^{-1} \) function is approximated with a single pole function

\[ \epsilon_{\text{GC}}^{-1}(q, \omega) \approx \frac{1}{\omega - \Omega_{\text{GC}}(q) + i0^+} - \left( \omega + \Omega_{\text{GC}}(q) - i0^+ \right)^{-1}, \]  

and the residuals \( \Omega_{\text{GC}} \) and energies \( \Omega_{\text{GC}} \) are found by imposing the PPA to reproduce the exact \( \epsilon^{-1} \) function at \( \omega = 0 \) and \( \omega = iE_{\text{PPA}} \), with \( E_{\text{PPA}} \) being a suitable user-defined parameter.

Using Eq. (2) and assuming \( f_{nk} \) to be either 1 or 0 we have that:

\[ (\omega - \epsilon_{nk}) G_{nk}(\omega) = 1 + [\Sigma_{nk}(\omega) - V_{\text{xc}}^{nk}] G_{nk}(\omega). \]  

The key approximation is now to take the first order Taylor expansion of the self-energy around \( \epsilon_{nk} \) (Newton approximation) in order to get

\[ G_{nk}(\omega) \approx \frac{f_{nk}}{\omega - \epsilon_{nk}^0 + i0^+} + \frac{1 - f_{nk}}{\omega - \epsilon_{nk}^0 + i0^+}, \]

with

\[ E_{\text{PPA}}^G = \epsilon_{nk} + \Sigma_{nk}(\epsilon_{nk} - V_{\text{xc}}^{nk}). \]

(11)

\[ Z_{nk} = \left[ 1 - \frac{d\Sigma_{nk}(\omega)}{d\omega} \right]_{\omega = \epsilon_{nk}}^{-1}. \]

(13)


It is important to note, at this stage, that by including explicitly the electronic occupations \( f_{nk} \), \( \text{yambo} \) can be equally applied to semiconductors, insulators and metals. In the latter case, however, the plasmon-pole approximation can be questionable when some of the valence orbitals are spatially localized (like in d or f metals) [12]. Nevertheless for metals in general the RPA is an excellent approximation to the calculation of optical properties, as the efficient screening occurring at the Fermi surface prevents the formation of excitonic states.

2.2. Optical properties: the Bethe–Salpeter equation

The evaluation of the response function \( \chi \) makes it possible to calculate the macroscopic dynamical dielectric function \( \epsilon_{M} \) and polarizability \( \alpha \). In particular the macroscopic dielectric function is defined in terms of the microscopic inverse dielectric function as [13]

\[ \epsilon_{M}(\omega) \equiv \lim_{q \to 0} \frac{1}{[\epsilon(q, \omega')^{-1}]_{G = 0} = \epsilon(\omega)}. \]

(14)

where \( \epsilon \) is the matrix in the space of reciprocal vectors \( G \) defined in Eq. (6). Eq. (14) implies that, in general, one cannot take the simple spatial macroscopic average of the dielectric function [13] since the charge redistribution induced by the interaction with light induces, in turn, the formation of local microscopic fields - the local field effects. Such effects are particularly important in nanoscale materials where confinement induces the formation of microscopic fields that counteract the external applied perturbation [2]. Similarly the dynamical polarizability of a zero-dimensional electronic system is defined as

\[ \alpha(\omega) = \frac{\Omega}{4\pi} \lim_{q \to 0} \frac{1}{q^2} \chi_{\text{GC} \to 0}(q, \omega). \]

(15)

where \( \Omega \) is the unit cell volume.

The RPA to Eqs. (14, 15) is often inadequate to describe the electronic correlations occurring in the response function. In practical applications the RPA does not yield optical absorption spectra in good agreement with experiments for several insulating and metallic systems [2]. For example, in the case of SiO2, this discrepancy has led to extensive debates over the past forty years about the nature of the four well-defined peaks observed in the experiment (see Fig. 2). The reason for the poor performance of the RPA is that the response function \( \chi \) measures the change in the electronic density induced by the external applied potential. In a noninteracting system the RPA for \( \chi \) is exact, but self-energy corrections modify the electronic density and, consequently, the RPA approximation is not valid anymore. Therefore, an estimation of the importance of corrections to the RPA can be obtained by looking at the value of the gap correction. The larger the gap, the less adequate is the RPA. The gap of SiO2, indeed, is \( \sim 10 \) eV and the RPA is not even qualitatively correct.

The drawbacks of the RPA are solved by using a more elaborate equation of motion for \( \chi \) that takes into account the effect...
of electron–electron correlations. This is the BS equation [10] that can be introduced by using the electron–hole (e–h) Green's function \( L \). First we note that the noninteracting \( q = 0 \) response function, Eq. (8), can be rewritten in terms of the noninteracting e–h Green's function \( L^0 \):

\[
\lim_{q \to 0} \chi_{GC}(q, \omega) = -i \sum_{nn'l'll'k} \int [\rho_{n'nk}(q, G)\rho_{l'll'k}(q, G')] L^0_{nn'll'l'}(\omega).
\]

To avoid the inversion of Eq. (14), we define a new interacting polarization [2] such that \( \epsilon_{\omega}(q, \omega) \equiv 1 - \nu(q)\chi_{GC,q=0}(q, \omega) \). This function defines a corresponding e–h Green's function \( \tilde{L} \):

\[
\lim_{q \to 0} \tilde{\chi}_{GC}(q, \omega) = -i \sum_{nn'l'll'k} \int [\rho_{n'nk}(q, G)\rho_{l'll'k}(q, G')] \tilde{L}_{nn'll'l'}(\omega).
\]

The BS equation naturally takes into account the electron–hole interaction in the response function as shown schematically in Fig. 3. The matrix \( \tilde{L}_{nn'll'l'} \) is the kernel of the BS equation composed of a direct electron–electron scattering term \( W \) plus an exchange interaction \( \tilde{V} \). Both \( W \) and \( \tilde{V} \) are integrals of Bloch functions

\[
W_{nn'll'l'} = \frac{1}{\Omega N_q} \sum_{GG'} \rho_{n'nk}(k, q = k - k_1, G)\rho_{l'll'k}(k_1, q = k - k_1, G')
\times \epsilon^{-1}_{GC}(q+G'),
\]

\[
\tilde{V}_{nn'll'l'} = \frac{1}{\Omega N_q} \sum_{G_{\text{phys}}} \rho_{n'nk}(k, q = 0, G)\rho_{l'll'k}(k_1, q = 0, G)\nu(G)
\]

with \( N_q \) the number of points in the BZ sampling.

It is important to observe that the BS equation is a Dyson-like equation that should be inverted at each frequency point. The dimension of the \( \tilde{L} \) matrix can be, however, quite large and the inversion of Eq. (18) practically impossible. However, for systems with a gap and at zero temperature the noninteracting e–h Green's function can be rewritten as

\[
y\left[ \tilde{L}_{nn'll'l'}(\omega) \right] = \frac{1}{\omega - \epsilon_{nk} + \epsilon_{n'k'}}.
\]

As a consequence it can be shown [2] that the BS equation can be reduced to an eigenvalue problem of the Hamiltonian \( H \):

\[
H_{nn'll'l'} = (\epsilon_{nk} - \epsilon_{n'k'})\delta_{nm}\delta_{ll'}\delta_{kk'}
+ (\epsilon_{nk} - \epsilon_{n'k'})[2\tilde{V}_{mm'll'} - W_{mm'll'}].
\]

The Hamiltonian in Eq. (22) is in general non-Hermitian. Nevertheless \( yambo \) adopts the standard Tamm–Dancoff approximation [16], in which only e–h pairs at positive energy are considered and the Hamiltonian \( H \) is Hermitian. Finally the dielectric function can be expressed in terms of the eigenstates \( |\lambda\rangle \) and eigenvalues \( E_\lambda \) of \( H \):

\[
\epsilon_{\omega}(\omega) \equiv 1 - \lim_{q \to 0} \frac{8\pi}{|q|^2}\sum_{nn'm'm'} \sum_{ll'm'm'} \rho_{n'nk}(q, G)\rho_{l'll'k}(q, G')
\times \sum_\lambda A_{n'll'}(A_{n'm'm'}^{\ast})_{\omega - E_\lambda}.
\]

with \( A_{n'll'} \) being the eigenvectors of \( H \). In the case of semiconductors the BS approach induces only a minor modification of the absorption spectrum. For wide-gap insulators, instead, the energies \( E_\lambda \) may fall within the single particle gap. In this case the eigenstates of the BS equation are called bound excitons [2]. A typical example is shown in Fig. 2 for the case of solid SiO\(_2\) [17,14].

2.3. Time-dependent density functional theory

Time-dependent density functional theory (TDDFT) [7] is gaining increasing popularity as an efficient tool for calculating electronic excitations in finite systems, thanks to its simplicity and moderate computational cost. In TDDFT the exact polarization function satisfies a Dyson-like equation that reads

\[
\chi_{GC}(q, \omega) = \chi_{GC}(q, \omega) + \sum_{G'} [\nu(q + G')
+ f_{xc}(q, G, G'; \omega)] \chi_{GC}(q, \omega).
\]

Eq. (24) is similar to Eq. (7) with an important addition, the xc kernel \( f_{xc} \) that accounts for the exchange and correlation effects. The exact form of the xc kernel is unknown, but the TDDFT success relies also in the fact that even using the simplest adiabatic local density approximation (ALDA) for \( f_{xc} \) a good accuracy in the evaluation of optical properties can be obtained [18].

We would like to mention here some common limitations of Eq. (24), associated with the use of plane-waves, when applied to low-dimensional electronic systems. As \( yambo \) is a plane-wave...

\[ \text{Fig. 2. The calculated absorption spectra of solid SiO}_2\text{ within the RPA and through solving the BS equation are compared with the experimental curve. Calculations taken from Ref. [14], experiment from Ref. [15].} \]

\[ \text{Fig. 3. Diagrammatic representation of the BS equation. The straight and wiggled lines represent the propagation of a KS electron and of the screened interaction. The dashed line represents the bare Columb interaction.} \]
code, it uses the super-cell approach to study small systems like molecules and nanoscale materials. This approach usually leads to two types of problems.

The first of these is the possibility of fictitious interactions between super-cell replicas (images). To treat this problem, yambo is capable of removing the long-range tail of Coulomb potentials following the method described in Ref. [19]. The second problem derives from the numerical instability of Eq. (24) that is induced by the presence of large regions of space with vanishing density, as occurs in large super-cells (see inset of Fig. 4). Unfortunately, this vanishing density induces some complications to Eq. (24) when \( f_{\text{xc}} \) is evaluated at the ALDA level. Indeed, the ALDA kernel is defined by:

\[
f^{\text{ALDA}}_{\text{xc}}(\mathbf{r}, \mathbf{r}'; t) = \delta(\mathbf{r} - \mathbf{r}') \frac{dV_{\text{HEG}}^{\text{nc}}(n)}{dn} |_{n=m(n, t)},
\]

where \( V_{\text{HEG}}^{\text{nc}}(n) \) is the exchange and correlation potential of the homogeneous electron gas. In the region of space with vanishing density we have that \( f_{\text{xc}}^{\text{HEG}}(n) \to \infty \) so that the evaluation of the term involving the \( f_{\text{xc}} \) in Eq. (24) cannot be directly calculated in reciprocal space, because the \( f_{\text{xc}}^{\text{ALDA}} \) is not well defined. To overcome this problem yambo can solve the TDDFT equation within the ALDA in the basis of the e–h pairs, instead of in reciprocal space [Eq. (24)]. In this case the TDDFT equation has the same form of the BS equation, Eq. (18), with the kernel \( \Sigma \) given by

\[
\Sigma_{mnk}^{\text{ALDA}} = -K_{mnk}^{\text{ALDA}} - \tilde{V}_{mnk}^{\text{ALDA}},
\]

with

\[
K_{mnk}^{\text{ALDA}} = 2 \int d\mathbf{r} d\mathbf{r}'' \phi_{m}^{\ast}(\mathbf{r}) \phi_{n}^{\ast}(\mathbf{r}) f_{\text{xc}}^{\text{ALDA}}(\mathbf{r}, \mathbf{r}'; t = 0) \times \phi_{m}^{\ast}(\mathbf{r}'') \phi_{n}^{\ast}(\mathbf{r}').
\]

In Fig. 4 we show, as an example, the ALDA dynamical polarizability along the x-axis of the ethylene molecule. The yambo result is compared with a calculation made with the code octopus [20] where all the quantities are defined in real-space, and the results are not affected by the presence of regions with zero density and of images due to the super-cell approach. We can see that yambo well reproduces the main excitation peak at 7.5 eV, that is composed by bound (localized) electron–hole states [21].

3. Some numerical aspects

The yambo code has been applied to a wide range of materials, from bulk compounds to molecules and nanostructures. As a consequence we have developed several ad hoc methods specifically designed to solve physical and numerical problems that can be commonly encountered.

3.1. The random integration method

The definition of the self-energy operator – and of many other quantities – requires an integration in the BZ. In practice this integral is replaced by some suitable grid of points. Let us consider for simplicity only the Hartree–Fock self-energy, given by Eq. (4).

Using a finite grid of transferred momenta \( \mathbf{q} \) it reads

\[
\Sigma_{\mathbf{k} \mathbf{q}} = -\frac{(2\pi)^3}{N_q \Omega} \sum_{\mathbf{m} \mathbf{G}} v(\mathbf{q} + \mathbf{G}) \rho_{\mathbf{m}}(\mathbf{k}, \mathbf{q}, \mathbf{G})^2 f_{\mathbf{m} \mathbf{k} - \mathbf{q}}.
\]

In approximating \( \Sigma_{\mathbf{k} \mathbf{q}} \) using a finite grid the key assumption is that the integrand of Eq. (4) must be a smooth function of \( \mathbf{q} \). While this is generally true for the oscillators \( \rho \) part, this is not so trivial for the Coulomb potential that, indeed, diverges for \( \mathbf{q} \to 0 \).

Nevertheless, in three-dimensional systems this divergence is not affecting the calculation. In fact, the phase space volume associated with the \( \Gamma \) point reduces as \( \mathbf{q} \to 0 \) and the divergence is de facto removed. In low-dimensional systems this cancellation holds only if a three-dimensional grid is used. When the Brillouin zone is sampled with lower-dimensional grid instability problems appear in the evaluation of the Coulomb integral. As shown in the right panel of Fig. 5, these instabilities may even grow as a function of the Brillouin zone sampling size. On the other hand using a three-dimensional grid is clearly inconvenient, and more importantly can make the calculations extremely cumbersome.

In order to avoid the use of a three-dimensional sampling yambo offers two methods to remove the divergence arising from the Coulomb integrals. The first is based on a cutoff Coulomb technique which is discussed in detail in Ref. [19]. The other is the so-called random integration method (RIM) [23]. In the RIM the HF self-energy is rewritten as

\[
\Sigma_{\mathbf{k} \mathbf{q}} \approx -\sum_{\mathbf{m} \mathbf{G}} \rho_{\mathbf{m}}(\mathbf{k}, \mathbf{q}, \mathbf{G})^2 f_{\mathbf{m} \mathbf{k} - \mathbf{q}} \times \int_{\mathbf{k}_F} \frac{d\mathbf{q}'}{(2\pi)^3} \sum_{\mathbf{G}} v(\mathbf{q} + \mathbf{q}' + \mathbf{G}).
\]
The integral of the Coulomb potential
\[
l_q(G) = \int_{R_F} d\mathbf{q}' (2\pi)^3 \sum_G v(\mathbf{q} + \mathbf{q}' + G)
\]
\[l_q(G) \approx \int_{R_F} d\mathbf{q}' (2\pi)^3 \sum_G v(\mathbf{q} + \mathbf{q}' + G)
\]
is evaluated in a region \(R_F\) around the \(F\) point. Representing as \(R_q\) the region \(R_F\) translated in the general \(q\) position, this region is chosen in such a way that \(R_F \cup R_q \cup R_{q_2} \cdots R_{q_{Nq}} = BZ\). The RIM is based again on the uniformity ansatz described above, but restricted only to the \(\rho_{nm}\) factors. The \(l_q\) integrals are calculated via a three dimensional Monte Carlo technique [24].

For practical purpose, it is necessary to evaluate only \(l_q(G = 0)\) because far from the origin the approximation leading to Eq. (28) is still accurate as shown in the right panel of Fig. 5. The importance of the RIM is exemplified in the left panel of Fig. 5 where we show the convergence of \(\Sigma^t\) with respect to the \(k\)-point sampling at the \(X\) point of a quasi one-dimensional trans-polyacetylene polymer.

### 3.2. The Lanczos–Haydock solver of the BS equation

Once the BS (or the TDFT) Hamiltonian \(H\) [Eq. (22)] has been calculated in the basis of \(e\)-\(h\) pairs \(|\mathbf{v}\mathbf{c}\mathbf{k}\rangle\), *yambo* offers two options for calculating the corresponding macroscopic dielectric function \(\epsilon_M(\omega)\) and related quantities (optical absorption, electron loss and dynamical polarizability); either via the diagonalization, or via the Lanczos–Haydock (LH) recursion method [25].

With the first option the program diagonalizes \(H\) using the standard serial or scalable BLAS/LAPACK routines [26] to find the eigenvalues \(E_i\) and eigenstates \(|\mathbf{v}\mathbf{k}\rangle\) that define the macroscopic dielectric function, Eq. (23). With the second option Eq. (23) is rewritten as,

\[
\epsilon_M(\omega) = 1 - |\langle P | (\omega - H)^{-1} | P \rangle|,
\]

where \(|P\rangle = \lim_{q\rightarrow 0} \frac{1}{\mathbf{q}} |\mathbf{v}\mathbf{k}\rangle (\mathbf{v}\mathbf{k} - \mathbf{q} | e^{-iq}\mathbf{r}\rangle (\mathbf{k})\). Then Eq. (31) is calculated using the LH method [25,27], a general algorithm to compute the matrix elements of the Green’s function \((\omega - H)^{-1}\) applied for the first time to solve the BS equation by Benedict and coworkers [28].

The LH algorithm recursively builds an orthonormal basis \(|q_i\rangle\) (Lanczos basis) in which \(H\) is represented as a real symmetric tridiagonal matrix,

\[
T_j = \begin{pmatrix}
    a_1 & b_2 & 0 & \cdots & 0 \\
    b_2 & a_2 & b_3 & \cdots & 0 \\
    0 & b_3 & a_3 & \cdots & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & \cdots & 0 & b_{j-1} & a_{j-1} \\
    0 & \cdots & 0 & b_j & a_j
\end{pmatrix}
\]

The first vector \(|q_1\rangle\) of the Lanczos basis is set equal to \(|P\rangle/||P||\). The next vectors are calculated from the three-term relation

\[
b_{j+1}|q_{j+1}\rangle = H|q_j\rangle - a_j|q_j\rangle - b_j|q_{j-1}\rangle.
\]

In the Lanczos basis Eq. (31) becomes

\[
\epsilon_M(\omega) = 1 - |\langle P | (\omega - 1) - \frac{1}{(\omega - a_1) - \frac{b_1^2}{(\omega - a_1 - \frac{b_1^2}{(\omega - a_2 - \frac{b_2^2}{(\omega - a_3 - \frac{b_3^2}{(\omega - a_4 - \frac{b_4^2}{(\omega - a_5 - \frac{b_5^2}{(\omega - a_6 - \frac{b_6^2}{(\omega - a_7 - \frac{b_7^2}{(\omega - a_8 - \frac{b_8^2}{(\omega - a_9 - \frac{b_9^2}{(\omega - a_{10})}}}}}}}}}}}}}}}}}}\rangle
\]

At each iteration the program computes a new vector \(|q_{j+1}\rangle\) [Eq. (33)], the matrix elements \(a_j, b_j, j = 1,\) and thus a better approximation \(\epsilon_M(\omega)\) from Eq. (34). The LH iteration procedure stops when the difference \(|\epsilon_M(\omega) - \epsilon_M(\omega - \frac{1}{N})|\) in the given range of frequencies is smaller than a user-defined threshold.

In practice, when interested in a finite range of frequencies one needs a number of iterations \(k\) much smaller than the dimension \(N\) of the Hamiltonian (corresponding to number of \(e\)-\(h\) pairs included in Eq. (22)) to get an accurate \(\epsilon_M(\omega)\). In the left panel of Fig. 6 this is exemplified for the dynamical polarizability calculated within the ALDA of the trans-azobenzene molecule: \(k \approx 50\) is enough for getting an accurate spectrum up to 6 eV, with \(N \approx 4000\). As a consequence, the LH method [\(O(K^{N^2})\) floating point operations] is usually much faster than the diagonalization procedure [\(O(N^4)\) floating point operations]. This is clearly shown in the right panel of Fig. 6: already for \(N \approx 1000\) the LH method starts to be more convenient, and for \(N \approx 4000\) it is about 70 times faster than the diagonalization procedure. The LH method is also more convenient in terms of memory size, in contrast with the diagonalization, only three vectors at a time need to be stored. Furthermore, the whole procedure has been efficiently parallelized in *yambo*. The LH algorithm is, therefore, the recommended method in *yambo* for the computation of the macroscopic dielectric function and related quantities, while the diagonalization should be used when the eigenvalues and eigenvectors of \(H\) are explicitly needed, for example for plotting the excitonic wavefunction via the post-processing tool *ypp*.

### 4. Overview of the software

The structure of the *yambo* package can be separated into a number of stages, schematically depicted in Fig. 7. In the preliminary stage (I), a C/Fortran driver passes control to the main *yambo* executable, or to the data converters (a2y, p2y, e2y). The purpose of the latter is to generate the core databases that contain the ground state data necessary for starting the code. A mostly procedural data initialization stage (II) follows, where some general-purpose databases are prepared for later use. The main physical
Fig. 7. Simplified schematic chart of the program. Diamond boxes denote some of the most important databases (see text).
calculations are performed in the third stage (III). Finally, databases created by \texttt{yambo} can be further manipulated using the post-processing tool \texttt{ypp} in a fourth stage (IV).

Operation of the code follows a series of functionally distinct 
runlevels. The main runlevels are activated by the user via the 
command-line interface (described in more detail in Section 5.2), 
and others are called automatically by the code where dependen-
cies are present. Runlevels have a modular structure, in the sense 
that each one performs specific physical tasks and terminates (in 
most cases) with the creation of one or several databases written
onto disk. These database files may then be accessed by differ-
ent runlevels. Runlevels may be skipped in subsequent runs if a 
database is found that is compatible with the user requirements 
on execution. A more thorough discussion of the databases, and 
the \texttt{yambo} I/O in general, can be found in Section 5.3.

The main runlevels are now described in more detail.

Stage I: (i) C driver: governs the actions taken by the rest of 
the code. \texttt{yambo} uses a standard \texttt{getopt} function [29] 
to parse the command line. This function is called by 
all executables to acquire the user-defined options passed at 
the command line. The syntax is described 
briefly in Section 5.2.

(ii) Data import/converter: the ground-state electronic 
structure of the system to be studied is imported from 
ground state codes (see Section 5.1), and 
converted into the core database files.

Stage II: (i) User input: if command line options were added in 
Stage I, the executable acts as an input file generator. 
On execution, the code reads default values for input 
parameters from existing databases and updates the values in 
the input file, after which the code terminates.

(ii) Data initialization: reorders $G$-vectors into spherical 
shells, calculates Fermi level and electronic occupa-
tions, sets up energy grids.

(iii) Brillouin-zone sampling: expands $k$-points to full BZ, 
generates $q$-point meshes, checks on uniformity of 
grids.

Stage III: (i) Hartree–Fock/Vxc: calculates the matrix elements of 
the Hartree–Fock exchange self-energy and of the 
DFT potential corresponding to the type of func-
tional used in the ground state code run.

(ii) Screening: calculates static and dynamical inverse 
dielectric functions, for use in the evaluation of the 
GW self-energy and of the BS/TDDFT kernel.

(iii) Quasiparticle: calculates quasiparticle corrections to 
the Kohn–Sham band structure within the GW ap-
proximation.

(iv) Linear response: optical properties within RPA and 
ALDA with and without local field effects.

(v) Bethe–Salpeter/TDDFT: creation of the BS/TDDFT 
Hamiltonian and subsequent diagonalization using 
scalar and scalable LAPACK routines or via Lanczos–
Haydock iterative procedure.

Stage IV: (i) Post-processing: contains routines for creating $k$-point 
grids, analyzing single-particle and excitonic wave-
functions and plotting the electronic wavefunctions and density.

5. Description of the individual software components

5.1. Main utilities

As described earlier, the \texttt{yambo} package is in fact composed of 
three separate utilities. The first of these is the set of converters 
(a2y, p2y and e2y) which generate the \texttt{yambo} core databases 
from the output of other ground state codes. The a2y converter 
imports data from the so-called KSS file as generated by the 
Abinit code [9], while p2y imports data written by the Quantum-
ESPRESSO/PWscf [8] code in the \texttt{iotk} file format [30]. Alterna-
tively, e2y can be used to import data from a netCDF formatted 
file written according to the ETSF file-format specifications [31]. 
As a set of high-level libraries are available [32] that are capable of 
reading and writing this format, it is relatively easy to interface 
\texttt{yambo} with other ground state codes.

The main computation tool is the \texttt{yambo} executable itself. De-
pending on the command line options used (see next section), it 
can act either as an input file generator or as a straightforward 
serial or parallel executable.

The last utility is the \texttt{ypp} post-processor, which is generally 
used to perform short analysis of pre-calculated databases.

5.2. Command line interface

Thanks to the C/Fortran driver routine, \texttt{yambo} offers a very 
user-friendly command-line interface for configuring the code at 
run-time and for creating and editing the main input file. An ex-
tended list of options can be displayed by using the \texttt{-H} option 
(see Table 1). \texttt{yambo} options can be lowercase and uppercase. 
Uppercase options may be added at run-time to specify input/output 
directories (-I/-O, see next Section), skip the MPI calls (-n), 
create a simple report of the existing database properties (-D), and so 
on. For instance, running 
\texttt{yambo -N -I /scratch/tests/silicon-bulk -D}
will ask for a report of databases in the /scratch/tests/
silicon-bulk directory, and force the parallel-compiled exe-
cutable to run in serial. Lower case options, instead, drive the input 
file editor. For example,
\texttt{yambo -i -o c -I ~/tests/silicon-bulk}
will generate an input file (the default being \texttt{yambo.in}) that can 
be used to run the initialization steps (-i) and calculate linear 
response optics at the RPA level (-c). A useful feature of the 
code is that default values for parameters are suggested based on 
their values in the most relevant database, if a value is not already 
present in the input file. Hence if 500 bands are written in the 
core databases, \texttt{yambo} will suggest a range of 1–500 bands for 
calculating the noninteracting response function.

Since \texttt{yambo} offers a huge range of tunable parameters, some 
of which are quite technical, it would be quite daunting for an 
average user to face the full list of parameters when running the 
code. Hence, an input-file verbosity flag (-v) lets the user decide 
how detailed the input file is to appear (the remaining parame-
ters are set to their default values). After checking the existing 
databases and input files, \texttt{yambo} invoked in this way will redirect 
the user to edit the newly-created \texttt{yambo.in} file.

The C parser used by \texttt{yambo} to process the input files is taken 
from the \texttt{octopus} [20] code.

5.3. I/O: the \texttt{yambo} databases

Files created and accessed by \texttt{yambo} are classified according to 
their purpose and identified by a specific prefix:

(i) Static database files (prefix \texttt{s}. \texttt{s}. otherwise known as the core 
databases) are generated in Stage I (see Fig. 7) by the a2y, 
p2y and e2y converters. They contain the information con-
cerning the geometry, basis set, wavefunctions and energies, etc.
Table 1
Command line options for the various yambo tools.

<table>
<thead>
<tr>
<th>yambo</th>
<th>a2y/p2y/e2y</th>
<th>ypp</th>
</tr>
</thead>
<tbody>
<tr>
<td>-h</td>
<td>Short Help</td>
<td>-h</td>
</tr>
<tr>
<td>-H</td>
<td>Long Help</td>
<td>-H</td>
</tr>
<tr>
<td>-J &lt;opt&gt;</td>
<td>Job string identifier</td>
<td>-N</td>
</tr>
<tr>
<td>-V &lt;opt&gt;</td>
<td>Input file verbosity</td>
<td>-P &lt;opt&gt;</td>
</tr>
<tr>
<td>-F &lt;opt&gt;</td>
<td>Input file</td>
<td>-O &lt;opt&gt;</td>
</tr>
<tr>
<td>-I &lt;opt&gt;</td>
<td>Core I/O directory</td>
<td>-S</td>
</tr>
<tr>
<td>-O &lt;opt&gt;</td>
<td>Additional I/O directory</td>
<td>-a &lt;real&gt;</td>
</tr>
<tr>
<td>-C &lt;opt&gt;</td>
<td>Communications I/O directory</td>
<td>-t</td>
</tr>
<tr>
<td>-N</td>
<td>Skip MPI initialization</td>
<td>-y</td>
</tr>
<tr>
<td>-D</td>
<td>Databases properties</td>
<td>-w</td>
</tr>
<tr>
<td>-S</td>
<td>Databases fragmentation</td>
<td>-K</td>
</tr>
<tr>
<td>-i</td>
<td>Initialization</td>
<td>-e &lt;opt&gt;</td>
</tr>
<tr>
<td>-o &lt;opt&gt;</td>
<td>Optics [opt=chi(hb)j]</td>
<td>-p &lt;opt&gt;</td>
</tr>
<tr>
<td>-t &lt;opt&gt;</td>
<td>The TDDFTs [opt=x/LDA]</td>
<td>-f</td>
</tr>
<tr>
<td>-c</td>
<td>Coulomb interaction</td>
<td>-S</td>
</tr>
<tr>
<td>-x</td>
<td>Hartree–Fock Self-energy and Vxc</td>
<td>-D</td>
</tr>
<tr>
<td>-b</td>
<td>Static Inverse Dielectric Matrix</td>
<td>-k</td>
</tr>
<tr>
<td>-p &lt;opt&gt;</td>
<td>GW approximations [opt=p/PA]</td>
<td>-t</td>
</tr>
<tr>
<td>-v &lt;opt&gt;</td>
<td>RS equation solver [opt=hd]</td>
<td>-l</td>
</tr>
</tbody>
</table>

(ii) Stable database files (prefix db.) are created by yambo at run-time, usually in Stage II. They are generally created once and used to store intermediate data designed to be re-read during subsequent executions.

(iii) Job-dependent database files (prefix db.) are also created at run-time but hold information that is usually specific to a particular runlevel (Stage III).

(iv) Output files (prefix o.) are usually created at the end of certain Stage III runlevels and are intended for human use (e.g., suitable for plotting or inspection).

If the netCDF libraries[33] have been configured for use, these database prefixes are further prefixed by n, e.g., ndb.kindx is the netCDF formatted version of db.kindx, the database containing the k/q-point grids. Users are strongly advised to use netCDF-linked executables, as the functionality of the code is enhanced. In addition there are auxiliary run-time report files (prefix r_.) containing the run-time log information, while standard output can be redirected onto disk (prefix l_).

Creation of each database is controlled by its own particular Fortran subroutine, e.g., src/io/IOQP.F creates the database of QP corrections db.QP. However, the actual writing of data is performed at a low level by some common modules, in order to minimize problems associated with portability. Some of the most important databases and their respective runlevels are indicated in Fig. 7 as diamond-shaped boxes.

In order to treat systems with large memory or disk requirements yambo offers the capability of fragmenting the larger databases into chunks (–S). This functionality is most frequently utilized in the splitting of the ground-state wavefunction files according to k-points and/or bands, and in the division of the Bethe–Salpeter Hamiltonian according to the k-point index.

By default, all databases are stored in the subfolder .SAVE of the working directory. More specific control of I/O directories may be achieved through the various uppercase command line options. For instance, it is common to store the static databases in a ‘core’ directory (yambo –J COREPATH), so that they can be shared by different processes. Dynamically-created databases can then be placed elsewhere (yambo –O OTHER). Furthermore, users may organize their work better according to a “job string” identifier (yambo –J JOBNAME), so that databases and output files are placed in a subdirectory with a name specified by the user. Finally, long jobs, like the creation or diagonalization of the Bethe–Salpeter Hamiltonian, place intermediate results in a RESTART folder, so that the job can be continued following a crash or if CPU time limits are exceeded.

6. Installation instructions

yambo makes use of the GNU autoconf suite (autoconf/autofilio) for installation. Hence, the standard procedure of

```
./configure
make all
```

should create executables for yambo, the ypp postprocessor and the basic Abinit converters a2y and place them in the bin/ folder of the yambo source directory. Detailed installation instructions are available in the manual, including how to enable the p2y and e2y converters, how to link with netCDF, BLACS and FFTW libraries, change installation options, so on. In short, a somewhat complete list of compile-time options can be inspected by running the standard command

```
./configure --help
```

7. Running yambo: excitonic effects in bulk silicon

In this section we outline the basic steps involved in a typical production run of yambo. Normally one would of course start by creating the core databases by importing the output data of some ground state code (see Section 5.1). For the purpose of illustration, however, we have included in the yambo source a pre-compiled set of core databases for bulk silicon in the doc/sample directory. Detailed installation instructions are available in the manual, including how to enable the p2y and e2y converters, how to link with netCDF, BLACS and FFTW libraries, change installation options, and so on. In short, a somewhat complete list of compile-time options can be inspected by running the standard command

```
./configure --help
```

Once the core databases (ns.db, ns.wf) are extracted, running yambo in the doc/sample/bulk_silicon/ directory produces as standard output:

```
> yambo
```

```bash
<--- [01] Job Setup
<--- [02] Input variables setup
<--- [02.01] K-grid lattice
<--- [02.02] RL shells
<--- Shells finder |100%
<--- (E) --(X)
<--- [02.03] Input (E)nergies[ev] & Occupations
```

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This is the Stage II run that yambo enters by default whenever, as in this case, no input file has been specified. The results of this setup run (BZ sampling indexes, G vector shells, etc.) are stored in two new database files, SAVE/ndb.gops and SAVE/ndb.kindx, that are to be re-used in subsequent runs. Besides the two databases, yambo writes a report file, r_setup, that contains a detailed list of information about the run and the system. Every runlevel generates an appropriate report file.

At this stage we can carry out a more interesting calculation: as an example we will calculate the optical absorption spectra of bulk silicon including excitonic effects. To solve the BS equation we will employ the LH algorithm described in Section 3.2. First we create the input with the command-line based user interface. From Table 1 we see that the options to use are:

```
--- [03] Transferred momenta grid
--- > indexes |-----------| 100% [X] - [X]
--- > Z indexes |-----------| 100% [X] - [X]
--- > Game over & Game summary
```

This command creates the yambo.in input file shown in Table 2 and opens it in the default text editor, vi. Note that, by reading the databases generated in the setup run, yambo already knows that there are 19 momenta permitted by the BZ sampling, and that 50 bands were calculated in the preceding ground-state run. To perform a test calculation we change some of the values in the input.

- In Eq. (17), we restrict the summation from band 2 to band 6:

  ```
  % BSEBands
  2 | 6 | # [BSK] Bands range
  %
  ```

- In the statically screened interaction we use just 51 RL vectors:

  ```
  BSEBands
  %
  ```

Calling yambo again, without command line options, will start the calculation, which should last for some minutes. The progress of the calculation (including expected/elapsed time for each time-consuming operation) can be followed from the standard output, or in case of background execution, read from the l_optics_bse_em1s_bss.log file.

At the end of the run several new files appear in the SAVE folder: the dielectric function ndb.emls, the BS Hamiltonian matrix ndb.Q1, and the information needed to restart the LH iterative procedure in ndb.Haydock_restart. Furthermore, the run generates two files in the working directory, the report file (r_optics_bse_em1s_bss) and the output file (o.eps_q001-bh).

The output file contains the calculated spectra (BS and RPA spectra) that can be visualized without further processing with standard plotting tools. Plotting the second versus the first column of the o.eps_q001-bh file gives the well-known absorption spectrum of bulk silicon within BSE. The result of the run is shown in Fig. 8, where it is compared with the independent particle (RPA) spectrum (fourth versus the first column of the same file), with the experimental spectrum [34] (included in the doc/sample/bulk_silicon/experiment.dat file) and with the result of a more converged calculation [37].

![Optical spectrum of bulk silicon.](image)

**Fig. 8.** Optical spectrum of bulk silicon. The result of the sample run described in the text is compared with a more converged calculation [37] and with the experiment [34]. Note that the result of the sample run has been blue-shifted by 1 eV to simulate the correct QP gap that, instead, is calculated in the converged spectrum [37].

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Appendix A

A.1. The $\chi^0$ poles accumulation

The noninteracting response function $\chi^0$ is a key ingredient of the yambo code. It enters, for example, in the definition of the RPA dielectric function and of the GW self-energy. Nevertheless the practical evaluation of $\chi^0$ is often a bottleneck in realistic calculations. The reason is that, as shown in Eq. (8), $\chi^0$ contains a triple summation over the $k$ points and the occupied and empty electronic levels. For systems with a large number of electrons this summation can easily reach millions of elements, that must be multiplied by the number of frequencies.

To provide a tunable and efficient tool to reduce the numerical effort in evaluating $\chi^0$ yambo follows the general idea of the algorithm proposed by Miyake [38] to rewrite $\chi^0$ as

$$
\chi^0_{G0}(q, \omega) = \frac{2}{\Omega N_k} \sum_p \left( \sum_{m n k} \rho^{m n k}_G(q, G) \rho^{n m k}_G(q, G^*) \right) \times F_p \left[ \frac{1}{\omega + E_p + i 0^+} - \frac{1}{\omega - E_p - i 0^+} \right]
$$

(35)

In Eq. (35) the $I_p$ are groups of e–h indexes (nm$k$) with similar e–h energies $E_p = \epsilon_m \epsilon_n - \epsilon_{kq}$. The latter are approximated with a single pole at $E_p$ with occupation $F_p$. The number of groups created can be controlled by the user by tuning the `G0rdSp` variable in the input file.

The important difference with Eq. (8) is that, in Eq. (35) the evaluation of the oscillators is partially decoupled from the energy dependence. As a consequence by decreasing the groups of e–h pairs it is possible to make the evaluation of $\chi^0$ almost independent of the number of frequencies.

A.2. Oscillator symmetries

The oscillators

$$
\rho_{nm}(k, q, G) = \langle nk | e^{i(q+G) r} | m k - q \rangle
$$

appear in almost all the quantities calculated in yambo. They are evaluated using efficient Fast Fourier Techniques (FFT) [39]. Nevertheless yambo uses symmetry arguments to reduce the number of calls to the FFT interface.

If we specify the symmetry operation by rewriting a general point in the BZ as $k = Rk_{IBZ}$, with $k_{IBZ}$ defined in the irreducible wedge of the BZ, Eq. (36) reads

$$
\rho_{nm}(k, q, G) = \int_{\Omega} \left[ e^{-i k_{IBZ} \cdot r} u^{n}_{k_{IBZ}}(r) e^{i(q+G) r} u^{*m}_{k_{IBZ}}(r) \right] \times \left[ u^{*m}_{R(k-k_{IBZ})}(r) e^{iG \cdot G_0} u^{n}_{mR(k-k_{IBZ})}(r) \right],
$$

(37)

with $G_0$ defined as $G_0 = k - q - (k - q)_{IBZ}$. Hence we find that

$$
\rho_{nm}(k, q, G) = \int_{\Omega} u^{n}_{k_{IBZ}}(r) e^{i(G - G_0) r} u^{*m}_{mR(k-k_{IBZ})}(r).
$$

(38)

In case of spatial symmetries (a similar procedure applies to the time-reversal symmetry) we can rewrite the left side rotated wavefunction as $u^*_m (k_{IBZ}) = u^*_m (R^{-1} k)$, so that

$$
\rho_{nm}(k, q, G) = \int_{\Omega} u^{*n}_{k_{IBZ}}(r) R^{-1} (G - G_0) u^{m}_{mR(k-k_{IBZ})}(r).
$$

(39)

Finally we notice that the symmetries constitute a group, and, consequently, $R^{-1} R = S$, with $S$ a symmetry operation. Thus, at difference with Eq. (36), Eq. (39) depends only on one symmetry index. By using Eq. (39) the computational cost of calculating all the oscillators at a given $k$ point is reduced by the number of symmetries in the star of $k$.

References

[21] The high energy peaks appearing in Fig. 4 correspond to the excitation of unlocalized orbitals whose different description in the `yambo` and `octopus` codes leads to the discrepancies observed in the figure. Nevertheless, these differences can be systematically removed by increasing the dimension of the basis size.


NetCDF [31] (network Common Data Form) is a set of software libraries to support the creation, access, and sharing of array-oriented scientific data. The key property of the netCDF databases is that they are platform-independent. For more information visit http://www.unidata.ucar.edu/software/netcdf/.


The sample run of the excitonic optical properties of bulk silicon described in Section 7 is introduced to briefly illustrate the steps needed to run yambo and, more importantly, is conceived to run in a few seconds on a typical PC. This sample run is not supposed to represent a realistic calculation because of the limited sampling of the BZ and because of the use of too few empty bands to perform a converged GW calculation. The more converged BSE spectrum shown in Fig. 8 uses 60(2048) points in the irreducible(reducible) wedge of the BZ (which corresponds to a $8 \times 8 \times 8$ Monkhorst–Pack (MP) [35] grid). The GW QP gap is calculated on the same $8 \times 8 \times 8$ MP grid but shifted to the origin in such a way as to contain the $\Gamma$ point. The GW gap obtained with yambo is 1.20 eV, in excellent agreement with the experimental value of 1.17 [36]. We have used a 181 x 181 plasmon-pole dielectric function $\epsilon_G$ which includes up to 60 bands. 150 bands, instead, have been included in Eq. (5). These converged BSE and QP calculations require a total CPU-time of the order of $\sim$24 hours. Interested users can download the relevant input files for these more converged calculations directly from the yambo web site http://www.yambo-code.org/publications.html.
