Introduction to Octopus: periodic systems

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Solids in Octopus

Solids are periodic objects

- Bloch theorem: wavefunctions are labeled by a band index and a $\mathbf{k}$-point index:

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}.\mathbf{r}}$$

  - We can have 1D periodic (like atomic chains), 2D periodic (slabs), 3D periodic (bulks).
  - Octopus treats properly these cases as mixed zero-boundary conditions and periodic boundary conditions
- We have two grids:
  - The real space is sampled by the real-space grid
  - The Brillouin zone is sampled by a $\mathbf{k}$-grid
- Only velocity gauge description in dipole approximation of the electromagnetic field is possible

Symmetries in Octopus

Crystals have well defined symmetries

- Space group and symmetries of periodic systems are identified using the *spglib* library.
- Symmetries are restricted to symmorphic symmetries (inversion, rotations, and mirror planes).
- Symmetry-breaking perturbations (kicks, vector potentials, strain, ...) can be used
- Octopus finds the small group of symmetries that are left invariant the perturbation direction.
  These symmetries are used for time-dependent calculations.
- Charge and current densities are also symmetrized (and other observables).
  $\Rightarrow$Important for numerical stability

Non-orthogonal cells

Octopus can work with non-orthogonal cells

- The grid points are generated along the non-orthogonal axis
  $\Rightarrow$The generated grid preserves rotations and mirror planes
- The stencil for finite differences contains cross-terms in the derivatives

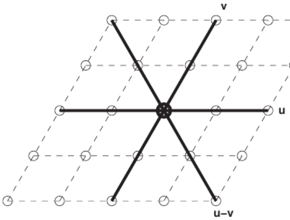

Figure: Hexagonal cell generated by u and v, and the corresponding discretization. Natan *et al.*, PRB 78, 075109 (2008)

Treatment of the velocity gauge in Octopus

Time dependent Kohn-sham equation within velocity gauge

$$i\frac{\partial}{\partial t}|\psi_{n,\mathbf{k}}(t)\rangle = \hat{H}_{\mathrm{KS}}(t)|\psi_{n,\mathbf{k}}(t)\rangle,$$

with

$$\langle\mathbf{r}|\hat{H}_{\mathrm{KS}}(t)|\mathbf{r}'\rangle = \left[\frac{1}{2}\left(-i\nabla - \frac{1}{c}\mathbf{A}(\mathbf{r},t)\right)^2 + v_{\mathrm{s}}(\mathbf{r},t)\right]\delta(\mathbf{r}-\mathbf{r}').$$

Treatment of the velocity gauge in Octopus

Within dipole approximation, Octopus uses an accelerated wavefunction

$$\psi^{\mathbf{A}}_{n,\mathbf{k}}(\mathbf{r},t) = e^{i\mathbf{A}(t).\mathbf{r}}\psi_{n,\mathbf{k}}(\mathbf{r},t).$$

It is easy to show that

$$e^{-i\mathbf{A}(t).\hat{\mathbf{r}}}\left[\frac{\hat{\mathbf{p}}^2}{2} + \hat{v}_{\mathrm{s}}\right]|\psi^{\mathbf{A}}_{n,\mathbf{k}}(t)\rangle = \left[\frac{1}{2}(\hat{\mathbf{p}} - \frac{1}{c}\mathbf{A}(t))^2 + \hat{v}_{\mathrm{s}}\right]|\psi_{n,\mathbf{k}}(t)\rangle.$$

The time-evolution of $|\psi_{n,\mathbf{k}}(t)\rangle$ is described using the ground-state Hamiltonian $\hat{H}_0 = \left[\frac{\hat{\mathbf{p}}^2}{2} + \hat{v}_{\mathrm{s}}\right]$ applied to the accelerated wavefunction.

Features related to solids

Octopus have many solid-dedicated features

- Density-of-states (DOS)
- Band-structure calculations
- Optical conductivity/dielectric function calculations
- Magnons and generalized Bloch theorem
- Band structure unfolding
- Phonons
- ...

The tutorials

You can find the tutorials under this link:
`https://octopus-code.org/documentation/13/tutorial/`

Periodic systems series:

- Lesson 1: Getting started with periodic systems
- Lesson 2: Wires and slabs
- Lesson 3: Optical spectra of solids (lengthy calculations!)
- Lesson 4: Band structure unfolding

The tutorials

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Have Fun !