

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:

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

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 - 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

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These symmetries are used for time-dependent calculations.
- Charge and current densities are also symmetrized (and other observables).
⇒ Important for numerical stability

Non-orthogonal cells

Octopus can work with non-orthogonal cells

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

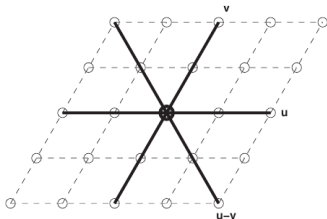


Figure: Hexagonal cell generated by u and v , and the corresponding discretization. Natan *et al.*, PRB 78, 075109 (2008)

Treatment of the velocity gauge in Octopus

Time dependent Kohn-sham equation within velocity gauge

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

with

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

Treatment of the velocity gauge in Octopus

Within dipole approximation, Octopus uses an accelerated wavefunction

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

It is easy to show that

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

The time-evolution of $|\psi_{n,\mathbf{k}}(t)\rangle$ is described using the ground-state Hamiltonian $\hat{H}_0 = \left[\frac{\hat{\mathbf{p}}^2}{2} + \hat{v}_s \right]$ 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/main/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

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Have Fun !

