Module
efaschroedinger

Module efaschroedinger{
  name = *somename*
  regions = *set_of_regions*
  ...

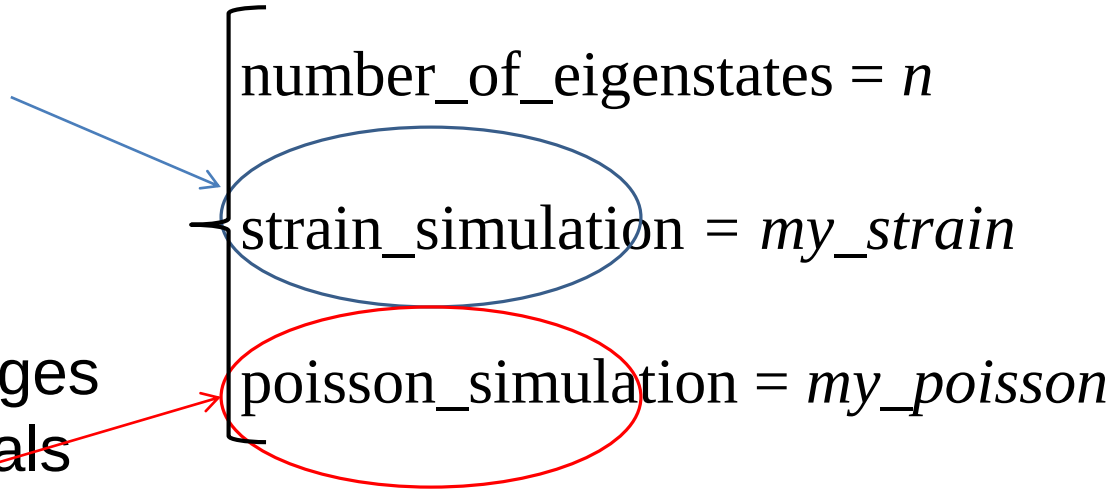
Dispersion {
}
Solver {}
Physics
 { *somemodel* { } }

Envelope Function Approximation

Module efaschroedinger

Options

for simulation on a strained system



for band edges and potentials

The particle (electron,hole) quantum density is calculated by default if the keyword ***QuantumDensity*** is present in the plot list:

plot = (ProbabilityDensity, EigenEnergy, ***QuantumDensity****)*

Envelope Function Approximation

Module
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Physics

Single CB or VB model
6-bands or 8-bands **k·p** model

For a single ***valence*** band

```
Physics
 {
   particle = el | hl

   model = single_band | 6x6 | 8x8

   [effective_mass = hole mass ]

 }
```

Module efaschroedinger

Quantum dispersion

```
Dispersion
{
  [k-path = G-K-M]
  number_of_nodes = 10
  k_max = 1
}
```

dispersion is calculated in 1D along a defined path P1-P2-P3, for example GKM.

1D k-space (for 1D and 2D Simulations)

The dispersion can be calculated in general in a k-space dimension between 1 and (3-simdim)

Envelope Function Approximation

Module ***opticskp***

Module opticskp
{
  name = *somename*
  regions = *set_of_regions*
  plot = *list_output_var*
  initial_state_model = *efa_sim*
  final_state_model = *efa_sim*
...
  k_integration{}
}

$$P(\hbar\omega) = \sum_{i,j} \frac{1}{2\pi^2} \frac{\omega_{ij}^2 e^2}{m^2 c^3} |\mathbf{M_{ij}e}|^2 f_i(E_i)(1 - f_j(E_j)) \frac{\Gamma/2}{(\hbar\omega_{ij} - \hbar\omega)^2 + (\Gamma/2)^2} d\Omega,$$

Envelope Function Approximation

Module opticskp

Options

spectrum energy range

- Emin = *3.1*
- Emax = *5.1*
- dE = *0.001*

Polarization = *(0,0,1)*

Envelope Function Approximation

Module opticskp

Integration in k space

With *plot = (optical_spectrum):*
integration of the optical spectrum in k-space

```
k_integration {
    k_max  = …
    number_of_elements= k-space grid,  e.g. (5,5)
    refine_k_space = true
    refine_fraction= 0.5
    refine_accuracy = 0.001
}
```

adaptive k-mesh refinement is enabled