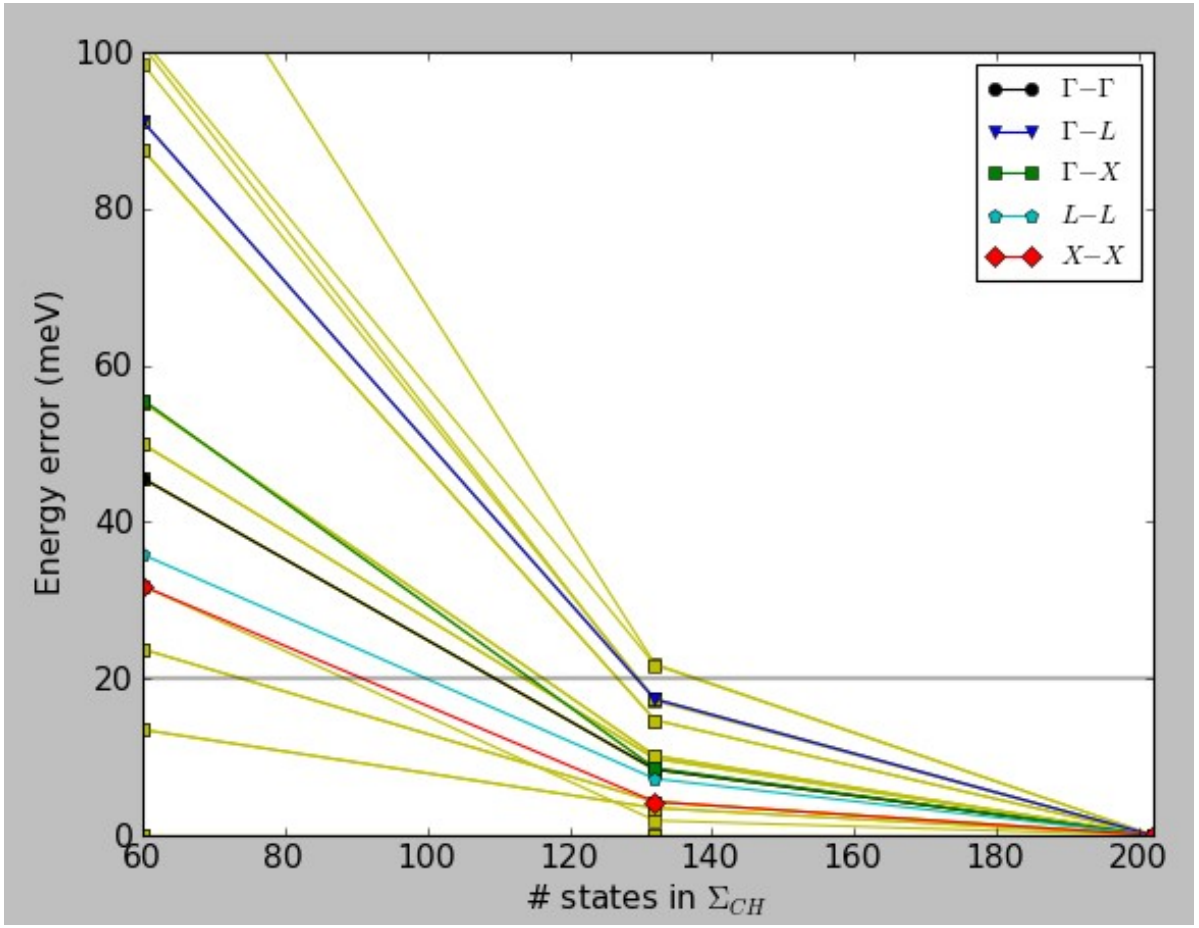
Tutorial 2: converging GW calculation on Si



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Scheme for converging bands and screened cutoff together

1. Calculate the dielectric matrix with “infinite” number of empty states and g-vectors, test error in QP gaps as you vary number of bands used in CH summation

1. Test error as you vary the number of g-vectors in your dielectric matrix while using an infinite number of empty states and and infinite number of bands in CH summation

1. Test error as you vary the number of empty states used in dielectric matrix while using an infinite number of g-vectors and an infinite number of bands in the CH summation

Workflow for tutorial

Generate ε^{-1} for number of bands, G-vectors = ∞

↓

Calculate QP energies with different numbers of bands in CH summation. Look at convergence plots

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Calculate QP energies with different values of screened cutoff, number of bands in CH summation = ∞. Look at convergence plots

↓

Generate ε^{-1} number of G-vectors = ∞, different numbers of bands in dielectric matrix calculation. Calculate QP energies with number of bands in CH summation = ∞. Look at convergence plots.

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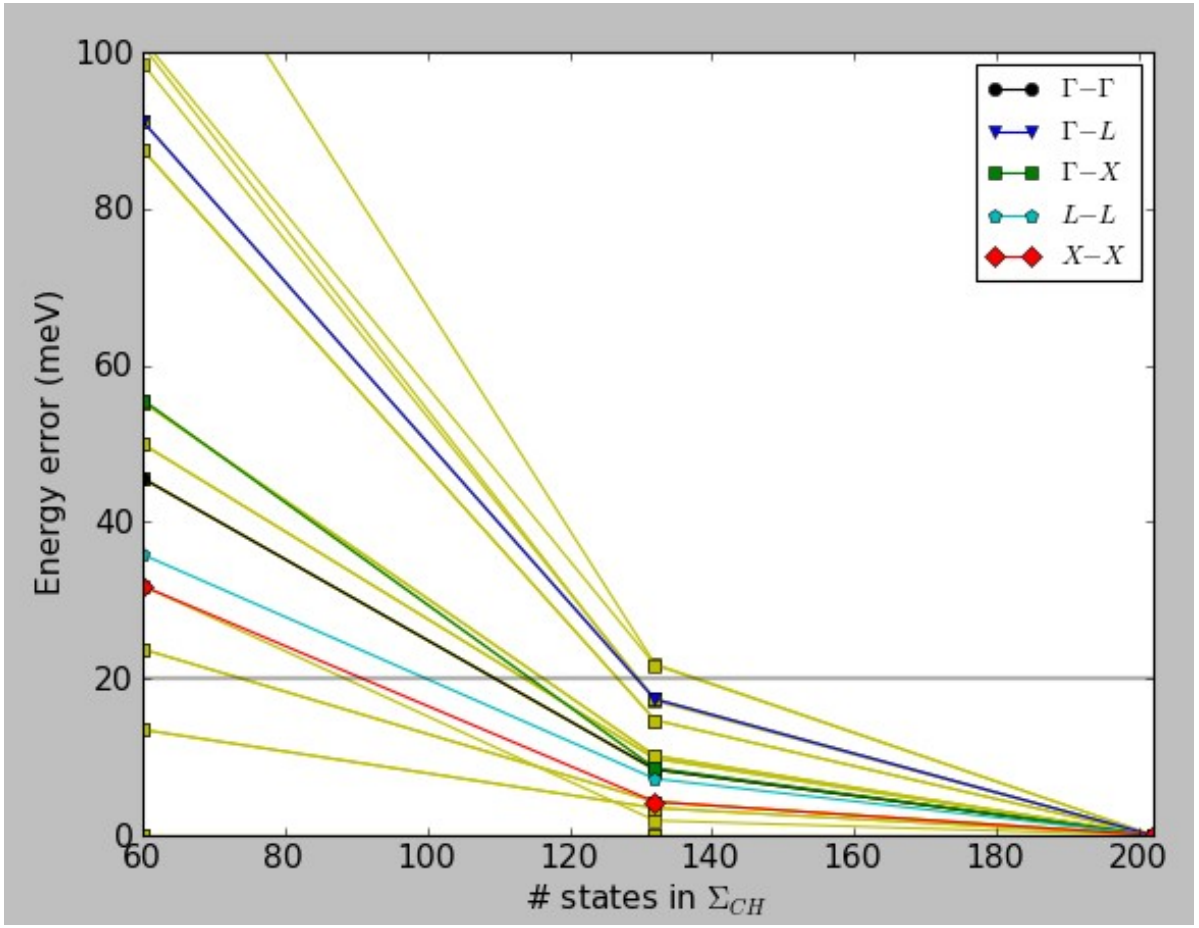
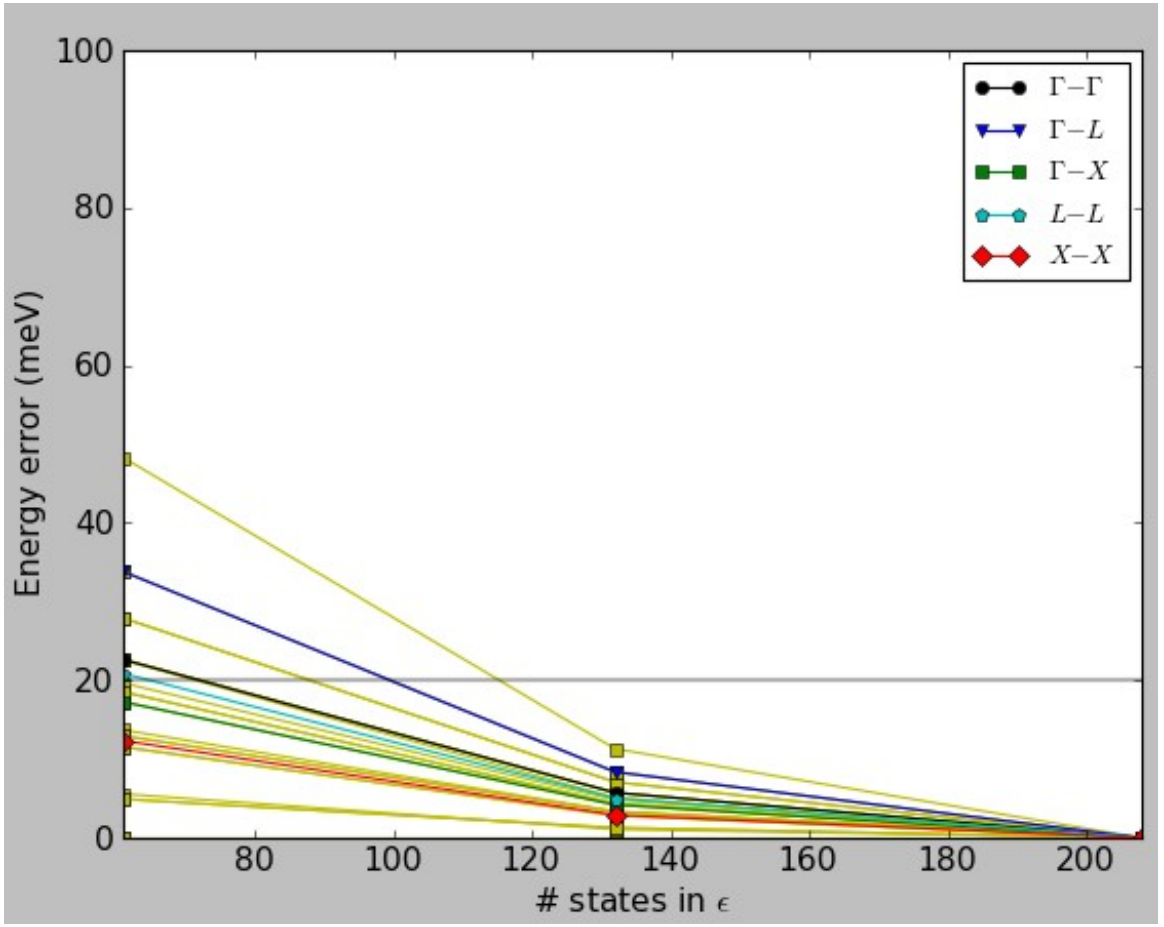
From convergence plots, determine screened cutoff, number of bands in epsilon, and number of bands in CH summation to give 100 meV error

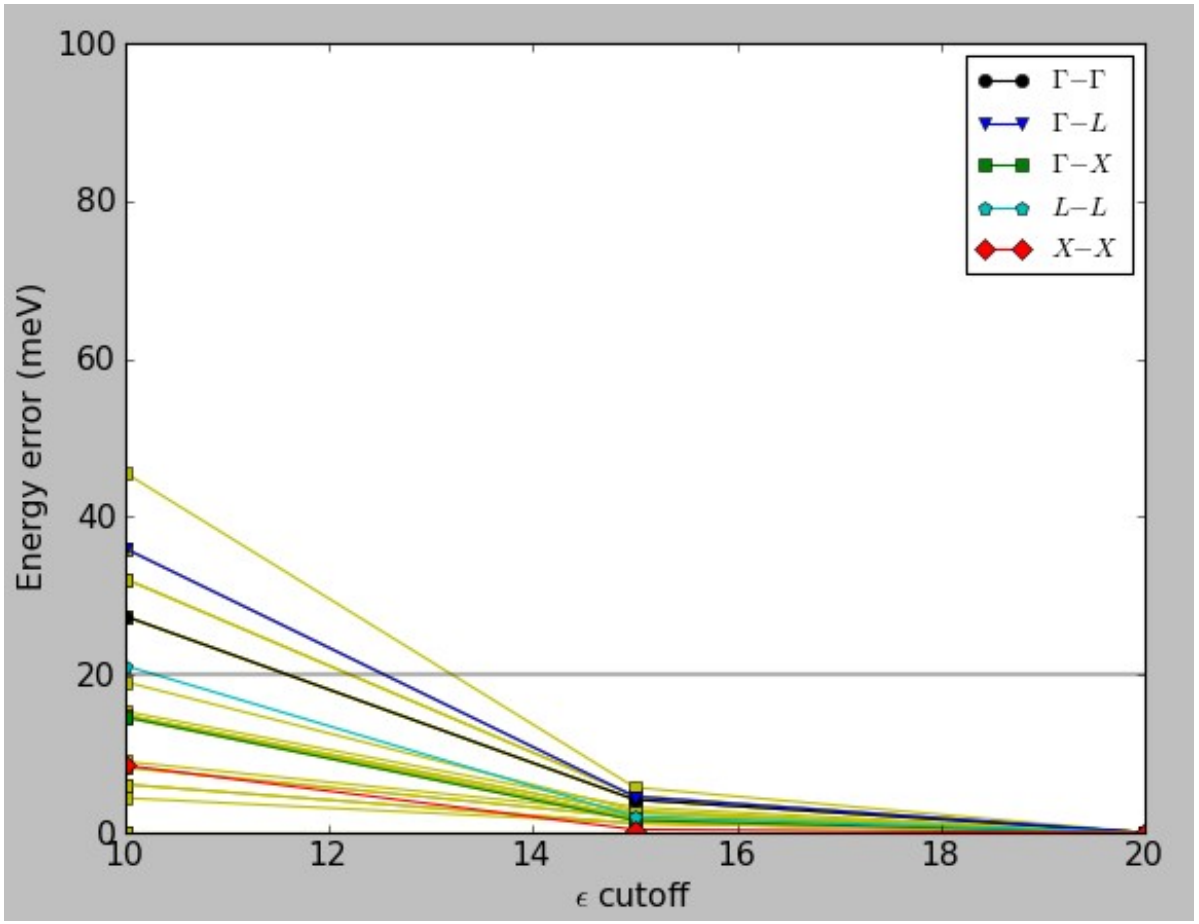
Convergence with bands in CH summation



Convergence with bands in epsilon calculation



Convergence with screened cutoff



Goals

The basic goals are the following:

1. Understand the steps of the convergence process.
2. Estimate the error from using a finite number of bands and G-vectors.

The stretch goals are:

1. Check convergence when using the static remainder
2. Check convergence with wavefunction cutoff.
3. Check convergence with q-grid.

```
cd $SCRATCH
cp -r /project/projectdirs/m1694/BGW-2014/2.1-silicon_convergence .
```