1 Symmetry Discussion

$k_{ij} = k_{ji}$ and $k_{ii} = kjj$ show using symmetry operations
$S = [-100; 010; 001]$
[**?**]

2 KPT symmetries

property(k) = property(-k) for all
show how kpts are reduced to first octant using just rotations
show how kpts in first octant are reduced.

3 Potential energy landscape

10-20 percent bond length? for a taylor series expansion?

For a dispersion curve, good enough to fit a 4-6th order polynomial. Test simple sin vs a dispersion like si really flat. What kind of simple function does that?

4 Taylor expansion

http://www.mathworks.com/help/symbolic/taylor.html

5 Eigvec mapping

take perfect eigvec and add rand element eigvec = eigvec + lambda*rand

6 How to Code: LJ Dispersion

6.1 Python w/o shared Memory

6.2 Python w/ shared Memory (Parallel Python)

6.3 Fortran Compiled Code w/ Python as a Wrapper

6.4 Accuracy Requirements

Fit with n-order polynomial: good for acoustic branches or simple dispersion systems.
Finite Difference: good for any system as long as branch crossings are avoided.
What resolution of the BZ can you expect? ALD (30x) vs NMD (12x)