

10/3/2023

PHY 245L: Modern Physics Lab

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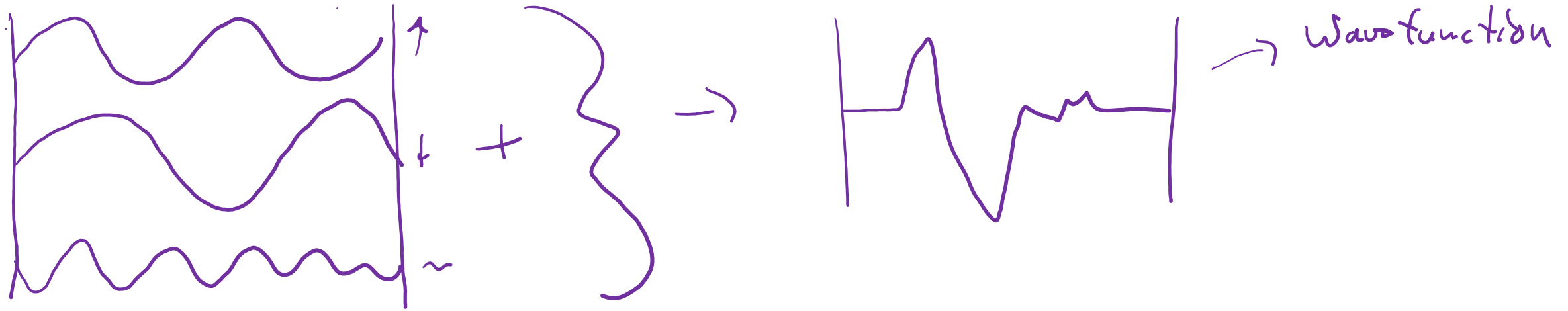
Lecture Topic(s): DFT Reminders

Reading for Next Class: Assigned on Moodle

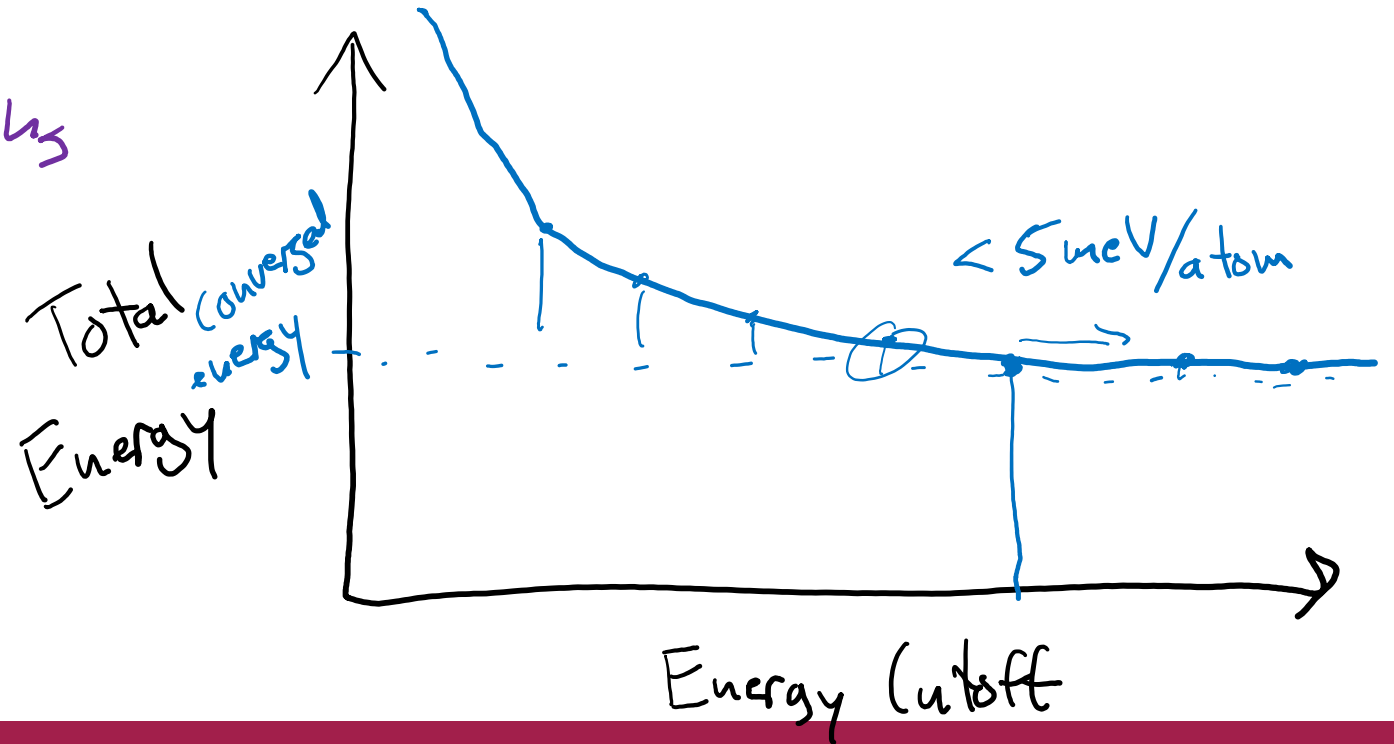
Logistics:

- Reflection 4 due Monday, 10/9 at midnight
- Lab Activity 4 due Monday, 10/9 at midnight

Plane Wave Basis – Energy Cutoff Convergence



Increasing Energy \rightarrow Shorter Wavelengths



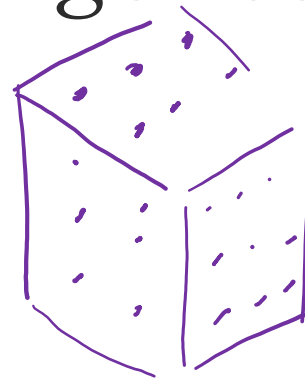
KPOINTS – Kpoint Convergence



$$y = A_1 \cos(k_1 x) + A_2 \cos(k_2 x) + A_3 \cos(k_3 x) + \dots$$

↓ Fourier Transform

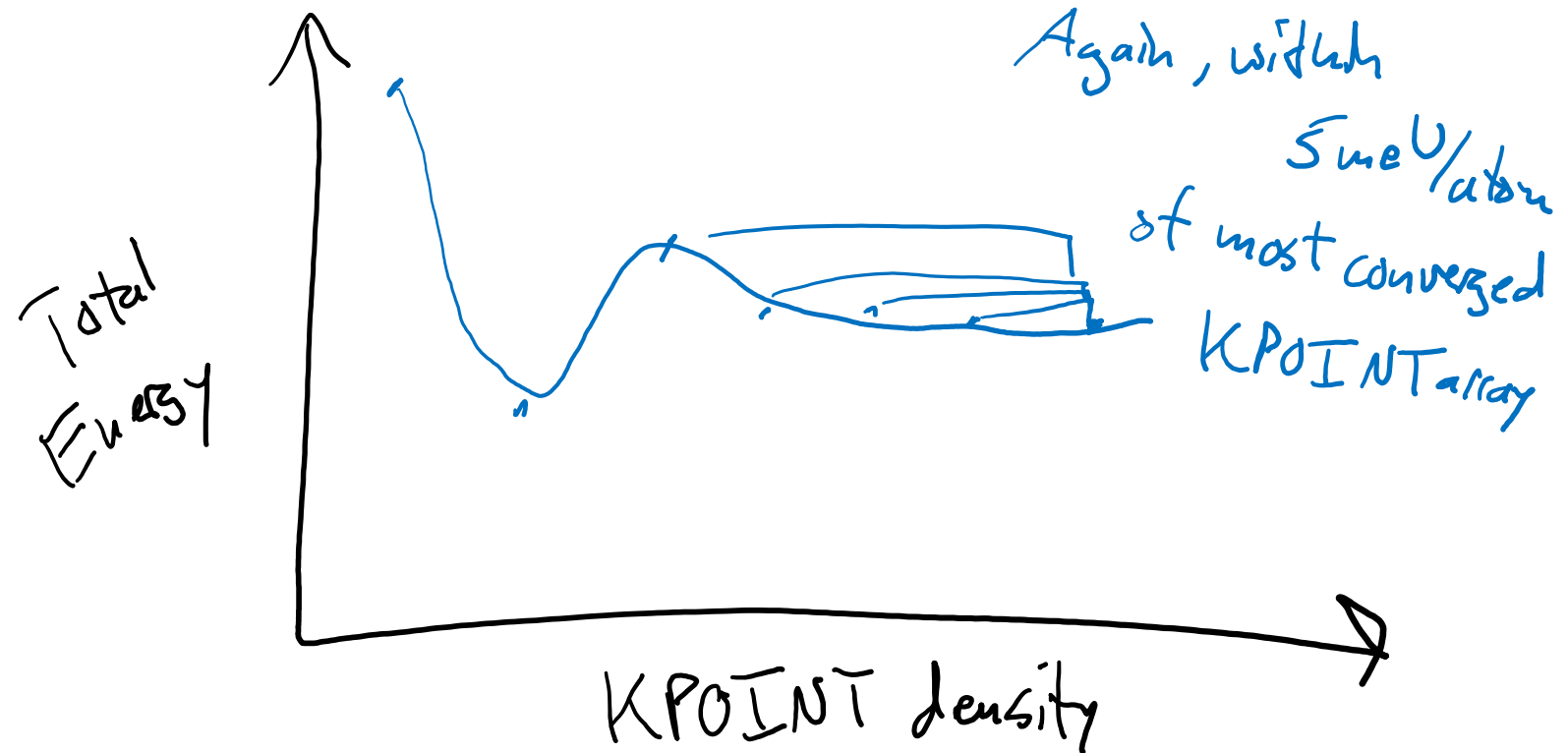
$f(k)$



Kpoints

$3 \times 3 \times 3$

$6 \times 6 \times 6$



Quantum Espresso – Anatomy of an Input File

What type of calculation, specify filenames/directories/etc...

Define the crystal lattice

electron mixing, Do not touch

positions

kpoints

```
&control
  calculation = 'scf'
  restart_mode='from_scratch'
  prefix='diamond'
  tstress = .true.
  tprnfor = .true.
  outdir = './'
  pseudo_dir = '/home/hickoxyo/CODE/QE/qe-7.1/pseudo'
/
&system
  ibrav= 2, celldm(1)=6.6, nat= 2, ntyp= 1
  ecutwfc =20
/
&electrons
  diagonalization='david'
  mixing_mode = 'plain'
  mixing_beta = 0.7
  conv_thr = 1.0d-8
/
ATOMIC_SPECIES
  C 12.011 C.pz-vbc.UPF
ATOMIC_POSITIONS
  C 0.00 0.00 0.00
  C 0.25 0.25 0.25
K_POINTS {automatic}
  10 10 10 0 0 0
```

"self-consistent field"

where output is printed/saved

pseudopotential directory
↳ limits # of electrons

lattice parameter (Bohr)

energy cutoff in Rydberg

Adding Locations to Your Path

- Recommendation: Do not attempt on your own unless you are confident in your abilities. I will demonstrate in class for those who are interested. [ADDENDUM: We will start with this next week]