10/3/2023

PHY 245L: Modern Physics Lab

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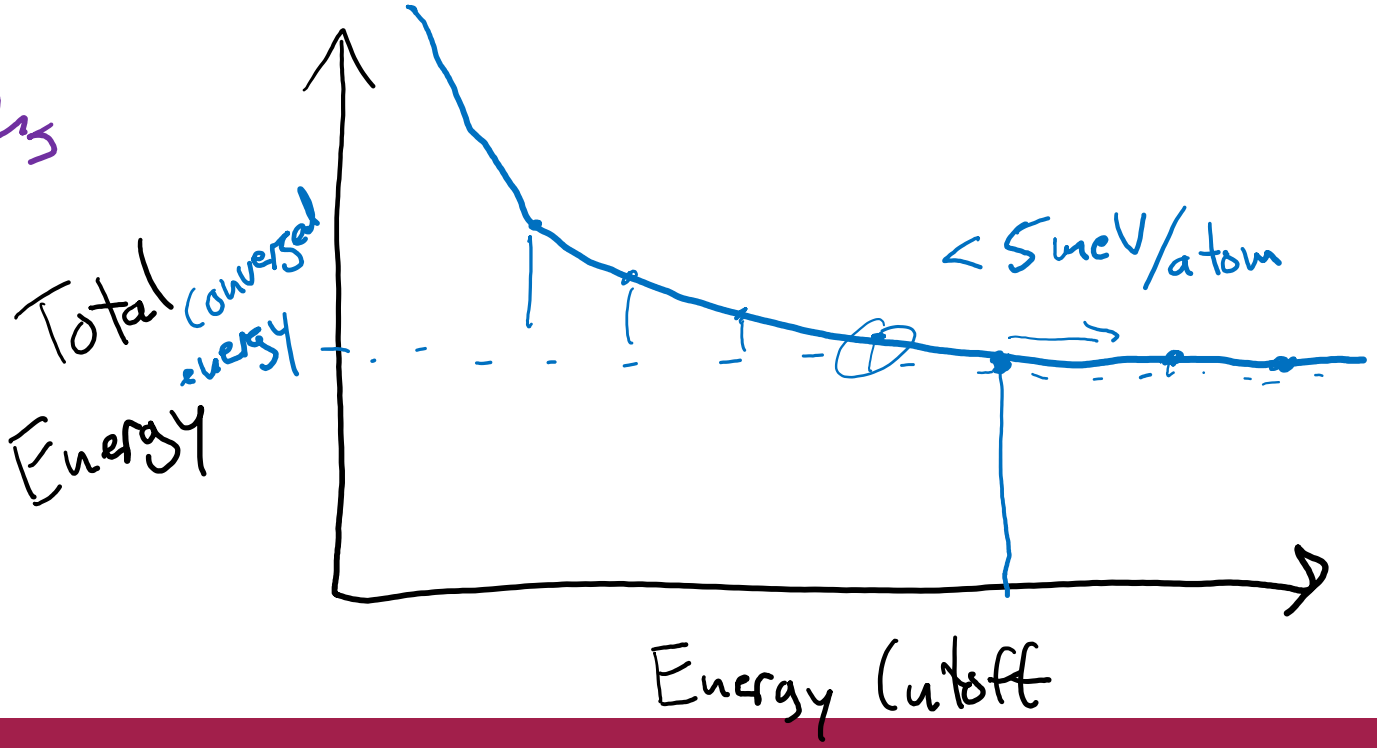
Lecture Topic(s): DFT Reminders
Reading for Next Class: Assigned on Moodle
Logistics:

- 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 → Shorter Wavelengths

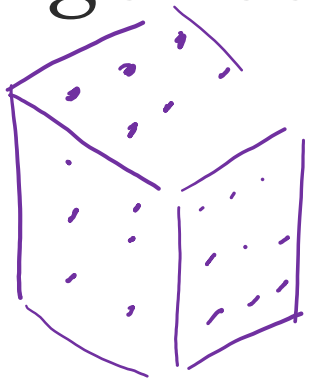


KPOINTS – Kpoint Convergence

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

↓ Fourier Transform

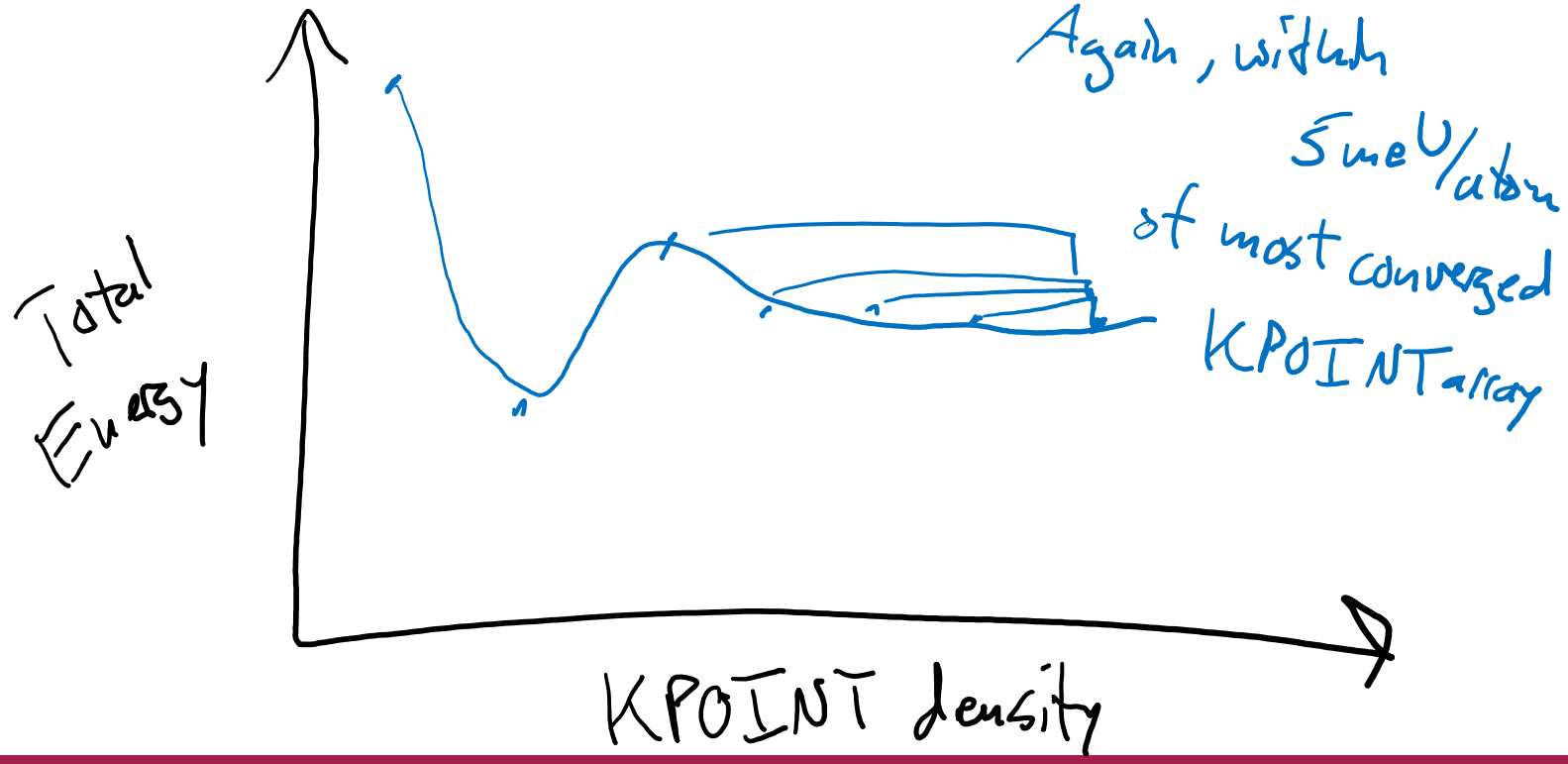
$f(k)$



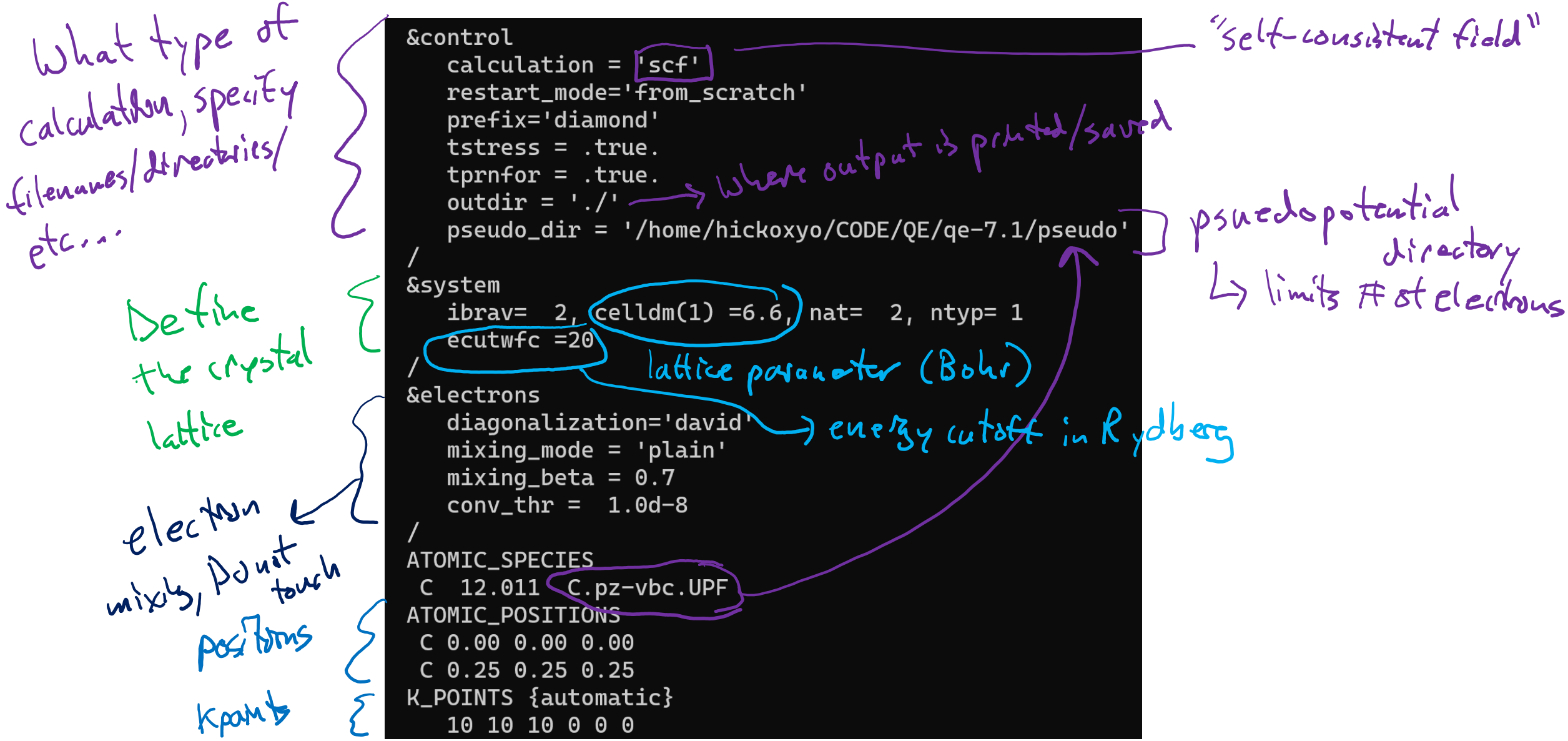
Kpoints

3 x 3 x 3

6 x 6 x 6



Quantum Espresso – Anatomy of an Input File



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]