Finite-T smearing scheme in ABINIT

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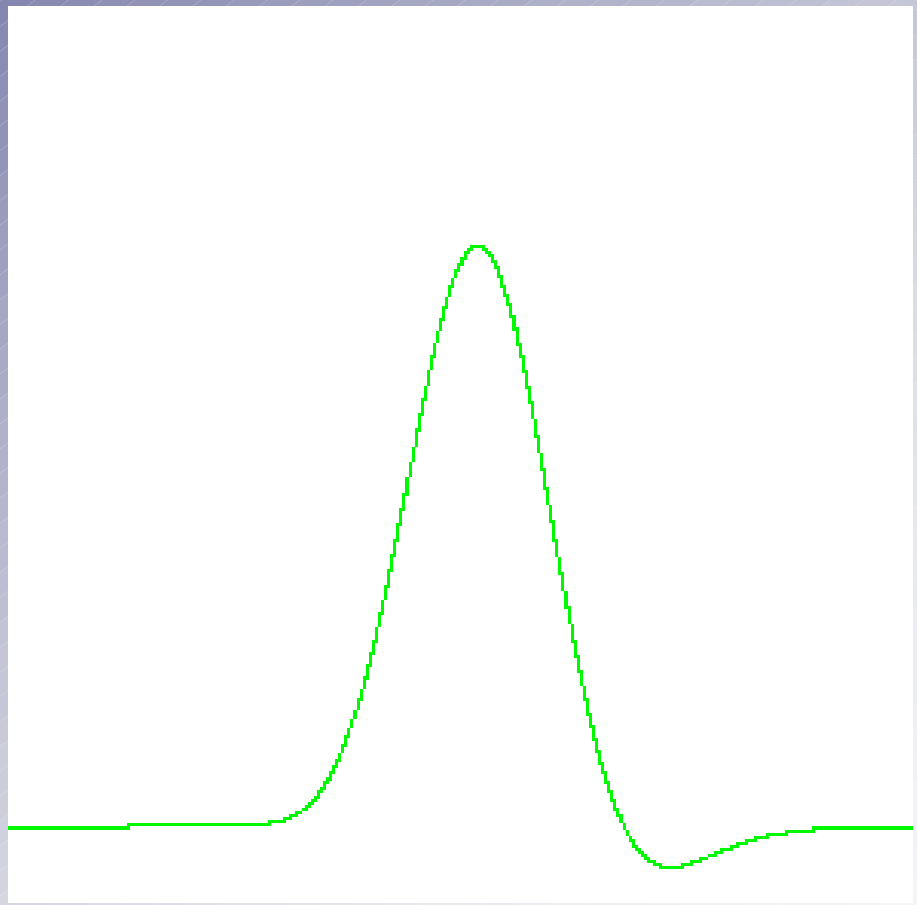


Overview (lots of stuff)

- Re-smearing scheme
  - The physical & simulation problems
  - Our solution: convolution
  - Coding in ABINIT: metallic occupations
- Angular momentum projection
  - The straightforward theory
  - Extension of cut3d
- Pseudopotential testing project

Re-smearing scheme: Two uses for smearing schemes (I)

- Finite-T physical free energy (Mermin)
- Entropic term which depends only on occupations.
- Electronic temperature T
- For fermions statistical mechanics gives the Fermi-Dirac f and S
- Recent work on variable occupation numbers to validate HKS extension

Re-smearing scheme: Two uses for smearing schemes (II)

- Accelerate the convergence wrt nkpt
- Why? The fermi surface is not well sampled:
  - K-points near the Fermi surface representative in energy but
  - Occupation is 1 or 0
  - Artificial smearing with gaussian-type occupation
  - Problems in MD (crossings)

Re-smearing scheme: Two uses for smearing schemes (III)

- How large should (can) the smearing be?
- Empirical convergence in kpoints for large smearing value
  - Reduce smearing and re-converge
- Intuitively, if the band is flat, □=infinity and nkpt=1

The problem

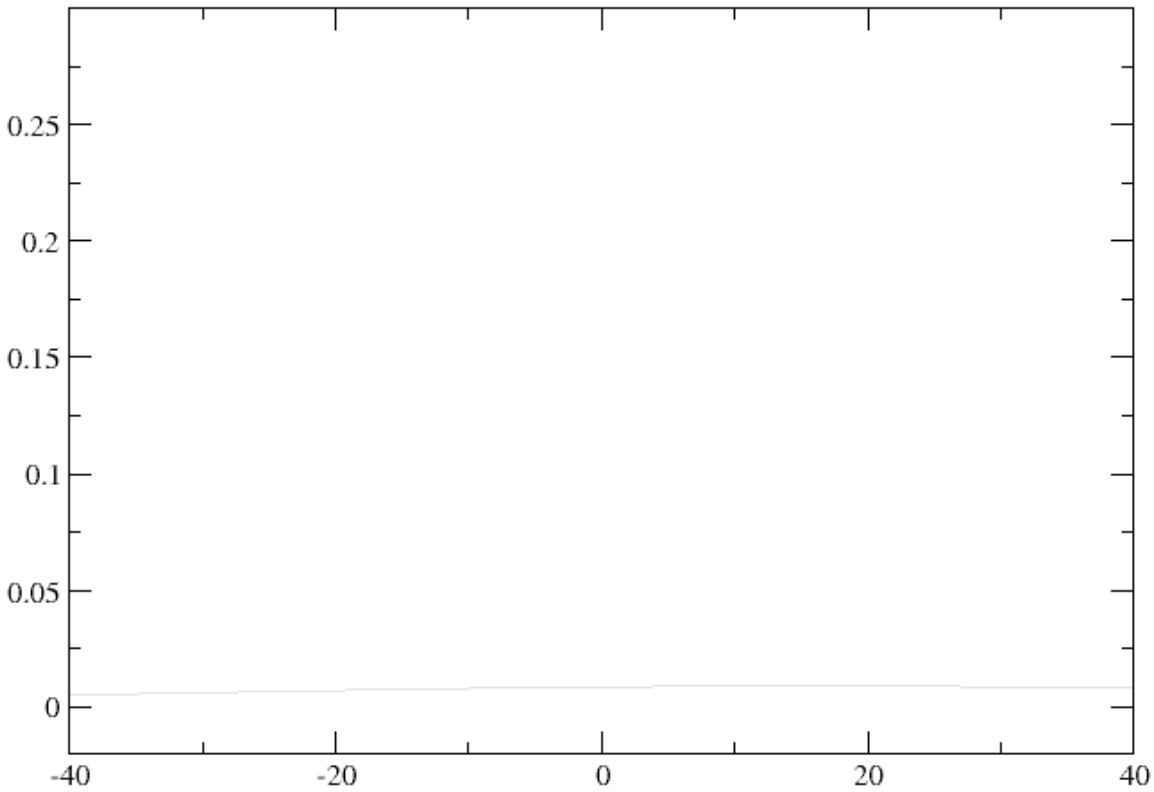
- FD only useful for kpoints at 2000 K
- For smaller T more k-points are needed
- Depends if you need
  - T related details, or
  - Just thermalisation (w ionic thermostat)

Combine the two:
finite T with faster convergence

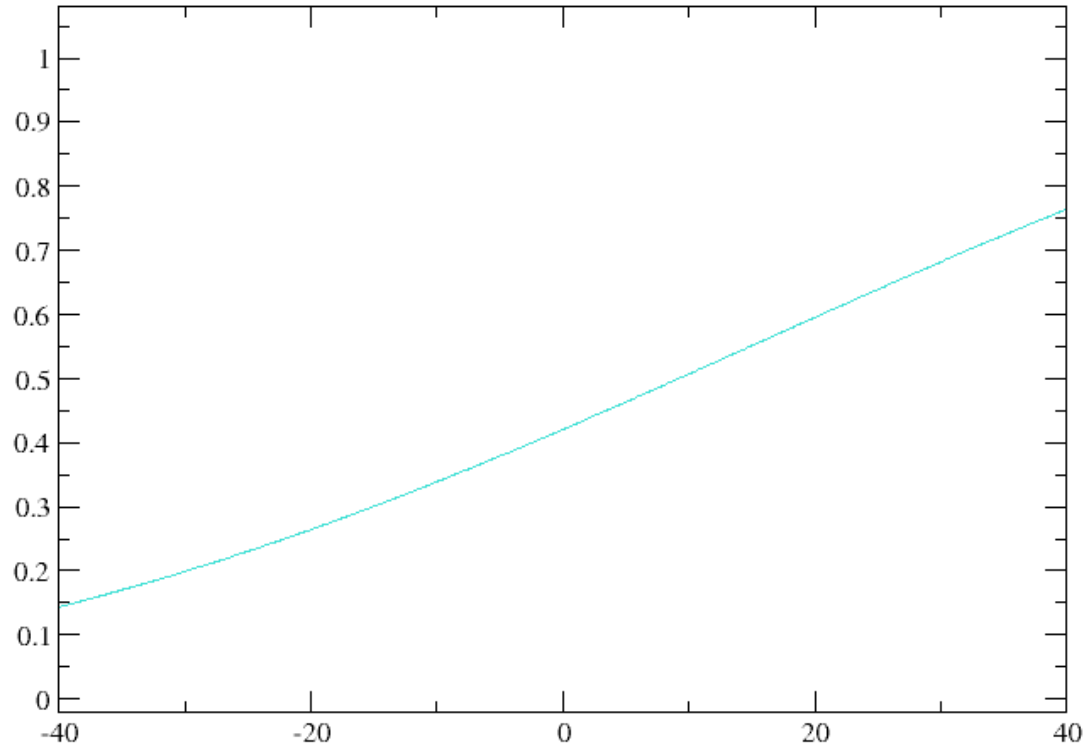
- Only at 2000 K FD occupation useful for kpoint
- For smaller T more k-points are needed

- Re-smear the occupation to accelerate convergence hence:
- Convolute the smearings
- Verstraete & Gonze PRB **46** 035111

What does the smearing delta look like?



What does the occupation look like?



Occupation functions in ABINIT

- Occopt = 3-7 with tsmear + tphysel

- getnel.f feeds the rest of ABINIT with
  - 1 splined occ function f and entropy function S
  - 1 fermi energy
- 1st pass: convolute deltas, obtain total f & S
- Smearing scheme transparent for rest of code.

Projection on angular momenta

- Projection on atomic-like states:

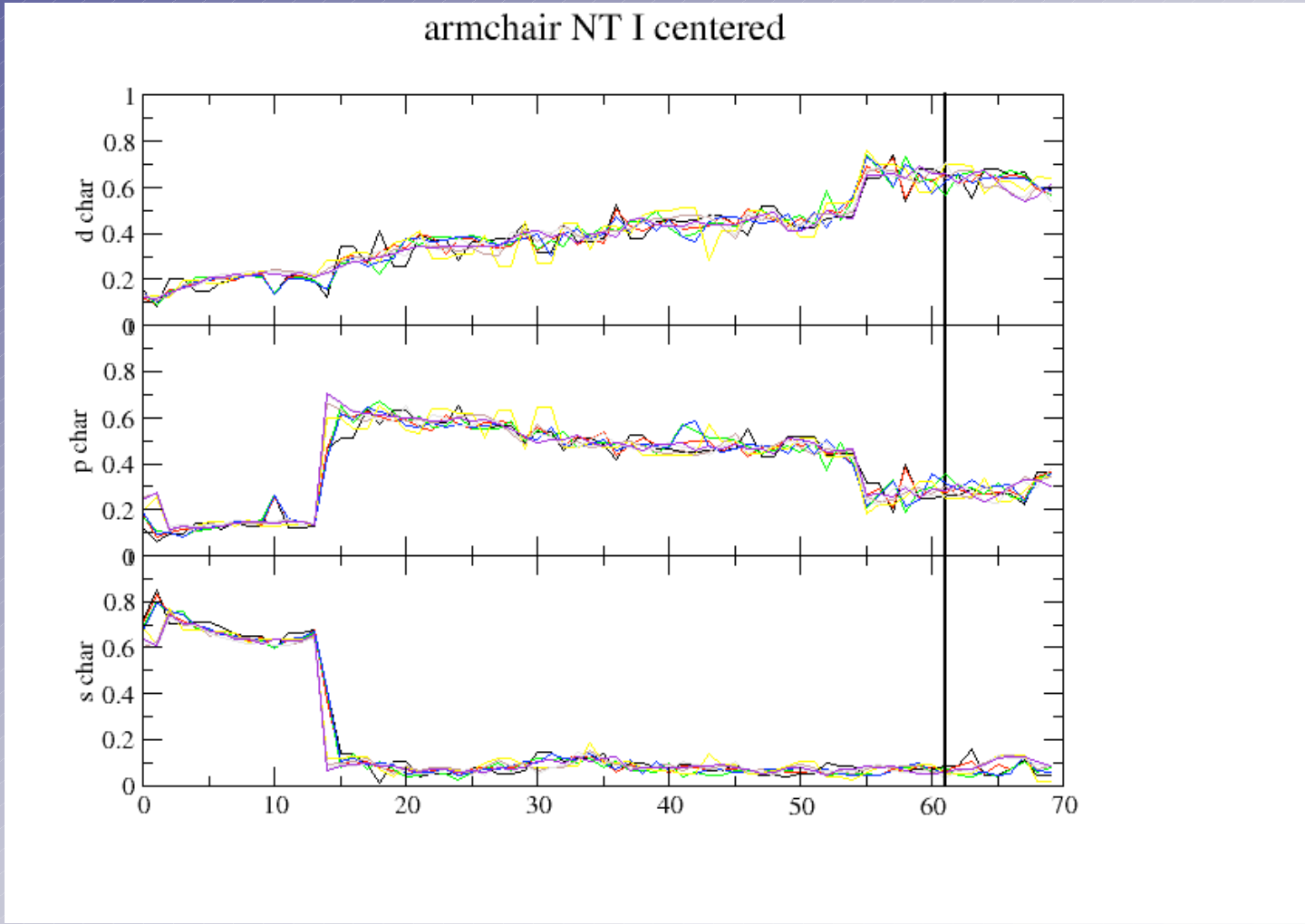
$$d^{\vec{k},n}_{at,l,m} = \left\langle Y_{lm}(\vec{r} - \vec{R}_{at}) \middle| \varphi^{\vec{k},n}(\vec{r}) \right\rangle$$

- Operate in reciprocal space
  - 1D integral over r: exp(ikr) gives Bessel fct
  - Sum over all G vectors

Changes to cut3d

- Jean-François Brière and Michel Côté added treatment of _WFK files to cut3d (wffile.f)
- 1) Initialize 1D real space integration
- 2) project state in reciprocal space
- 3) output proportions of s,p,d, for each atom
- Local change to wffile.f, encapsulated code
- Quick because wfk treated in reciprocal space

An application
because Xavier said no applications



Pseudopotential testing and benchmarking: a proposal (I)

- Many types of pseudopotentials
- Reliability, hardness, transferability problems
- Systematic comparison of different
  - schemes (HGH, TM flavors)
  - XC functionals PBE, PW…
  - Codes? SIESTA, VASP, or vs. Gaussian

Pseudopotential testing and benchmarking (II)

- Generate and test whole tables
  - Atomic case is simple
  - Solids (+ oxides?)
- Systematize tests of pseudopotentials on small fast but pertinent systems.
- Output: ecut, expected acell for bulk, transferability quality…

- Oh, and the users may like it too

Pseudopotential testing and benchmarking (III)

What's been done so far:

- Table of HGH psp
- Perl scripts for making
  - All FHI psps
  - Testing them in simple systematic ways (needs more work)
- Q: how much of this is useful if we have PAW?