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FROM RESEARCH TO INDUSTRY

Speeding-up the ground state Hamiltonian in real space

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PLANE-WAVE DFT HAMILTONIAN

- $H\psi = \epsilon\psi \qquad H = -\Delta + V_l + Vnl$
- ψ is discretized on a *plane-wave basis* with a cut-off e_{cut}

In a plane-wave formalism:

- $-\Delta$ is $^1/_{G^2}$ ➢ $O(N_{pw})$
- V_l is a convolution, applied as a FFT ➢ $O(N_{pw} ln(N_{pw}))$
- $V_{nl} = \sum |pi > Dij < pj|$ ➢ $O(N_{proj} N_{pw})$

- Typical values : $N_{pw} \sim 10^5$; $N_{proj} \sim 2N_{atom}$ … $32N_{atom}$
- V_{nl} is a bottleneck on large systems!

NON-LOCAL OPERATOR

- $\langle G|V_{nl}|\psi\rangle = \sum\langle G|p_i\rangle\, D_{ij}\, \langle p_j|\psi\rangle$
- The projectors are localized on the atoms!
- Goal : compute $\langle p_j|\psi\rangle$ on the real space grid
  Not so simple!

- ψ is only known on a coarse grid.
  This is not so simple as to compute a 3D integral

$$\int_{|x-c|<r_c} \psi(x)p(x)dx$$

- $p(r)$ is not limited in frequency.
  Aliasing problem : $\frac{1}{N}\sum_r p(r)\,\Psi(r) \neq \sum_G p(G)\Psi(G)$

ALIASING

$$I = \frac{1}{N}\sum_{r} p(r)\,\Psi(r)$$

$$= \frac{1}{N}\sum_{j=0}^{N-1} p(\frac{j}{N})\Psi(\frac{j}{N}) = \frac{1}{N}\sum_{j=0}^{N-1}\sum_{m\in\mathbf{Z}} e^{im2\pi j/N} p(2\pi m) \sum_{n\in[|-n_{max},n_{max}|]} \Psi(2\pi n) e^{in2\pi j/N}$$

$$= \frac{1}{N}\sum_{m\in\mathbf{Z}}\sum_{n\in[|n_{max},n_{max}|]} p(2\pi m)\Psi(2\pi n)\sum_{j=0}^{N-1}(e^{i(m+n)2\pi/N})^j$$

$$= \sum_{k\in\mathbf{Z},g\in\Omega^*} p(g-kN)\Psi(g) = \sum_{g\in\Omega^*} p(g)\Psi(g) + \sum_{k\neq 0\in\mathbf{Z},g\in\Omega^*} p(g-kN)\Psi(g)$$

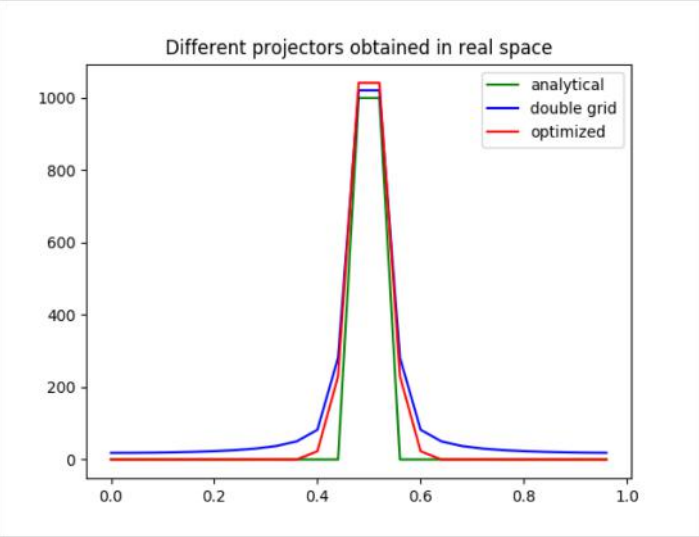
exact aliasing

- First idea: cut *p* in frequency (project on the PW basis)
  Not a good idea because we loose localization in real space
- We search for a accuracy/locality compromise

REFERENCE METHOD BY KING-SMITH, PAYNE, LIN

King-Smith, Payne, Lin, Phys. Rev. B **44**, 13063 (1991)

1. Densify the real space grid
   i.e.: add plane wave components for p and ψ: $(e_{cut} \rightarrow emax)$
2. Put zero in the these new components for ψ
3. Optimize the new p components in order to localize the projector a much as possible
   ➢ p support is enlarged but not too much!



$$I = \frac{1}{N} \sum_{r<\alpha r_c} p(r)\,\Psi(r)$$

$$= \sum_{g^2<ecut^2} p(g)\,\Psi(g) + \sum_{e_{cut}{}^2<g^2<e_{max}^2} p(g)\,\Psi(g)$$

optimized zero

REFERENCE METHOD BY KING-SMITH, PAYNE, LIN

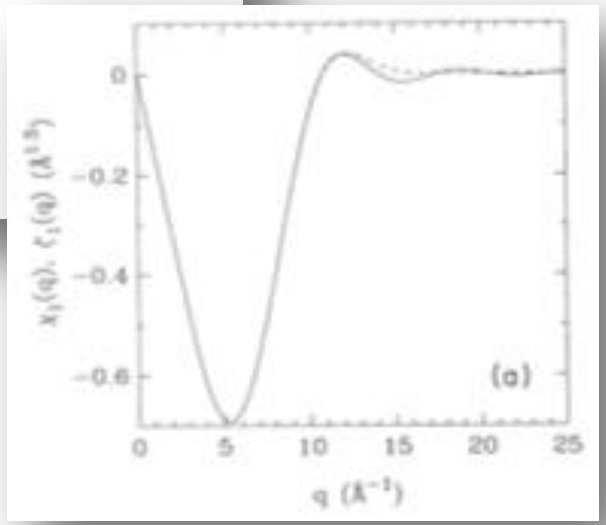
King-Smith, Payne, Lin, Phys. Rev. B **44**, 13063 (1991)

1. Fix $p(g)$ for $\frac{1}{2}g^2 \leq e_{cut}$
2. Set $p(g) = 0$ for $\frac{1}{2}g^2 > \frac{1}{2}G_{max}^2 \approx e_{cut}$

   $p(r)$ support is enlarged: $r \leq r_c \longrightarrow r \leq \alpha r_c$
3. Optimize $p(g)$ for $e_{cut} \leq \frac{1}{2}g^2 \leq \frac{1}{2}G_{max}^2$

   Minimize $\mathrm{I} = \int_{\alpha r_c}^{\infty} r^2 p(r) dr$

   i.e. solve a least squares problem



CAN WE IMPROVE?

- Several improvements proposed:

  Tafipolsky & Schmid, J. Chem. Phys. 124, 174102 (2006)
  Soler & Anglada, Comp. Phys. Comm. 180, 1134 (2009)

- Our proposal:
  Add a degree of freedom for the optimization of *p*

$$Err = | < p, \Psi >_{\Omega^*} - < p_{opt}, \Psi >_{\Omega_\alpha} |$$

$$Err \leq | < p, \Psi >_{\Omega^*} - < p_{opt}, \Psi >_{\Omega^*} | + | < p_{opt}, \Psi >_{\Omega} - < p_{opt}, \Psi >_{\Omega_\alpha} |$$

$$Err \leq \lambda \sqrt{\int_0^{G_{max}} |p - p_{opt}|^2 w(q) dq} \; + \; \beta \sqrt{\int_{\alpha r_c}^{\infty} |p_{opt}|^2 dr}$$

Not considered in KS method

Frequency distribution of ψ

FIRST IMPLEMENTATION IN ABINIT

- Modification of `pawtab` and `hamiltonian` datastructures
  `rs_proj` class added
- `nonlop` flowchart changed
  `opernla` $\langle p_j|\psi\rangle$ in real space
  `opernlb` $\langle r|V_{nl}|\psi\rangle = \sum\langle r|p_i\rangle\, Dij\, \langle p_j|\psi\rangle$

```
 ----------------------------------------------------------
 Components of total free energy (in Hartree) :

    Kinetic energy  =  8.01939344934234E+00
    Hartree energy  =  1.43804953659833E+00
    XC energy       = -3.69674579734631E+00
    Ewald energy    = -1.27864121210521E+01
    PspCore energy  =  5.41017918797015E-01
    Loc. psp. energy= -6.46801177206690E+00
    Spherical terms =  2.52029293426270E+00
    >>>>>>>>> Etotal= -1.04324158514649E+01

 "Double-counting" decomposition of free energy:
    Band energy     =  2.24902810048924E+00
    Ewald energy    = -1.27864121210521E+01
    PspCore energy  =  5.41017918797015E-01
    Dble-C XC-energy= -2.99873374296493E-01
    Spherical terms = -1.36170881133375E-01
    >>>> Etotal (DC)= -1.04324103571957E+01

  >Total energy in eV           = -2.83880472321360E+02
  >Total DC energy in eV        = -2.83880322814691E+02
```

```
 Components of total free energy (in Hartree) :

    Kinetic energy  =  8.01762316556784E+00
    Hartree energy  =  1.43933530912141E+00
    XC energy       = -3.69708237303331E+00
    Ewald energy    = -1.27864121210521E+01
    PspCore energy  =  5.41017918797015E-01
    Loc. psp. energy= -6.47578427317843E+00
    Spherical terms =  2.52915037374109E+00
    >>>>>>>>> Etotal= -1.04321520000365E+01

 "Double-counting" decomposition of free energy:
    Band energy     =  2.24489285542259E+00
    Ewald energy    = -1.27864121210521E+01
    PspCore energy  =  5.41017918797015E-01
    Dble-C XC-energy= -3.01051828219876E-01
    Spherical terms = -1.36631411242319E-01
    >>>> Etotal (DC)= -1.04381845862947E+01

  >Total energy in eV           = -2.83873292558859E+02
  >Total DC energy in eV        = -2.84037447579199E+02
```

Toy model:
Diamond
ecut=15 Ha

TODO

- Add precision control 😐
- Add parallelism (grid points, projector indexes) 🙂
- Implement forces and stress tensor 🙂

- Mix with the application of the local operator 🙁

  Idea : add a pointer to function in fourwf

  $func \rightarrow V_{local}$ (standard)

  $func \rightarrow V_{local} + V_{nl}$

- Target application: molecular dynamics

Commissariat à l’énergie atomique et aux énergies alternatives - www.cea.fr