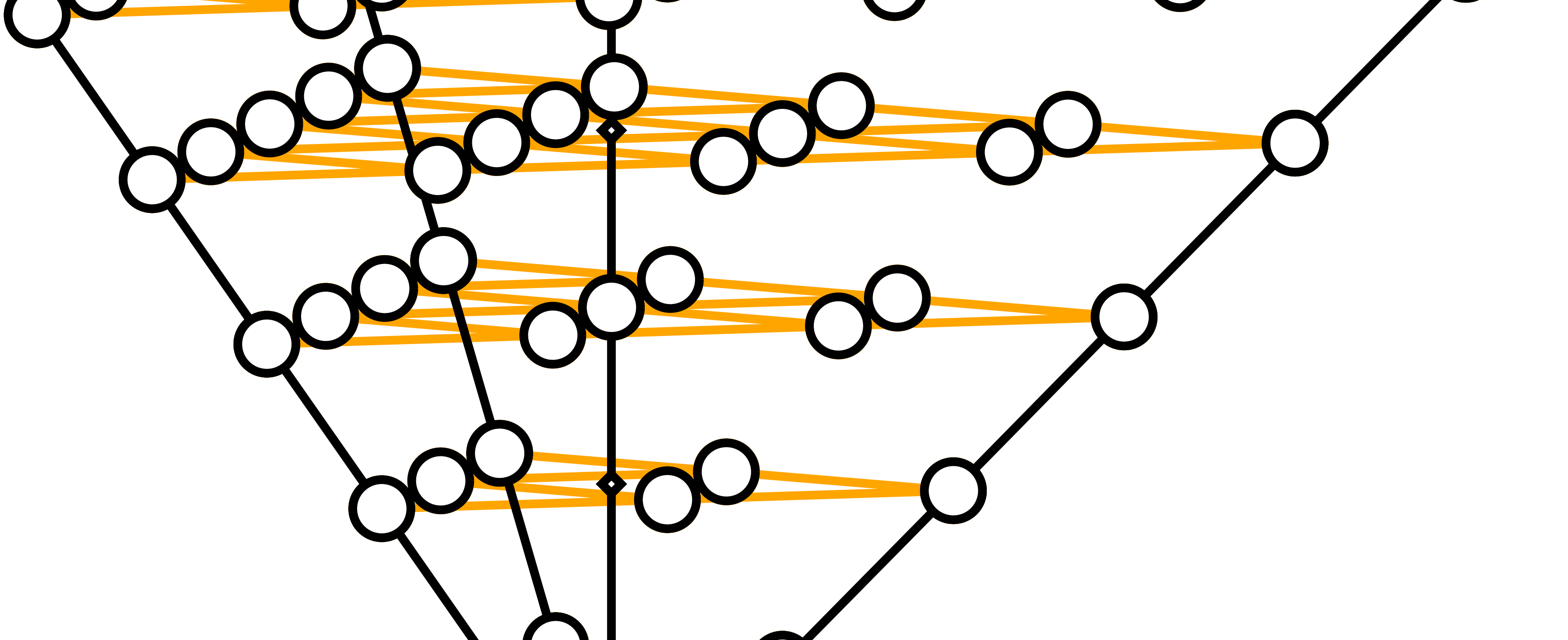

Analytical PAW Projector Functions for Reduced Bandwidth Requirements

2019 June 12 | Paul F Baumeister (JSC), Shigeru Tsukamoto (PGI)
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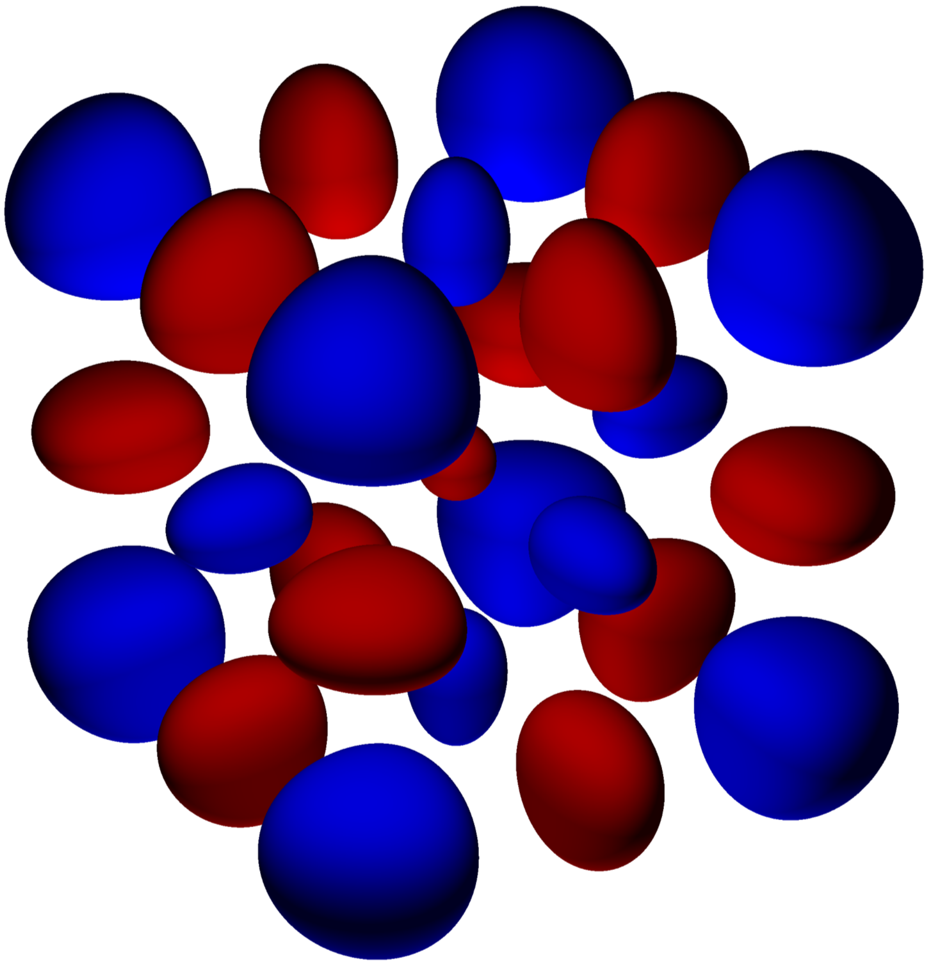
Overview

- Bandwidth Issue in PAW
- Tensor decomposition
- 1D Harmonic Oscillator
- Spherical Harmonic Oscillator
  - Cartesian vs. Radial Solution
- Bandwidth Saving
- Representation Quality
- Adapted PAW Datasets
- Advantages and Drawbacks
- GPU Speedup Results

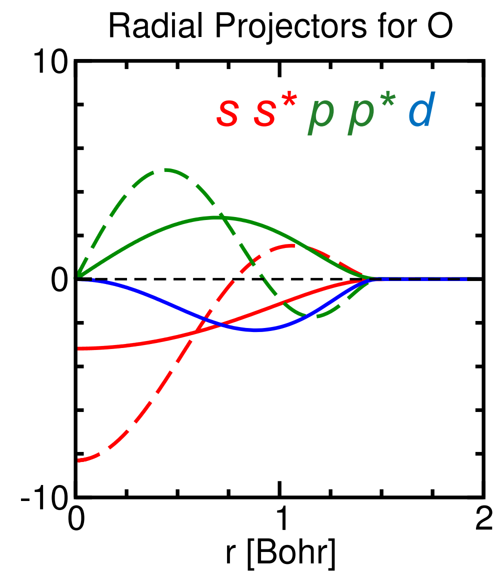


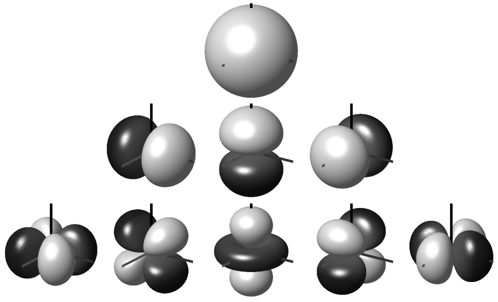
Density Functional Theory

Projector Augmented Wave (PAW) method

- DFT: workhorse methodology for materials science
- PAW: all-electron accuracy at pseudopotential costs
- PAW can be applied to plane-wave basis sets or real-space grid-based implementations of DFT
- Projector functions are represented in real-space, for reasons of scalability also in plane-wave codes

$$\tilde{p}_i(\vec{r}) = \tilde{P}_{n\ell}(r) \cdot Y_{\ell m}(\vartheta, \varphi)$$



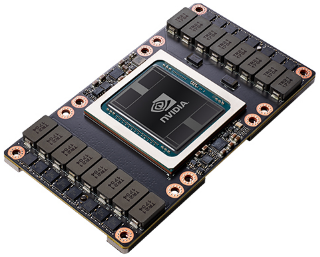


Bandwidth Issues in PAW Codes

Projection and Expansion operations are expensive

The non-local potential of the PAW Hamiltonian

$$\hat{V}_{\text{ion}} = |\tilde{p}_i\rangle\, D_{ij}\, \langle\tilde{p}_j|$$



V100 GPU
7.5 TFlop/s
0.9 TByte/s

requires computing the inner product

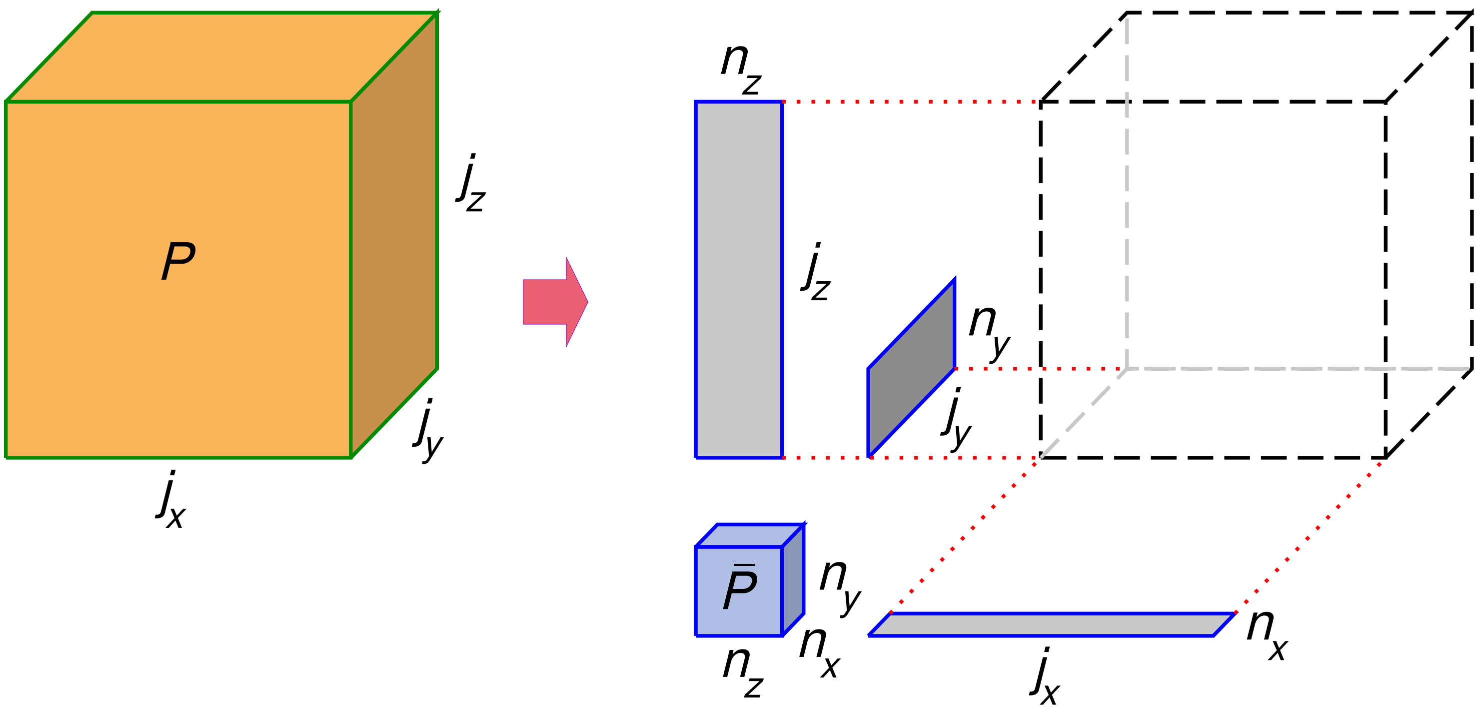
$$\langle\tilde{p}_j|\,\Psi_k\rangle$$

For more than one wave function (*k*-index) this can be mapped to matrix-matrix multiplications but the projectors are localized, so the *p*-operañd is sparse.

➔ Limited by memory bandwidth

Bandwidth Savings in PAW Codes

Rank-3 tensor decomposition: Data compression

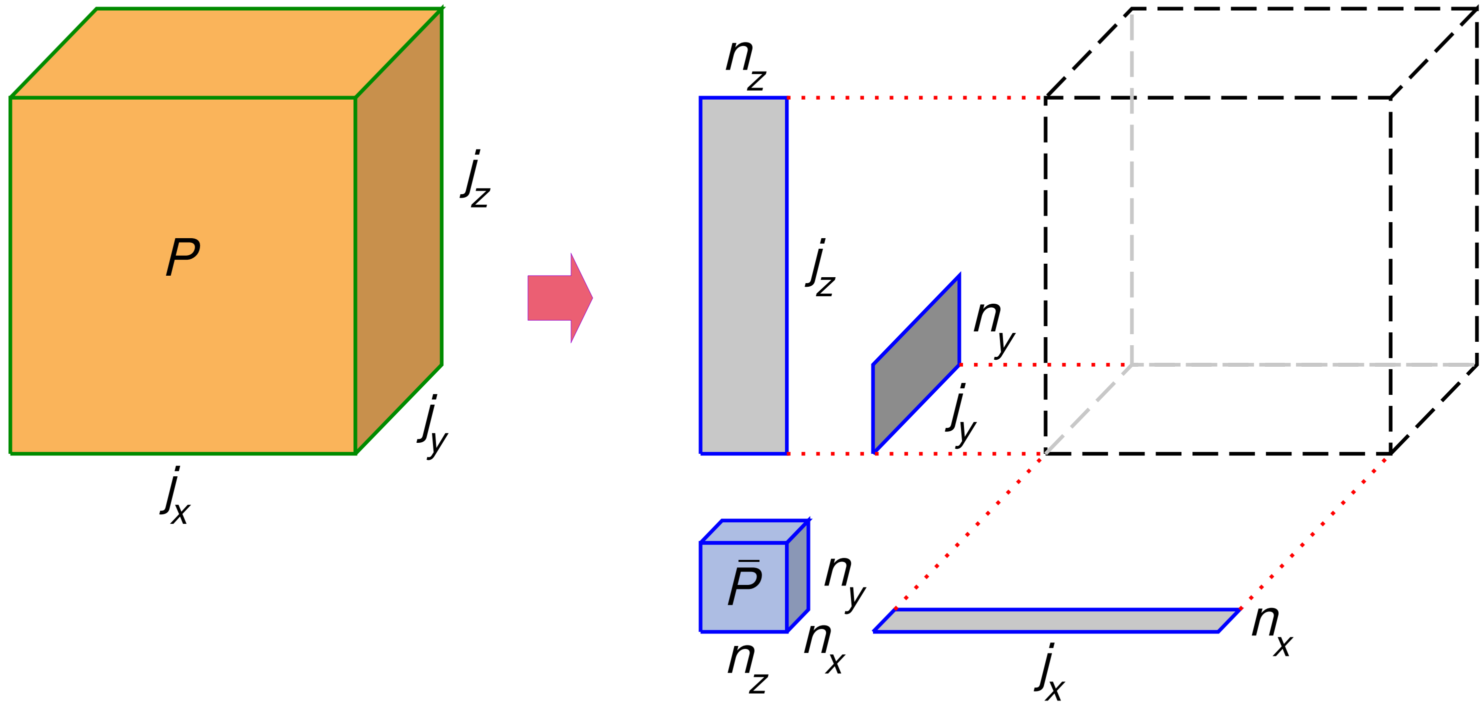


$$P_{j_x j_y j_z} \approx \sum_{n_x n_y n_z} \bar{P}_{n_x n_y n_z} \, v^{[x]}_{n_x j_x} \, v^{[y]}_{n_y j_y} \, v^{[z]}_{n_z j_z}$$

Inspired by
Khoromskaia and Khoromskij

Bandwidth Savings in PAW Codes

Rank-3 tensor decomposition: Data compression



$$P(x,y,z) \approx \sum_{n_x n_y n_z} \bar{P}_{n_x n_y n_z}\, \psi_{n_x}(x)\, \psi_{n_y}(y)\, \psi_{n_z}(z)$$

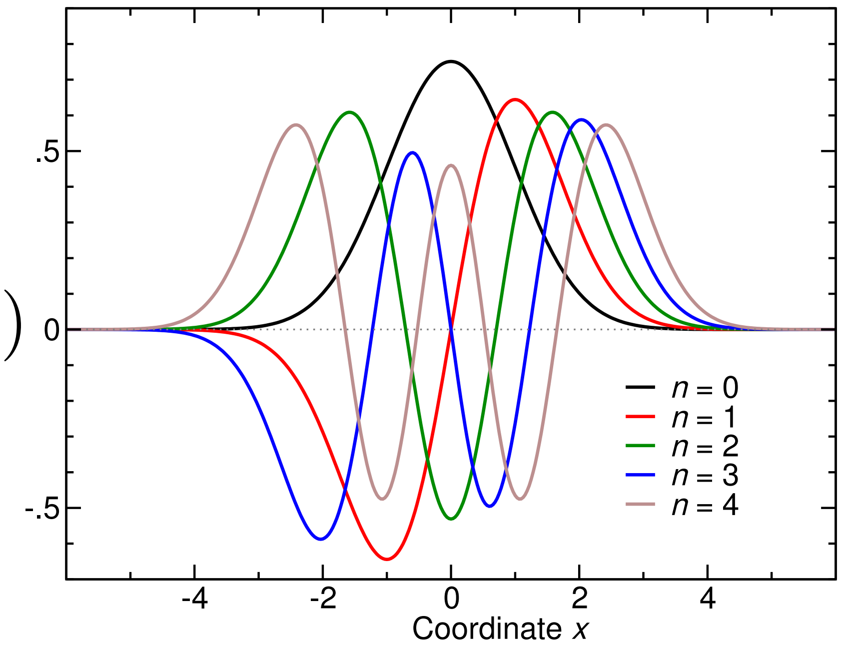
1D Harmonic Oscillator

Hamiltonian $$\hat{H}_{1\mathrm{D}} = -\frac{\partial^2}{\partial x^2} + x^2$$

Quantum # $$n \in \mathbb{N}_0$$

Eigenvalue $$E_{1\mathrm{D}} = (2n+1)$$

Eigenstates $$H_n(x)\exp(-\frac{x^2}{2})$$



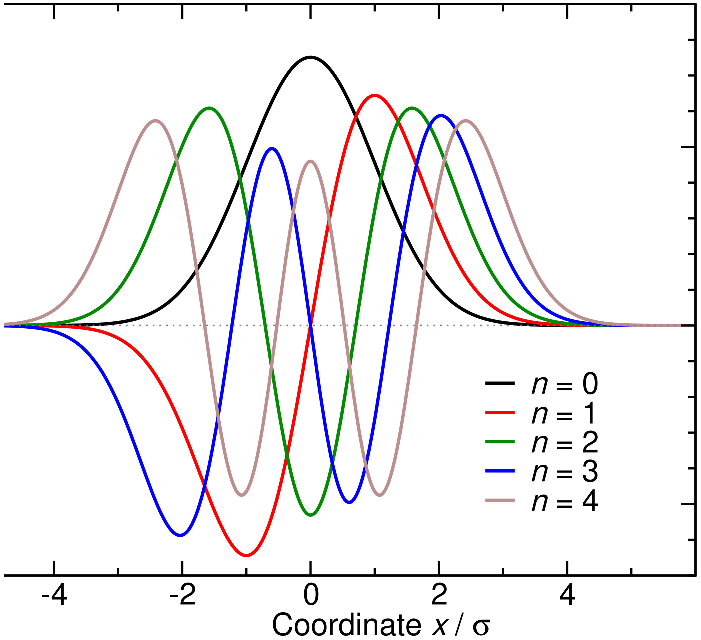
1D Harmonic Oscillator

Hamiltonian $$\hat{H}_{1\mathrm{D}} = -\frac{\partial^2}{\partial x^2} + x^2\sigma^{-4}$$ Length scale parameter $\boldsymbol{\sigma}$

Quantum # $$n \in \mathbb{N}_0$$

Eigenvalue $$E_{1\mathrm{D}} = (2n+1)\sigma^{-2}$$

Eigenstates $$H_n\left(\frac{x}{\sigma}\right)\exp(-\frac{x^2}{2\sigma^2})$$



Spherical Harmonic Oscillator

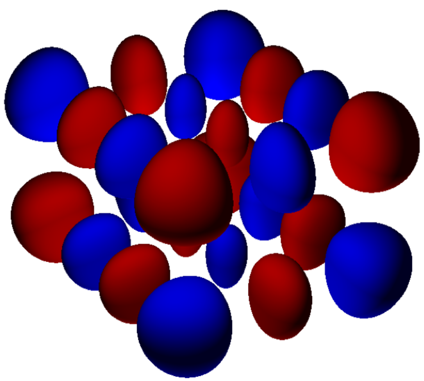
3D Isotropic Harmonic Oscillator: Solution in Cartesian Coordinates

Hamiltonian $$\hat{H}_{\mathrm{SHO}} = -\vec{\nabla}^2 + \vec{r}^2 = \hat{H}^{[x]}_{\mathrm{1D}} + \hat{H}^{[y]}_{\mathrm{1D}} + \hat{H}^{[z]}_{\mathrm{1D}}$$

Quantum #s $$(n_x, n_y, n_z) \in \mathbb{N}_0^3$$

Eigenvalue $$E_{\mathrm{SHO}} = 2(n_x + n_y + n_z) + 3$$

Eigenstates $$\Psi_{n_x n_y n_z}(x, y, z) = \psi_{n_x}(x)\,\psi_{n_y}(y)\,\psi_{n_z}(z)$$



$n_x = 3$
$n_y = 2$
$n_z = 1$

Spherical Harmonic Oscillator

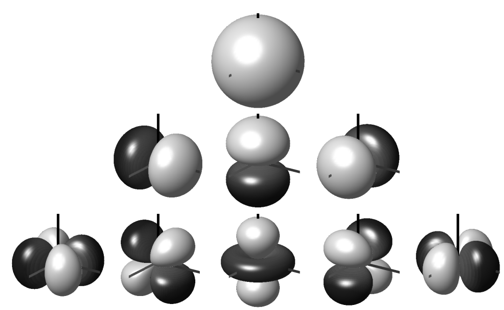
3D Isotropic Harmonic Oscillator: Solution in Spherical Coordinates

Hamiltonian $$\hat{H}_{\mathrm{SHO}} = -\vec{\nabla}^2 + \vec{r}^2 = -\Delta + r^2$$

Quantum #s $$(\ell, m) \text{ and } n_r \in \mathbb{N}_0$$

Eigenvalue $$E_{\mathrm{SHO}} = 2(\ell + 2n_r) + 3$$

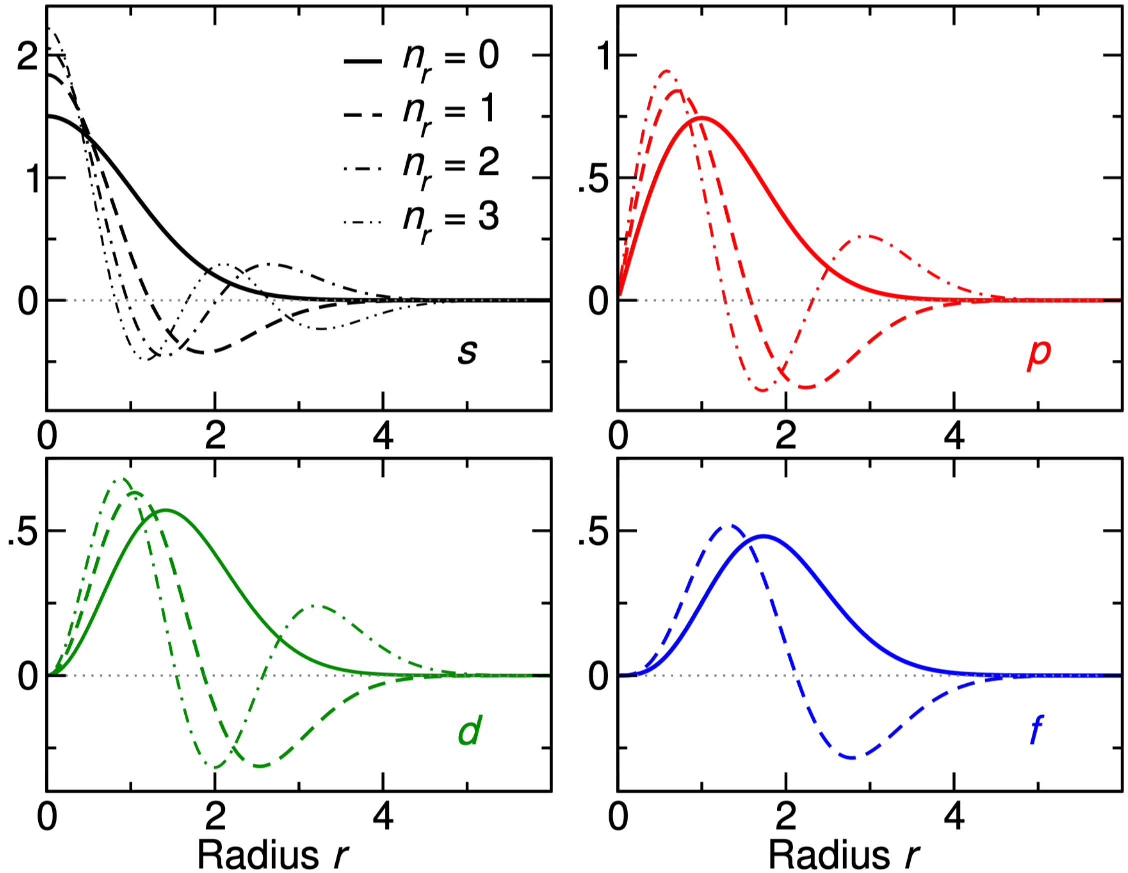
Eigenstates $$\Psi_{n_r \ell m}(r, \vartheta, \varphi) = R_{n_r \ell}(r)\, Y_{\ell m}(\vartheta, \varphi)$$



Spherical Harmonic Oscillator

Solution in Spherical Coordinates: Radial eigenstates

$$R_{n_r\ell}(r) \;\sim\; r^{\ell} L_{n_r}^{(\ell+\frac{1}{2})}(r^2)\exp(-\frac{r^2}{2})$$



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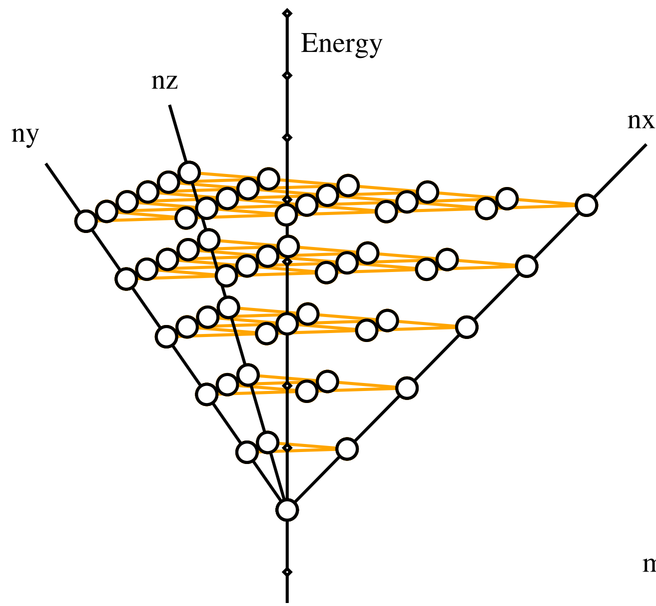
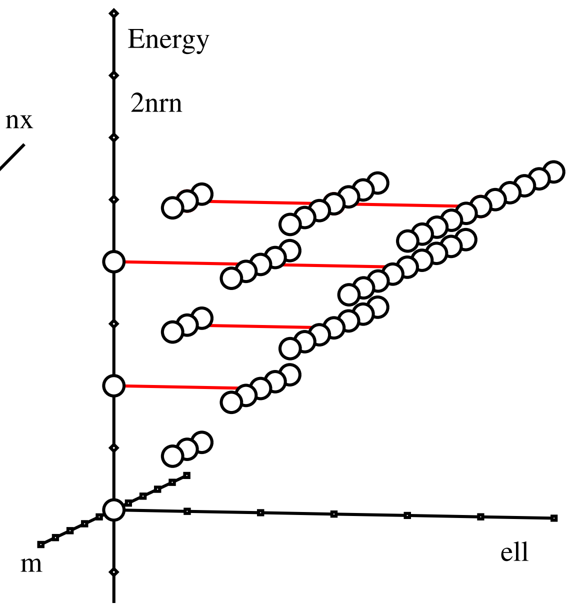
Spherical Harmonic Oscillator

Degenerate energy levels between Cartesian and Radial match

$$n_x + n_y + n_z = \ell + 2n_r$$





$$E_{\mathrm{SHO}} = 2(n_x + n_y + n_z) + 3 \qquad E_{\mathrm{SHO}} = 2(\ell + 2n_r) + 3$$

Spherical Harmonic Oscillator

Degenerate energy levels between Cartesian and Radial match

$$n_x + n_y + n_z = \ell + 2n_r := \nu$$

➔ there is a unitary transform $\hat{U}$ connecting the subspaces indexed by $\boldsymbol{\nu}$

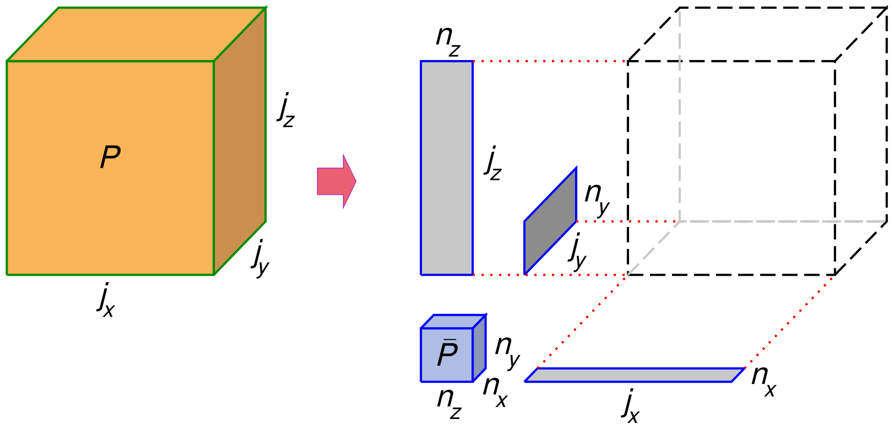
$$\Psi_{n_x n_y n_z}(x,y,z) \equiv \sum_{n_r \ell m} U^{n_r \ell m}_{n_x n_y n_z} \, \Psi_{n_r \ell m}(r,\vartheta,\varphi)$$

$$\hat{U}_{\nu=2} = \begin{pmatrix} \sqrt{1/6} & 0 & -\sqrt{1/2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ -\sqrt{1/6} & 0 & -\sqrt{1/6} & 0 & 0 & \sqrt{2/3} \\ 0 & 1 & 0 & 0 & 0 & 0 \\ \sqrt{1/3} & 0 & \sqrt{1/3} & 0 & 0 & \sqrt{1/3} \end{pmatrix}$$

Bandwidth Savings in PAW Codes

Apply tensor decomposition to PAW projectors

Expand the set of PAW projectors in a SHO basis



$$\tilde{p}_i(x,y,z) \approx \sum_{n_x n_y n_z} \bar{p}_{i\, n_x n_y n_z}\, \psi_{n_x}(x)\, \psi_{n_y}(y)\, \psi_{n_z}(z)$$

Cartesian SHO basis

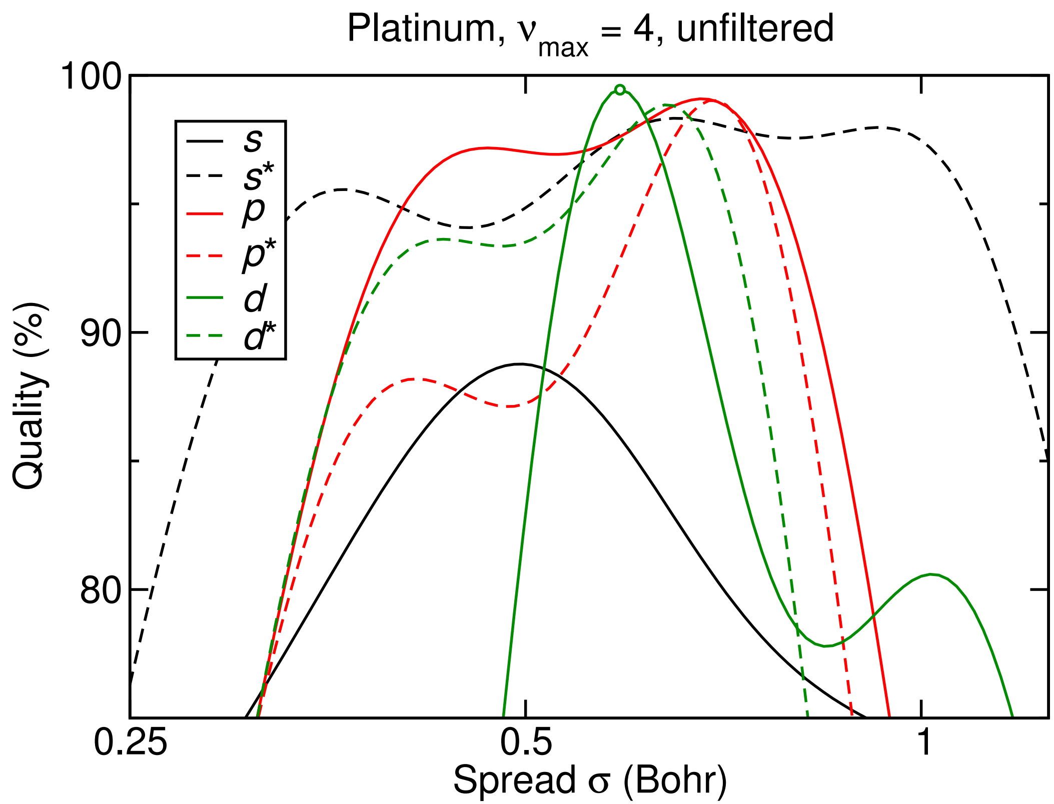
Can be computed in radial representation

$$\left\langle \tilde{P}_{n\ell} \middle| R_{n_r \ell} \right\rangle$$

Quality of Representation

Expanding GPAW projector functions in a radial SHO basis

Quality as a function of **σ** for all projector functions of an element



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Quality of Representation

Minimum SHO basis size

The projector function with the highest kinetic energy decides the minimal ν_{max}

Number of coefficients

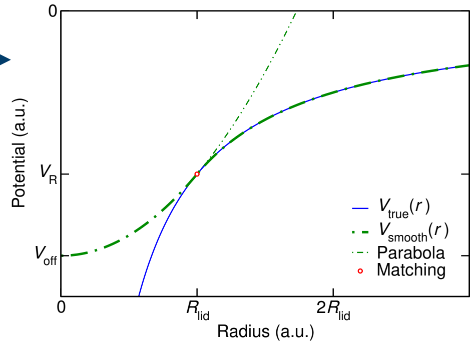
56	p** f* h	5
35	s** d* g	4
20	p* f	3
10	s* d	2
4	p	1
1	s	0

H	2																				2	He
Li	2	2																		3	3	Ne
Na	3	3											3	3	3	3	3	3	3	3	3	3	Ar
K	3	3	4				4	4	4	4	4	4	4	4	4	3	3	3	3	3	3	Kr
Rb	3	3	4				4	4	4	–	4	4	4	4	4	4	4	4	3	3	3	Xe
Cs	3	4	4	5	...	5	4	4	4	4	4	4	4	4	4	4	4	4	–	–	3	Rn

PAW Projector Generation

The original recipe suggested by P. Blöchl

1. Pseudize the potential →



2. Choose energy parameters
3. Find true partial waves
4. Create smooth partial waves
5. Get preliminary projectors:

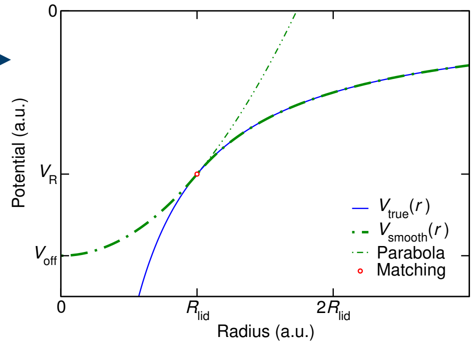
$$|\tilde{p}_{n\ell}\rangle = \left(\hat{T} + \tilde{V}_{\text{eff}} - \varepsilon_{n\ell}\right)\left|\tilde{\phi}_{n\ell}\right\rangle$$

➔ Many tuning parameters

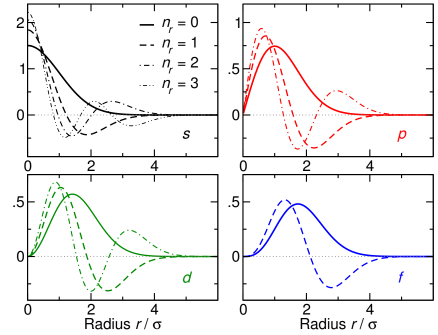
PAW Projector Generation

A modified recipe adjusted to given analytical SHO projector functions

1. Pseudize the potential
2. Choose energy parameters
3. Find true partial waves
4. Set projectors to radial SHO basis functions
5. Get smooth partial waves:



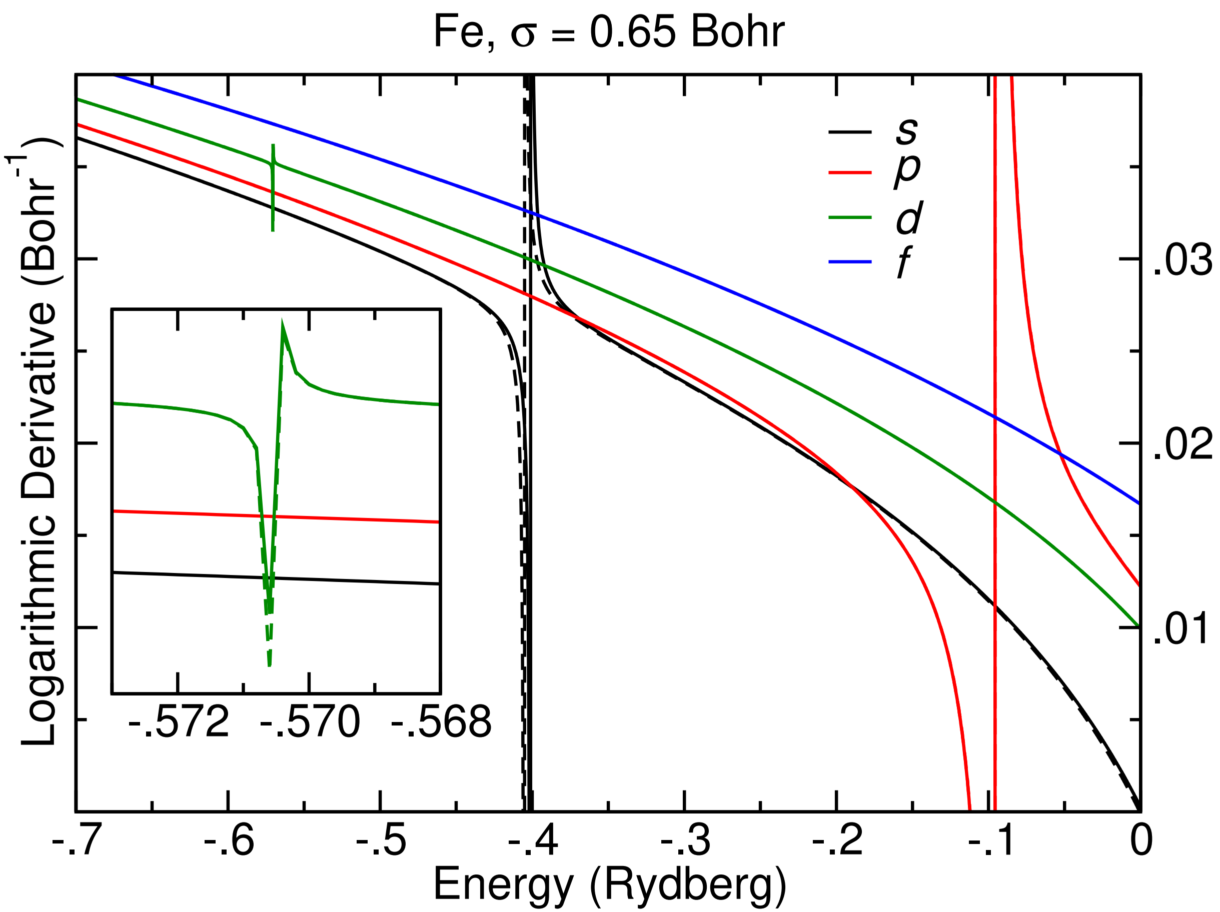
$$\left|\tilde{\phi}_{n\ell}\right\rangle = \left(\hat{T} + \tilde{V}_{\text{eff}} - \varepsilon_{n\ell}\right)^{-1} \left|R_{n\ell}\right\rangle$$



➔ Recipe has less freedom

Modified PAW Generation

Compare scattering properties of true (solid lines) and PAW (dashed lines)

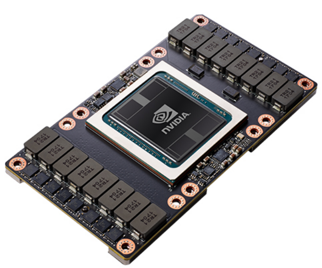


Pro and Contra

Advantages and Drawbacks of a SHO basis for projection operations

Pro: A SHO basis

- factorizes in coordinates (x,y,z)
- has a radial representation (n_r,ℓ,m)
- can be represented on uniform grids without Fourier-filtering
- has only 2 parameters: $\boldsymbol{\sigma}$ and $\boldsymbol{\nu}_{\mathrm{max}}$
- is known analytically, no requirement for memory capacity and bandwidth



Contra: A SHO basis

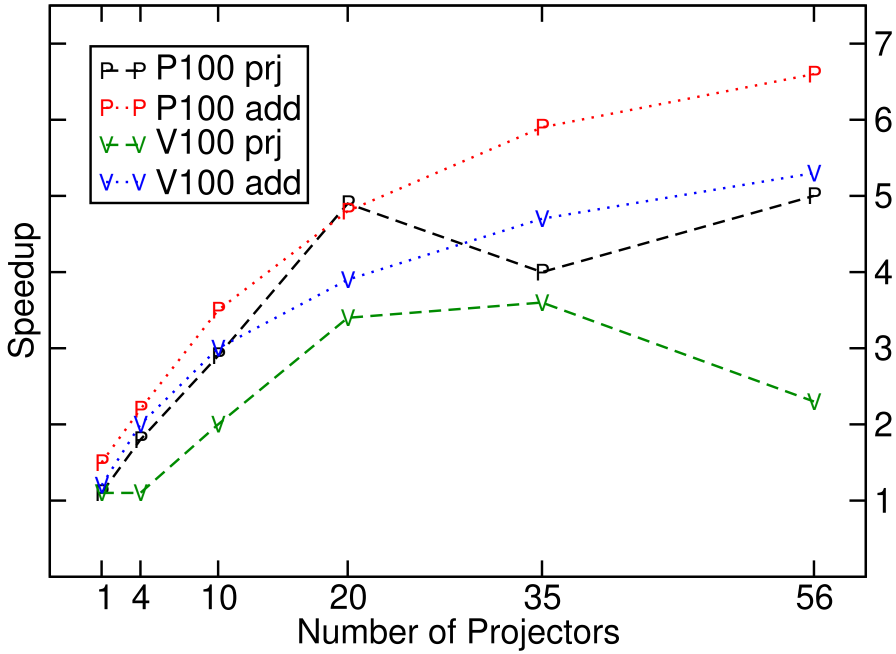
- may be larger than usual sets:
  PAW: $s_2\ p_2\ d_2$ → 18 coeff.
  SHO: $s_3\ p_2\ d_2\ f_1\ g_1$ → 35 coeff.
  but maybe better transferability
- is not perfect for existing projectors
  but we can adjust the PAW data

Performance Results on GPUs

Prototype for Projection (`prj`) and Expansion (`add`) operations

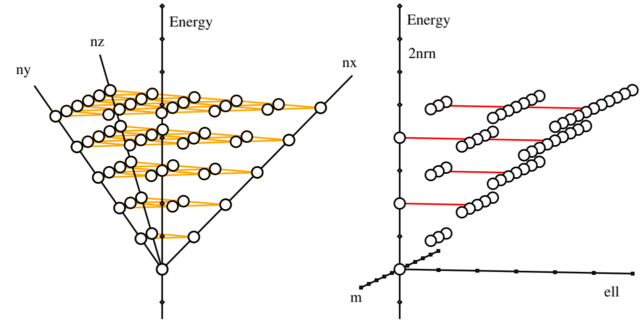
$$c_{jk} = \langle \tilde{p}_j | \Psi_k \rangle \qquad\qquad |\Psi_k\rangle \mathrel{+}= |\tilde{p}_i\rangle\, d_{ik}$$

1D Hermite polynomials times Gaussians evaluated on-the-fly on NVIDIA GPUs



	P100		V100	
#	prj	add	prj	add
1	1.1	1.5	1.1	1.2
4	1.8	2.2	1.1	2.0
10	2.9	3.5	2.0	3.0
20	4.9	4.8	3.4	3.9
35	4.0	5.9	3.6	4.7
56	5.0	6.6	2.3	5.3

Summary



Spherical Harmonic Oscillator (SHO)

- Radial representation with sharp (ℓ,m)
- Cartesian representation factorizing in (x,y,z)
- Uniform transform, Radial ⇄ Cartesian

Bandwidth and Memory Savings using 3D factorizable PAW projectors

- On-the-fly evaluation of 1D Hermite-Gauss basis suitable for GPUs
- No filtering of PAW projector functions needed

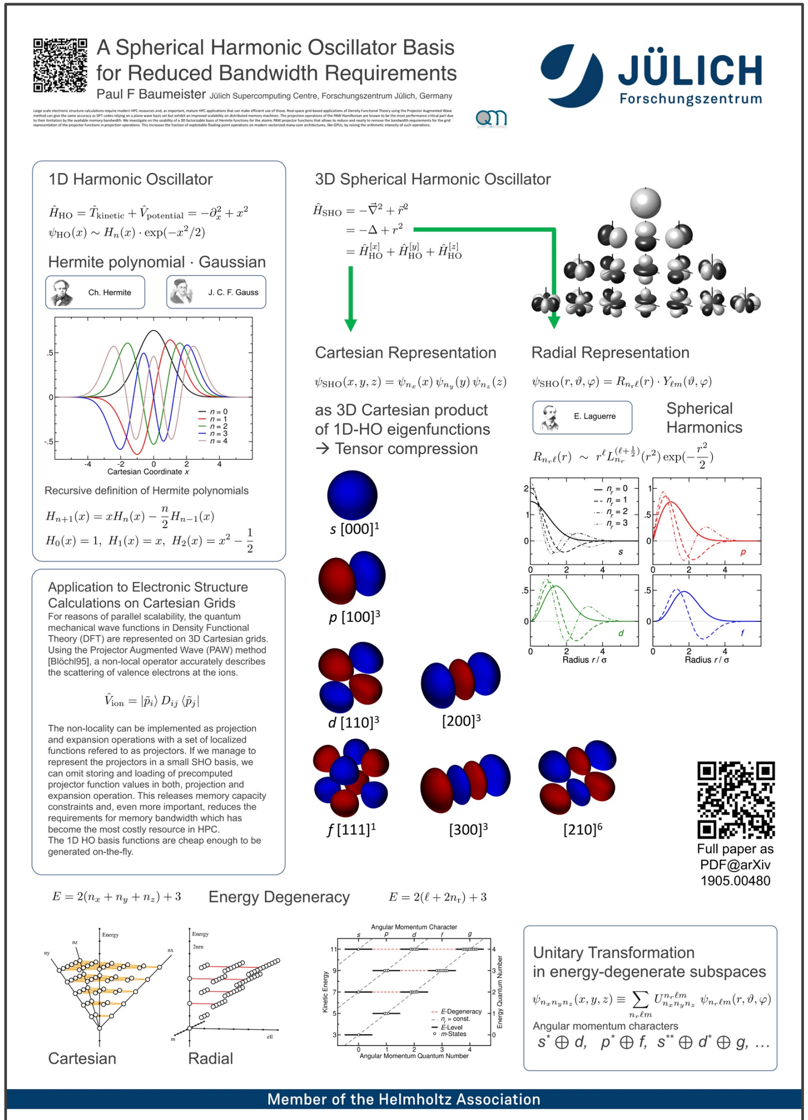
Quality Analysis for GPAW projection functions represented in a SHO basis

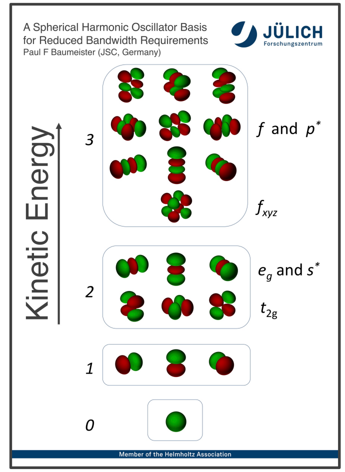
- Minimum SHO basis sizes: 10 ($Z < 5$), 20 (non-metal), 35 (d-metal)
- Minimal SHO basis is not suitable for all existing PAW sets

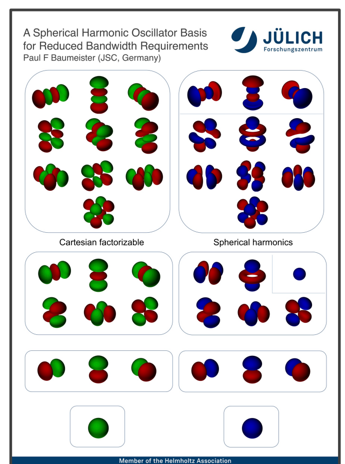
Modification of PAW projector generation scheme

- Use a single (analytically given) radial SHO basis function as projector
- Smooth partial waves are generated from projectors

More discussion? – Poster CSM05







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Thursday
8pm
HG E0 Nord