A Circular Harmonic Oscillator Basis

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Polar coordinates are frequently used to transform 2D images appearing in 4D scanning transmission electron microscopy (4D-STEM) as the dominant feature of the ronchigram is a central spot where the undeflected electron beam hits the detector. The information of interest resides in the deviations from a circular shape of the spot. The function basis of the quantum mechanical harmonic osciallator consists of Hermite polynomials and a Gaussian envelope function for the one-dimensional problem. For the two-dimensional isotropic problem, the basis can be represented either as a Cartesian product of two 1D basis functions or in polar coordinates.
A unitary transformation connects both representations. To allow fast and affordable compression of STEM images, we incorporate the Cartesian product representation as it leads to two successive matrix-matrix multiplications. This compression method is particularly suitable for single-side-band (SSB) ptychography.
We present the explicit shape of the associated radial functions of a circular harmonic oscillator and compression factors in relation to computational costs for a typical SSB ptychography application.

1D Harmonic Oscillator

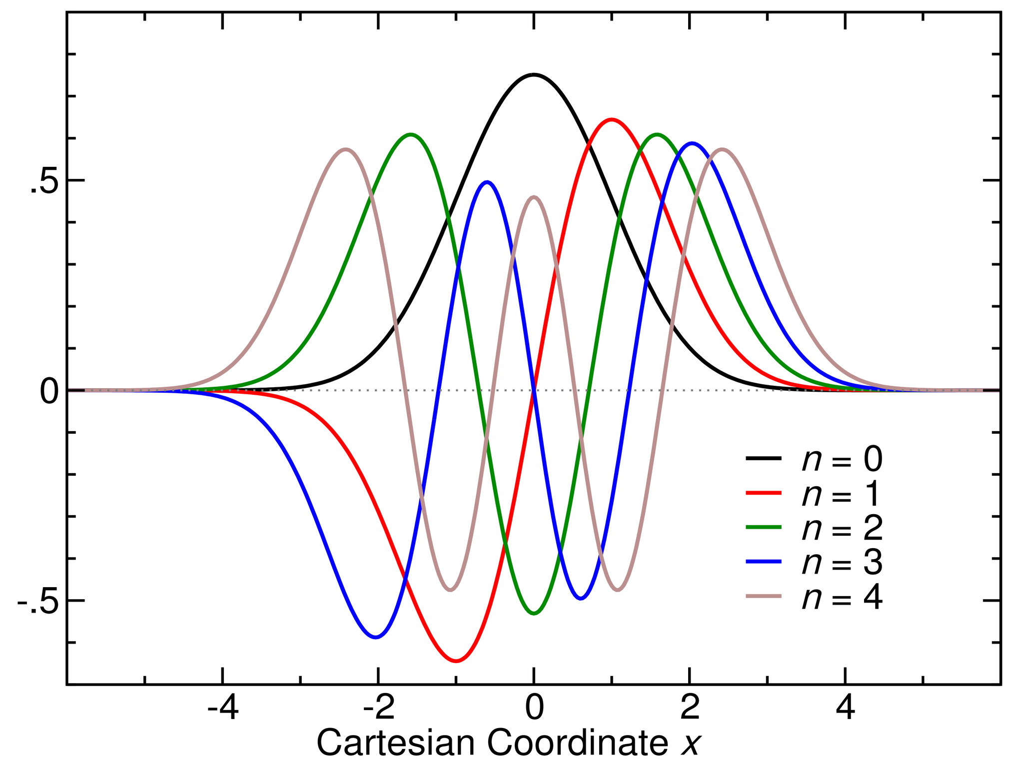
$$\hat{H}_{\text{HO}} = \hat{T}_{\text{kinetic}} + \hat{V}_{\text{potential}} = -\frac{\partial^2}{\partial x^2} + x^2$$

$$\psi_{\text{HO}}(x) \sim H_n(x) \cdot \exp(-x^2/2)$$

Hermite polynomial · Gaussian


Ch. Hermite


J. C. F. Gauss



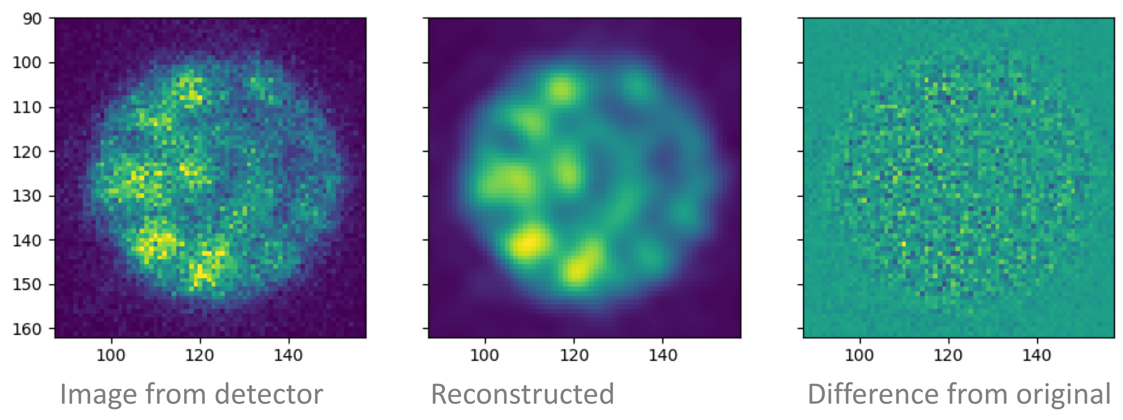
Recursive definition of Hermite polynomials

$$H_{n+1}(x) = xH_n(x) - \frac{n}{2}H_{n-1}(x)$$

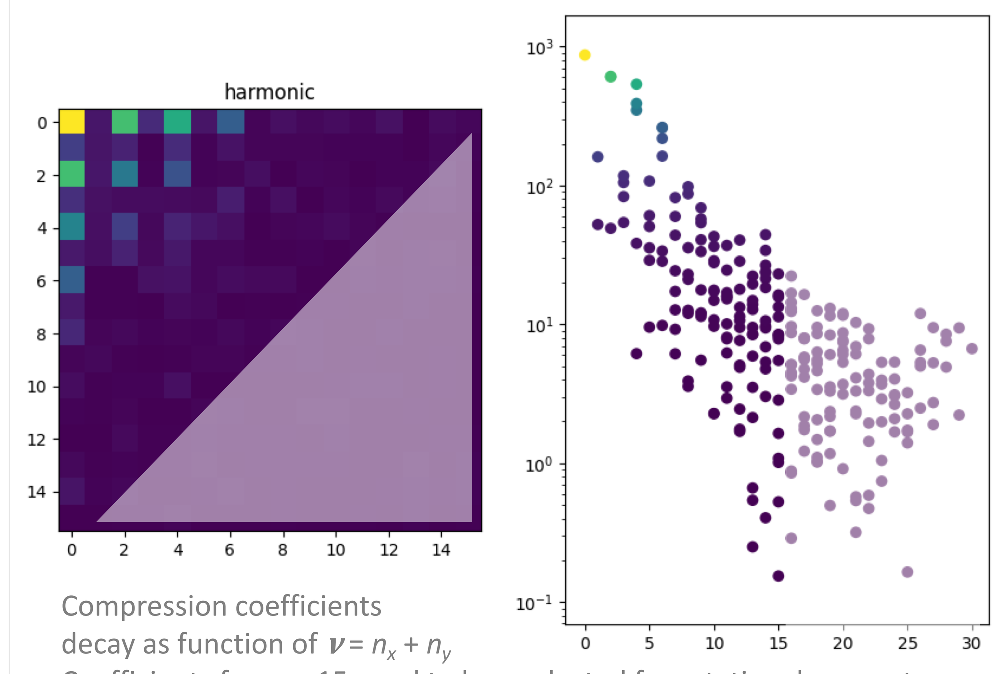
$$H_0(x) = 1,\ H_1(x) = x,\ H_2(x) = x^2 - \frac{1}{2}$$

Application to Image Compression in STEM

Scanning Transmission Electron Microscopy



Represent detector frame in 16✕16 HO-basis



Compression coefficients
decay as function of $\nu = n_x + n_y$
Coefficients for $\nu > 15$ need to be neglected for rotational symmetry

Compare to other methods/radial functions

	Speedup	Compression	RMS deviation	Max deviation
Harmonic oscillator	4.5x	25x	0.050	0.082
Cylindrical harmonics	0.87x	34x	0.059	0.09
Cropping & binning	4.1x	13x	0.16	0.19
Fourier transform	3.0x	13x	0.31	0.33
Sectored	3.8x	20x	0.086	0.14

Fast & strong compression using 2D-HO basis

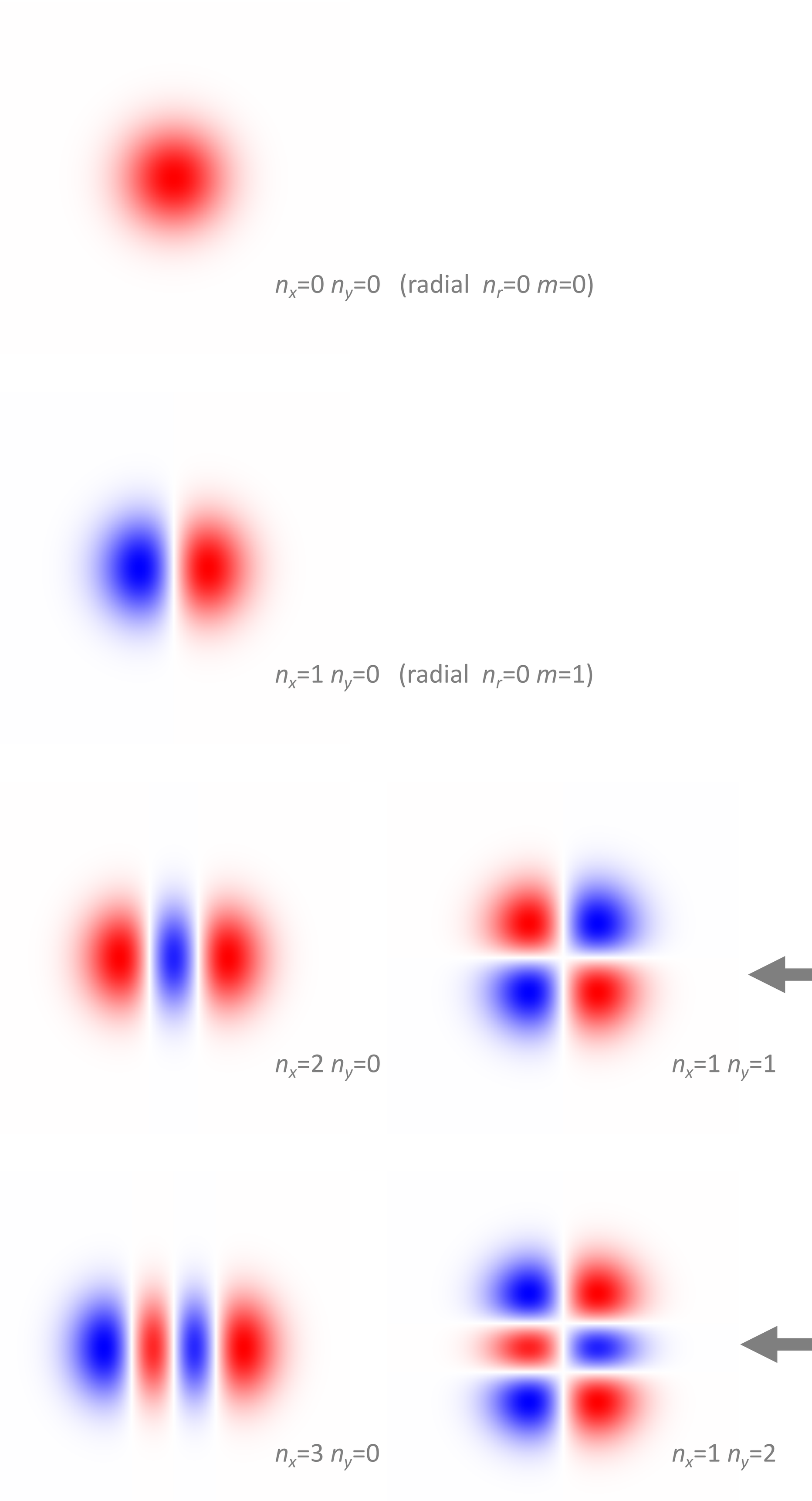
2D Isotropic Harmonic Oscillator

$$\hat{H}_{\text{SHO}} = -\vec{\nabla}^2 + \vec{r}^2$$
$$= -\Delta + r^2$$
$$= \hat{H}^{[x]}_{\text{HO}} + \hat{H}^{[y]}_{\text{HO}}$$

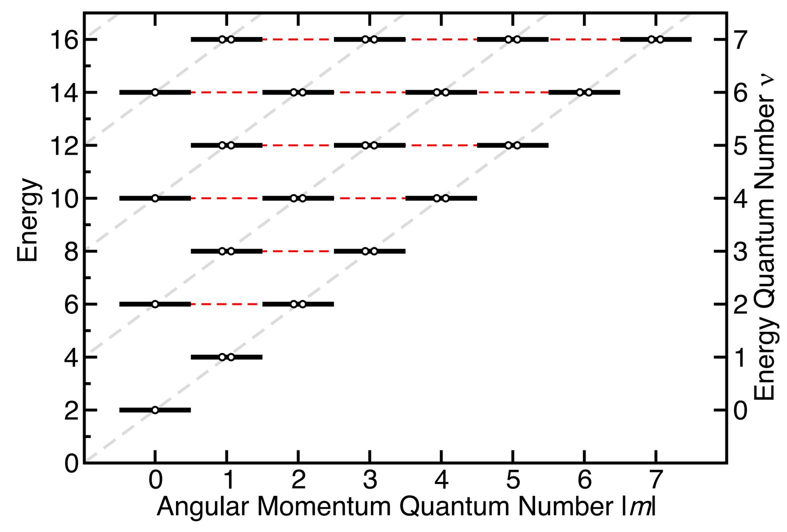
Cartesian Representation

$$\Psi_{\text{CHO}}(x,y) = \psi_{n_x}(x)\psi_{n_y}(y)$$

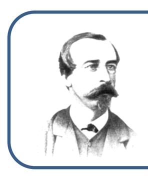
as 2D Cartesian product of 1D-HO eigenfunctions
→ Tensor compression



Radial Representation



$$\Psi_{\text{CHO}}(r,\varphi) = R_{n_r|m|}(r) \cdot \exp(\imath m\varphi)$$

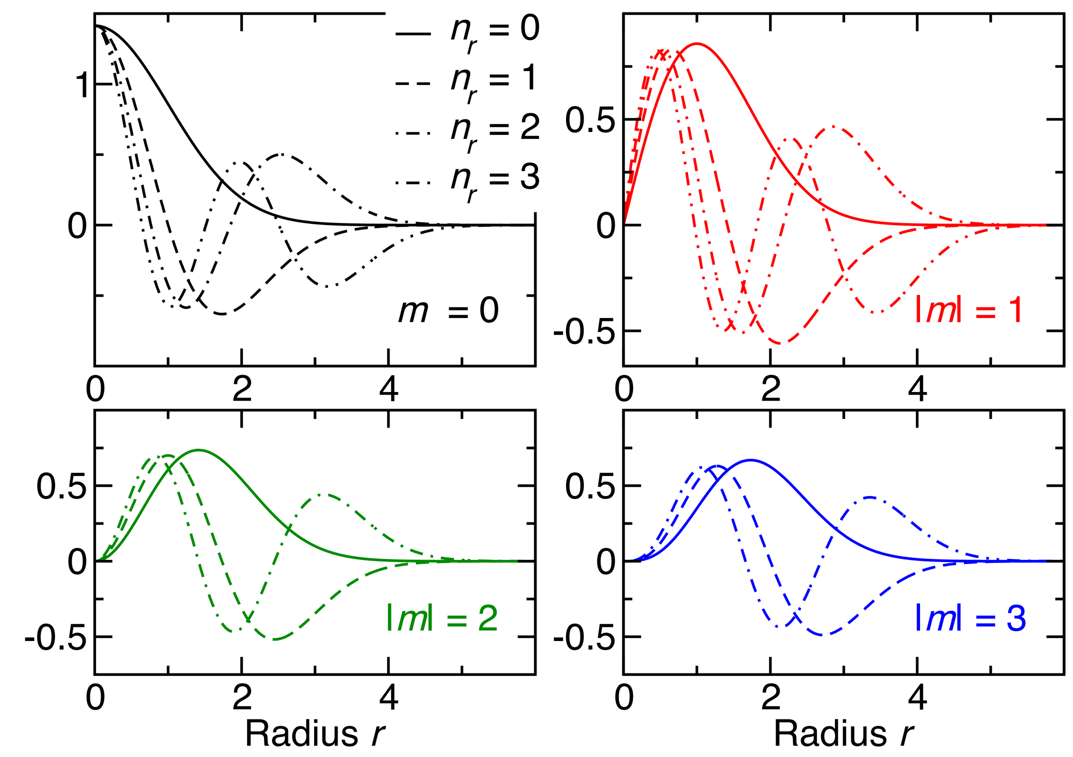

E. Laguerre

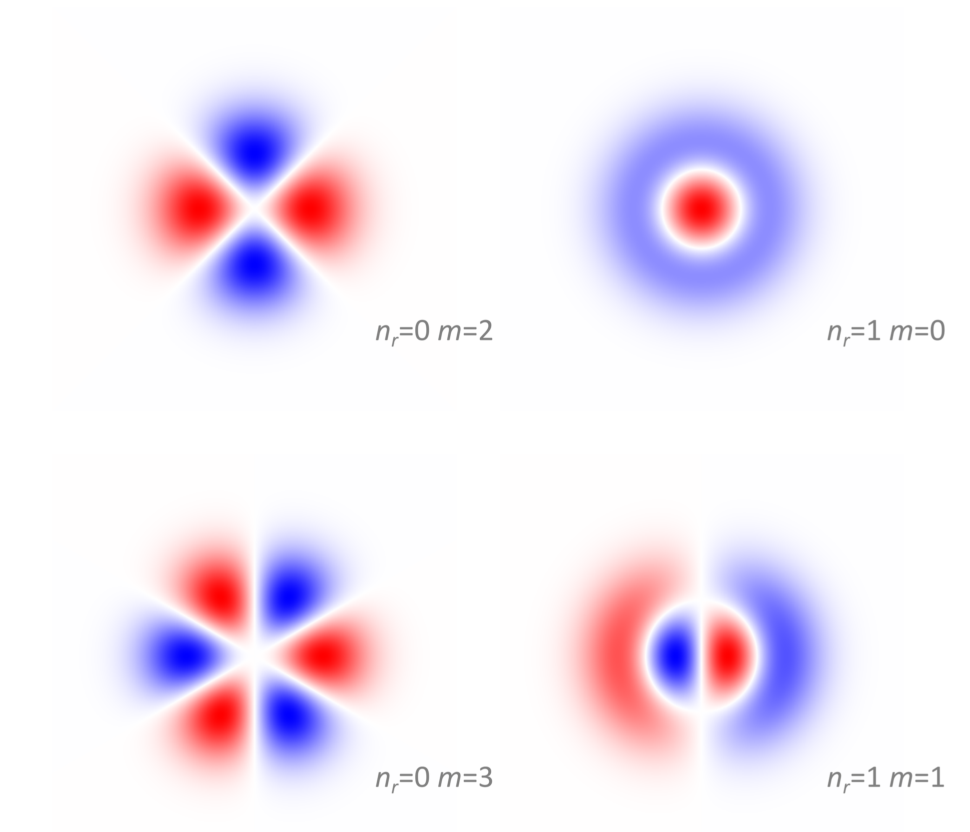
Circular Harmonics

Associated Laguerre polynomials

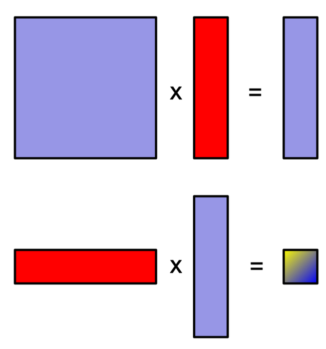
$$R_{n_r|m|}(r) \propto r^{|m|} \sum_{k=0}^{n_r} c_k r^{2k} \quad \text{with}$$

$$(k+1)(k+1+|m|)c_{k+1} = (k-n_r)c_k$$





Compress 2D images using the factorization property



Unitary Transformation in degenerate subspaces

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

Data set available at
doi.org/10.26165/JUELICH-DATA/WDRGAX