# Solving for the low-rank tensor components of the wave function in scattering problems with multiple ionization

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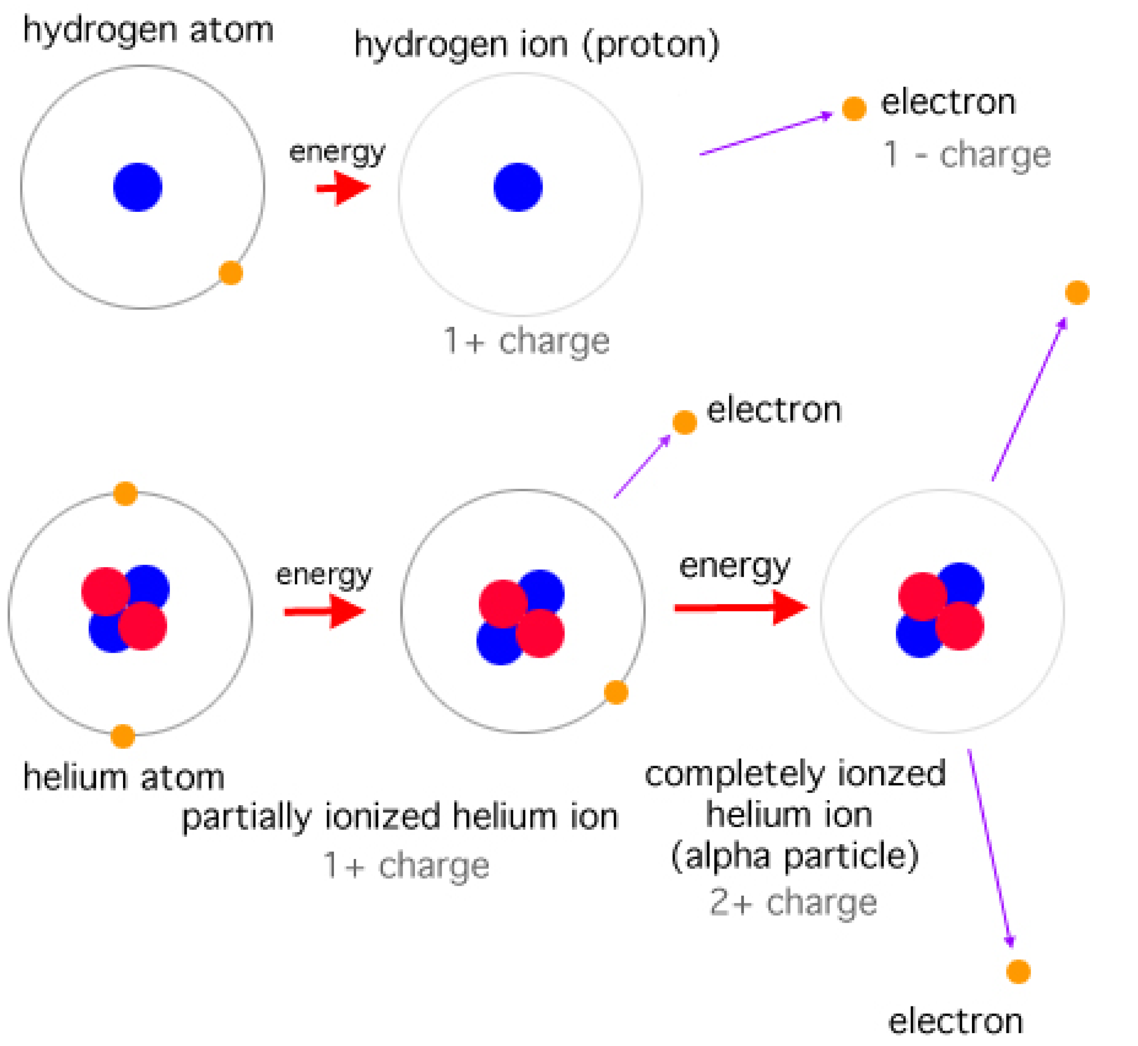
## Ionization & scattering problems

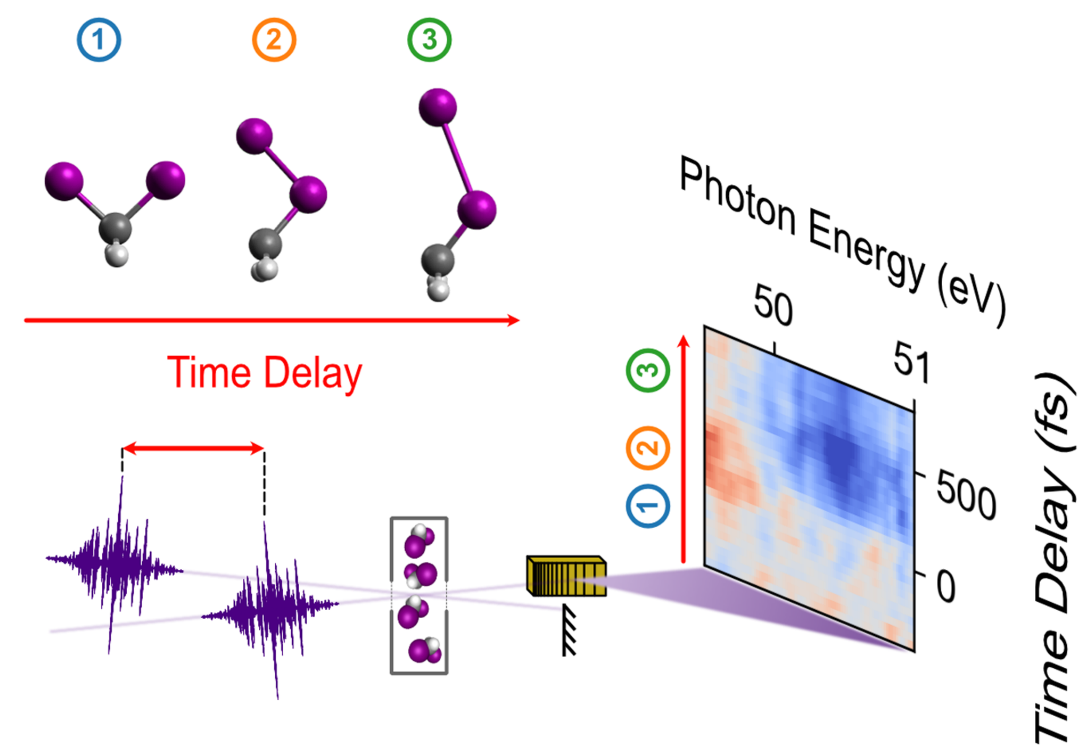
Information about microscopic systems comes from experiments where electrons scatter from an object.




## Molecular movie

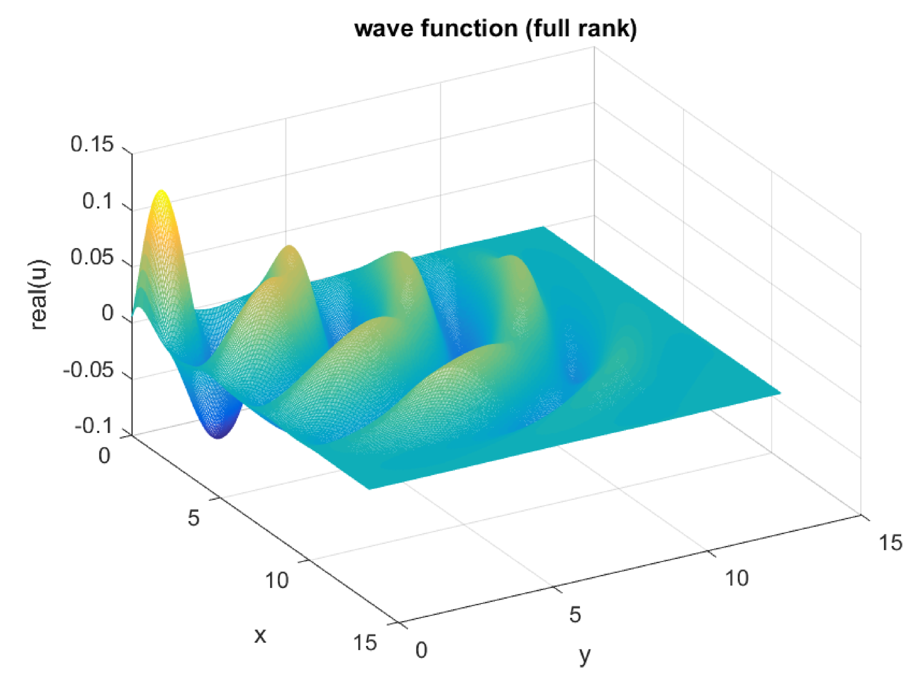
Electrons are emitted along angles that can be measured. This results in a probability distribution, called the ***far field map***. This corresponds the the amplitude of the wave in the emitting direction.

In new experiments, based on a far field map, the original state of molecules will be reconstructed.



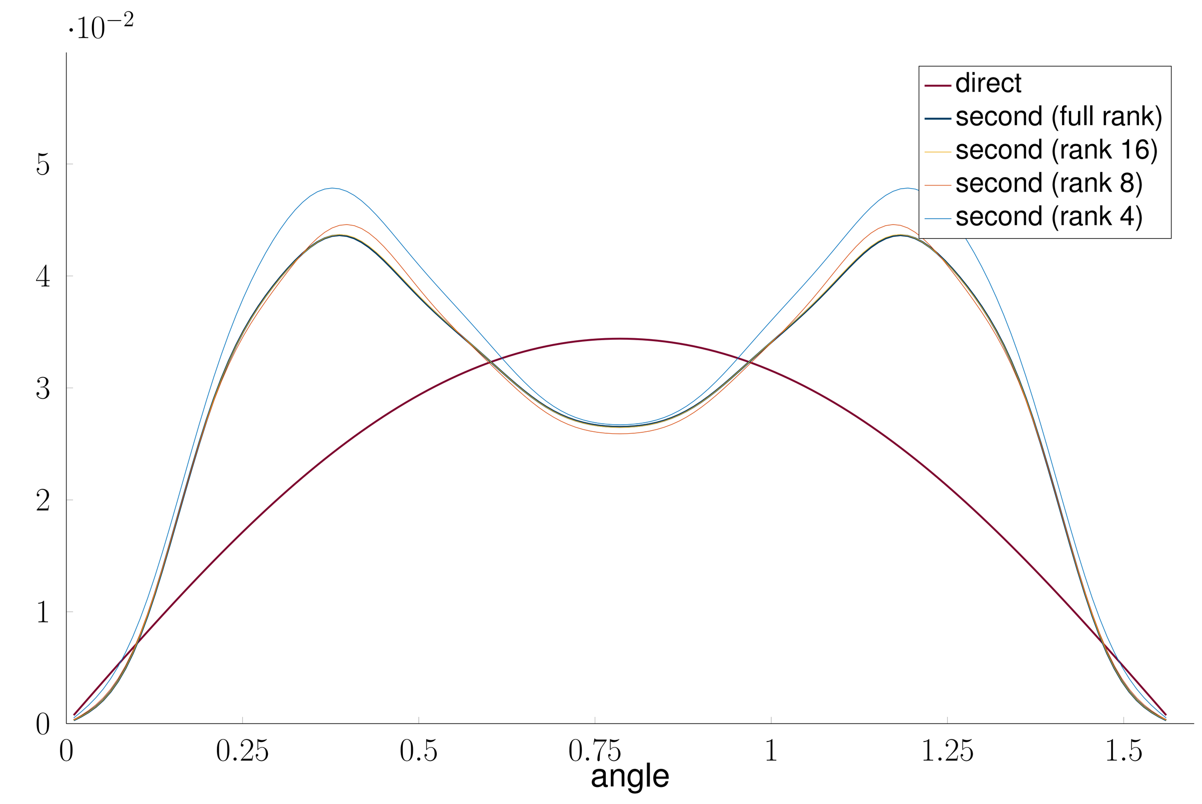

## Wave function

- 2D Helmholtz equation with $(x, y) \in (0,\ 10)^2$ and extended with ECS, $E = 4$,
  $\omega^2(x, y) = \exp\left(-|(x-y)^4|\right) - E$,
  $f(x, y) = \exp\left(-x^2 - y^2\right)$.
- Discretization: FD grid of 200 grid points and ECS layer with 67 points rotated over $\pi/6$.

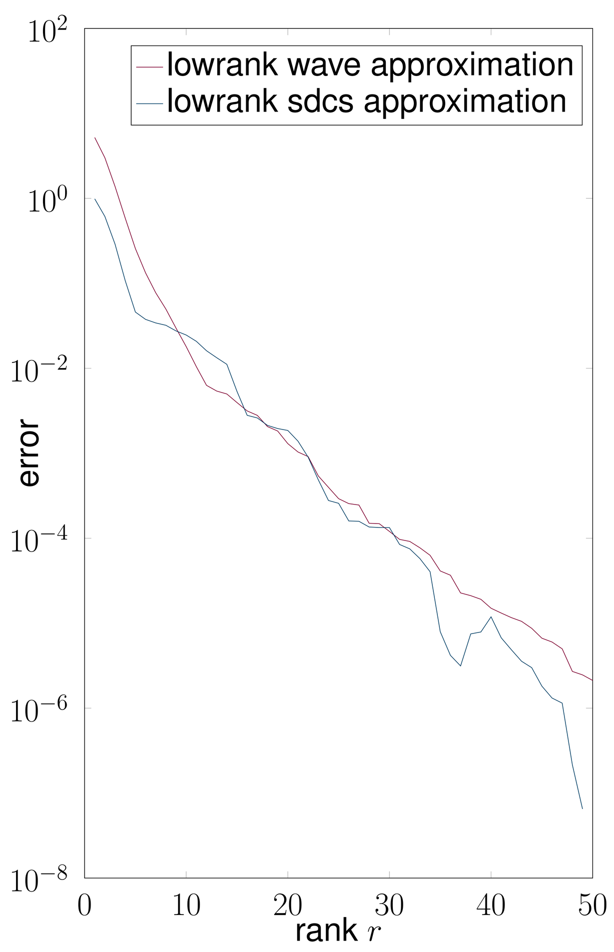



## Differential cross section

$$\frac{d\sigma}{d\Omega}(\theta) = \int_0^b \int_0^b \sin(\omega_0 \sin\theta x) \sin(\omega_0 \cos\theta\, y) \left[f + \omega_0^2 \chi u_{sc}\right] dx dy$$




## Error SDCS




## Observation (2D)

To get a good apprixmination for the SDCS a ***low rank*** approximation to the Helmholtz equation is sufficient.

Discretization of Helmholtz equation on a 2D cartesian grid with $n_x \times n_y$ unknowns leads to the following matrix equation:

$$\boldsymbol{D}_{xx}\boldsymbol{A} + \boldsymbol{A}\boldsymbol{D}_{yy}^{\mathsf{T}} - \boldsymbol{W} \circ \boldsymbol{A} = \boldsymbol{F} \qquad (1)$$

where $\boldsymbol{A}, \boldsymbol{F}$ and $\boldsymbol{W}$ are $n_x \times n_y$ matrices that describe the unknown solution $u_{sc}(x, y)$, $f$ and $\omega^2$ on the discretized mesh.

Assuming that $\boldsymbol{A}$ has low rank this matrix can be written as $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{V}^{\mathsf{H}}$ with $\boldsymbol{U} \in \mathbb{C}^{n_x \times r}$ and $\boldsymbol{V} \in \mathbb{C}^{n_y \times r}$ both with orthogonal columns and $r \ll \min(n_x, n_y)$ is the rank of matrix $\boldsymbol{A}$:

$$\boldsymbol{D}_{xx}\boldsymbol{U}\boldsymbol{V}^{\mathsf{H}} + \boldsymbol{U}\boldsymbol{V}^{\mathsf{H}}\boldsymbol{D}_{yy}^{\mathsf{T}} - \omega^2\boldsymbol{U}\boldsymbol{V}^{\mathsf{H}} = \boldsymbol{F} \qquad (2)$$

Derive equations to solve for the factors $\boldsymbol{U}$ and $\boldsymbol{V}$:

$$\begin{aligned}\boldsymbol{D}_{xx}\boldsymbol{U} + \boldsymbol{U}\boldsymbol{V}^{\mathsf{H}}\boldsymbol{D}_{yy}^{\mathsf{T}}\boldsymbol{V} - \omega^2\boldsymbol{U} &= \boldsymbol{F}\boldsymbol{V} \\ \boldsymbol{U}^{\mathsf{H}}\boldsymbol{D}_{xx}\boldsymbol{U}\boldsymbol{V}^{\mathsf{H}} + \boldsymbol{V}^{\mathsf{H}}\boldsymbol{D}_{yy}^{\mathsf{T}} - \omega^2\boldsymbol{V}^{\mathsf{H}} &= \boldsymbol{U}^{\mathsf{H}}\boldsymbol{F}\end{aligned} \qquad (3)$$

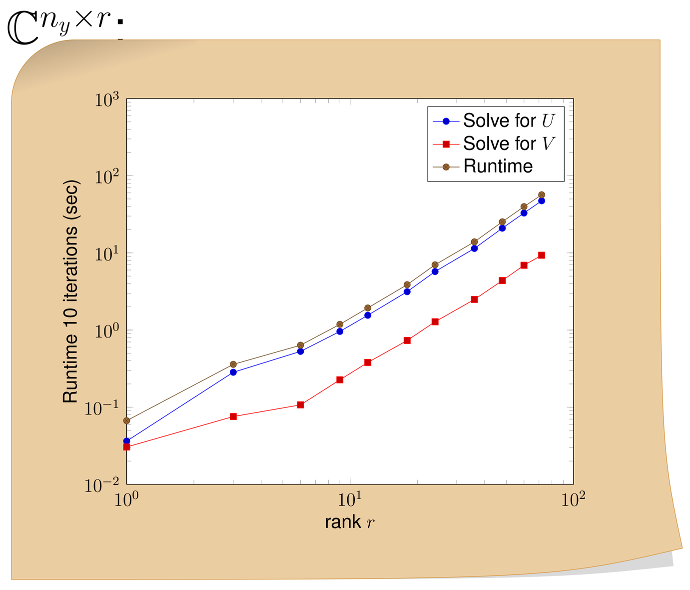
## The algorithm (2D)

We have update equations for $\boldsymbol{U}$ and $\boldsymbol{V}$:

$$\left[\left(\boldsymbol{I} \otimes (\boldsymbol{D}_{xx} - \omega^2\boldsymbol{I})\right) + \left(\boldsymbol{V}^{\mathsf{T}}\boldsymbol{D}_{yy}\overline{\boldsymbol{V}} \otimes \boldsymbol{I}\right)\right] \operatorname{vec}[\boldsymbol{U}] = \operatorname{vec}[\boldsymbol{F}\boldsymbol{V}].$$

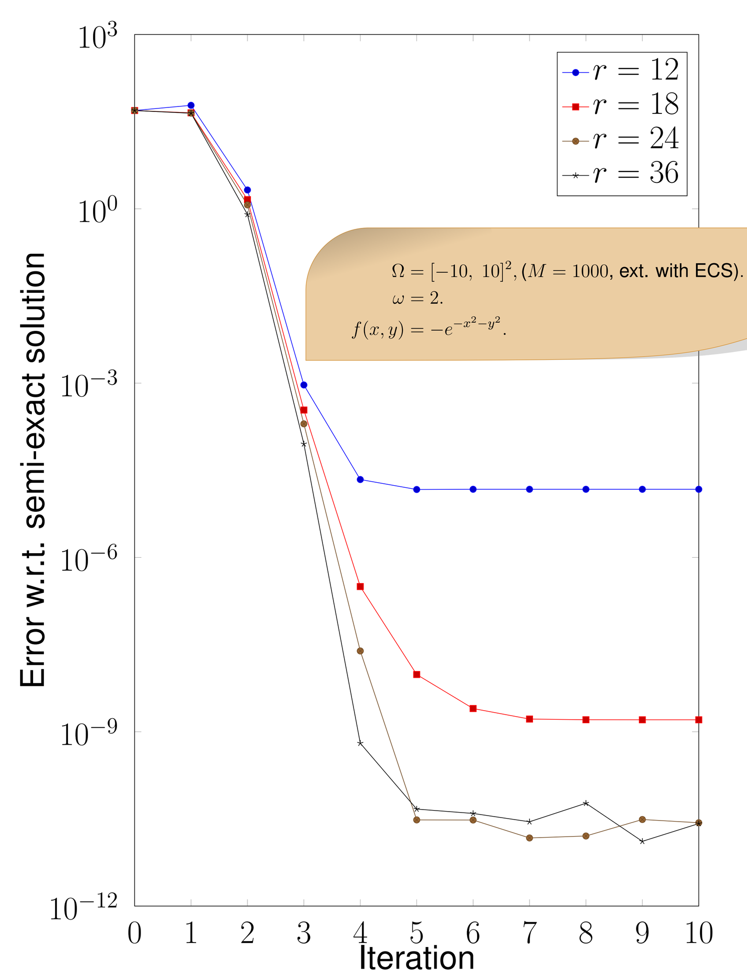
$$\left[\left(\boldsymbol{I} \otimes \boldsymbol{U}^{\mathsf{H}}\boldsymbol{D}_{xx}\boldsymbol{U}\right) + \left((\boldsymbol{D}_{yy} - \omega^2\boldsymbol{I}) \otimes \boldsymbol{I}\right)\right] \operatorname{vec}\left[\boldsymbol{V}^{\mathsf{H}}\right] = \operatorname{vec}\left[\boldsymbol{U}^{\mathsf{H}}\boldsymbol{F}\right].$$

Given: initial guess $\boldsymbol{V}_0 \in \mathbb{C}^{n_y \times r}$;
$[\boldsymbol{V}, \boldsymbol{R}] = \operatorname{qr}[\boldsymbol{V}_0]$;
**while** *not converged* **do**
 Solve for $\boldsymbol{U}$;
 $[\boldsymbol{U}, \widetilde{\boldsymbol{R}}] = \operatorname{qr}[\boldsymbol{U}]$;
 Solve for $\boldsymbol{V}^{\mathsf{H}}$;
 $[\boldsymbol{V}, \boldsymbol{R}] = \operatorname{qr}[\boldsymbol{V}]$;
**end**
$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{R}^{\mathsf{H}}\boldsymbol{V}^{\mathsf{H}}$;




- Solving for $\boldsymbol{U}, \boldsymbol{V}$ can be interpreted as a ***projection operator*** applied on residual.
- The successive application of these projection operators doesn't result in a new projection operator. But it can be seen as a ***perturbation*** of a projection operator.
- This perturbation is typical ***small and bounded***, which leads to convergence.

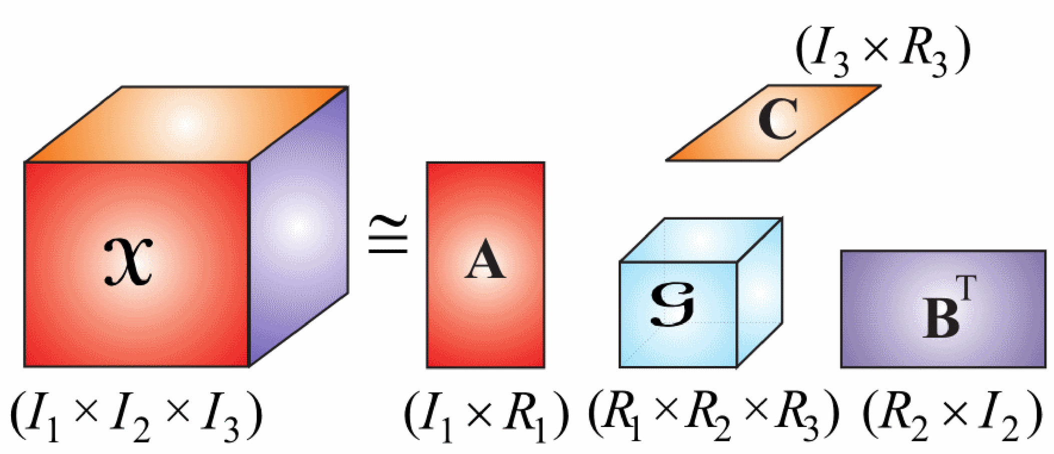
## Errors per iteration




## Tucker tensor decomposition

A matrix SVD is generalized by a ***Tucker tensor decomposition*** which represents an $d$-th order tensor $\boldsymbol{\mathcal{X}} \in \mathbb{R}^{I_1 \times I_2 \times \ldots \times I_d}$ as a multilinear transformation of a dense core tensor $\boldsymbol{\mathcal{G}} \in \mathbb{R}^{R_1 \times R_2 \times \cdots \times R_d}$ by orthonormal matrices $\boldsymbol{U}_n = \boldsymbol{U}^{(n)} \in \mathbb{R}^{I_n \times R_n}$:

$$\begin{aligned}\boldsymbol{\mathcal{X}} &= \boldsymbol{\mathcal{G}} \times_1 \boldsymbol{U}^{(1)} \times_2 \boldsymbol{U}^{(2)} \ldots \times_d \boldsymbol{U}^{(d)} \\ &= \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \cdots \sum_{r_d=1}^{R_d} g_{r_1 r_2 \cdots r_d} \left(\boldsymbol{u}_{r_1}^{(1)} \circ \boldsymbol{u}_{r_2}^{(2)} \circ \cdots \circ \boldsymbol{u}_{r_d}^{(d)}\right)\end{aligned} \qquad (4)$$




## Helmholz on tensors

Application of Helmholz opr. $\mathcal{L}$ on $\boldsymbol{\mathcal{M}}$:

$$\begin{aligned}\mathcal{L}\boldsymbol{\mathcal{M}} = \boldsymbol{\mathcal{F}} = \;& \boldsymbol{\mathcal{G}} \times_1 \boldsymbol{D}_{xx}\boldsymbol{U}_1 \times_2 \boldsymbol{U}_2 \times_3 \boldsymbol{U}_3 \\ &+ \boldsymbol{\mathcal{G}} \times_1 \boldsymbol{U}_1 \times_2 \boldsymbol{D}_{yy}\boldsymbol{U}_2 \times_3 \boldsymbol{U}_3 \\ &+ \boldsymbol{\mathcal{G}} \times_1 \boldsymbol{U}_1 \times_2 \boldsymbol{U}_2 \times_3 \boldsymbol{D}_{zz}\boldsymbol{U}_3 \\ &- \boldsymbol{\mathcal{W}} \circ (\boldsymbol{\mathcal{G}} \times_1 \boldsymbol{U}_1 \times_2 \boldsymbol{U}_2 \times_3 \boldsymbol{U}_3).\end{aligned}$$

where $\boldsymbol{U}_i^H \boldsymbol{U}_i = \boldsymbol{I}$, for $i = 1, 2, 3$.

## The algorithm (3D)

To derive an update equation for $\boldsymbol{U}_1$ multiply with $\boldsymbol{U}_2$ and $\boldsymbol{U}_3$ in the second and third dimension, respectively:

$$\mathcal{L}\boldsymbol{\mathcal{M}} \times_2 \boldsymbol{U}_2^H \times_3 \boldsymbol{U}_3^H = \boldsymbol{\mathcal{F}} \times_2 \boldsymbol{U}_2^H \times_3 \boldsymbol{U}_3^H.$$

Unfolding in first mode leads to a matrix equation for $\overline{\boldsymbol{U}_1}\boldsymbol{G}_{(1)}$.

## Conclusions

- In certain cases the solution to Helmholtz can be described by a ***limited number of singular values***. Low rank approximations are sufficient and ***reduce computational cost*** to construct a far field map.
- The presented algorithm has ***good contractiity properties***. In practice only a ***small number of iterations*** are needed (also for low rank space dependent wave numbers).
- Using Tucker decompositions the presented algorithm can be ***extended to*** $n$**D**.