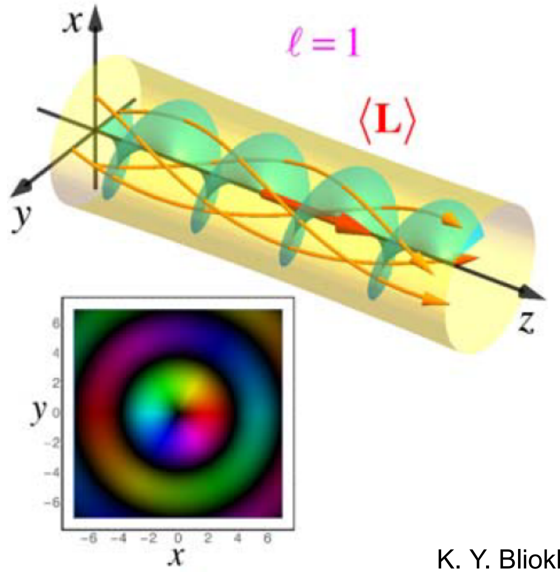
Vortex electron scattering by atomic targets

Sophia Strnat, Vortex states in nuclear and particle physics, Zhuhai

Vortex electrons and their production

Wave function

$$\Psi^{tw}_{p_z|\mathbf{p}_\perp|m}(\mathbf{r},t) = e^{-i\omega t + ip_z z} e^{im\varphi_r} \cdot \sqrt{|\mathbf{p}_\perp|} J_m(|\mathbf{p}_\perp| r_\perp)$$

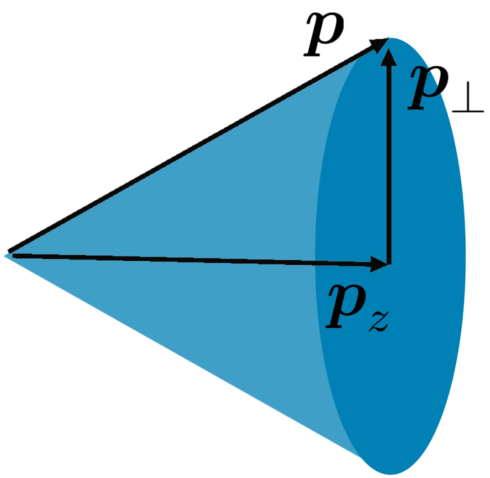


K. Y. Bliokh *et al*. Physics Reports,Volume 690, (2017)

Vortex electrons and their production

Wave function

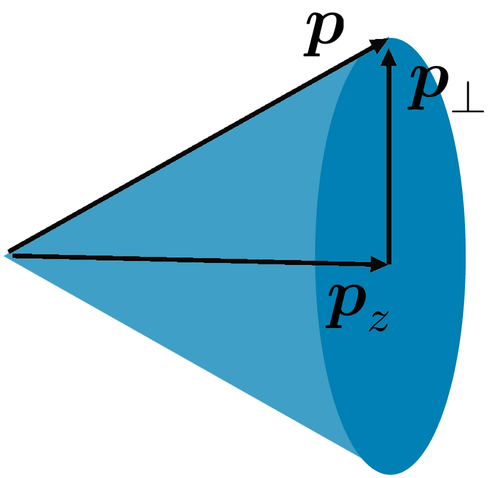
$$\Psi^{tw}_{p_z|\mathbf{p}_\perp|m}(\mathbf{r},t) = \int d^3\mathbf{p}\; a_{p_z|\mathbf{p}_\perp|m}(\mathbf{p}) e^{-i\omega t + i\mathbf{pr}}$$



Vortex electrons and their production

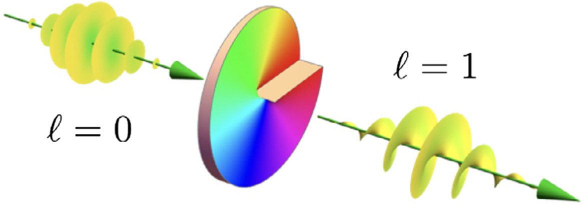
Wave function

$$\Psi^{tw}_{p_z|\mathbf{p}_\perp|m}(\mathbf{r}, t) = \int d^3\mathbf{p}\; a_{p_z|\mathbf{p}_\perp|m}(\mathbf{p})\, e^{-i\omega t + i\mathbf{pr}}$$

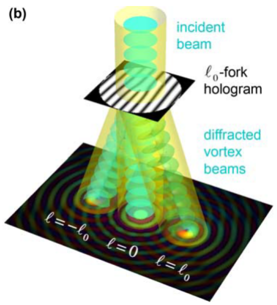


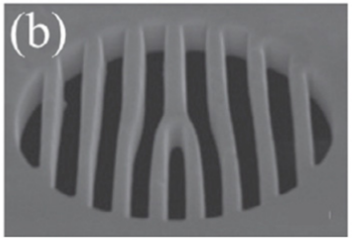
Production

- spiral phase plates[1]

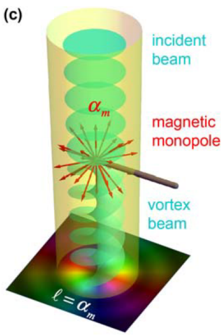


- diffraction grating with an edge dislocation[1,2]





- magnetic quasi-monopoles[2]

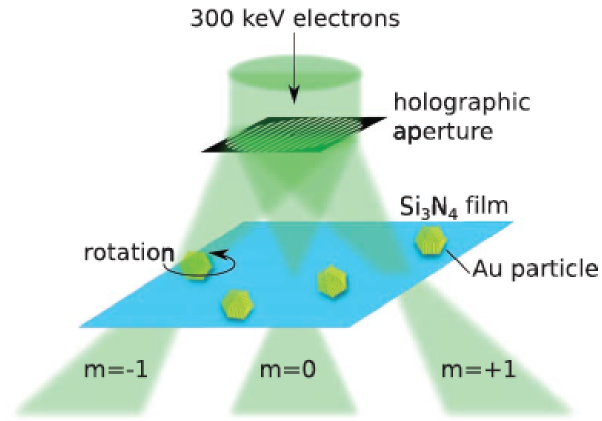


[1] H. Larocque *et al.* (2018): ‘Twisted’ electrons, Contemp. Phys., DOI: 10.1080/00107514.2017.1418046
[2] K. Y. Bliokh *et al.* Physics Reports, Volume 690, 24 May 2017

Applications of vortex electrons

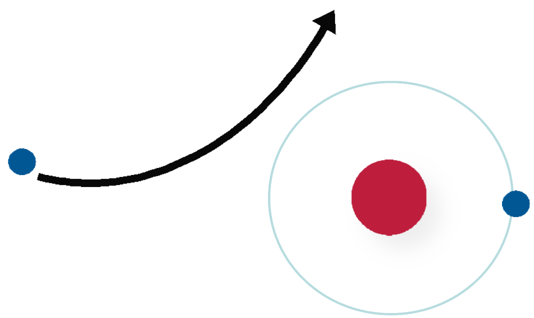
Applications

- spintronic applications
- manipulation of nanoparticles
- magnetic-dependent EELS
- access chiral-dependent electronic excitations



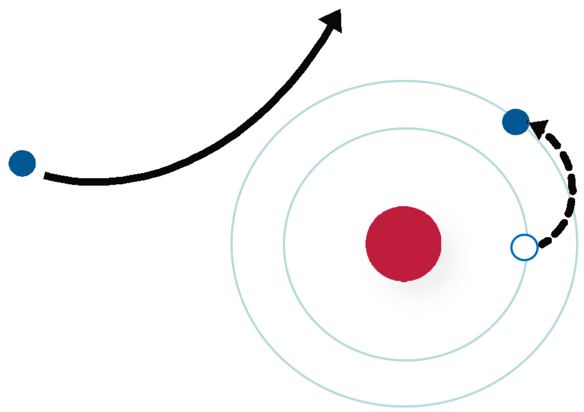
Verbeeck et al. Adv. Mater. **25**, 1114–1117 (2012)

Knowledge about electron scattering is required



elastic scattering

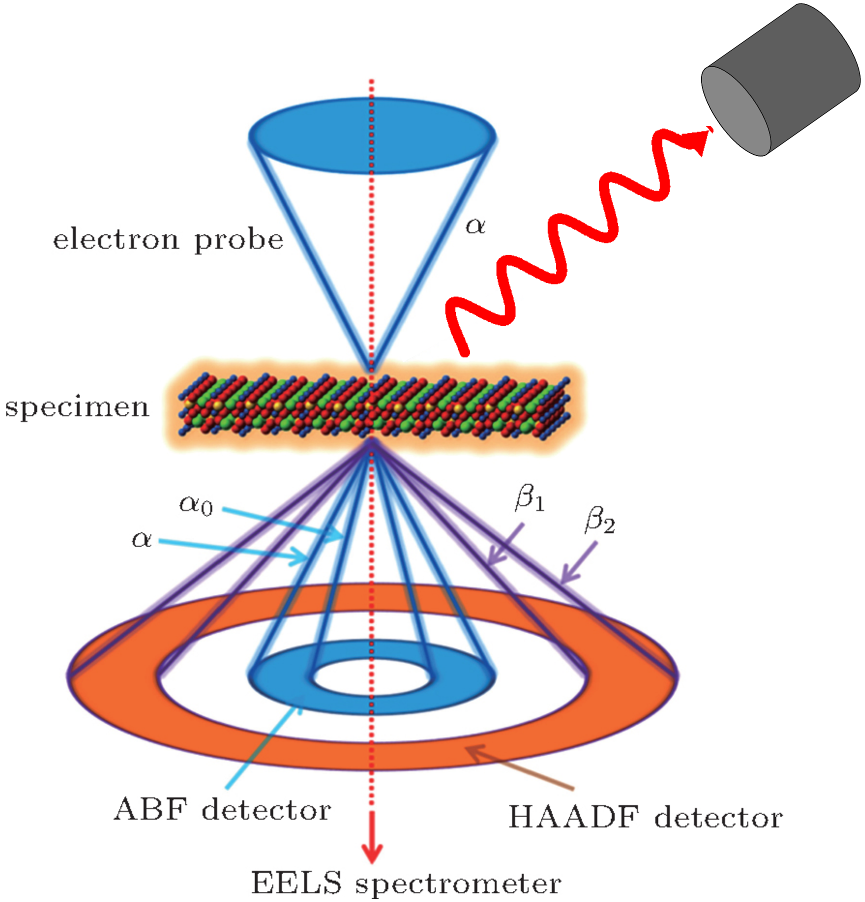
See for instance: D. V. Karlovets, Phys. Rev. A **95**, 032703; A. V. Maiorova, Phys. Rev. A **98**, 042701; V. P. Kosheleva, Phys. Rev. A **98**, 022706; V. Serbo, Phys. Rev. A **92**, 012705...



inelastic scattering

Electron impact excitation and decay

D. Park @ LENA (TU BS)



modified from Z. Qing-Hua, Xiao, Chinese Physics B **25**(6): 066803 (2016)

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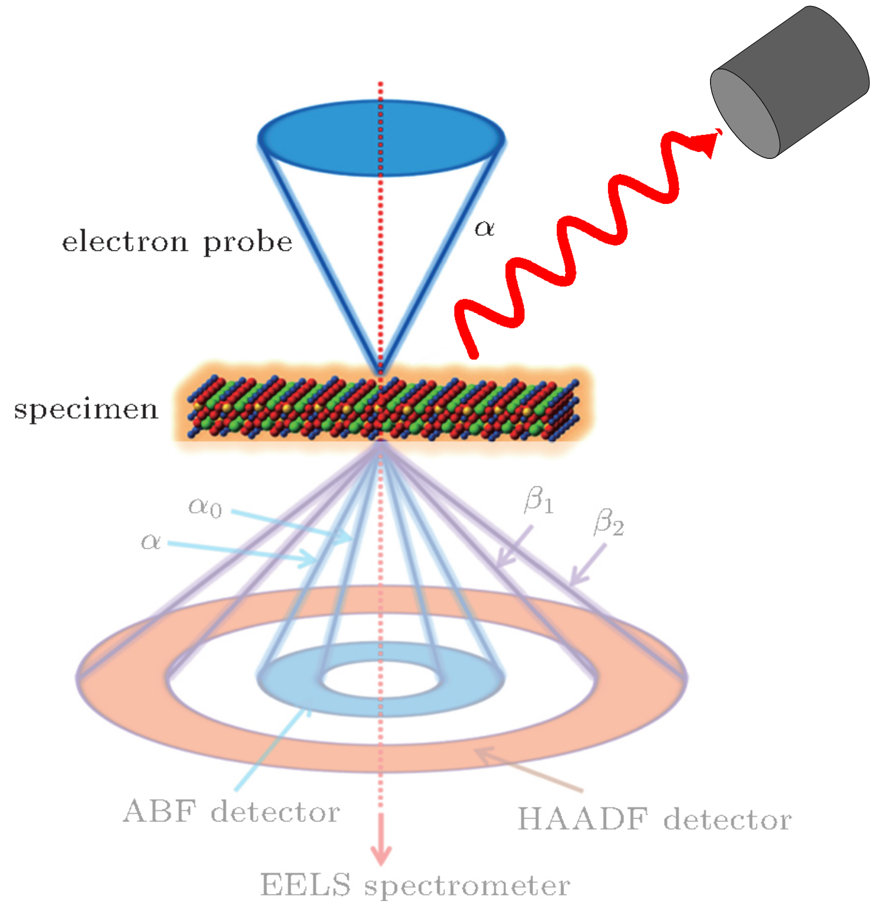
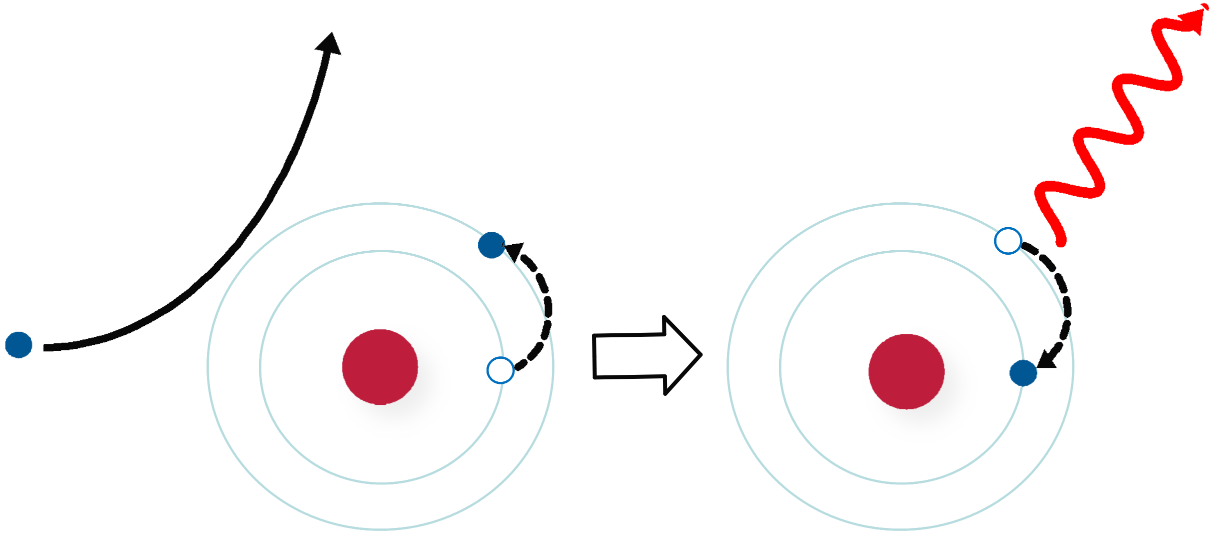


modified from Z. Qing-Hua, Xiao, Chinese Physics B **25**(6): 066803 (2016)

Electron impact excitation and decay

D. Park @ LENA (TU BS)

Two step process



excitation

decay

Photon emission can be observed!

How to describe the photon emission pattern?

The angular distribution of the emitted photons is

$$W(\theta,\phi) = \frac{W_{tot}}{4\pi}\left(1 + \alpha_2^{\gamma}\sqrt{\frac{4\pi}{5}}\sum_{q=-2}^{2} A_{2q}(J_f)\, Y_{2q}(\theta,\phi)\right)$$

Excitation probability

$$W_{\mathrm{tot}}(\alpha_f J_f M_f) = \frac{1}{2J_i+1}\sum_{M_i}\sum_{m_{s'}}\int d\Omega_{p'}\, |f^{(tw)}_{m_{\mathrm{TAM}}}|^2$$

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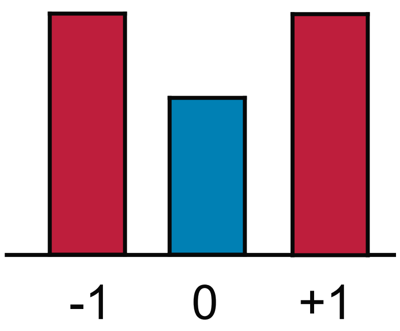
Alignment parameters

$$A_{20} \neq 0$$



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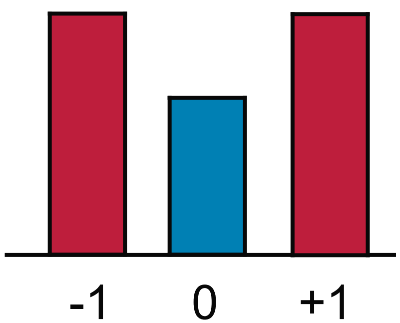
$$W(\theta, \phi) = \frac{W_{tot}}{4\pi} \left(1 + \alpha_2^{\gamma} \sqrt{\frac{4\pi}{5}} \sum_{q=-2}^{2} A_{2q}(J_f) Y_{2q}(\theta, \phi) \right)$$

Excitation probability

$$W_{\text{tot}}(\alpha_f J_f M_f) = \frac{1}{2J_i + 1} \sum_{M_i} \sum_{m_{s'}} \int d\Omega_{p'} \, |f^{(tw)}_{m_{\text{TAM}}}|^2$$

Alignment parameters

$$A_{20} \neq 0$$

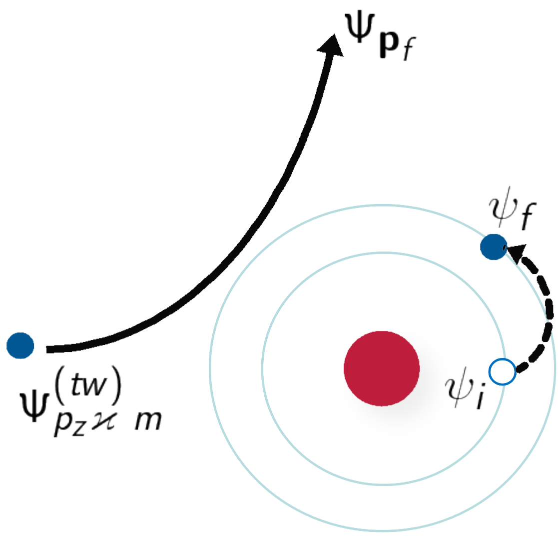


The scattering amplitude needs to be evaluated!

State of the art - theory

Non-relativistic Born approximation for vortex electrons scattered off hydrogen:

$$f^{(tw)}_{m\text{TAM}}(p_z, \varkappa, m, \mathbf{p}') \simeq \left\langle \Psi_{\mathbf{p}_f}\psi_f \left| \frac{1}{r_{12}} \right| \psi_i \Psi^{(tw)}_{p_z\varkappa\; m} \right\rangle$$



Source: R. Van Boxem, Phys. Rev. A 91 (2015) 032703.

State of the art - theory

Non-relativistic Born approximation for vortex electrons scattered off hydrogen:

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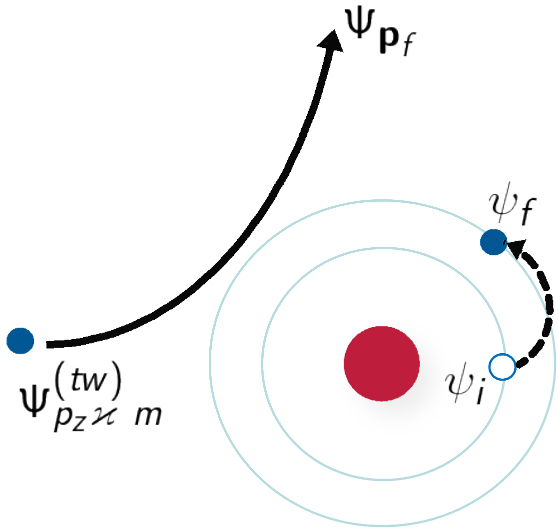
Above, the theory includes...

- Non-relativistic approach
- Born approximation
- Only Coulomb interaction
- Only hydrogen atoms



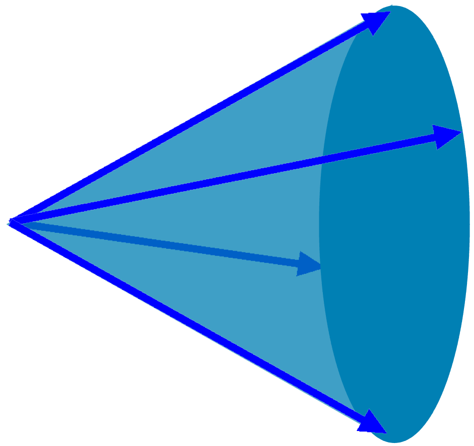
We want to extend this to a relativistic, **distorted wave** and many-electron theory!

Source: R. Van Boxem, Phys. Rev. A 91 (2015) 032703.

Vortex electrons: free vs. distorted basis

free twisted wave

$$\Psi^{(tw)}_{\varkappa m_{\mathrm{TAM}} p_z m_s}(\mathbf{r}) = \int d^3\mathbf{p}\; a_{\varkappa m_{\mathrm{TAM}}}(\mathbf{p}) u_{\mathbf{p} m_s} e^{i\mathbf{pr}}$$

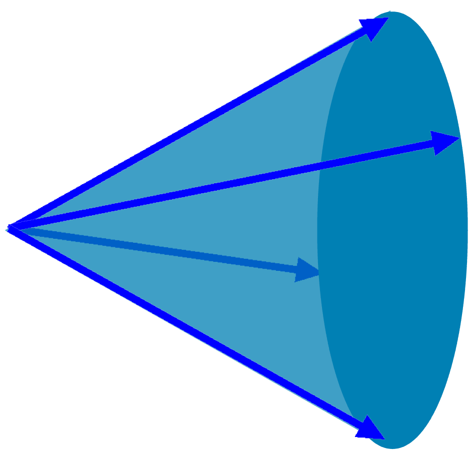


momentum vec. of a plane wave

Vortex electrons: free vs. distorted basis

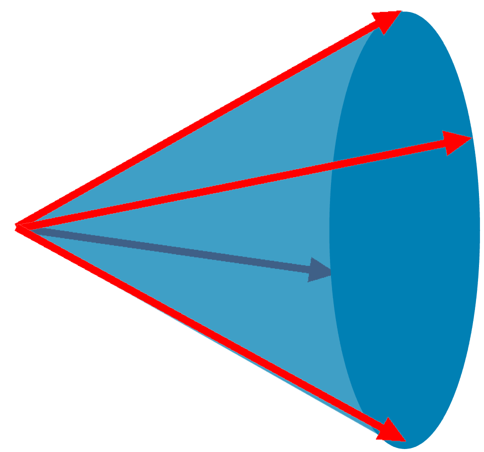
free twisted wave

$$\Psi^{(tw)}_{\varkappa m_{\mathrm{TAM}} p_z m_s}(\mathbf{r}) = \int d^3\mathbf{p}\; a_{\varkappa m_{\mathrm{TAM}}}(\mathbf{p})\, u_{\mathbf{p} m_s} e^{i\mathbf{pr}}$$



distorted twisted wave

$$\Psi^{(tw)}_{\varkappa m_{\mathrm{TAM}} p_z m_s}(\mathbf{r}) = \int d^3\mathbf{p}\; a_{\varkappa m_{\mathrm{TAM}}}(\mathbf{p})\, F^{+}_{\mathbf{p} m_s}(\mathbf{r})$$



→ (blue) momentum vec. of a plane wave

→ (red) momentum vec. of a distorted wave

Relativistic Distorted Wave Approximation

Instead of plane wave solutions, we use the distorted wave function to construct our vortex electron wave function

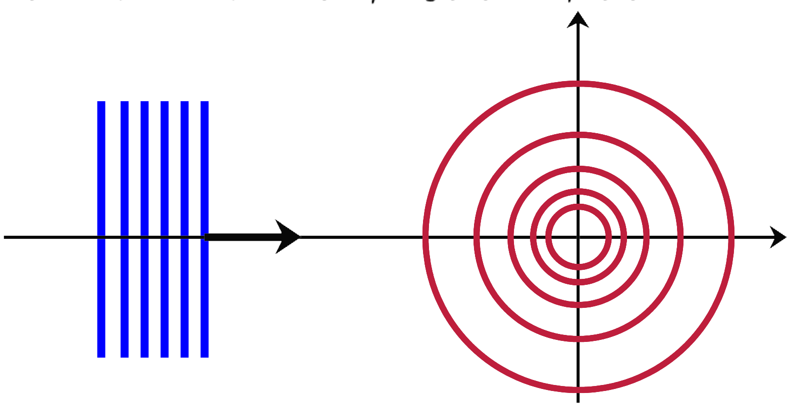
$$\Psi^{(tw)}_{\varkappa m_{\mathrm{TAM}} p_z m_s}(\mathbf{r}) = \int d^3\mathbf{p}\; a_{\varkappa m_{\mathrm{TAM}}}(\mathbf{p}) F^{+}_{\mathbf{p} m_s}(\mathbf{r})$$

The well-known continuum solution of the Dirac equation is

$$F^{\pm}_{\mathbf{p} m_s}(\mathbf{r}) = \frac{1}{\sqrt{4\pi\epsilon p}} \sum_{\kappa\mu} i^l e^{\pm i\Delta_\kappa} \sqrt{2l+1} (l\, 0\, 1/2\, m_s | j\, m_s) D^j_{\mu m_s}(\hat{p}) \varphi_{\epsilon\kappa\mu}(\mathbf{r})$$

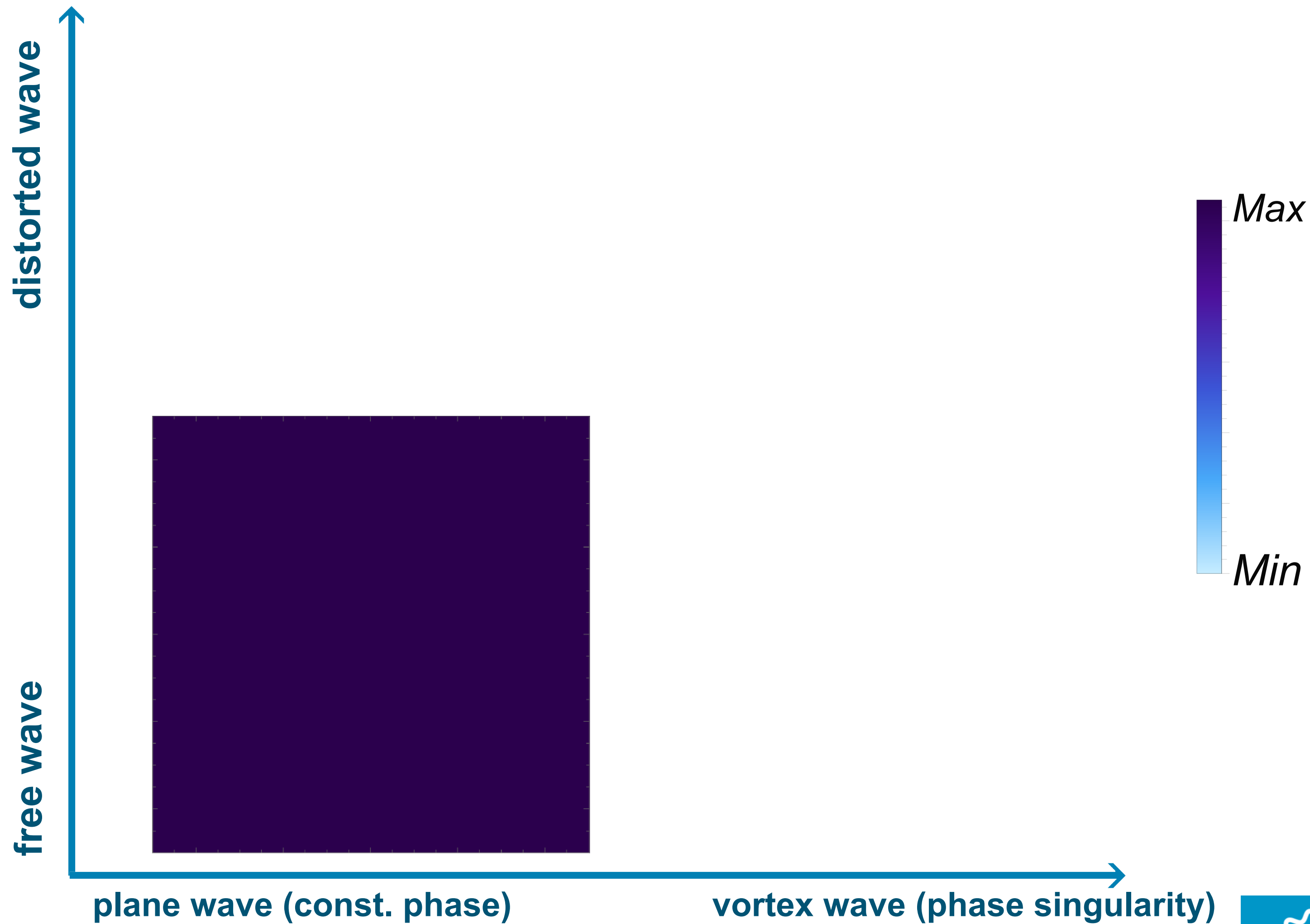
with the asymptotics for big distances

$$\Psi^{(tw)}_{\varkappa m_{\mathrm{TAM}} p_z m_s} \simeq \psi_{free} + f^{(tw)}_{m_{\mathrm{TAM}}} \psi_{spher}$$

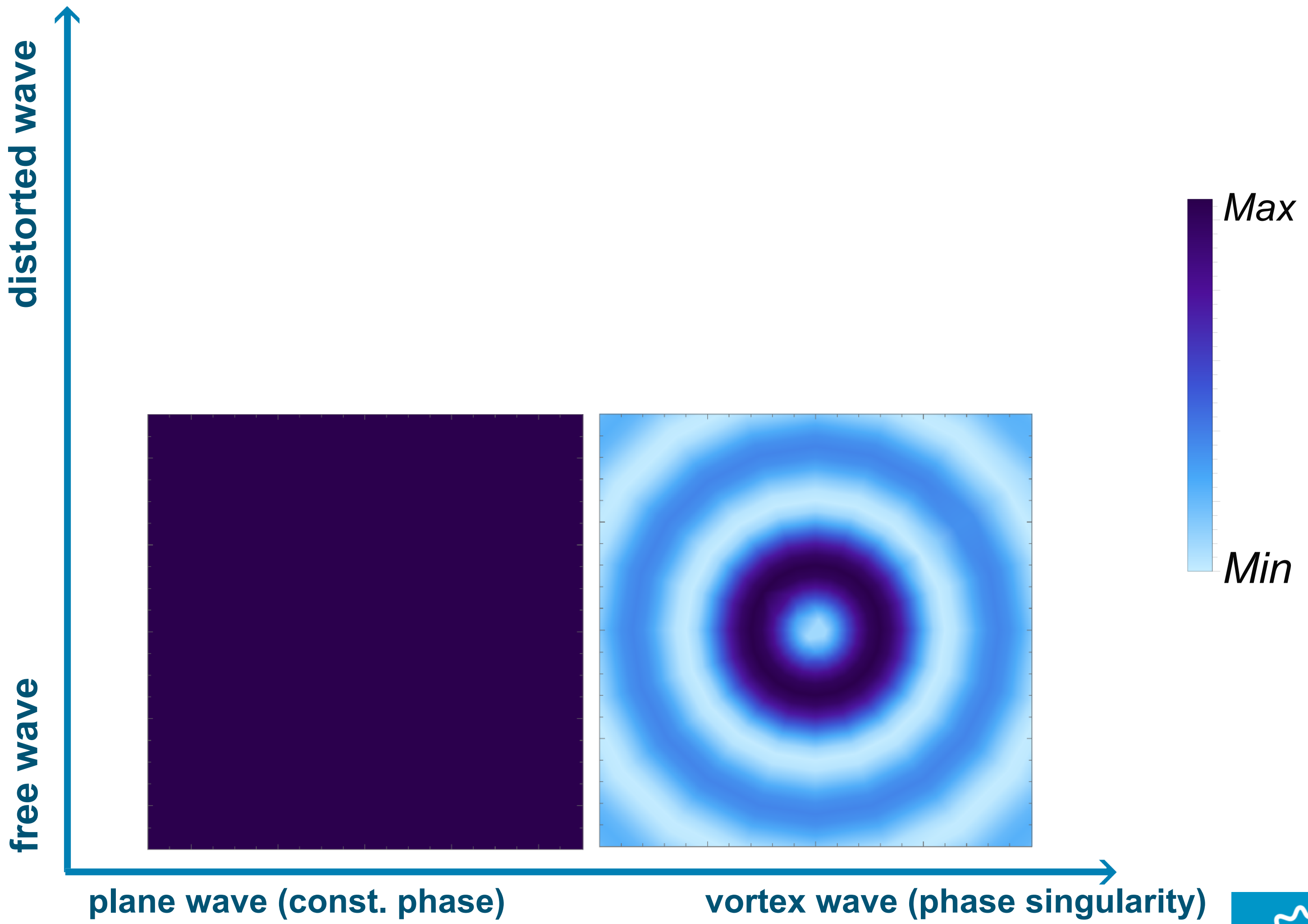


V. A. Zaytsev, V. G. Serbo, and V. M. Shabaev, Phys. Rev. A **95**, 012702

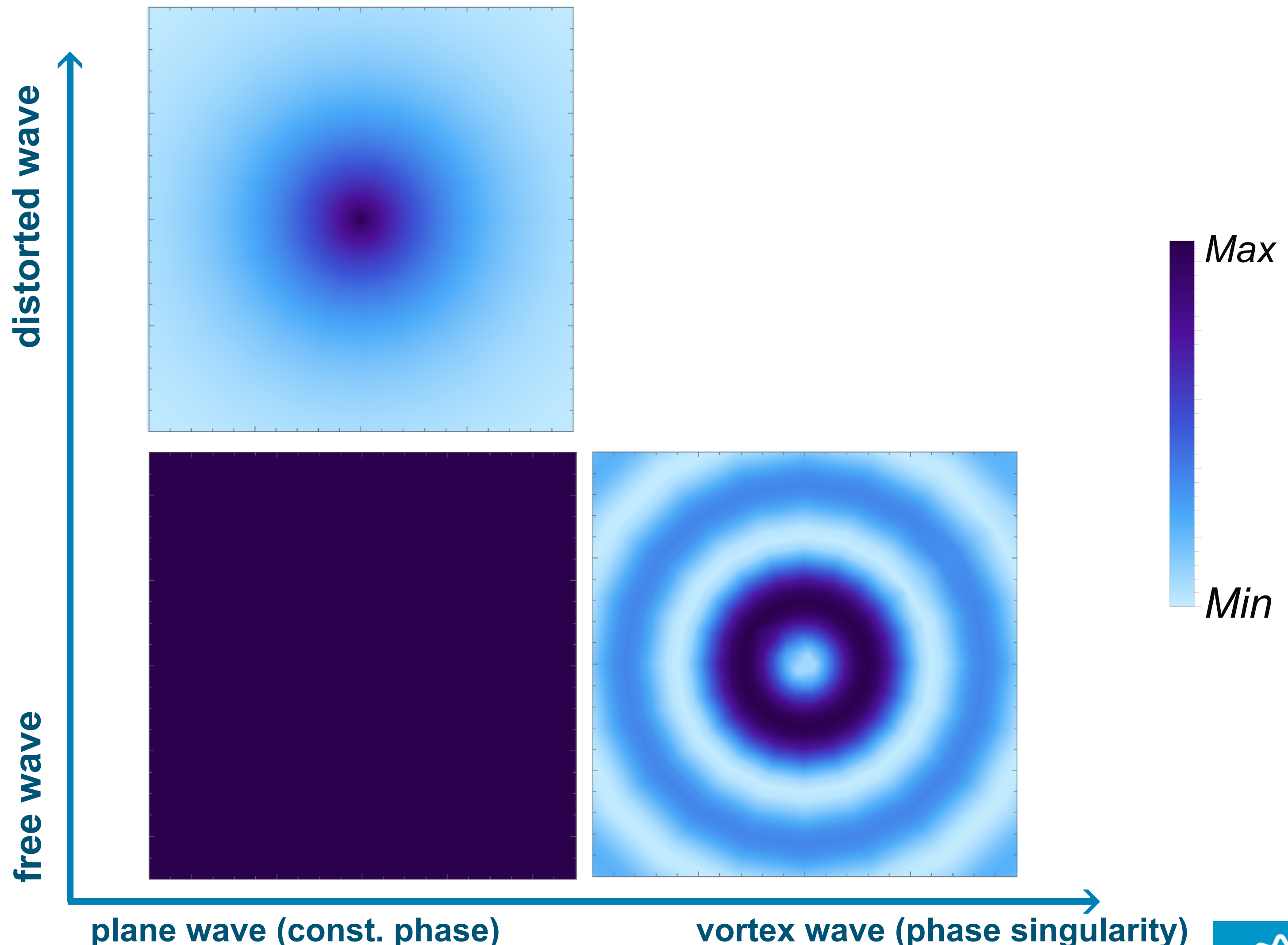
Probability density - free vs. distorted vortex electrons



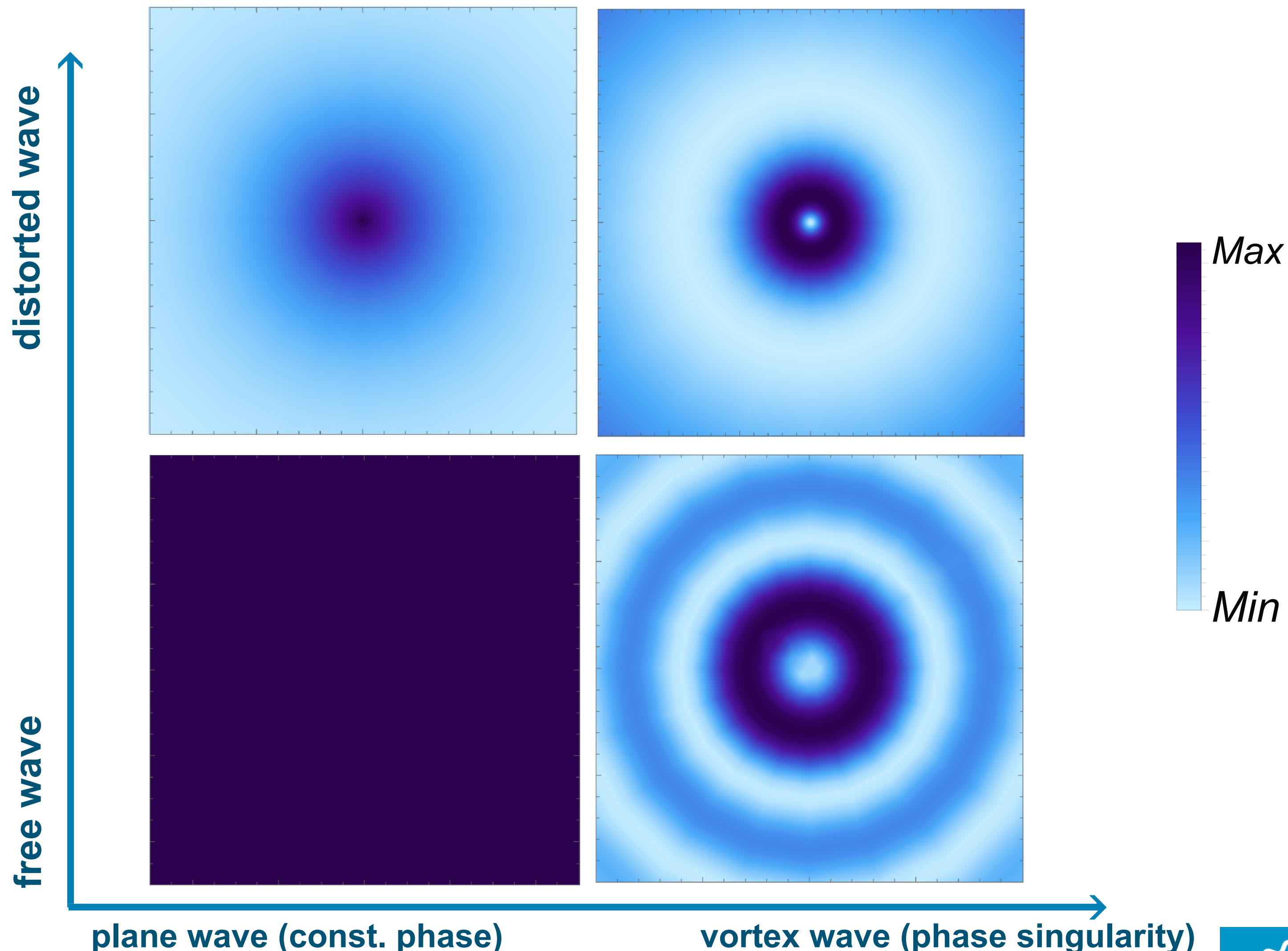
Probability density - free vs. distorted vortex electrons



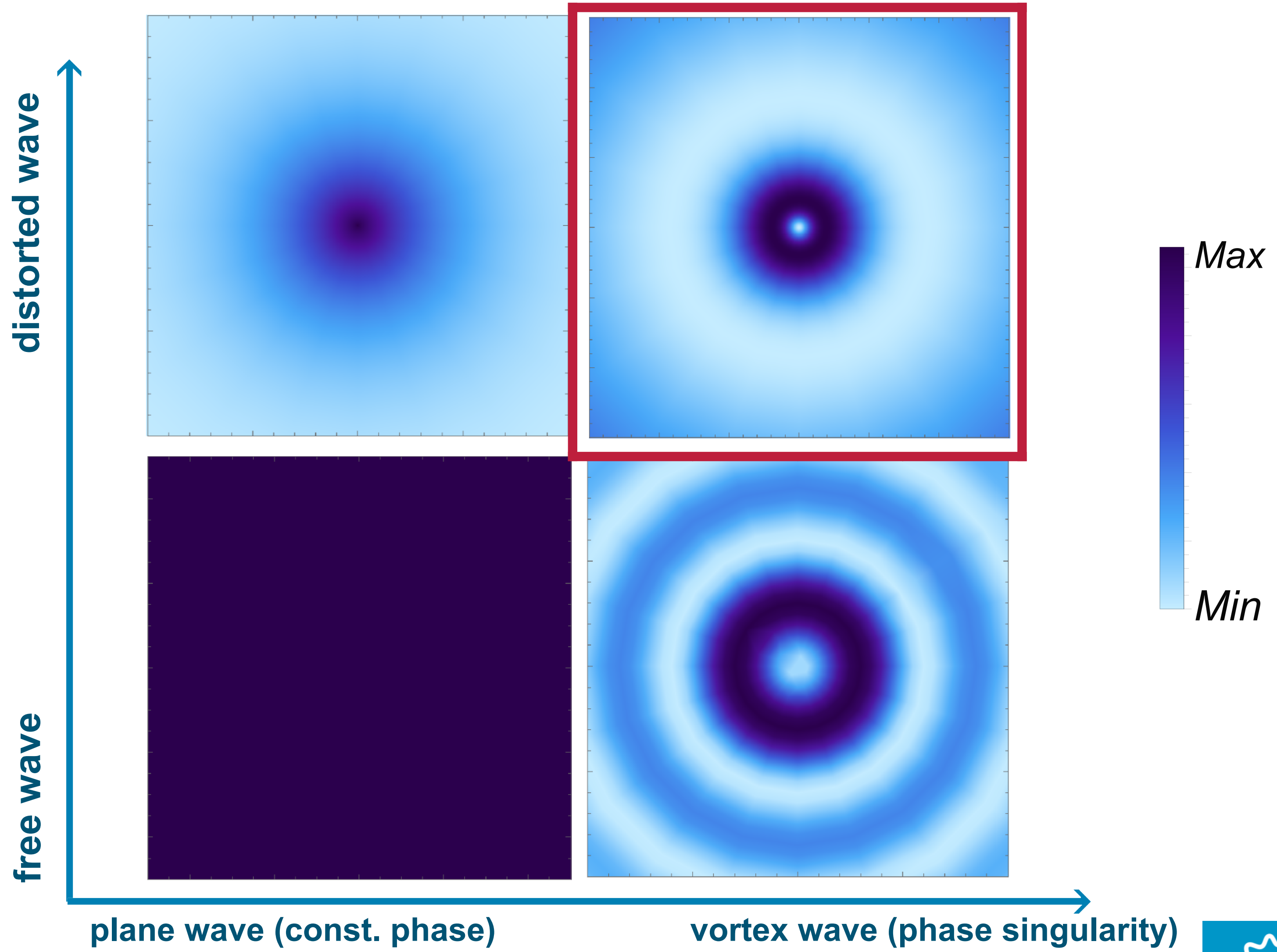
Probability density - free vs. distorted vortex electrons



Probability density - free vs. distorted vortex electrons



Probability density - free vs. distorted vortex electrons



Scattering amplitude - Relativistic Distorted Wave Approximation

"Building-block" of our theory is the scattering amplitude

$$f^{(tw)}_{m_{\mathrm{TAM}}}(\alpha_i, J_i, M_i, \alpha_f, J_f, M_f; p_z, \varkappa, \mathbf{p}') =$$
$$(2\pi)^2 \sqrt{\frac{p'}{p}} \left\langle \psi_{\alpha_f J_f M_f} F^{-}_{\mathbf{p}' m_s'} \middle| \hat{V} \middle| \psi_{\alpha_i J_i M_i} \Psi_{p_z \varkappa\ m_{\mathrm{TAM}}} \right\rangle$$

With the potential

$$\hat{V} = \hat{V}_C + \hat{V}_B - \hat{V}_d$$
$$= \sum_{i<j} \left(\frac{1}{r_{ij}} - \alpha_i \alpha_j \frac{1}{r_{ij}} + \frac{1}{2} (\alpha_i \nabla_i)(\alpha_j \nabla_j) r_{ij} \right) - \hat{V}_d$$

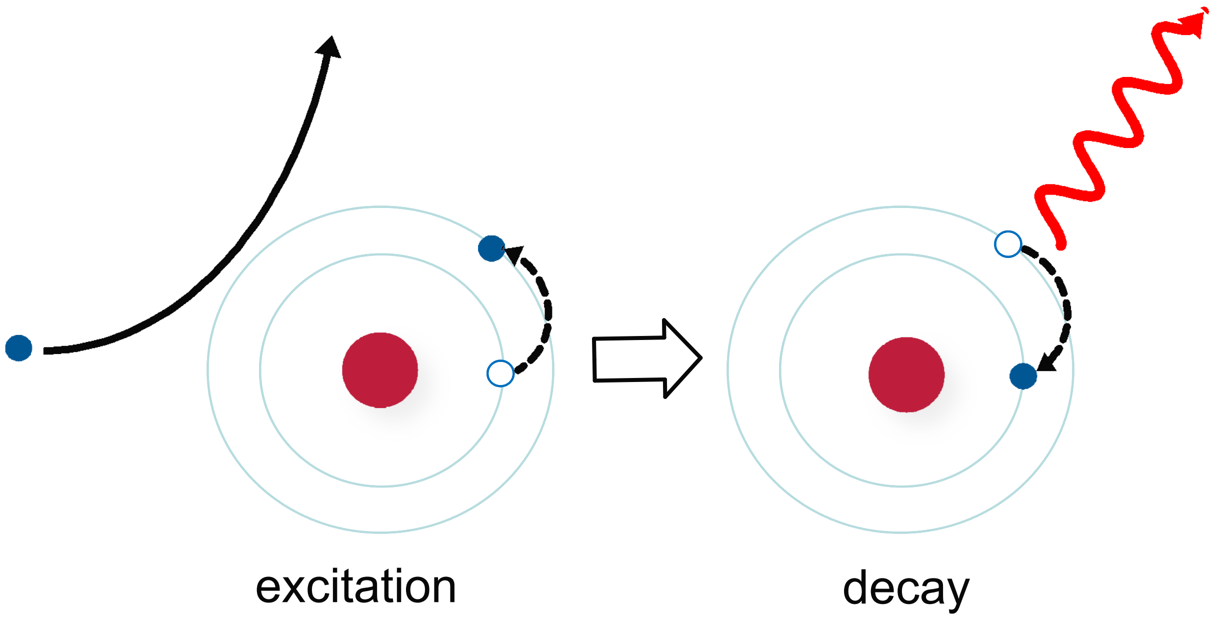
where $|\alpha_i J_i M_i\rangle$ and $|\alpha_f J_f M_f\rangle$ are the initial and final atomic states and $\hat{V}_d$ is the distortion potential.

L. Sharma, Phys. Rev. A **83**, 062701 (2011)

Electron impact excitation and decay

D. Park @ LENA (TU BS)

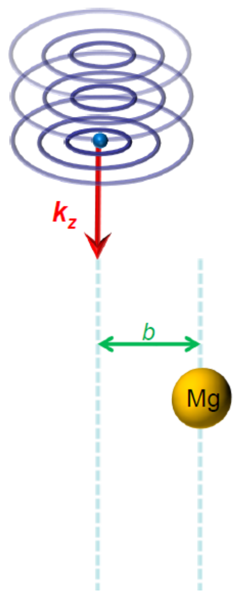
Two step process



Photon emission can be observed!

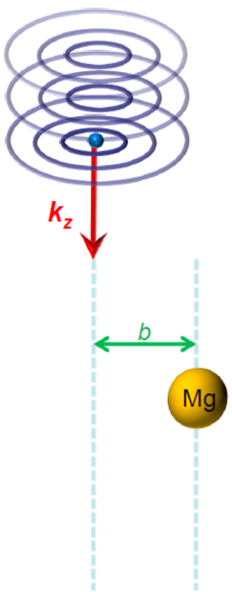
Geometry of the process

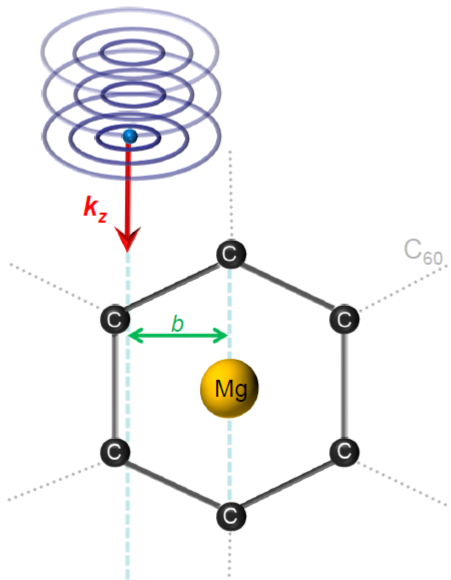
isolated



Geometry of the process

isolated vs. **confined atom**

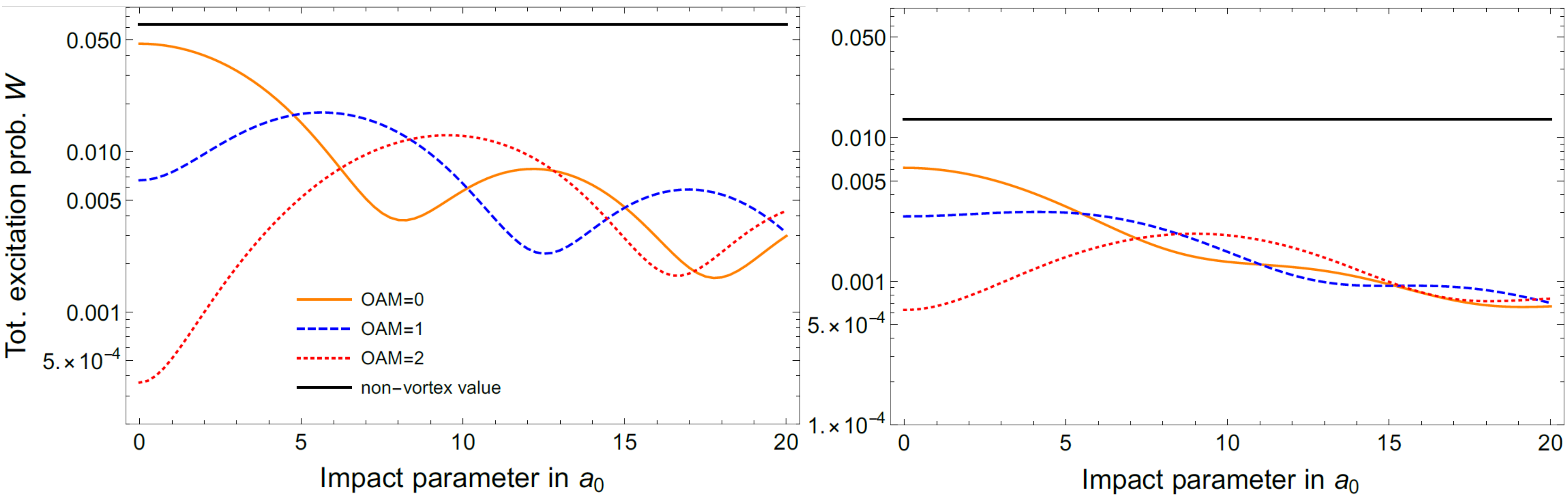




Effect of the environment on the scattering - total ex. rate

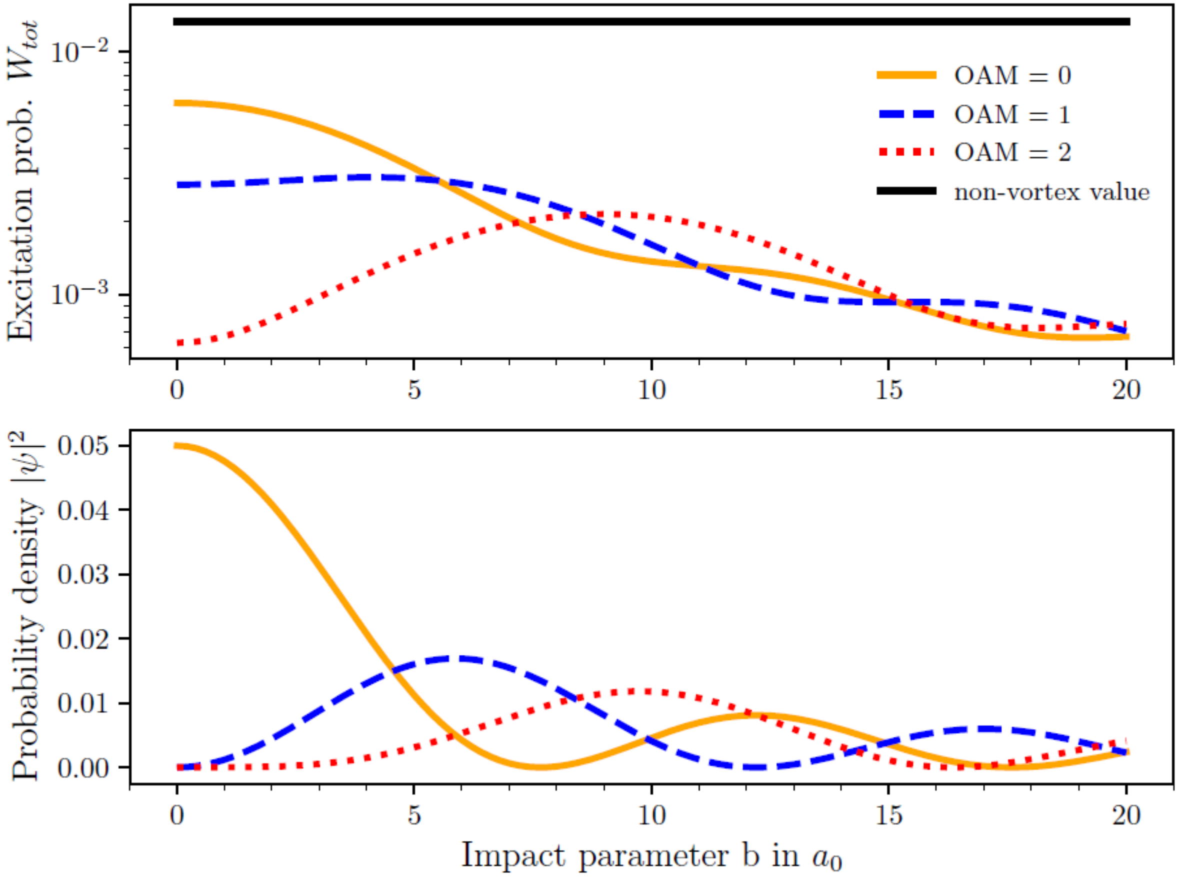
$^1S_0 \rightarrow {}^3P_1$ transistion in Mg, incident electron energy 20 eV, $\theta_k = 15°$

isolated vs. **confined atom**



Oscillations of the probability density (free vortex electron)

$^1S_0 \rightarrow {}^3P_1$ transistion in Mg, incident electron energy 20 eV, $\theta_k = 15°$

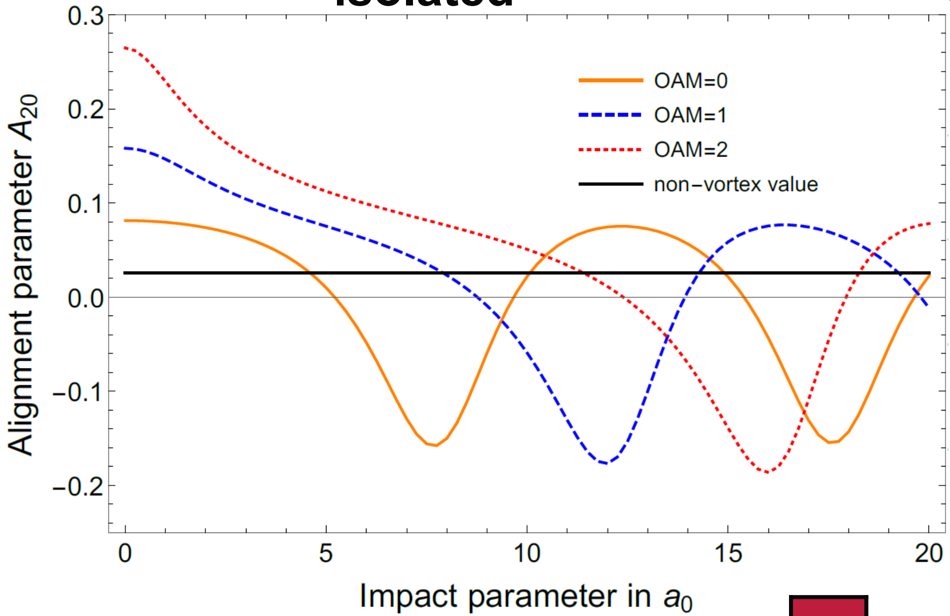


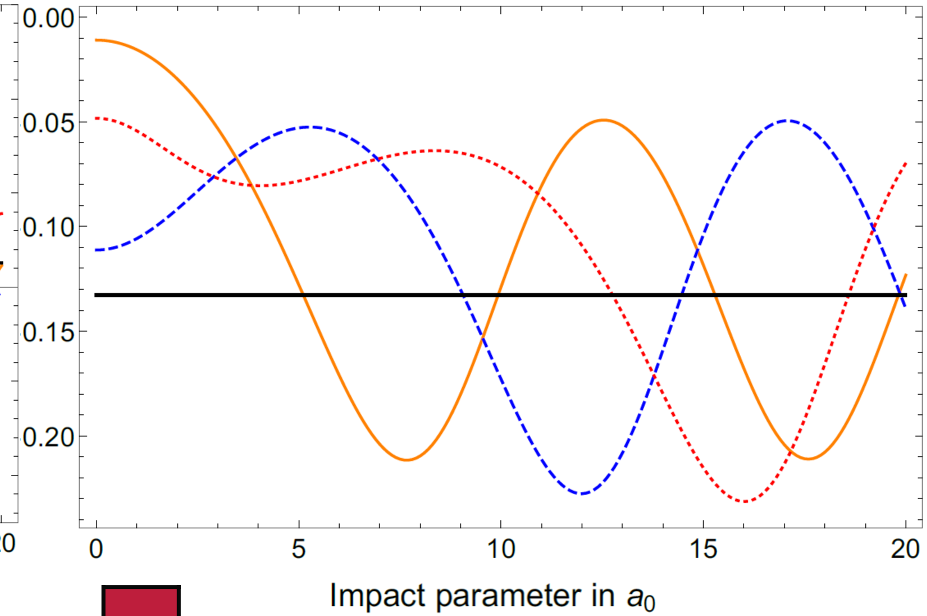
Alignment parameters

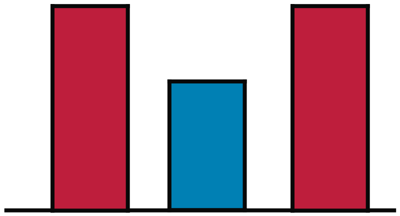
$^1S_0 \rightarrow {}^3P_1$ transistion in Mg, incident electron energy 20 eV, θ_k = 15°

$$A_{20}(J_f = 1) = \frac{\frac{1}{\sqrt{6}} W_{-1} - \sqrt{\frac{2}{3}} W_0 + \frac{1}{\sqrt{6}} W_1}{W_{-1} + W_0 + W_1}$$

isolated vs. **confined atom**

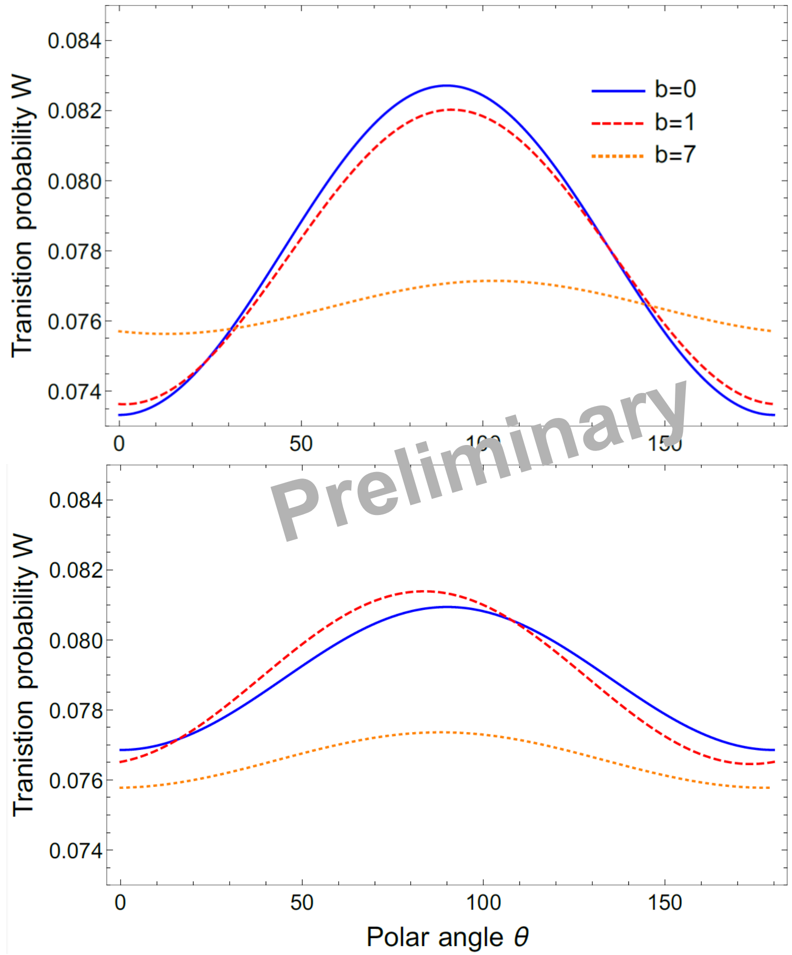






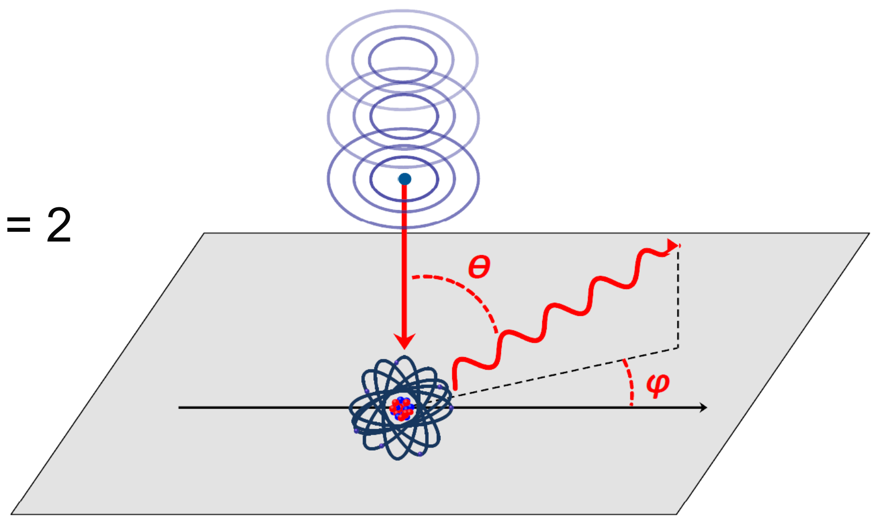
Sebsequent decay of the excited state - θ dependence

Angular distribution of the radiative decay ($^3P_1 \rightarrow {}^1S_0$)



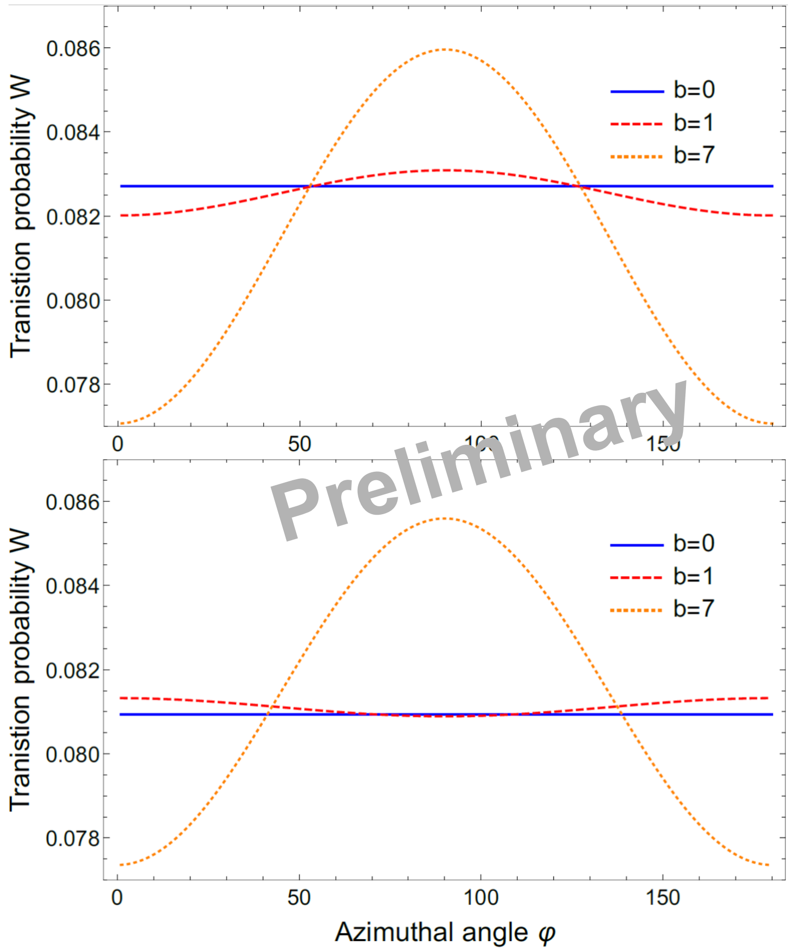
OAM = 1

OAM = 2



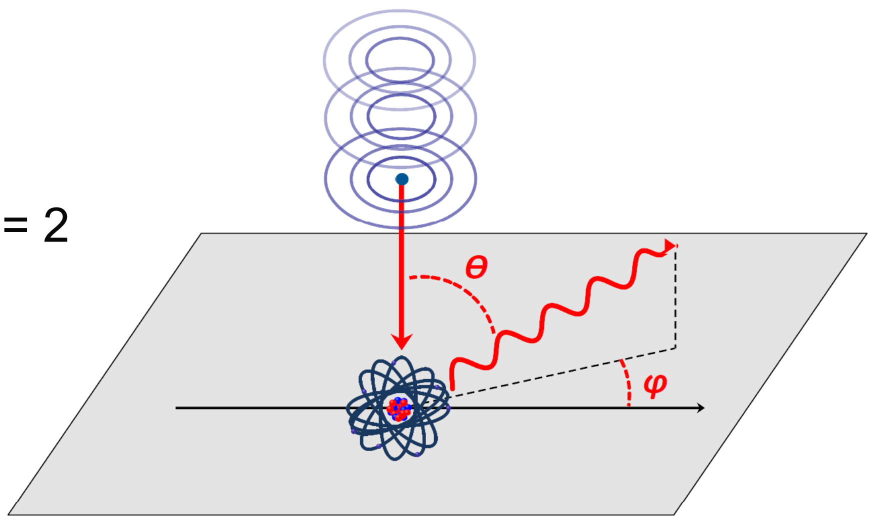
Sebsequent decay of the excited state - φ dependence

Angular distribution of the radiative decay ($^3P_1 \rightarrow {}^1S_0$)



OAM = 1

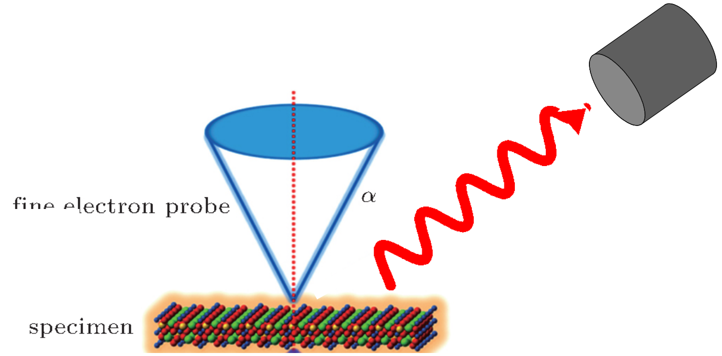
OAM = 2



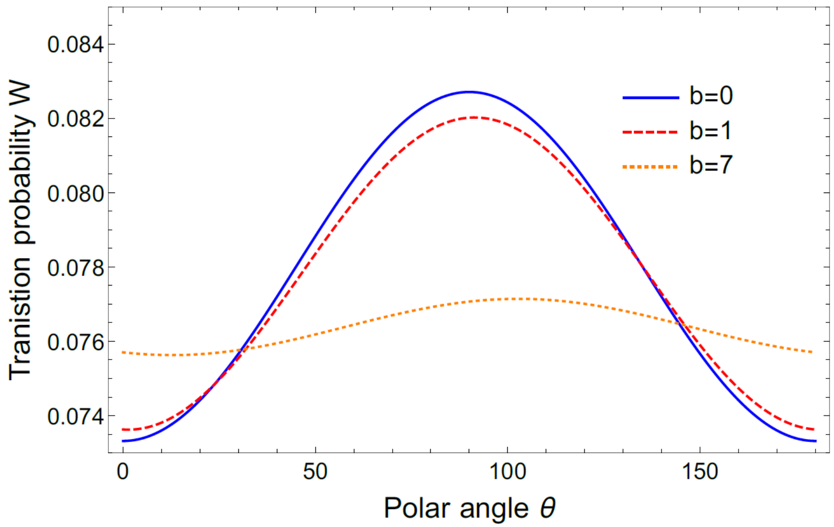
Summary and Outlook

- Development of the scattering theory of relativistic twisted electrons beyond the Born approximation
- Scattering off isolated and confined Mg has been analyzed
- Alignment/orientation of the atom with spatial dependence has been calculated
- Investigation of subsequent decay

- Implementation of twisted electron wave packets
- Higher energies



modified from Z. Qing-Hua, Xiao, Chinese Physics B **25**(6): 066803 (2016)



Acknowledgements

L. Sharma[1], A. Peshkov, R. Schmidt, J. Sommerfeldt, D. Park, D. Hüser, C. Bick and A. Surzhykov

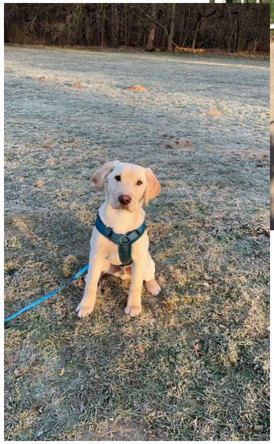
[1] Department of Physics, Indian Institute of Technology, Roorkee 247667, India

all others: Physikalisch Technische Bundesanstalt, Braunschweig D-38116, Germany and

Technische Universität Braunschweig,

Braunschweig D-38106, Germany

... and the FPM group from PTB!



Thank you for your attention!

Relativistic Distorted Wave Approximation

Instead of plane wave solutions, we use the continuum solution of the Dirac equation to receive our vortex electron wave function

$$\Psi^{(tw)}_{\varkappa m_{\mathrm{TAM}} p_z m_s}(\mathbf{r}) = \int d^3\mathbf{p}\; a_{\varkappa m_{\mathrm{TAM}}}(\mathbf{p}) F^{+}_{\mathbf{p} m_s}(\mathbf{r})$$

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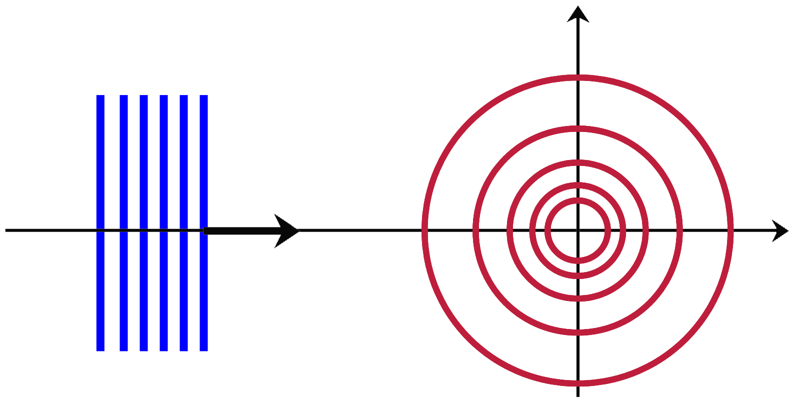
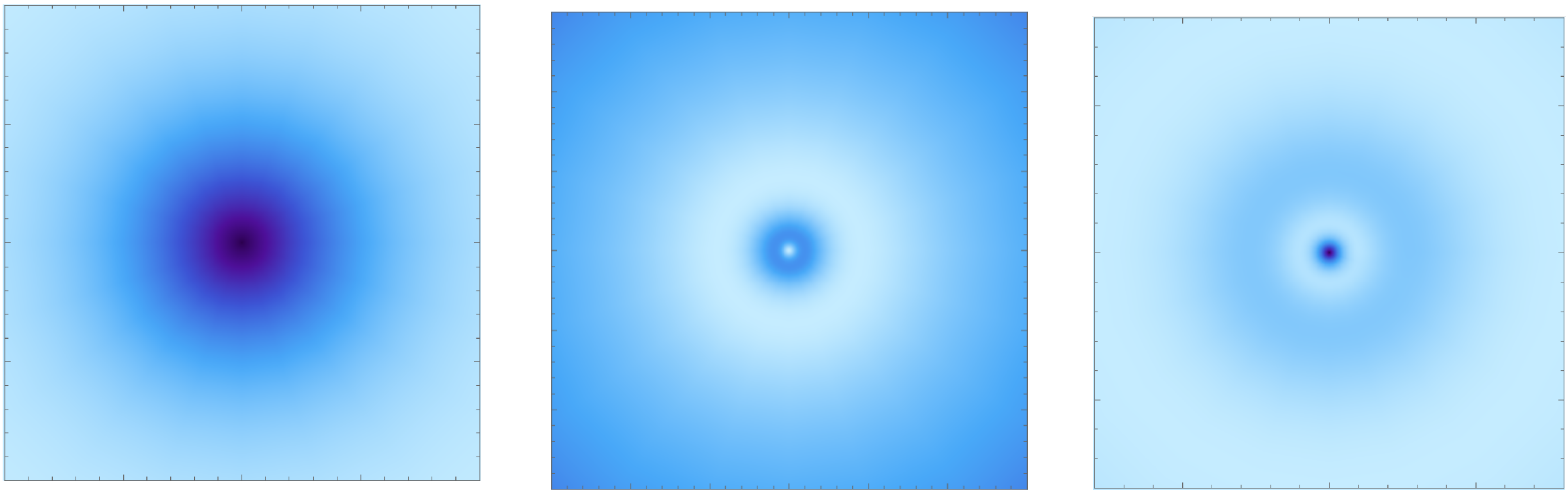
with the asymptotics

$$\psi \simeq \psi_{pw} + f\psi_{spher}$$



Relativistic Distorted Wave Approximation

b = 1.5



continuum | continuum+vortex | continuum+vortex+ displacement

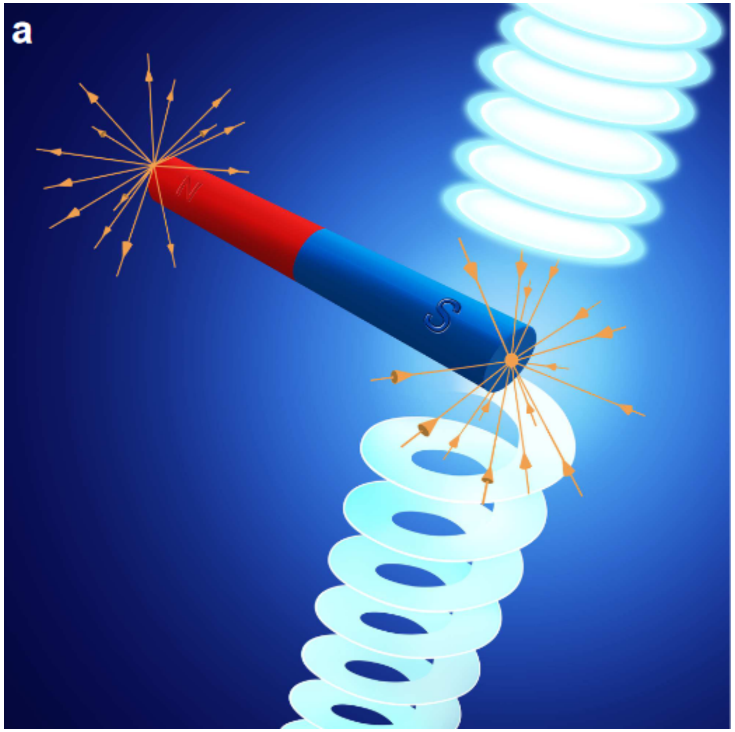
Alignment/orientation

$$\mathcal{A}_{kq}(\alpha J;\mathbf{p}_0,\mathbf{p}) = \rho^f_{kq}(\alpha J;\mathbf{p}_0,\mathbf{p})\,/\rho^f_{00}(\alpha J;\mathbf{p}_0,\mathbf{p})$$
$$= \hat{J}\sum_{MM'}(-1)^{J-M'}\left(JM,J-M'\,|\,kq\right)$$
$$\times \frac{\sum_{M_0\mu_0\mu} T_{M_0\mu_0\to M\mu}(\mathbf{p}_0,\mathbf{p})T^*_{M_0\mu_0\to M'\mu}(\mathbf{p}_0,\mathbf{p})}{\sum_{MM_0\mu_0\mu}|T_{M_0\mu_0\to M\mu}(\mathbf{p}_0,\mathbf{p})|^2}$$

$$\mathcal{A}_{k0}(\alpha J;\mathbf{p}_0) = \frac{1}{\sigma(\alpha J)}\sum_{M=-J}^{J}(-1)^{J-M}(JM,J-M\,|\,k0)\,\sigma(\alpha JM)$$

V. V. Balashov,et al., Polarization and Correlation Phenomena in Atomic Collisions (Kluwer Academic, 2000).

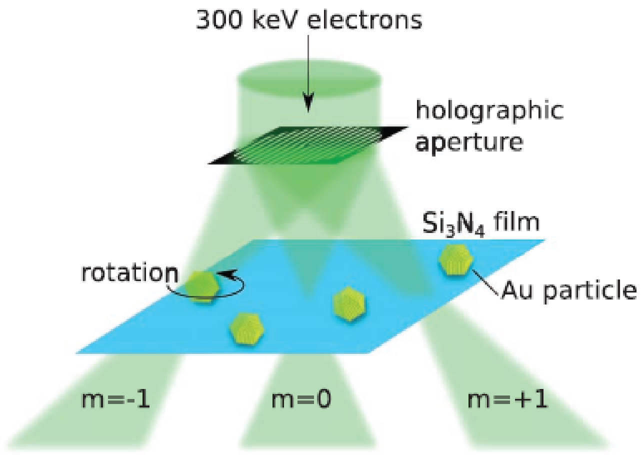
Magnetic quasi-monopoles



Source: A. Béché, arXiv:1305.0570v2

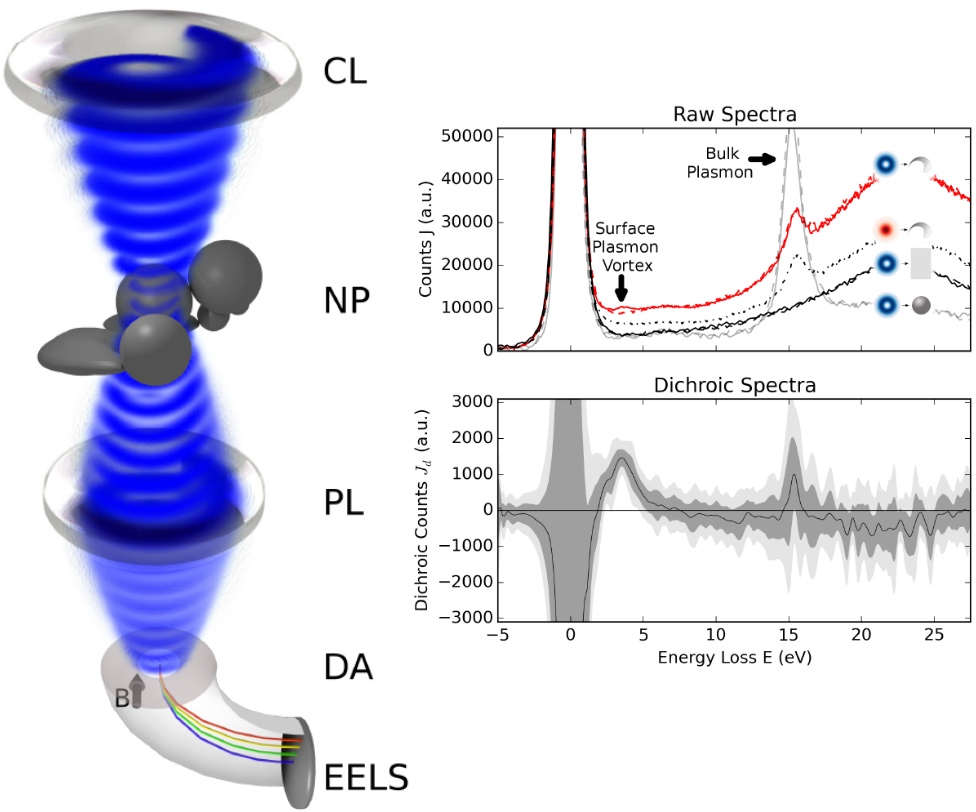
Manipulation of nanoparticles

angular momentum can be transferred to nanoparticles setting them into a rotating motion



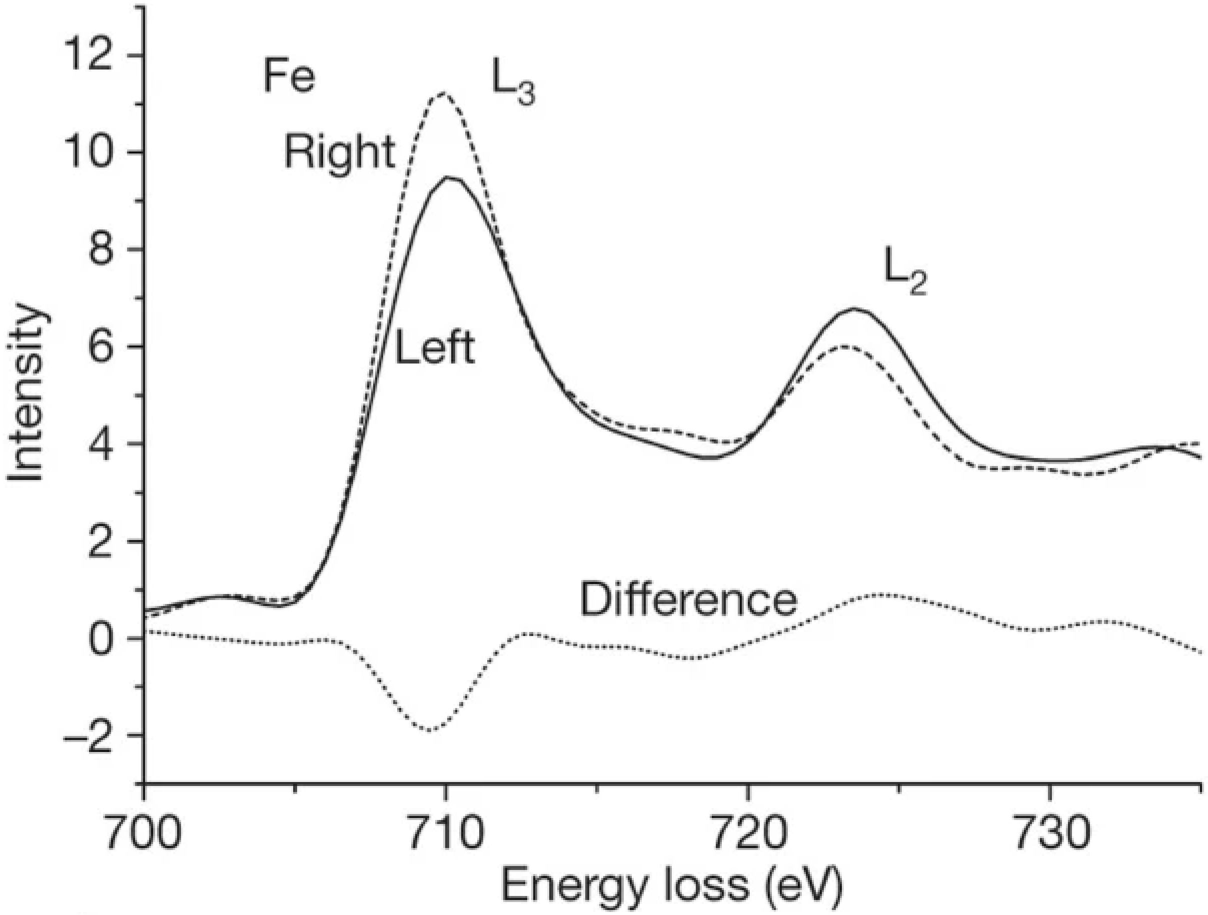
Source: Verbeeck et al. Adv. Mater. **25**, 1114–1117 (2012)

Probing chirality with vortex electrons



Source: Tyler R. Harvey et al., arXiv:1507.01810v1 (2015)

Magnetic Electron Energy Loss Spectroscopy



Source: Verbeck et al. Nature volume 467, pages 301–304 (2010)

Spintronic applications

- characterization of spintronic devices
- employing spin-polarized current injection

Source: Yuan et al. PRA **88**, 031801(R) (2013)

Distortion Potential

L. Sharma ,Phys. Rev. A **83**, 062701 (2011)

$$V_d(r) = V_{\text{st}}(r) + V_{\text{ex}}(r)$$

$$V_{\text{st}}(r) = -\frac{Z-N}{r} + \sum_{j\in \text{all subshells}} \mathcal{N}_j \int_0^\infty \left[P^2_{n_j\kappa_j}(r_j) + Q^2_{n_j\kappa_j}(r_j)\right]\frac{1}{r_>}dr.$$

$$V_{\text{ex}}(r) = \frac{1}{2}\left[\left(\frac{1}{2}k^2 - V_{\text{st}}(r) + \frac{3}{10}[3\pi^2\rho(r)]^{\frac{2}{3}}\right) - \left\{\left(\frac{1}{2}k^2 - V_{\text{st}}(r) + \frac{3}{10}[3\pi^2\rho(r)]^{\frac{2}{3}}\right)^2 + 4\pi\rho(r)\right\}^{\frac{1}{2}}\right]$$

$$\rho(r) = \frac{1}{4\pi r^2}\sum_{j\in \text{all subshells}} \mathcal{N}_j\left[P^2_{n_j\kappa_j}(r_j) + Q^2_{n_j\kappa_j}(r_j)\right]$$

Distortion Potential

Y. Itikawa, PHYSICS REPORTS (Review Section of Physics Letters) 143, No. 2 (1986) 69—108

One of the simplest derivations of DWM is based on the standard first-order perturbation theory. The total Hamiltonian of the system of an electron and an atom (ion) is (atomic units being used throughout the present paper unless otherwise stated)

$$\mathscr{H} = \mathscr{H}_{\mathrm{T}}(1, \ldots, N) + \mathscr{J}(N+1) + V(1, \ldots, N+1)\,, \tag{3.1}$$

where $\mathscr{H}_{\mathrm{T}}$ is the Hamiltonian of the target (N being the number of the bound electrons), $\mathscr{J}(N+1)$ is the kinetic energy operator for the incident ($(N+1)$th) electron, and V is the interaction between the electron and the target. We denote by $\mathscr{H}_0$ the Hamiltonian for the target and the non-interacting electron:

$$\mathscr{H}_0 = \mathscr{H}_{\mathrm{T}}(1, \ldots, N) + \mathscr{J}(N+1)\,. \tag{3.2}$$

This describes the asymptotic region of the collision system. When the target is an ion, the Coulomb interaction with the ionic charge is usually included in $\mathscr{H}_0$ (see section 3.4.3).

Now introduce a distortion potential, U, and assume that the eigenfunction of the Hamiltonian

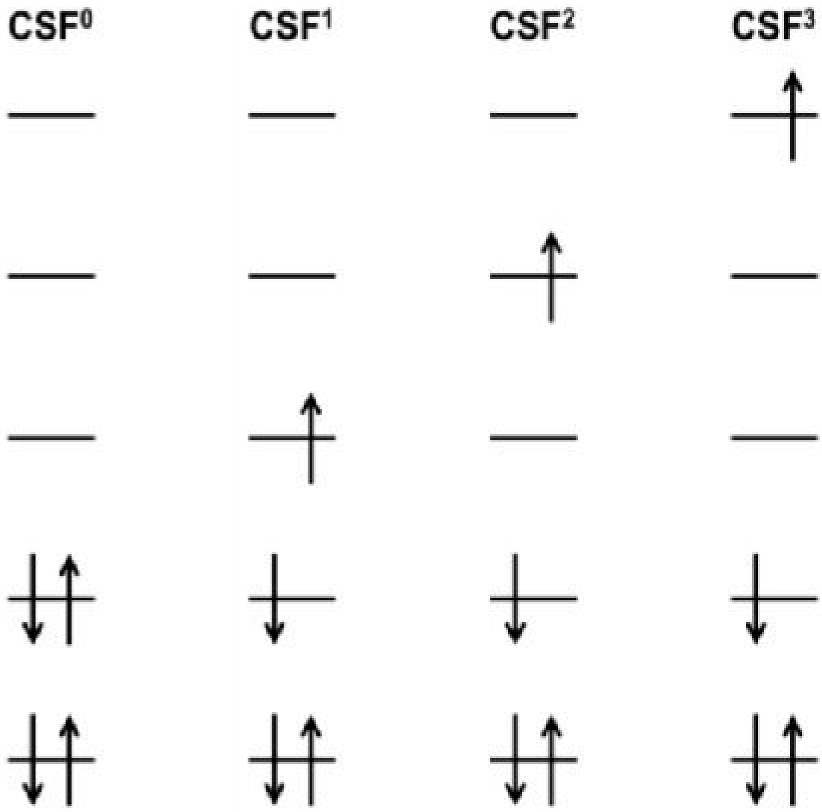
$$\bar{\mathscr{H}} = \mathscr{H}_0 + U \tag{3.3}$$

is already known. Taking the difference, $V - U$, as a perturbation, we employ the first-order perturbation theory. The transition matrix for the excitation process a→b is given by (electron exchange being neglected for the moment)

$$T^{\mathrm{DW}}(\mathrm{a}\to\mathrm{b}) = \langle \chi_{\mathrm{b}}^{(-)} | V - U | \chi_{\mathrm{a}}^{(+)} \rangle\,. \tag{3.4}$$

General-purpose Relativistic Atomic Structure (GRASP)

- Multiconfiguration self-consistent-field calculations based on the Dirac-Coulomb Hamiltonian



Source: https://www.gloriabazargan.com/blog/ci-calculations

Elastic scattering by crystals

Atoms are described by a sum of Yukawa potentials

$$V(r) = \sum_i \frac{A_i}{r} e^{-\alpha_i r}$$

With the well-known scattering amplitude (Born approximation):

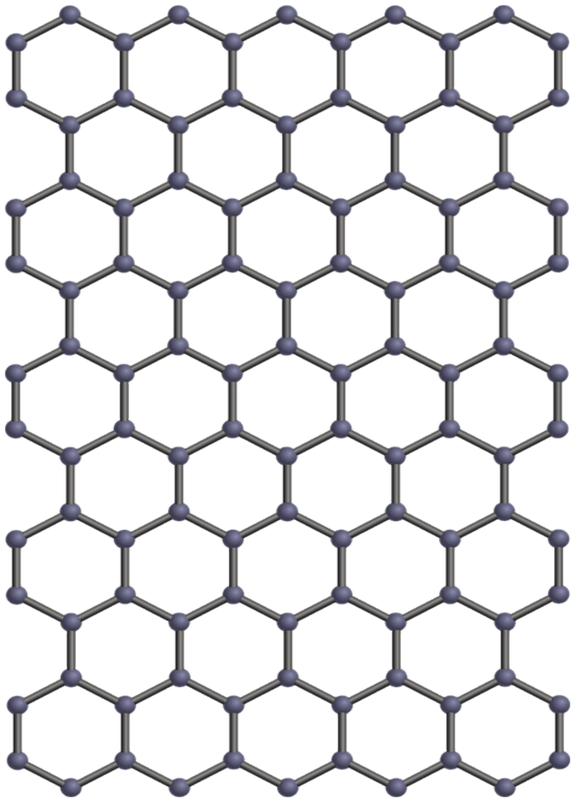
$$f(\boldsymbol{q}) = \sum_i \frac{2ZA_i}{\mu_i^2 + \boldsymbol{q}^2}$$

F. SALVAT, J. D. MARTÍNEZ, R. MAYOL, AND J. PARELLADA

TABLE I. Parameters of the analytical screening function $\phi_a(r)$. Elements indicated with an asterisk have DHFS radial expected values inconsistent with conditions (15).

Element	A_1	A_2	α_1	α_2	α_3
H 1*	−184.39	185.39	2.0027	1.9973	
He 2*	−0.2259	1.2259	5.5272	2.3992	
Li 3*	0.6045	0.3955	2.8174	0.6625	
Be 4*	0.3278	0.6722	4.5430	0.9852	
B 5*	0.2327	0.7673	5.9900	1.2135	
C 6*	0.1537	0.8463	8.0404	1.4913	
N 7*	0.0996	0.9004	10.812	1.7687	
O 8*	0.0625	0.9375	14.823	2.0403	

Source: Salvat *et al*. PRA **36** 467 (1987)



$$V(\boldsymbol{r}) = \sum_j V(\boldsymbol{r} + \boldsymbol{R}_j)$$