New results on vortex electron photoemission and scattering by atomic targets

Alisa Chaikovskaia

ITMO University, Saint-Petersburg

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Vortex states in nuclear and particle physics
Zhuhai, China


City of fountains, City of culture


City of youth, City of vigour

What the talk is about

Vortex electron
photoemission

Vortex electron
"applications"

There are many well-known works in

- photoionization

  O. Matula, A. Hayrapetyan, V. Serbo, A. Surzhykov, S. Fritzsche. Atomic ionization by twisted photons: Angular distribution of emitted electrons. J. Phys. B: At. Mol. Opt. Phys., 2013,

  A. Peshkov, D. Seipt, A. Surzhykov, S. Fritzsche. Photoexcitation of atoms by Laguerre-Gaussian beams. PRA, 2017,...

- scattering of vortex electrons

  V. Serbo, I. P. Ivanov, S. Fritzsche, D. Seipt, and A. Surzhykov. Scattering of twisted relativistic electrons by atoms. PRA, 2015,

  D. V. Karlovets, G. L. Kotkin, V. G. Serbo, and A. Surzhykov. Scattering of twisted electron wave packets by atoms in the Born approximation. PRA, 2017, ...

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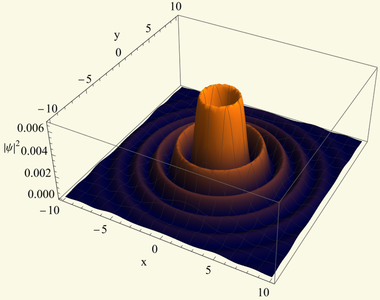
But there would be smth new

- evolved state formalism (see D. Karlovets talk on Thursday)
- somewhat exotic LG state
- vortex electrons of high energies
- focus on getting information about an electron beam

Vortex photo-electron

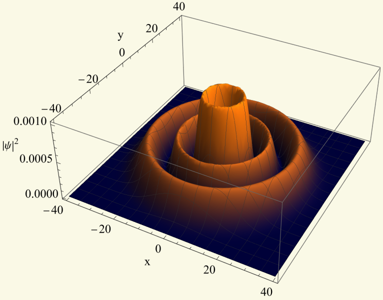
(preliminary results)



Bessel profile, $l = 2$

$$\boldsymbol{A}^{B}_{\kappa\ell k_z\Lambda}(\boldsymbol{r}) = \int \frac{\mathrm{d}^2 \boldsymbol{k}_\perp}{(2\pi)^2} a_{\kappa\ell}(\boldsymbol{k}_\perp) \boldsymbol{A}_{\boldsymbol{k}\Lambda}(\boldsymbol{r}) e^{-i\boldsymbol{k}_\perp \boldsymbol{b}}$$

$$a_{\kappa\ell}(\boldsymbol{k}_\perp) = \sqrt{\frac{2\pi}{\kappa}} (-i)^\ell e^{i\ell\varphi_k} \delta(|\boldsymbol{k}_\perp| - \kappa)$$



Laguerre - Gaussian profile, $l = 2$, $n = 2$

$$\boldsymbol{A}^{LG}_{lnk_z\Lambda}(\boldsymbol{r}) = \int \frac{\mathrm{d}^2 \boldsymbol{k}_\perp}{(2\pi)^2} U_{ln}(\boldsymbol{k}_\perp) \boldsymbol{A}_{\boldsymbol{k}\Lambda}(r) e^{-i\boldsymbol{k}_\perp \boldsymbol{b}}$$

$$U_{ln}(\boldsymbol{k}_\perp) = (-1)^{\ell+n} \pi 2^{l/2} i^\ell w_0^{\ell+1} k_\perp^\ell \exp\left[-\frac{k_\perp^2 w_0^2}{4}\right] \times L_n^\ell\left(\frac{k_\perp^2 w_0^2}{2}\right) \exp[i\ell\varphi_k]$$

Evolved state

$$|ev\rangle = \hat{S}\,|i\rangle = \int \frac{\mathrm{d}^3 p_{f'}}{(2\pi)^3}\,|f'\rangle \underbrace{\langle f'|\,\hat{S}\,|i\rangle}, \quad |ev\rangle = \int \frac{\mathrm{d}^3 p_{f'}}{(2\pi)^3}\,|f'\rangle\, S_{fi}$$

Then the final state wave function in the momentum representation is

$$\psi_{\mathbf{ev}}(\boldsymbol{p}_f) \equiv \langle \boldsymbol{p}_f | ev\rangle = \int \frac{\mathrm{d}^3 p_{f'}}{(2\pi)^3}\,\langle \boldsymbol{p}_f | \boldsymbol{p}_{f'}\rangle\, S_{fi} = \int \frac{\mathrm{d}^3 p_{f'}}{(2\pi)^3}\delta(\boldsymbol{p}_f - \boldsymbol{p}_{f'}) S_{fi} = S_{fi}(\boldsymbol{p}_f)$$

- state as it is $\Rightarrow$ no dependence on detection scheme
- we keep phase in S_{fi}

OAM operator action in the momentum representation

$$\langle \boldsymbol{p}|\,\hat{L}_z\,|ev\rangle = -i\frac{\partial}{\partial \varphi_p}\,\langle \boldsymbol{p}|ev\rangle = -i\frac{\partial}{\partial \varphi_p}\psi_{ev}(\boldsymbol{p})$$

In relativistic theory:

$$S_{fi}^{(1)} = ie \int \psi_f^*(\boldsymbol{r},t)\boldsymbol{\alpha}\boldsymbol{A}(\boldsymbol{r},t)\psi_i(\boldsymbol{r},t)\mathrm{d}^4x = 2\pi i\delta(\varepsilon_i + \omega - \varepsilon_f)M_{fi}$$

In the non-relativistic limit $\boldsymbol{\alpha} \Longrightarrow -i\nabla/m$. Then

$$M_{fi} = -i\frac{e}{m}\int \psi_f^*(\boldsymbol{r})\boldsymbol{A}\nabla\psi_i(\boldsymbol{r})\,\mathrm{d}^3x, \quad \boldsymbol{A}_{\boldsymbol{k}\Lambda}(\boldsymbol{r}) = \boldsymbol{e}_{\boldsymbol{k}\Lambda}e^{i\boldsymbol{k}\boldsymbol{r}}$$

Initial matter state – an electron in the “hydrogen"-like atom. Final – plane wave.

$$\psi_i(\boldsymbol{r}) = \frac{Z^{3/2}e^{-Zr/a}}{\sqrt{\pi a^3}}, \quad a = \frac{1}{me^2}, \quad \psi_f(\boldsymbol{r}) = e^{i\boldsymbol{p}\boldsymbol{r}}$$

For the ground 1s state of electron we obtain the plane wave scattering amplitude

$$M_{fi} = \mathcal{N}p\frac{\boldsymbol{n}\boldsymbol{e}_{\boldsymbol{k}\Lambda}}{\left(\frac{Z^2}{a^2} + q^2\right)^2}, \quad \boldsymbol{q} = \boldsymbol{p} - \boldsymbol{k}, \quad \boldsymbol{n} = \boldsymbol{p}/p$$

Evolved state has OAM $= \ell$ (incident Bessel photon)

Twisted amplitude: $$M_{fi}^{\mathbf{TW}} = \int \frac{\mathrm{d}^2 k_\perp}{(2\pi)^2} a_{\kappa\ell}(\boldsymbol{k}_\perp) e^{-i\boldsymbol{k}_\perp \boldsymbol{b}}(\boldsymbol{k}_\perp) M_{fi}$$

$$M_{fi}^{TW} = \mathcal{N}\sqrt{\frac{\kappa}{2\pi}}(-i)^\ell e^{i\ell\varphi_p}\left[\frac{p_\perp}{\sqrt{2}}\left[d^1_{-1\Lambda} I_{\ell+1}(\alpha,\beta,\boldsymbol{b},\varphi_p) - d^1_{1\Lambda} I_{\ell-1}(\alpha,\beta,\boldsymbol{b},\varphi_p)\right] + p_z d^1_{0\Lambda} I_\ell(\alpha,\beta,\boldsymbol{b},\varphi_p)\right],$$

$$\alpha \equiv \frac{Z^2}{a^2} + p^2 + k^2 - 2p_z k_z, \quad \beta \equiv 2p_\perp k_\perp, \quad \tilde{\varphi} = \varphi_k - \varphi_p$$

$$I_\ell(\alpha,\beta,\boldsymbol{b},\varphi_p) \equiv \int \frac{\mathrm{d}\tilde{\varphi}}{2\pi} e^{i\ell\tilde{\varphi} - i\kappa b\cos(\tilde{\varphi}+\varphi_p-\varphi_b)} \frac{1}{(\alpha - \beta\cos\tilde{\varphi})^2}$$

where I_ℓ here equals $-\frac{\partial}{\partial\alpha}\tilde{I}_\ell$ in Serbo et al, PRA, 2015.

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where I_ℓ here equals $-\frac{\partial}{\partial\alpha}\tilde{I}_\ell$ in Serbo et al, PRA, 2015.

$\boxed{\boldsymbol{b} = 0}$ $\Longrightarrow$ $I_\ell(\alpha,\beta,0)$ does not depend on φ_p. Thus,

$$-i\frac{\partial}{\partial\varphi_p} M_{fi}^{TW} = \ell M_{fi}^{TW}, \quad -i\frac{\partial}{\partial\varphi_p} S_{fi}^{TW} = \ell S_{fi}^{TW}, \quad \boxed{-i\frac{\partial}{\partial\varphi_p}\psi^{ev}(\boldsymbol{p}) = \ell\psi^{ev}(\boldsymbol{p})}$$

Types of targets

To model a target we average the scattering characteristic (amplitude, cross section) f with some distribution function $n(\mathbf{b})$:

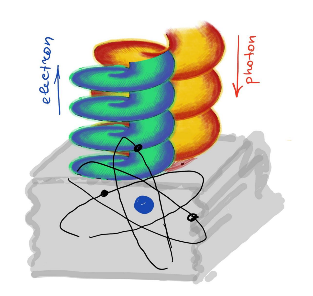
$$F_\ell(\mathbf{p},\mathbf{k},\mathbf{b}) = \int \mathrm{d}^2\mathbf{b}\, n(\mathbf{b}) f_\ell(\mathbf{p},\mathbf{k},\mathbf{b}).$$

$$n^{single}(\mathbf{b}) = \delta(\mathbf{b}-\mathbf{b}_0)$$

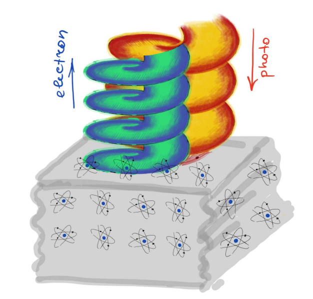
$$n^{macro}(\mathbf{b}) = \frac{1}{\pi R^2}\theta(R-|\mathbf{b}|),\ R\to\infty$$

$$n^{meso}(\mathbf{b}) = \frac{1}{2\pi\sigma_b^2} e^{-\frac{1}{2}\left(\frac{\mathbf{b}-\mathbf{b}_0}{\sigma_b}\right)^2},$$

call σ_b effective size of a target



single atom target



mesoscopic/macroscopic target

Non-zero impact parameter

$$e^{-i\kappa b\cos(\tilde{\varphi}+\varphi_p-\varphi_b)} \approx 1 - \frac{i\kappa b}{2} e^{-i\varphi_b} e^{i(\tilde{\varphi}+\varphi_p)} - \frac{i\kappa b}{2} e^{i\varphi_b} e^{-i(\tilde{\varphi}+\varphi_p)}$$

In the matrix element we replace

$$I_\ell(\alpha,\beta,\boldsymbol{b},\varphi_p) \to I_n(\alpha,\beta,0) - \frac{i\kappa b}{2} e^{-i\varphi_b} e^{i\varphi_p} I_{\ell+1}(\alpha,\beta,0) - \frac{i\kappa b}{2} e^{i\varphi_b} e^{-i\varphi_p} I_{\ell-1}(\alpha,\beta,0)$$

$\Rightarrow$ final state electron is a superposition of states with l, $l \pm 1$, $l \pm 2$, $\ldots$

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$\Rightarrow$ final state electron is a superposition of states with l, $l \pm 1$, $l \pm 2$, $\ldots$
Consider **coherent** averaging over the *axially symmetric* mesoscopic target

$$\widetilde{M}_{fi}^{TW} = \int \mathrm{d}^2 b \; n(\boldsymbol{b}) M_{fi}^{TW} = \int b \, \mathrm{d}b \, \mathrm{d}\varphi_b n(\boldsymbol{b}) M_{fi}^{TW}$$

Integration over φ_b eliminates any term containing the factor $e^{in\varphi_b}$ in the amplitude.
$\Rightarrow$ final state electron has OAM ℓ

Density matrix approach

Define the density matrix of the evolved state $\boxed{\hat{\rho}_{ev} = |ev\rangle\langle ev|}$

$$\langle L_z \rangle = \frac{1}{\mathrm{Tr}(\hat{\rho}_{ev})} \mathrm{Tr}\left(\hat{L}_z \hat{\rho}_{ev}\right)$$

Check:

$$\langle L_z \rangle = \frac{1}{\mathrm{Tr}(\hat{\rho}_{ev})} \int \frac{\mathrm{d}^3 q \mathrm{d}^3 q'}{(2\pi)^6} \underbrace{\sum_{\tilde{\ell}} \tilde{\ell} (2\pi)^2 e^{i\tilde{\ell}(\varphi_q - \varphi'_q)} \delta(q_\perp - q'_\perp) \delta(q_z - q'_z) \frac{1}{q_\perp}}_{\langle \boldsymbol{q} | \hat{L}_z | \boldsymbol{q}' \rangle} \psi^*_{ev}(\boldsymbol{q}) \psi_{ev}(\boldsymbol{q}') = \ell$$

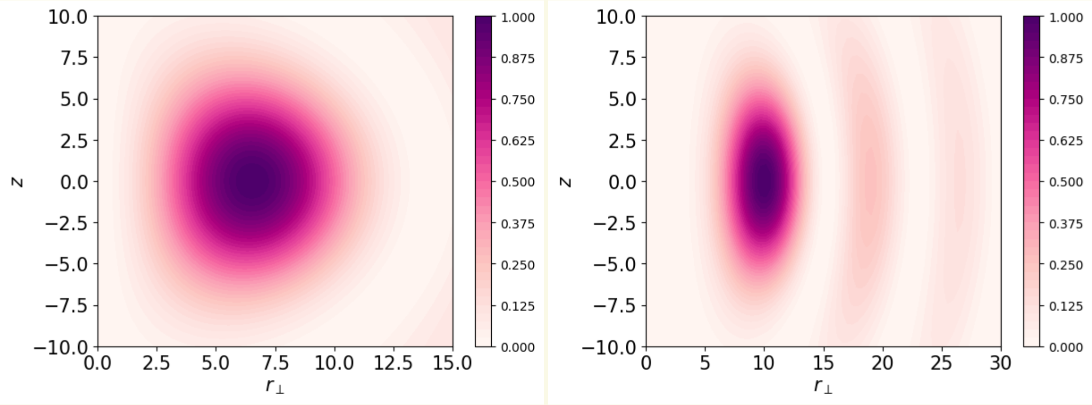
Introduction of small impact parameter preserves $\langle L_z \rangle = \ell$.
For the (**incoherent** approach) – introduce the averaged density matrix

$$\hat{\rho}'_{ev} = \int \mathrm{d}^2 b \, n(\boldsymbol{b}) \hat{\rho}_{ev}(\boldsymbol{b})$$

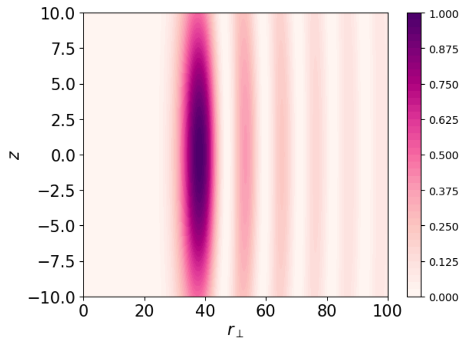
Pro's: information on phase remains (not necessarily so for cross sections)

Probability density of photoelectron

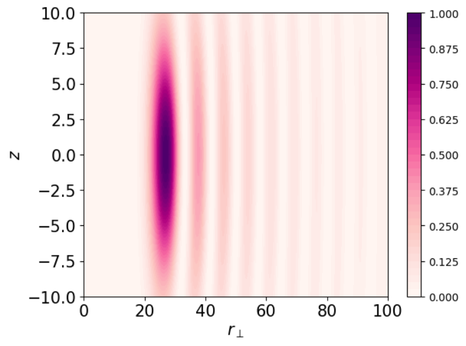
Incident Bessel beam, $\ell = 1$, $E = -1.2E_i$:   Incident LG beam, $\ell = 3$, $n = 1$, $E = -1.2E_i$:



Incident LG beam, $\ell = 10$, $n = 1$, $E = -1.1E_i$:

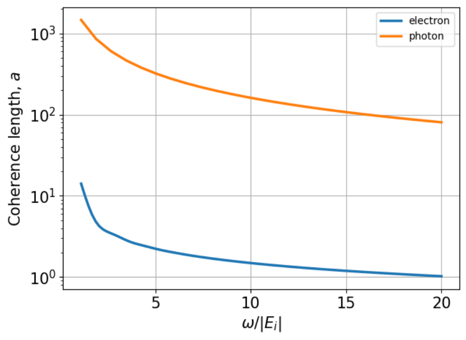


Incident LG beam, $\ell = 10$, $n = 1$, $E = -1.2E_i$:

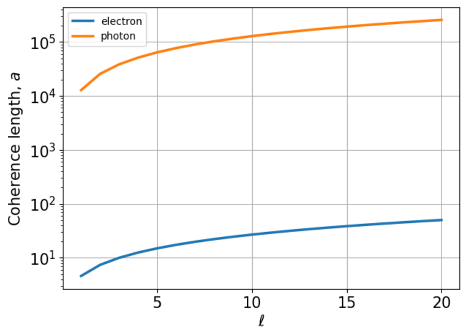


Transverse coherence length (Bessel beam)

For $\ell = 3,\ \theta_k = 1$ deg:



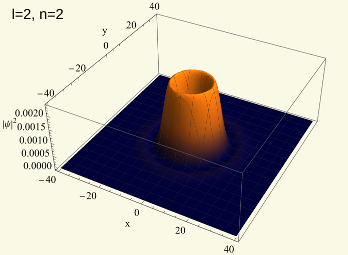
$E = -1.2E_i,\ \theta_k = 1$ deg:

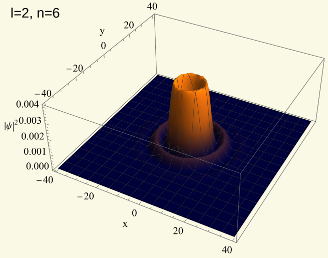


Scattering of non-relativistic LG electron packets

(arXiv:2404.11497)

Introducing Elegant Laguerre-Gaussian (eLG) beams



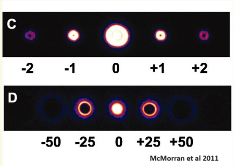


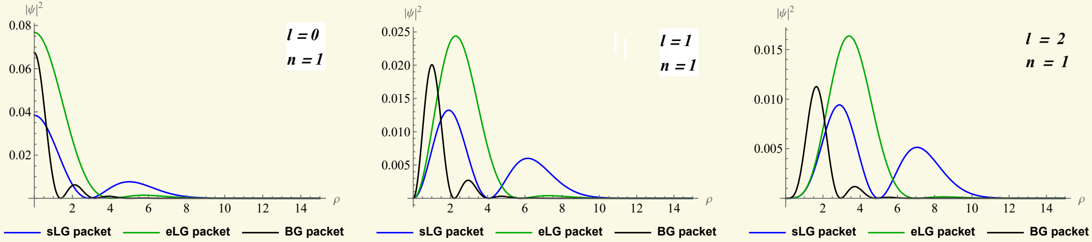
$$\Psi_\perp^{eLG}(\rho) = N_{eLG}\frac{\rho^{|\ell|}}{\sigma_\perp^{|\ell|+1}} L_n^{|\ell|}\left(\frac{\rho^2}{2\sigma_\perp^2}\right)\exp\left(i\ell\varphi - \frac{\rho^2}{2\sigma_\perp^2}\right)$$

Key properties:

- introduced by Siegman (1973) in laser optics
- good for optical micro manipulation
- exact solution of the Schrödinger equation
- form a complete set of solutions BUT are not orthogonal

eLG electrons?





Bessel-Gaussian (BG) wave packet has the Gaussian wave function, in the momentum representation:

$$Ce^{-(\varkappa-\varkappa_0)^2/(2\sigma_\varkappa^2)}$$

Scattering characteristics

Number of events for single atom scattering

$$\frac{d\nu}{d\Omega} = \frac{N_e}{\cos\theta_k}|F(\boldsymbol{Q},\boldsymbol{b})|^2,\ \boldsymbol{Q} = \boldsymbol{p}' - \boldsymbol{p},\ \boldsymbol{p} = \langle \mathbf{k} \rangle$$

$$F(\boldsymbol{Q},\boldsymbol{b}) = -\frac{m_e}{2\pi}\int \mathcal{V}(r)\Psi_\perp(\boldsymbol{r}+\boldsymbol{b})e^{-i\boldsymbol{Q}\boldsymbol{r}}d\boldsymbol{r}$$

$$\Psi_\perp(\boldsymbol{r}+\boldsymbol{b}) = \int e^{i(\boldsymbol{r}+\boldsymbol{b})\boldsymbol{k}_\perp}\Phi_\perp(k_\perp)\frac{d^2\boldsymbol{k}_\perp}{2\pi}.$$

Average cross section for macroscopic target

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{1}{N_e}\int \frac{d\nu}{d\Omega}d^2\boldsymbol{b}.$$

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{1}{\cos\theta_k}\int |f(\boldsymbol{Q}-\boldsymbol{k}_\perp)|^2|\Phi_\perp(\boldsymbol{k}_\perp)|^2 d^2k_\perp$$

Hydrogen-like targets:

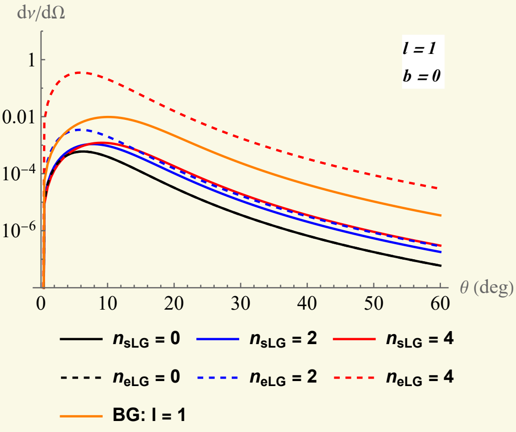
$$\mathcal{V}_H(r) = -\frac{e^2}{r}\left(1+\frac{r}{a}\right)e^{-2r/a}$$

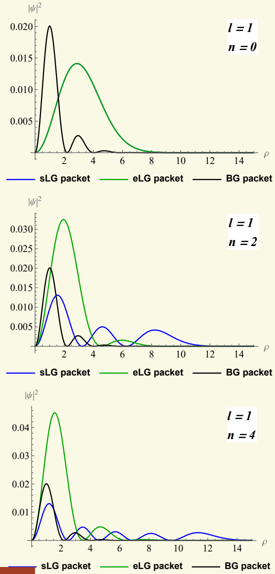
Heavy elements (Fe, Ag, Au):
take the potential field as the
superposition of three Yukawa terms

$$\mathcal{V}_Y(r) = -\frac{Ze^2}{r}\sum_{j=1}^{3}A_j e^{-\mu_j r},$$

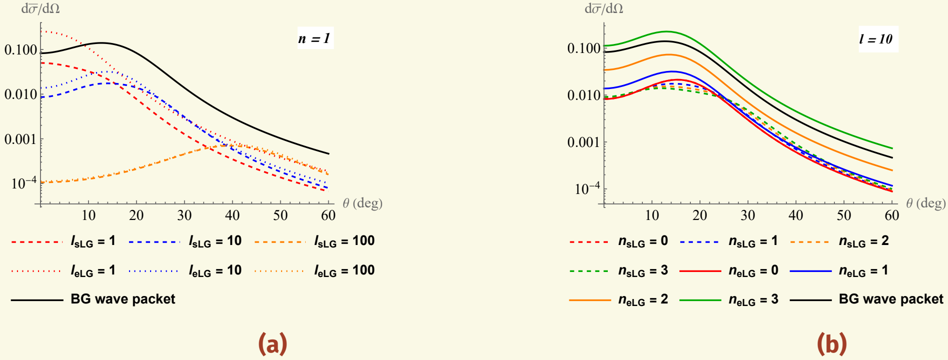
See akin calculations in *V. Serbo et al (2015)*

Scattering on a single hydrogen-like atom



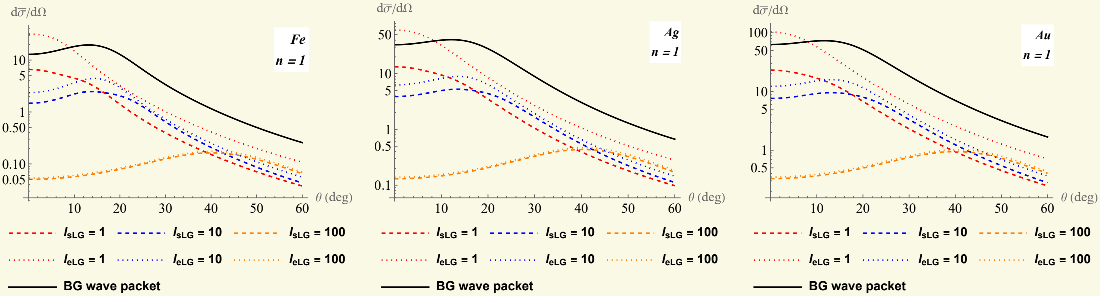


$p = 10/a$ ($\varepsilon = 1.4$ keV), $\sigma_\varkappa = \varkappa/5$, $\theta_k = 10^\circ$



The average cross section $d\bar{\sigma}/d\Omega$ for different values of OAM (a) and n (b). Results are presented for the width of the incident packet $\sigma_\varkappa = \varkappa_0/3$ and opening angle $\theta_k = 15^\circ$.

Macroscopic target of heavy elements



(a) **(b)** **(c)**

Scattering of sLG (solid lines), eLG (dashed lines), and BG (black line) packets on Fe (a), Ag (b), and Au (c) macroscopic targets: The average cross section $d\bar{\sigma}/d\Omega$ for different values of l. Width of the incident packets $\sigma_{\varkappa} = \varkappa_0/3$, opening angle $\theta_k = 15^{\circ}$, and $n = 1$.

Scattering of highly relativistic vortex electrons

(PRA A 108, 062803 (2023))

The Mott scattering description is given in terms of the scattering amplitude:

$$f_{\lambda,\lambda'}(\mathbf{p},\mathbf{p}') = -\int \psi^{\dagger}_{\mathbf{p}'\lambda'}(\mathbf{r})\mathcal{V}_{at}(\mathbf{r})\psi_{\mathbf{p}\lambda}(\mathbf{r})\mathrm{d}^3r,$$
$$S_{fi} = i2\pi\delta(\varepsilon-\varepsilon')f_{\lambda,\lambda'}(\mathbf{p},\mathbf{p}')$$

The resulting cross-section is

$$\left.\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right|_{(PW)} = \frac{1}{16\pi^2}\left|f_{\lambda,\lambda'}(\mathbf{p},\mathbf{p}')\right|^2$$

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)^{(single)} = J^2_{m-\lambda}(\kappa b_0)\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)^{(PW)}$$

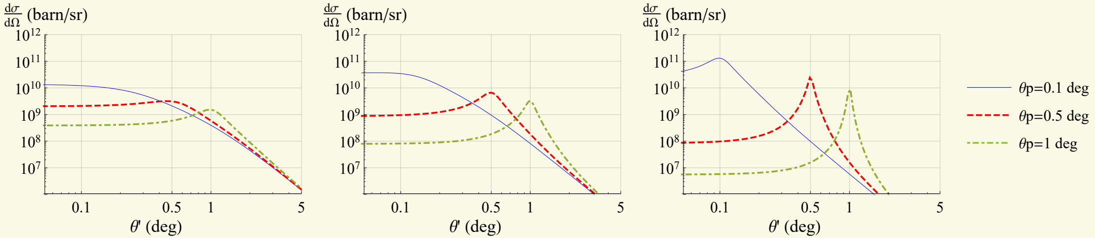
Here we consider scattering of Bessel beam with **TAM** m on different targets:

$$\lim_{\theta_p\to 0}\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)^{(macro)} = \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)^{(PW)} \quad \theta_p \lesssim 5^\circ$$

$$\left|F^{(meso)}_{m,\lambda,\lambda'}(\mathbf{p},\mathbf{p}',\mathbf{b}_0)\right|^2 = \int \mathrm{d}^2b\,\left|F(\mathbf{p},\mathbf{p}',\mathbf{b})\right|^2 \frac{e^{-\frac{1}{2}\left(\frac{\mathbf{b}-\mathbf{b}_0}{\sigma_b}\right)^2}}{2\pi\sigma_b^2}$$

$$\tan\theta_p = \frac{\kappa}{p_z}$$

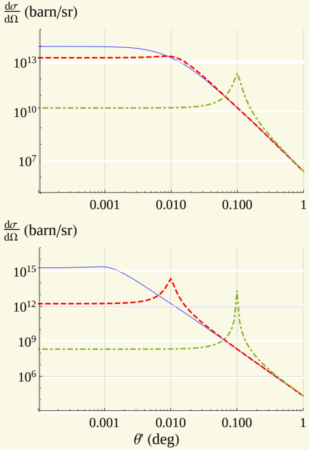
For various widths r_{beam} and TAM m at $\varepsilon = 2m_e$: typical θ_p ($\lesssim 1$ deg). $\theta_p \propto \varepsilon^{-1}$



Macroscopic Fe target. *Left*: $\varepsilon = 2m_e$, blue $\theta_p = 0.1^\circ$ ($\kappa = 1.5$ keV), red $\theta_p = 0.5^\circ$ ($\kappa = 7.7$ keV), green $\theta_p = 1^\circ$ ($\kappa = 15$ keV); *Middle*: $\varepsilon = 5m_e$, blue $\theta_p = 0.1^\circ$ ($\kappa = 4.4$ keV), red $\theta_p = 0.5^\circ$ ($\kappa = 21.9$ keV), green $\theta_p = 1^\circ$ ($\kappa = 43$ keV); *Right* : $\varepsilon = 20m_e$, blue $\theta_p = 0.1^\circ$ ($\kappa = 17.8$ keV), red $\theta_p = 0.5^\circ$ ($\kappa = 89$ keV), green $\theta_p = 1^\circ$ ($\kappa = 178$ keV).

$$\boxed{\text{Peak at } \theta' = \theta_p \Longrightarrow \kappa}$$

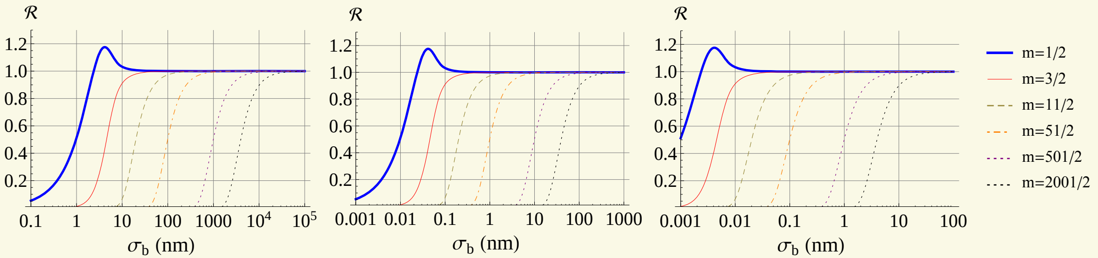
The peak is distinguishable only for values of $\kappa \gtrsim 10$ keV.



Macroscopic Au target and ultra-relativistic electron energies. *Top panel*: $\varepsilon = 100m_e$, blue solid $\theta_p = 0.001^\circ$ ($\kappa = 0.89$ keV), dashed red $\theta_p = 0.01^\circ$ ($\kappa = 8.9$ keV), dot dashed green $\theta_p = 0.1^\circ$ ($\kappa = 89$ keV); *Bottom panel*: $\varepsilon = 1000m_e$, blue solid $\theta_p = 0.001^\circ$ ($\kappa = 8.9$ keV), dashed red $\theta_p = 0.01^\circ$ ($\kappa = 89$ keV), dot dashed green $\theta_p = 0.1^\circ$ ($\kappa = 891$ keV).

Problem: no sensitivity to OAM with macroscopic target

$$\mathcal{R}_{m-\lambda}(\sigma_b, \kappa) \equiv \left(\frac{d\nu}{d\Omega}\right)^{(meso)} \Big/ \left(\frac{d\nu}{d\Omega}\right)^{(macro)}$$



Parameters: $\varepsilon = 5\,m_e$, $\lambda = 1/2$.
Left panel: $\theta_p = 0.001$ deg, κ = 44 eV; *middle panel*: $\theta_p = 0.1$ deg, κ = 4.4 keV; *right panel*: $\theta_p = 1$ deg, κ = 44 keV.

On results with mesoscopic target

A finite size target can be used to retrieve information about OAM $m - \lambda$.
However, we need realistic target sizes $\sigma_b > 1$ nm.

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Introduce OAM detuning:

$$\delta = \frac{(m_2 - \lambda_2) - (m_1 - \lambda_1)}{m_2 - \lambda_2}$$

and necessary accuracy in the scattering amplitude measurement $\mathcal{D}$:

$$\mathcal{D} = \max_{\sigma_b, \kappa \in \mathbb{R}_+} \left(\mathcal{R}_{m_2 - \lambda_2}(\sigma_b, \kappa) - \mathcal{R}_{m_1 - \lambda_1}(\sigma_b, \kappa) \right)$$

A two times difference between the OAM values ($\delta = 0.5$) – $\mathcal{D} \approx 0.45$.
For closer OAM values (smaller δ), $\mathcal{D}$ also decreases: for $\delta \approx 0.08$ – $\mathcal{D} \approx 0.064$, and for $\delta \approx 0.01$ – $\mathcal{D} \approx 0.007$.
For example, to distinguish $m_1 - \lambda_1 = 11$ and $m_2 - \lambda_2 = 12$ (detuning $\delta = 0.083$) one must have experimental setup resolution better than $\mathcal{D} = 0.064$.

Summary

On photoelectron emission

- evolved state gets OAM ℓ
- OAM of incident photon is preserved
- coherent / incoherent approach

On scattering of LG electrons

- OAM dependent (target -averaged) cross sections
- info on beam characteristics

On scattering of highly-relativistic electrons

- OAM from scattering on targets of varying sizes
- measuring κ of a Bessel beam

Thank you!