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Elimination of spurious oscillations on photoemission spectra

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INTRODUCTION & AIM

We present a method to accurately compute transition probabilities in one-dimensional photoionization problems by solving the time-dependent Schrödinger equation (TDSE) and projecting the solution onto scattering states with proper incoming or outgoing boundary conditions [1,2]. By using our new **Scattering Projection Method (SPM)**, our approach avoids spurious oscillations [3] and allows for the calculation of directional emission, enabling the study of asymmetries. We analyze partial differential photoionization probabilities of Al(111) metallic surfaces under short, grazing-incidence laser pulses.

METHOD

TDSE:

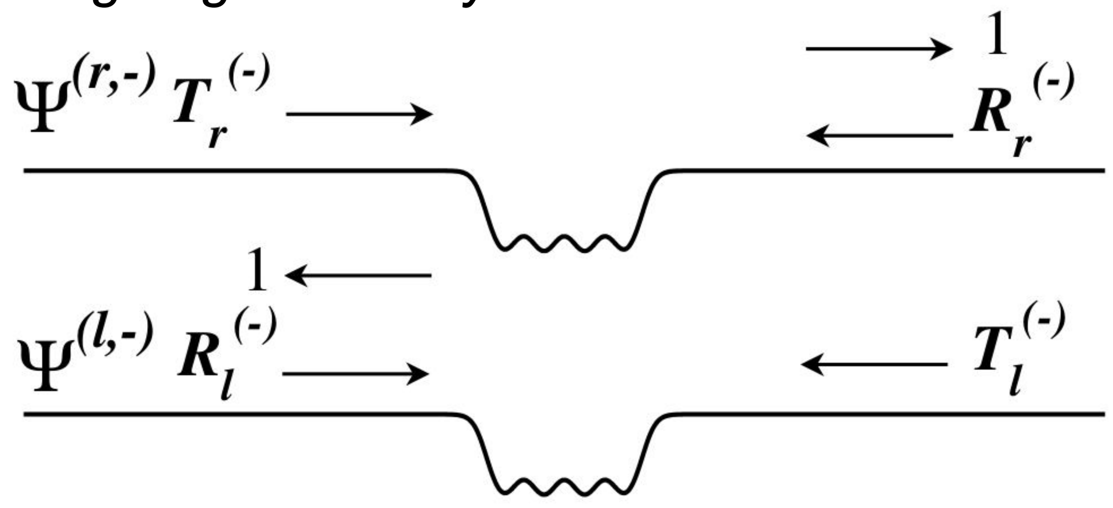
$$i\frac{\partial \Psi(z,t)}{\partial t} = \hat{H}(z,t)\,\Psi(z,t)$$

$$\hat{H}(z,t) = -\frac{1}{2}\frac{\partial^2}{\partial z^2} + \underbrace{V(z)}_{\text{Confinement potential}} + \underbrace{z\,F(t)}_{\text{e-pulse interaction}}$$

Spectrum calculation methods

- **Stationary:** Projection onto eigenstates of potential
- **Window Operator Method (WOM):** Smoothing of prior spectra based on [4]
- **Scattering Projection Method (SPM):** New basis of continuum scattering states [1,2]

Outgoing boundary conditions:

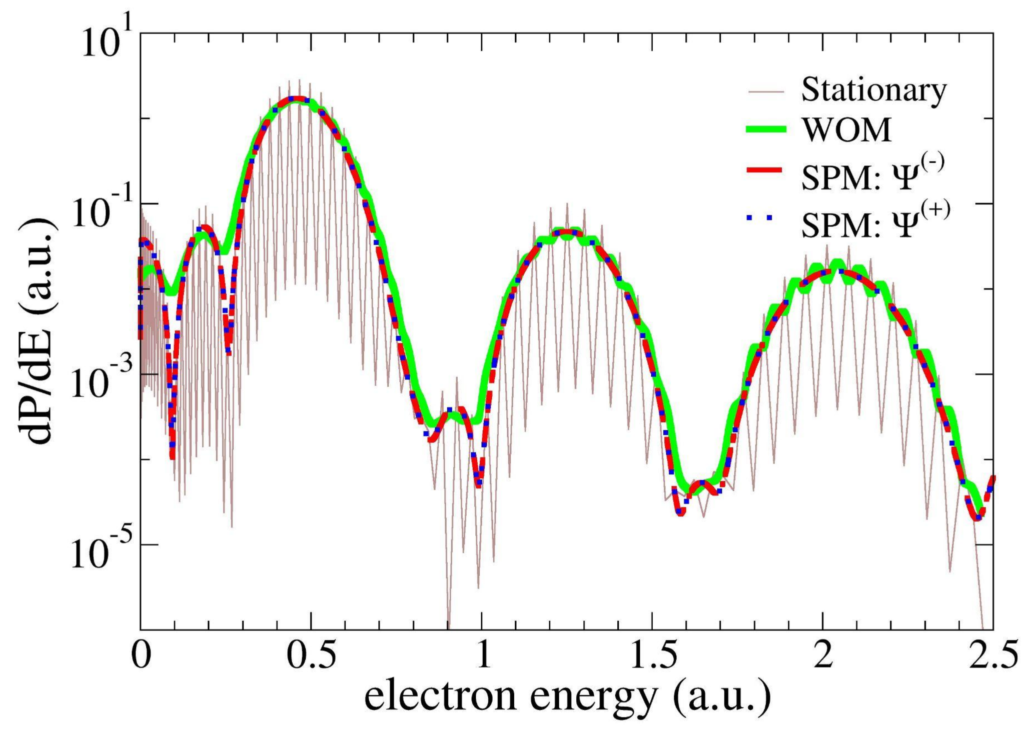


RESULTS & DISCUSSION

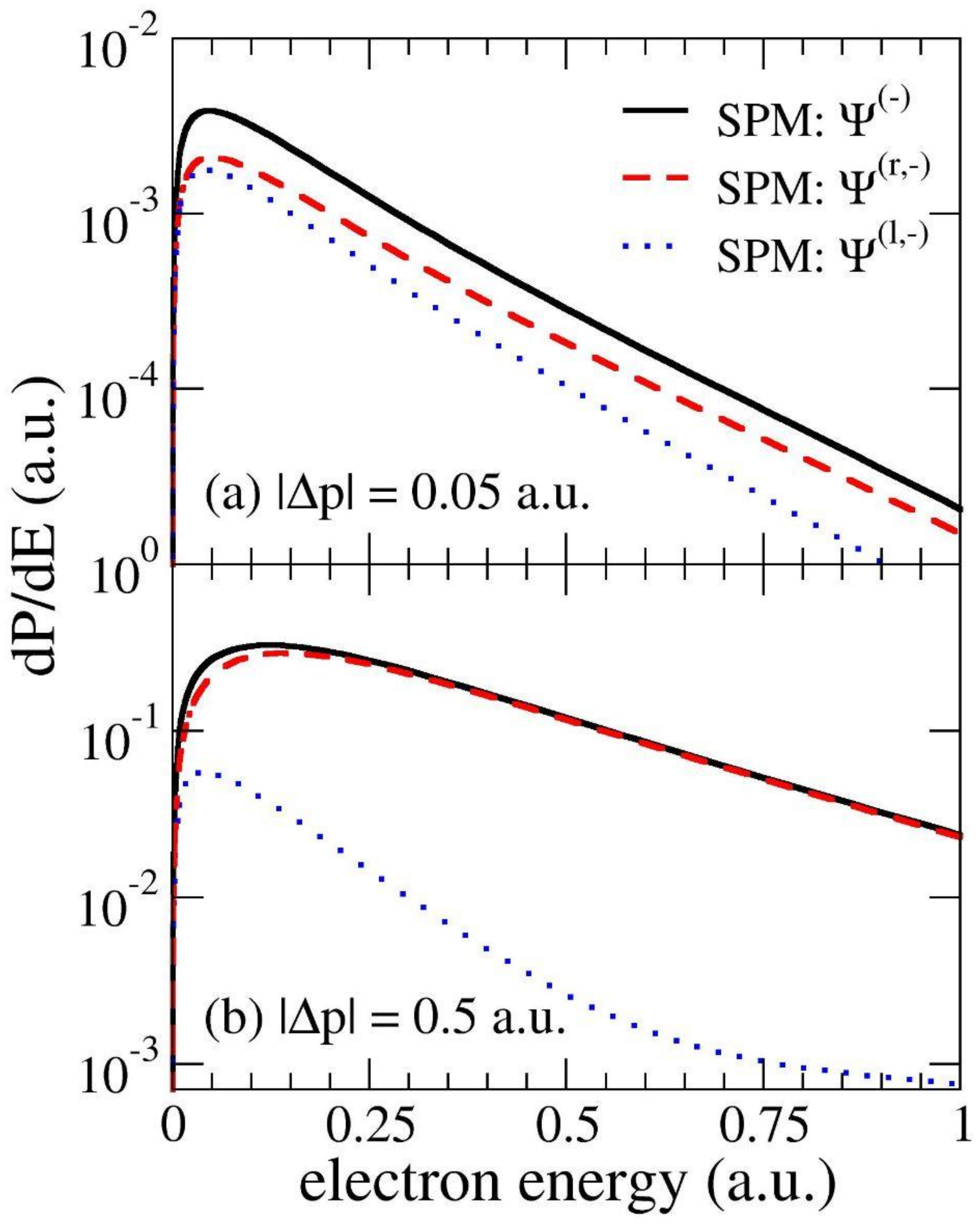
Square-well

(width=3, depth=0.5)

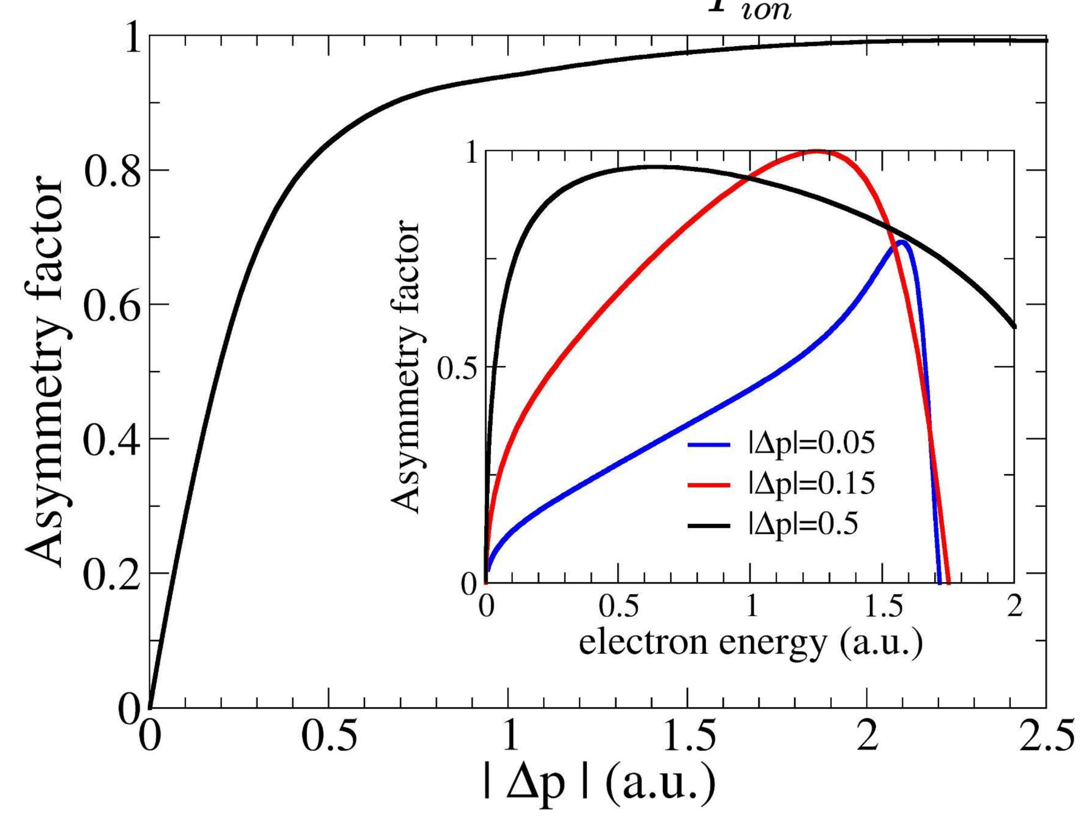
6-cycle pulse



Half-cycle pulse: directional emission

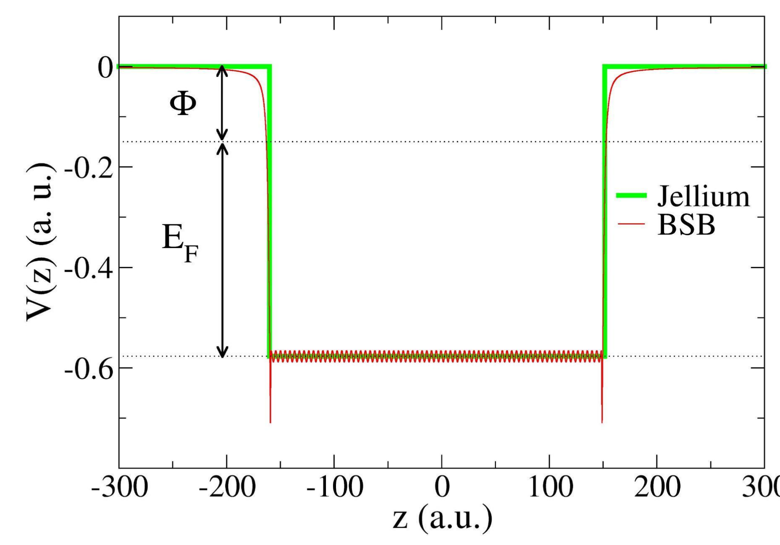


$$\text{Asym factor} = \frac{(P_{ion})_r - (P_{ion})_l}{P_{ion}}$$



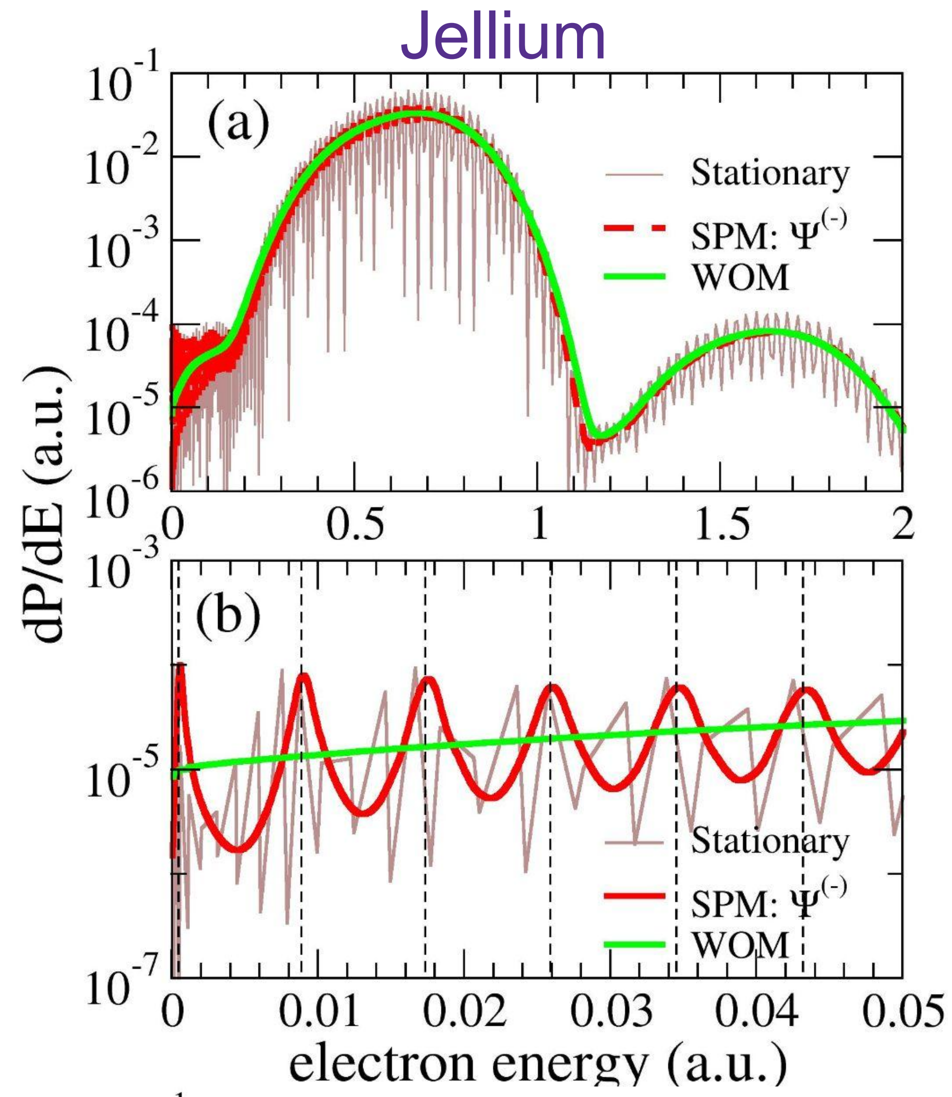
Surface Al(111)

Jellium vs Band-Structure-Based [5,6]

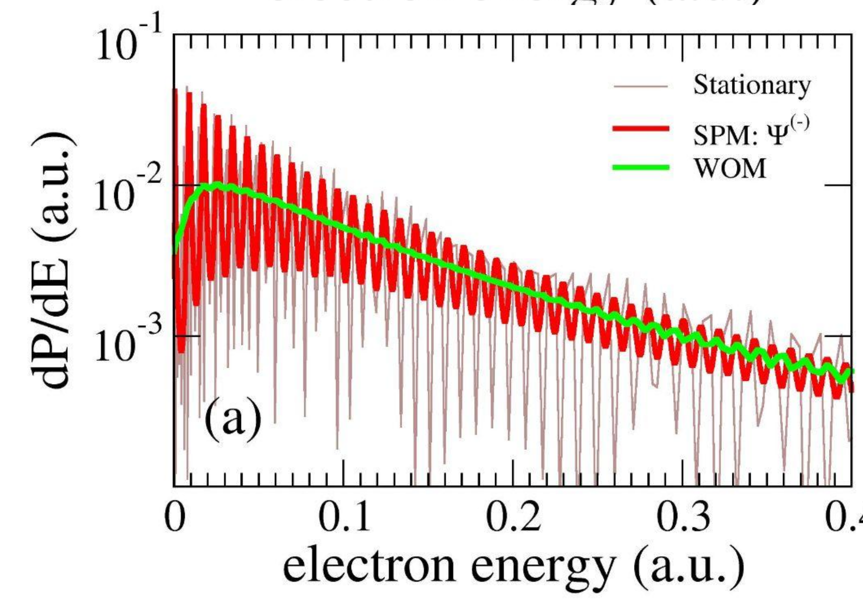


Jellium

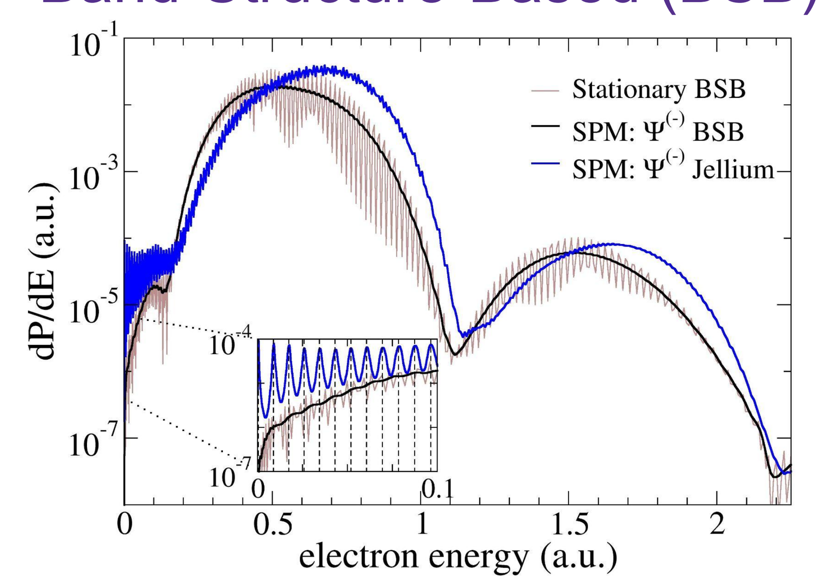
6-cycle pulse



Half-cycle pulse



Band-Structure-Based (BSB)



CONCLUSION

- SPM **reduces spurious oscillations** in ionization spectra more effectively than the WOM.
- SPM **preserves physical oscillations** arising from real quantum interference, avoiding the over-smoothing seen in WOM.
- SPM allows for **directional emission analysis**, enabling the study of asymmetries.
- In photoemission **from metal surfaces** under grazing-incident laser pulses, SPM successfully captures physical features previously obscured by noise (stationary projection).

[1] Barlari et al., Eur. Phys. J. D. **79**,93 (2025).
[2] Barlari, Bachelor's thesis (2018).
[3] Garriz et al, Eur. J. Phys. **31**, pp. 785-799 (2010).
[4] Schafer et al, Comp. Phys. Comm **63**, pp. 427–434 (1991).
[5] Chulkov et al, Surf. Science **437**, pp. 330–352 (1999).
[6] C.A. Ríos Rubiano et al, Phys. Rev. A. **95**, 033401 (2017).