Quantum Metrology with Photoelectrons Vol. 3: *Analysis methodologies*

Notes for proposal (following outline doc “IOP ebook proposal form v010920.docx”)
02/09/21, v1

General overview:

Vol. 3. will focus on analysis techniques for quantum metrology with photoelectrons, including:

- Interpreting experimental data.
- Extraction/reconstruction/determination of quantum mechanical properties (matrix elements, wavefunctions, density matrices) from experimental data.
- Comparison of experimental and theoretical data.
- New analysis methodologies & techniques.
- Introduction to newly-developed software platform (see below).

Provisional contents:

Part 1: theory & software (general review & update of the topic, including recent theory developments)

1. Introduction
    a. Topic overview.
    b. Context of vol. 3 (following vols. 1 & 2).
    c. Aims: Vol. 3 in the series will continue the exploration of quantum metrology with photoelectrons, with a focus on numerical analysis techniques, forging a closer link between experimental and theoretical results, and making the methodologies discussed directly accessible via a new software platform/ecosystem.
2. Quantum metrology software platform/ecosystem overview
    a. Introduction to python packages for simulation, data analysis, and open-data.
    b. Photoelectron metrology toolkit (PEMtk) package/platform for experimental data processing & analysis. (See pemtk.readthedocs.io.)
    c. ePSproc package for theory & simulation. (See epsproc.readthedocs.io.)
    d. ePSdata platform for data/results library (https://phockett.github.io/ePSdata/about.html#Motivation).
3. General method development: geometric tensor treatment of photoionization, fitting & matrix-inversion techniques
    a. Theory development overview - tensor methods (e.g. https://epsproc.readthedocs.io/en/latest/methods/geometric_method_dev_pt3_AFBLM_090620_010920_dev_bk100920.html)
    b. Direct molecular frame reconstruction via matrix-inversion methods (see Gregory, Margaret, Paul Hockett, Albert Stolow, and Varun Makhija. “Towards Molecular Frame Photoelectron Angular Distributions in Polyatomic Molecules from Lab Frame Coherent Rotational Wavepacket Evolution.” *Journal of Physics B: Atomic, Molecular and Optical Physics* 54, no. 14 (July 2021): 145601. https://doi.org/10.1088/1361-6455/ac135f.)
4. Numerical implementation & analysis platform tools
    a. Tensor methods implementation in ePSproc/PEMtk.

    b. Information content analysis (inc. basis-set exploration, e.g. https://pemtk.readthedocs.io/en/latest/fitting/PEMtk_fitting_basis-set_demo_050621-full.html), see also vol. 2, sect. 12.1.
    c. Density matrix analysis. (e.g. https://epsproc.readthedocs.io/en/dev/methods/density_mat_notes_demo_300821.html)
    d. Generalised bootstrapping implementation in PEMtk (see vol. 2, sects. 11.3 & 12.3)

Part 2: numerical examples (open-source worked examples using the new software platform)

5. Quantum metrology example: generalised bootstrapping for a homonuclear diatomic scattering system (N2)*
    a. Experimental data overview & simulation.
    b. Matrix element extraction (bootstrap protocol, see vol. 2, sects. 11.3 & 12.3) & statistical analysis.
    c. Direct molecular frame reconstruction via matrix-inversion methods.
    d. Comparison of methods.
    e. Information content/quantum information analysis. (See vol. 2, sect. 12.1.)
6. Quantum metrology example: generalised bootstrapping for a heteronuclear scattering system (CO)*
    a. Experimental data overview & simulation.
    b. Matrix element extraction (bootstrap protocol, see vol. 2, sects. 11.3 & 12.3) & statistical analysis.
    c. Direct molecular frame reconstruction via matrix-inversion methods.
    d. Comparison of methods.
    e. Information content/quantum information analysis. (See vol. 2, sect. 12.1.)
7. Quantum metrology example: generalised bootstrapping and matrix-inversion methods for a complex/general asymmetric top scattering system (C2H4 (ethylene))*
    a. Experimental data overview & simulation.
    b. Matrix element extraction (bootstrap protocol, see vol. 2, sects. 11.3 & 12.3) & statistical analysis.
    c. Direct molecular frame reconstruction via matrix-inversion methods.
    d. Comparison of methods.
    e. Information content/quantum information analysis.
8. Future directions & outlook
9. Summary & conclusions

* Exact choice of “simple” and “complex” systems may change, but should include a homonuclear diatomic and/or heteronuclear diatomic, and symmetric and asymmetric top polyatomic systems. May also include an atomic example.