Publ. Astron. Obs. Belgrade No. 84 (2008), 145 *Progress Report*

DECOHERENCE IN THE DIFFRACTION OF HELIUM AT SURFACES

F. AIGNER[1], N. SIMONOVIĆ[2], B. SOLLEDER[1] and J. BURGDÖRFER[1]

[1]*Institute for Theoretical Physics, Vienna University of Technology, A-1040 Vienna, Austria, EU*
E–mail: aigner@concord.itp.tuwien.ac.at

[2]*Institute of Physics, P.O. Box 57, 11001 Belgrade, Serbia*
E–mail: simonovic@phy.bg.ac.yu

Abstract. Scattering of fast neutral atoms with keV kinetic energies at alkali-halide surfaces under grazing angles displays intriguing diffraction patterns (Schüller, Wethekam and Winter 2007, Roisseau et al. 2007). In spite of the impulsive interaction with a surface at elevated temperature, which results in phonon excitation, quantum coherence evidently persists. To quantitatively study this remarkable survival of coherence, we present an ab initio simulation of the quantum diffraction of fast helium beams at a LiF (100) surface in the $\langle 110 \rangle$ direction and compare with recent experimental diffraction data.

Decoherence is analyzed employing a quantum trajectory Monte Carlo method (Minami, Reinhold and Burgdörfer 2003), calculating the ensemble average over solutions of a stochastic linear Schrödinger equation. The evolution of the atomic wavepacket is governed by a sequence of stochastic collisions and continuous propagation in the He-LiF surface potential. We find near-perfect agreement between the resulting diffraction patterns and experimental results (Schüller, Wethekam and Winter 2007) without using any adjustable parameters.

The question, whether the LiF surface features "buckling", (i.e. vertical surface reconstruction where the F atoms are displaced relative to the Li atoms) has been addressed in the past (de Wette, Kress and Schröder 1985). However, experimental uncertainties were of the same order as the displacement amplitude itself. In atom-surface diffraction at a grazing angle, surface reconstruction drastically changes the diffraction patterns. By comparison of numerical and experimental results, the buckling amplitude can be determined with unprecedented accuracy.

References

de Wette, F., Kress, W. and Schröder, U.: 1985, *Phys. Rev. B*, **32**, 4143.
Minami, T., Reinhold, C. and Burgdörfer, J.: 2003, *Phys. Rev. A*, **67**, 022902.
Rosseau, P., Khemliche, H., Borisov, A. and Roncin, P.: 2007, *Phys. Rev. Lett.*, **98**, 016104.
Schüller, A., Wethekam, S. and Winter, H.: 2007, *Phys. Rev. Lett.*, **98**, 016103.