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Ab initio 2D computations for quantum reflection from metallic surfaces

Abstract**:** The numerical study of scattering problems finds a wide range of applications in surface science, and in particular quantum reflection (QR). We present a highly optimised, norm-preserving method to compute QR of slow atoms from metallic surfaces by solving numerically the Time-Dependent Schrödinger Equation in 2D. The aim of our study is to provide a proof of principle that QR from 2D uni-axially periodic potential structures can be investigated in a time-dependent fashion. To this end, the numerical procedures used are presented, as well as comparisons with 1D results for QR from static and oscillating 1D potentials and first order results for QR from a truly 2D non-separable periodic potential. This enables the first systematic time-dependent investigations of atom-surface potentials, where Casimir interactions are relevant, as well as numerical tests of matter wave diffraction.