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Diffraction of atoms through a crystalline grating with sub-nm period

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Abstract

We report on a theoretical study exploring the possibility to diffract atomic matter-waves through crystalline materials. Using molecular dynamics (MD) simulations based on time-dependent density functional theory (TDDFT), we find a high chance for atomic hydrogen at 120'000 m/s to be coherently transmitted through a single layer of graphene. The natural lattice period of the membrane amounts to only 246 pm, resulting in wide diffraction angles in the 10 mrad regime. We discuss how this can be used for novel applications in force sensing and studies of ultra-thin membranes.

Interference of electrons and neutrons plays a critical role in the analysis, characterization, and visualization of materials in condensed-matter research. This is complemented by atomic and molecular interference, which allows to study surfaces and their interaction with the matter-waves in great detail [1, 2]. Transmission of massive matter-waves through crystalline materials, however, has not yet been demonstrated.

Here we discuss the coherent diffraction of fast atomic hydrogen through crystalline single-layer graphene based on TDDFT/MD simulations [3]. In order to overcome the transmission barrier of graphene [4], we consider atomic hydrogen with a velocity of up to 120'000 m/s. While the atoms couple only weakly to the phonons in the membrane during transit, we predict significant energy-loss to the electronic system. However, these couplings are not strong enough to localize the atom to a single hexagon in the membrane and are thus found to be compatible with coherent transmission. This suggests that atoms can be diffracted through the natural lattice spacing of 246 pm, leading to diffraction angles in the 10 mrad regime.

The proposed setting is an important limiting case for quantum physics in several aspects. On the one hand, we predict coherent diffraction although the matter-wave loses a considerable amount of energy to the grating structure. On the other hand, the large momentum transfer allows for atomic coherence functions which are predicted to stretch over meters on reasonable length scales. This can give rise to novel applications in force sensing, tests of the foundations of quantum mechanics, and studies of ultra-thin membranes. Our approach might be particular important for studying effects which scale with velocity [5].

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