This thesis discusses important questions of the beam dynamics in the proton-lead operation in the Large Hadron Collider (LHC) at CERN in Geneva. In two time blocks of several weeks in the years 2013 and 2016, proton-lead collisions have so far been successfully generated in the LHC and used by the experiments at the LHC. One reason for doubts regarding the successful operation in proton-lead configuration was the fact that the beams have to be accelerated with different revolution frequencies. There is long-range repulsion between the beams, since both beams share the beam chamber around the interaction points. Because of the different revolution frequencies, the positions of the interaction between the beams shift each revolution. This can lead to resonant excitation and to an increase in the transverse beam emittance, as was observed in the Relativistic Heavy-Ion Collider (RHIC). In this thesis, simulations for the LHC, RHIC and the High-Luminosity Large Hadron Collider (HL-LHC) are performed with a new model. The results for RHIC show relative growth rates of the emittances of the gold beam in gold-deuteron operation in RHIC from 0.1 %/s to 1.5 %/s. Growth rates of this magnitude were observed experimentally in RHIC. Simulations for the LHC show no significant increase of the emittance of the lead beam for different intensities of the counter-rotating beam. The simulation results confirm the measured stability of the beams in the LHC and the issue of strongly increasing emittances in RHIC is reproduced. Also, no significant increase of the emittance is predicted for the Future Circular Collider (FCC) and the HL-LHC.

Using a frequency-map analysis, this work verifies whether the interaction of the lead beam with the much smaller proton beam in the proton-lead operation of the LHC leads to diffusion within the lead beam. Experiences at HERA at DESY in Hamburg and at SppS at CERN have shown that the lifetime of the larger beam can rapidly decrease under certain circumstances. The results of the simulation show no chaotic dynamics near the beam centre of the lead beam. This result is supported by experimental observation.

A program code has been developed which calculates the beam evolution in the LHC by means of coupled differential equations. This study shows that the growth rates of the lead beam due to intra-beam scattering is overestimated and that particle bunches of the lead beam lose more intensity than assumed in the model. The analysis also shows that bunches colliding in a detector suffer additional losses that increase with decreasing crossing angle at the interaction point.

In this work, 2016 data from beam-loss monitors in combination with the luminosity and the loss rate of the beam intensity are used to determine the cross section of proton-lead collisions at the center-of-mass energy of 8.16 TeV. Beam-loss monitors that mainly detect beam losses that are not caused by the collision process itself are used to determine the total cross section via regression. An analysis of the data recorded in 2016 at the center-of-mass energy of 8.16 TeV resulted in a total cross section of σ=(2.32±0.01(stat.)±0.20(sys.)) b. This corresponds approximately to a hadronic cross section of σ(had)=(2.24±0.01(stat.) ±0.21(sys.)) b. This value deviates only by 5.7 % from the theoretical value σ(had)=(2.12±0.01) b.

The simulation code for determining the beam evolution is also used to estimate the integrated luminosity of a future one-month run with proton-lead collisions. The result of the study shows that in the future the luminosity in the ATLAS and CMS experiments will increase from 15/nb per day in 2016 to 30/nb per day, which is a significant increase in terms of the performance. This operation, however, requires the use of the TCL collimators to protect the dispersion suppressors at ATLAS and CMS from collision fragments.

This work also gives an outlook on the expected luminosity production in proton-nucleus operation using ion species lighter than lead ions. For example, a change from proton-lead to proton-argon collisions would increase the integrated luminosity from monthly 0.8/nb to 9.4/nb in ATLAS and CMS. This is an increase of one order of magnitude and approximately a doubling of the integrated nucleon-nucleon luminosity. There may be a test operation with proton-oxygen collisions in 2023, which will last only a few days and will be operated with a low luminosity. The LHCf experiment (LHCb experiment) would achieve the desired integrated luminosity of 1.5/nb (2/nb) within 70h (35h) beam time.