Density functional theory calculation of ionization in antiproton-helium collisions

TOM KIRCHNER, Department of Physics and Astronomy, York University, Toronto, Ontario M3J 1P3, NILS HENKEL, Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany, MATTHIAS KEIM, HANS JÜRGEN LÜDDE, Institut fuer Theoretische Physik, Goethe-Universitaet, D-60438 Frankfurt, Germany — Probabilities and total cross sections for ionization in antiproton-helium collisions are calculated in a time-dependent density functional theory approach. The Kohn-Sham potential is approximated as the sum of the Hartree-exchange potential and a correlation potential that was proposed in the context of laser-induced double ionization. Furthermore, some approaches to the problem of calculating the ionization probabilities from the density are investigated. We find that the correlation potential yields no obvious improvement of the results over the exchange-only approximation where the correlation potential is neglected. Furthermore, we find the problem of calculating the desired observables crucial, introducing errors of at least the same order of magnitude as the correlation potential. At small energies we find that trajectory effects play an important role: the ionization cross sections are enlarged significantly if curved instead of straight-line trajectories are used to describe the projectile motion.