Abstract Submitted for the DAMOP06 Meeting of The American Physical Society

Numerical study of charge transfer in ion-ion collisions using the lattice time-dependent Schrödinger equation method T. MINAMI, M.S. PINDZOLA, Auburn University, T.-G. LEE, University of Kentucky, D.R. SCHULTZ, ORNL — Bräuning, et.al. (J. Phys. B, 38, p2311) recently measured cross sections of charge transfer in collisions of He^{2+} with Li^{2+} . At the same time, they also performed calculations of the cross sections of this collision system and of collisions of H⁺ with He⁺ using the basis generator method (BGM). For the former system, BGM seems to overestimate the cross sections compared to their experiment, while for the latter system, BGM provides excellent agreement with past experiments. Since both are ion-ion collision with asymmetrical nuclear charges involving one electron, BGM agreeing one system but the other points to a situation requiring further study. Motivated by this question, we have performed atomic orbital coupled channel (AOCC) calculations for both systems. When we use our most complete basis set for the calculations, we obtain results close to BGM on both systems. However, results from AOCC do not readily converge with regard to the size of the basis sets and therefore results were not conclusive. We also have performed the lattice time-dependent Schrödinger equation (LTDSE) calculations. Preliminary results for both systems by LTDSE are close to BGM. In this presentation, we compare BGM, AOCC and LTDSE with the experiment. This research used resources of NCCS at ORNL and NERSC, and was supported by DOE OFES.

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Date submitted: 06 Feb 2006

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