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Charge Hopping in an Optical Tweezer Array of Sr Atoms: An Application of Generalized Local Frame Transformation Theory T. J. PRICE, CHRIS H. GREENE, Purdue University, J. P. COVEY, MANUEL EN-DRES, California Institute of Technology — Tunneling of a Rydberg electron in highly excited states of Sr_2^+ is investigated. This work will complement an experiment to be performed by the Endres group involving an array of Sr atoms in optical tweezers. In the tweezer array, the distance between the Sr atoms is on the order of a micrometer. The large internuclear separation and high energies of the Sr_2^+ states lead to electronic wave functions that can't be treated with conventional quantum chemistry. Instead, we apply a generalized local frame transformation theory [Giannakeas et al., Phys. Rev. A. 94, 013419 (2016)] to determine tunneling rates in Sr_{2}^{+} in part from wave functions that we have calculated for H_2^+ . This technique is based on the idea that near each nucleus the electronic wave function of H_2^+ is locally that of a hydrogen atom. We determine a local frame transformation matrix between H wave functions in spherical coordinates and H_2^+ wave functions in spheroidal coordinates. Then, we incorporate the effect of scattering from the Sr cores by using Green's functions and quantum defects of Sr.

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