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Gauge transformations in multichannel laser-interaction Hamiltonians G.S.J. ARMSTRONG, B.D. ESRY, J. R. Macdonald Laboratory, Kansas State University, Manhattan, KS 66506, USA — In our previous studies of molecular photodissociation, we solved the time-dependent Schrödinger equation in full dimensionality, casting the laser-molecule interaction in a length-gauge form. The nuclear wave function is then expanded on a basis of symmetric top functions in the angular coordinates. However, a velocity gauge representation of the nuclear motion may be advantageous, and may reduce the number of partial waves required in the angular basis expansion. In molecular problems, the standard transformation between length and velocity gauge must take account of the presence of short-range non-linear radial dependence of the dipole. In problems involving a single channel, the short-range behavior is not removed by the gauge transformation, leading to a short-range mixed-gauge Hamiltonian. Having derived the form of this Hamiltonian, we extend our analysis to multichannel problems, where the gauge transformation is further complicated by off-diagonal dipole terms. We examine the impact of this transformation in full-dimensional calculations, particularly its effectiveness in reducing the required size of the angular basis. This work is supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U.S.A.

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