Treatment of anomalous long range derivative couplings in atom-atom collisions

BERNARD ZYGELMAN, University of Nevada, Las Vegas —

In the multi-channel Born-Oppenheimer approximation the system wavefunction is expanded in a basis of adiabatic states. In such a description, non-adiabatic derivative couplings (or gauge potentials) may arise and which do not vanish in the asymptotic region. Traditionally, electron translation factors are introduced in the multi-channel expansion to eliminate such couplings. Here we present an alternative method that involves a series of gauge transformations. We apply and illustrate this technique in the H-H system where one of the collision partners is in the n=2 excited state. In addition, a fully solvable model is introduced that illustrates the physical basis for these transformations.

1This work was supported by NSF-PHY-0758140