PRAMANA
—journal of
physics

Vol. 48, No. 2,
February 1997
pp. 411–424

Resonances and chaos in the collinear collision system (He, H_2^+) and its isotopic variants

SUSANTA MAHAPATRA[a], N SATHYAMURTHY[a] and
RAMAKRISHNA RAMASWAMY[b]
[a] Department of Chemistry, Indian Institute of Technology, Kanpur 208 016, India
[b] School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110 067, India

Abstract. The collinear atom-diatom collision system provides one of the simplest instances of chaotic or irregular scattering. Classically, irregular scattering is manifest in the sensitive dependence of post-collision variables on initial conditions, and quantally, in the appearance of a dense spectrum of dynamical resonances. We examine the influence of kinematic factors on such dynamical resonances in collinear (He, H_2^+) collisions by computing the transition state spectra for collinear (He, HD^+) and (He, DH^+) collisions using the time-dependent quantum mechanical approach. The nearest neighbor spacing distribution $P(s)$ and the spectral rigidity $\Delta_3(L)$ for these resonances suggest that the dynamics is predominantly *irregular* for collinear (He, HD^+) and predominantly *regular* for collinear (He, DH^+). These findings are reinforced by a significantly larger "correlation hole" in ensemble averaged survival probability $\langle\langle P(t)\rangle\rangle$ values for collinear (He, HD^+) than for collinear (He, DH^+). In addition we have also examined measures of classical chaos through the dependence of the final vibrational action, n_f, on the initial vibrational phase ϕ_i of the diatom, and Poincaré surfaces–of–section. They show that (He, HD^+) collisions are partly chaotic over the entire energy range (0–2.78 eV) while (He, DH^+) collisions, in contrast, are highly regular at collision energies below the classical threshold for reaction. Above the threshold, the scattering remains regular for initial vibrational states $v = 0$ and 1 of DH^+.

Keywords. Dynamical resonances; irregular scattering; collinear collisions.

PACS Nos 05.45; 34.10; 34.50

1. Introduction

Dynamical resonances in atom-molecule collisions [1] have been of great interest since they give rise to unusual variations in the scattering amplitude and related quantities. Reactive scattering resonances, which have been identified in a number of systems, one of which is (He, H_2^+) in collinear as well as noncollinear configurations [2], are characterized by oscillations in the reaction probability P^R as a function of the collision energy E. Many of them are of the Feshbach type and can be interpreted in terms of bound states supported by vibrational adiabatic potentials in hyperspherical coordinates [2(d),3]. A closer examination of $P^R(E)$ curves for collinear (He, H_2^+), for example, reveals that there are additional oscillations [2(h)] that are irregularly spaced as a function of the energy and which can not be assigned easily. The connection between such (quantal) resonances and the features of the classical dynamics is the subject of this article.