PRAMANA
—journal of
physics

© Indian Academy of Sciences

Vol. 50, No. 6,
June 1998
pp. 535–545

Calculation of highly excited eigenstates of chaotic quantum systems

V B SHEOREY and M S SANTHANAM*
Physical Research Laboratory, Navrangpura, Ahmedabad 380 009, India
* Present address: IBM Solutions Research Centre, Block 1, Indian Institute of Technology, Hauz Khas, New Delhi 110 016, India

Abstract. Computational methods for the calculation of a large number of eigenstates of coupled oscillator system are developed and discussed. These calculations have enabled us to identify and investigate properties of an infinite set of states sharply localized in configuration space in this system. Some of the results and their significance are discussed. Extensions to three-dimensional systems are also briefly considered.

Keywords. Quantum chaos; wave functions; excited states.

PACS Nos 05.45; 31.50

1. Introduction

The classical dynamics of generic time independent Hamiltonian systems with two or more degrees of freedom exhibits chaos, i.e., its phase space dynamics shows extreme sensitivity to initial conditions. Quantum systems for which the underlying classical dynamics is chaotic are an active area of research and atomic and molecular systems provide numerous examples of such quantum systems. One of the simplest of chaotic quantum systems is a one electron atom in an external magnetic field. For Rydberg states of the atom, however, the external field strength can become comparable with the attractive electrostatic field felt by the electron and this results in chaotic classical dynamics for the electron. The spectra of Rydberg states of such systems have been measured as a function of the external field strength [1, 2]. Experiments have also been performed on many electron atoms in high external magnetic fields and involve detection of Rydberg atoms after laser excitation [3] and recently some new experiments using many-electron atoms have been suggested to study quantum chaos in such systems [4]. On the theoretical side the Hamiltonian for the hydrogen atom in an external magnetic field can be transformed using semi-parabolic coordinates to that for two nonlinearly coupled harmonic oscillators [1]. Another problem which has been extensively studied is that of two coupled quartic oscillators [5, 6, 7]. In both these problems the accurate eigen-energies and eigenfunctions of highly excited states are required to be calculated in order to elucidate the effect of classical chaos in quantum systems. The eigenvalues and eigen-functions are obtained by diagonalizing the Hamiltonian matrix in a suitable complete set of basis states. The choice of basis states is dictated by physical considerations and by