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WAVEPACKETS AND PERIODIC ORBITS FOR ANHARMONICALLY RESONANT SYSTEMS

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The classical periodic orbits of non–linear dynamical systems play an important role in organising the structure of the classical phase space, which becomes increasingly complicated as the energy increases. Two types of quantum mechanical wavepacket calculation will be reported, to elucidate the influence of these orbits on the quantum mechanical eigenstates.
The first is a model study of the stretching modes of H2O which supports three types of periodic orbit. Type A (symmetric stretch) is unstable to small perturbations at energies above the fundamentals, while types B (generalised asymmetric stretch) and C (local mode) are stable. Wavepackets initiated along the stable orbits yield simple eigenvalue progressions up to the dissociation limit, but the unstable type A gives rise to a more complicated eigenvalue pattern.
The second investigation involves wavepackets initiated along the unstable periodic orbit of a non–linear 1:2 Fermi resonance. A Husimi phase space representation is used to relate features of the autocorrelation function to the time evolution of the wavepacket and to the classical phase space structure. It is shown that the subsequent motion, after initiation along the orbit, is governed by the separatrix attached to the orbit in cases when the local motion is both regular and near chaotic. The regular case gives rise to two types of recurrence pattern in the autocorrelation function, which are associated with two distinct branches of the separatrix. The near chaotic case shows a richer eigenvalue pattern and weaker recurrences, which are attributed to the more complicated structure of the now broken separatrix. No global smearing of the wavepacket is observed in either case, during the time of observation.