orbits are close to the exact orbits, even after an unlimited number of timesteps. The equivalence between the discrete-time and continuous-time dynamics holds only for sufficiently small of the timestep Δ. For intermediate values of Δ (sufficiently large that the conservation law does not hold, but sufficiently small that the numerical orbits are not chaotic) a new "super-adiabatic" invariant A is derived, and it is shown that conservation of A forces the numerical orbits to lie on smooth closed curves. If the potential energy varies rapidly over a small region, it is shown that very high-order resonances between the timestep and the orbital period T, (i.e., $T/\Delta = n$, where n is a large integer) produce large deviations of these closed curves from the exact orbit. Such resonances also cause extreme sensitivity of the numerical orbit to the timestep.

BOUNDARY ELEMENT SOLUTION OF HEAT CONVECTION–DIFFUSION PROBLEMS. B. Q. Li, *Massachusetts Institute of Technology, Cambridge, Massachusetts, USA*; J. W. Evans, *University of California, Berkeley, California, USA*.

A boundary element method is described in detail for the solution of two-dimensional steady-state convective heat diffusion problems in homogeneous and isotropic media with both linear and nonlinear boundary conditions. Through an exponential variable transformation, the introduction of fundamental solutions and the use of Green's theorem, the problem is reduced to one involving values of temperature and/or heat flux in the form of an integral only along the boundary. The integral is solved numerically for three examples. Two of them have linear boundary conditions and their numerical results are compared with the corresponding analytical solutions. The other has a nonlinear boundary condition due to heat radiation and an iterative procedure is applied to obtain the numerical solution. The fictitious source formulation leading to the boundary element solution of the same problems is discussed as an alternative. The extension of the method to formulate transient and/or three-dimensional convective heat diffusion problems is also described, and the relevant fundamental solutions are given. Finally, the exponential variable transformation is applied to construct a functional of variational principle which leads to developing a finite element formulation of the problems with a banded, symmetric stiffness matrix.

CLOSED FORM SOLUTION FOR LOCALIZED MODES ON A POLYMER CHAIN WITH A DEFECT. V. K. Saxena, *Universidade Federal de Santa Catarina, Florianopolis, SC, BRAZIL*; L. L. Van Zandt and W. K. Schroll, *Purdue University, West Lafayette, Indiana, USA*.

The problem of localized vibration modes on a polymer chain with a symmetry breaking defect is formulated as a finite sum of exponentially decaying waves on the polymer. Applying a set of similarity and unitary transformations, and using the singular value decomposition technique, the size of the problem is reduced to relatively small dimensions as compared to the large size of the original set of equations for propagating modes on the chain. A modification of the polynomial eigenvalue problem converts the algebraic system to a simple eigenvalue problem which may be diagonalized to give eigenvectors of different decaying waves for an expansion set to describe general localized excitations. Application of proper boundary conditions at the site of broken symmetry leads to determination of the frequencies of the localized modes and corresponding eigenvector expansion. Possible applications of the algorithm to various defect problems on a polymer chain are discussed and some preliminary results on a particular defect are presented.

RUNGE–KUTTA SMOOTHER FOR SUPPRESSION OF COMPUTATIONAL-MODE INSTABILITY OF LEAP FROG SCHEME. Akira Aoyagi, *Kyushu Industrial University, Fukuoka, JAPAN*; Kanji Abe, *The University of Tokyo, Tokyo, JAPAN*.

The Runge–Kutta smoother is applied to suppress nonlinear numerical instabilities in the leap-frog scheme for time integration of the Korteweg–de Vries equation. The accuracy of integration is compared