RECENT DEVELOPMENTS IN THE QUANTUM NONLINEAR DIMER: HOPF BIFURCATIONS, TIME EVOLUTION, AND THERMAL STABILITY

V. M. Kenkre

Department of Physics and Astronomy
University of New Mexico
Albuquerque, NM 87131, USA

1. INTRODUCTION AND SOME EXACT RESULTS

A simple but rich nonlinear structure that has received a great deal of attention in the last few years is the quantum nonlinear dimer [1] in which a quasiparticle, such as an electron or an excitation, shuttles back and forth between two sites while interacting so strongly with a boson field, e.g. the vibrations of the system, that the quasiparticle evolution becomes nonlinear. The discrete nonlinear Schroedinger equation in various forms has served as the evolution equation for this structure [2]. The advantage of studying this small system lies in the fact that insights into many issues of interest on extended systems can be gained without having to grapple with the considerable additional complexities which extended systems introduce into the problem. Much work has been done on the nonlinear dimer [3-6]. Here we report on a few developments that have occurred recently in our investigation of the system. They are (i) exact solutions for the quantum nonlinear dimer in the absence of dissipation, (ii) a new approach we have constructed to analyze the thermal stability of nonlinear structures, and (iii) bifurcation behaviour we have encountered in the interaction of the dimer with a heat reservoir. The first two will be mentioned in the rest of this section and the third in section 2.

The Hamiltonian of the quantum dimer is, in terms of standard quasiparticle operators,

$$H = V\hat{r} + g\omega\hat{p}\left(b^{+} + b\right) + \omega\left(b^{+}b + \frac{1}{2}\right) \tag{1}$$

where V denotes the interaction matrix element for the quasiparticle transfer between the two sites of the dimer, and g measures the coupling strength with the vibration of frequency ω, the destruction operator for the vibration quantum being b. We have put the (identical) site energy of the two sites equal to zero and have put $\hbar = 1$. In the semiclassical approximation, in which the vibration is denoted by the purely classical quantity y one can show [5] that (1) results in :

$$\frac{dp}{dt} = 2Vq; \qquad \frac{dq}{dt} = -2Vp - \chi pr; \qquad \frac{dr}{dt} = \chi qy \tag{3a}$$

$$\frac{d^2y}{dt^2} = -\omega^2(y-p) \tag{3b}$$

where $p = \rho_{11} - \rho_{22}$; $q = i(\rho_{12} - \rho_{21})$; $r = \rho_{12} + \rho_{21}$. Among results reported earlier regarding (1),(3) are stationary states [3], and the time evolution for the case of disparate time scales between the vibrations and the quasiparticle: both for special initial conditions, and for arbitrary initial conditions [4]. One of the new results we wish to comment on here is solutions for the case when the time scale disparity *does not* exist. While valid only for restricted values of the dimer parameters, they are exact. The technique of obtaining them [7] is based on writing p as a function of y : $p = f(y)$. The specific form of p as a three-term series, allows the solution for the vibrational amplitude to be found in the form $y = y_0 \mathrm{cn}(\Omega\tau|k)$ in terms of appropriate dimer parameters, and

$$p = a\mathrm{cn}(\Omega\tau|k) + b\mathrm{cn}^3(\Omega\tau|k) \tag{4a}$$

$$q = -\Omega \mathrm{sn}(\Omega\tau|k)\mathrm{dn}(\Omega\tau|k)\left[a + 3b\mathrm{cn}^2(\Omega\tau|k)\right] \tag{4b}$$

$$r = c_0 + c_1\mathrm{cn}^2(\Omega\tau|k) + c_2\mathrm{cn}^4(\Omega\tau|k) \tag{4c}$$

We do not describe the meaning of the various parameters in (4) here but only draw attention to the interesting form of the solution.

An important undertaking is the exploration of the effects of a coupling between the quantum nonlinear dimer and a heat reservoir. Two quite different methods of attack suggest themselves. One of them consists of a Langevin equation analysis: Computer simulations [8,9] or analytic treatments [10,11] may be used to augment (3) through the introduction of random noise terms. One of the new outcomes of such a Brownian motion analysis of treating thermal reservoir interactions is the subject of section 2 below. A quite different treatment has been developed recently by us in collaboration with Cruzeiro-Hansson and Raghavan [12]. The basic idea is to evaluate the equilibrium partition function (and related quantities) of the semiclassical quantum dimer, and follow a Gibbs approach to thermal stability. Space considerations permit us only to point out that the partition function, which is proportional to the integral Q

$$\mathrm{Q} = \int_{-\infty}^{+\infty} dy \; e^{-\frac{1}{2}by^2} \cosh\left(b\sqrt{\mathrm{v}^2 + y^2}\right) \tag{5}$$

where the dimensionless temperature b is half the ratio of the polaronic binding energy to the thermal energy kT while v is the ratio of the band splitting to the binding energy. Equation (5) possesses a very rich structure and leads to a powerful approach to the thermal stability problem on the basis of an unexpected analogy to magnetic systems [12].

2. BIFURCATIONS

The Brownian motion analysis of interactions with the heat reservoir reat situations has resulted in the fascinating prediction [13] of Hopf bifurcations. With the notation that r_{eq} is the thermal equilibrium value of r, and α is a rate which attempts to drive the system to the thermal state, the underlying equations of motion are [11]:

$$\frac{dp}{dt} = 2Vq \tag{6a}$$

$$\frac{dq}{dt} = -2Vp - \chi pr + \frac{2V\chi}{\Gamma} qr - \alpha q \tag{6b}$$

$$\frac{dr}{dt} = \chi pq - \frac{2V\chi}{\Gamma} q^2 - \alpha(r - r_{eq}) \tag{6c}$$

A high temperature expression for the rate representing fluctuations is $\alpha = (2\chi / \Gamma)kT$.

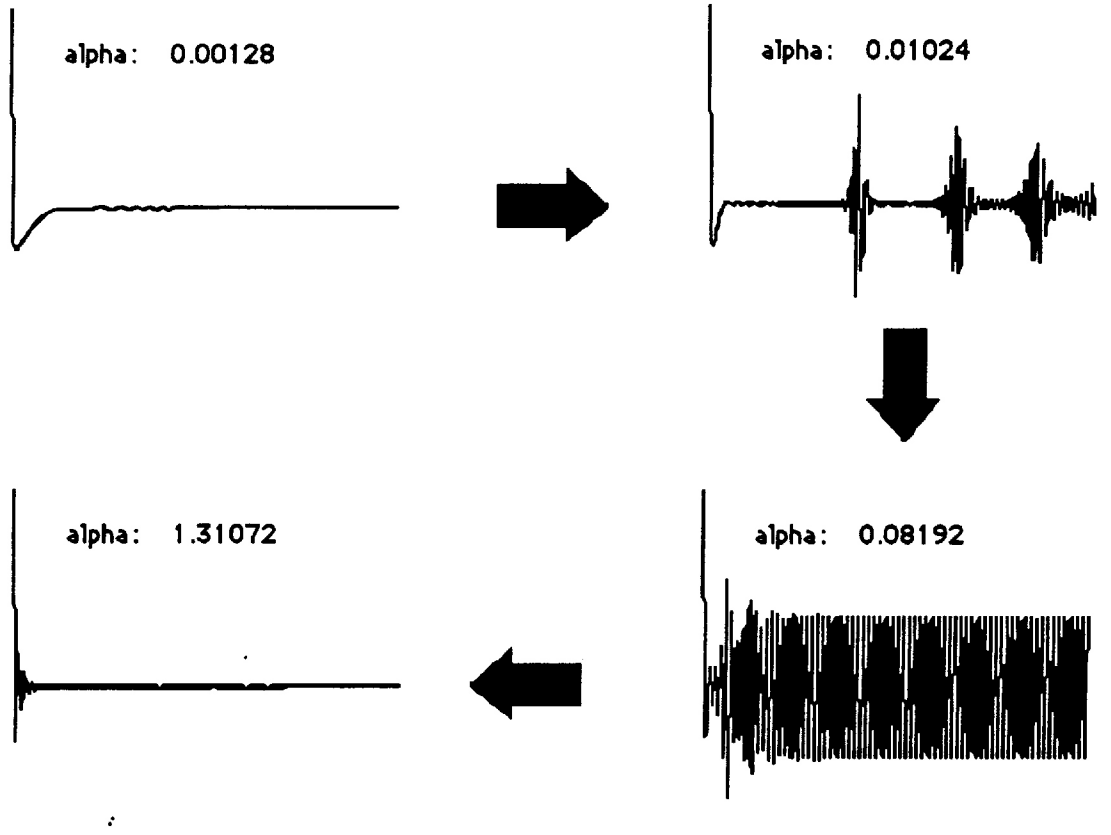

FIG. 1: Time evolution of the probability difference p(t) describing curious effects of thermal reservoir interactions. The horizontal axis in all four frames is the time. The nonlinearity $\chi / 2V$ is larger than 1. There are thus selftrapped states. The values of $\alpha / 2V$ are as denoted by alpha in the four frames. As $\alpha / 2V$ is increased, one sees the appearance of bursts in the evolution of probability difference. These burst On further increasing $\alpha / 2V$, the bursts disappear at a critical value.

For vanishing α, the probability difference p oscillates and then tends to the stationary value. As α increases, p tends to 0 at larger times even for large nonlinearities. This represents destruction of the selftrapped structure by thermal fluctuations. As α increases further, a rather interesting burst of p occurs for a short time, and the burst recurs after a time period. The bursts become more frequent with further increase of α and behaviour that *appears* chaotic occurs. There is a limit cycle here which is destroyed by a further increase in α. Stable dissipative behaviour is recovered. Stability analysis shows that the destruction of limit cycles occurs for $\alpha > r_{eq}\chi / \Gamma$. This bifurcation behaviour is reflected in predicted features of several observables such as fluorescence polarization in stick dimers.

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