Classical and quantum analysis of chaos in the discrete self-trapping equation

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We study the discrete self-trapping model, for three degrees of freedom. The fraction of the energy shell of the phase space that is chaotic is evaluated directly from the classical motion and also from the exact energy levels of the corresponding quantum system. The correspondence between classical and quantum results is discussed.

I. INTRODUCTION

Several years ago the discrete self-trapping (DST) equation was introduced as a potentially interesting model of nonlinear dynamics.[1] In simplest terms, the system comprises f anharmonic oscillators (freedoms), which are coupled through linear dispersive interactions. More specifically, it takes the form

$$\left[i\frac{d}{dt}-\omega_0\right]\overline{A}+\epsilon M\overline{A}+\gamma \, \mathrm{diag}(|A_1|^2,\ldots,|A_f|^2)\overline{A}=0 ,$$

(1.1)

where $\overline{A}$ is the column vector

$$\overline{A}=\mathrm{col}(A_1,A_2,\ldots,A_f)$$

(1.2)

of complex components. With the *dispersive* parameter ϵ and the *anharmonic* parameter γ both equal to zero, Eq. (1.1) represents a system of f noninteracting, harmonic oscillators each of frequency ω_0. In the general case ($\epsilon\neq 0$ and $\gamma\neq 0$), the dynamics of Eq. (1.1) exhibits the effects of both anharmonicity and dispersion. This interaction can lead to either *self-trapping* (i.e., local modes or solitons) or *chaos* or a mixture of self-trapping and chaos depending upon the parameters and initial conditions that are chosen.[1]

The original motivation for studying the DST equation arose from theoretical studies of vibrational energy self-trapping in protein[2,3] and related experimental studies in hydrogen bonded, polypeptide crystals.[4,5] In these applications the number of degrees of freedom (f) is rather large: ca. 200 for a typical protein and much greater for an experimental polypeptide crystal. In order to gain theoretical perspective, initial attention was directed toward the DST with a few degrees of freedom, which is closely related to the study of anharmonic vibrations in small molecules [water, ammonia, methane, benzene, etc. (Refs. 6 and 7)]. During the course of these "chemical" investigations a quantum theory for the DST equation was developed[8,9] and has proven to be remarkably accurate and straightforward to apply.[10]

Our aim in this paper is twofold. First we augment previous studies of classical chaos exhibited by the DST equation;[1,11-13] and, second, we relate these studies to the corresponding quantum analysis. Thus our work should be considered in the context of growing interest in "quantum chaology",[14-20] but we believe that it is of particular interest for the following reasons. (i) The DST equation is a good model for anharmonic molecular vibrations[4-9] and is therefore of considerable technical interest. (ii) As will be explained in the following, the quantum DST system can be analyzed without truncating infinite wave function expansions;[8-10] thus the only errors in computing energy levels are numerical. (iii) The quantum DST system has an anharmonic parameter—γ in Eq. (1.1)—which can be independently varied as one approaches the correspondence limit. These last two properties are shared by the spin system analyzed recently by Nakamura and Bishop.[19] Motivated by the known mapping between an integrable nonlinear Schrödinger equation and an integrable spin system,[21] Bishop has suggested that a mapping may exist between his nonintegrable spin system and the DST equation.[22] We have studied this question in some detail and have been unable to find such a mapping. Even if one were to be found, however, we feel that property (i) of the DST system would be sufficient to justify the results presented here.

To appreciate the ease with which the DST system can be quantized,[8,10] we note that it has two conserved quantities, the *number*

$$N= \sum_{i=1}^{f} |A_i|^2$$

(1.3)

and the *energy*

$$H=\omega_0 N-\tfrac{1}{2}\gamma \sum_{i=1}^{f} |A_i|^4-\epsilon \sum_{i\neq j}^{f} m_{ij} A_i^* A_j .$$

(1.4)

Under quantization, the complex mode amplitudes (A_i^* and A_i) become boson creation and annihilation operators ($\hat{B}_i^{\dagger}$ and $\hat{B}_i$).

With full symmetrization of the operator products Eq. (1.3) becomes the *number operator*

$$\hat{N}= \sum_{i=1}^{f} (\hat{B}_i^{\dagger}\hat{B}_i+\tfrac{1}{2})$$

(1.5)

and Eq. (1.4) becomes the *energy operator*

$$\hat{H} = (\omega_0 - \tfrac{1}{2}\gamma)\hat{N} - \tfrac{1}{2}\gamma \sum_{i=1}^{f} \hat{B}_i^\dagger \hat{B}_i \hat{B}_i^\dagger \hat{B}_i$$

$$- \epsilon \sum_{i \neq j}^{f} m_{ij} \hat{B}_i^\dagger \hat{B}_j \ . \tag{1.6}$$

$\hat{H}$ and $\hat{N}$ operate upon wave functions of the form $|n_1\rangle|n_2\rangle \ldots |n_f\rangle$ which, for typographical convenience, we write as $[n_1,n_2,\ldots n_f]$.

Thus the quantized discrete self-trapping (QDST) equation describes an assembly of bosons.[23] It has been discussed in some detail for nearest-neighbor interactions in the limit $\gamma \ll \epsilon$ and $f \to \infty$.[24-26] This is the limit in which the classical DST reduces to the nonlinear Schrödinger equation.[27]

Stationary states of the QDST equation must be eigenfunctions of both $\hat{N}$ and $\hat{H}$. As in Refs. 7 and 8, the wave function, $|\psi_n\rangle$, is chosen to be a linear combination of all possible states of n particles, leading to a matrix equation for the column vector consisting of the coefficients in this expansion.

It is now well established that classical solution trajectories of Eq. (1.1) for three or more degrees of freedom ($f \geq 3$) can be either chaotic or quasiperiodic for appropriate values of the dispersive and anharmonic parameters, ϵ and γ.[1,6,11-13] Here we study the system for $f = 3$ with the dispersion matrix

$$\epsilon M = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \tag{1.7}$$

from the perspectives of both classical and quantum dynamics.

Results of the classical studies are presented in the following section. Here we estimate the fraction of phase space occupied by chaotic trajectories, which we call ρ_c. Quantum results are presented in Sec. III. We use tools that have been developed by Berry to estimate again the chaotic fraction of phase space, called ρ_q.[20] If these tools are valid we expect $\rho_q \to \rho_c$ as $n \to \infty$, the correspondence limit. The degree to which we are able to confirm such a correspondence is discussed in the concluding section.

II. CLASSICAL ANALYSIS

The DST equation for one degree of freedom reduces to a nonlinear oscillator and the solution is sinusoidal. For two degrees of freedom, we have two conserved quantities and again the system is integrable. Indeed, it has been shown that it can be reduced to the pendulum equation.[28,29] Here we shall confine ourselves to the three degrees of freedom DST which are not integrable. Indeed, chaotic trajectories have been found.[1,11-13] The latter studies were done fixing a specific initial condition and varying the nonlinearity parameter γ. In a particular case, by varying γ, regular trajectories were encountered in a narrow window amidst chaotic ones.[13] However, because these results are valid for one particular initial condition, one cannot claim that such a regular window is a generic feature for this narrow range of values. To do so, one must use a global indicator which probes the

entire energy shell. Such an indicator is ρ_c, which is defined as the fraction of the energy shell E, which is chaotic.[30]

In the case of DST, the phase space must be restricted to the constant N surface as well as the energy shell E when the classical results are compared with quantum results.

Two methods of evaluating ρ_c have been investigated. Meyer relates an integral over the energy surface to an integral over the Poincaré section.[30] Implicit in his derivation is the assumption that *all* trajectories on the energy surface intersect the Poincaré section. We have not found any Poincaré section for which this assumption is valid in our system and suspect that in general it is not true.[31] For this reason we have adopted a second method to evaluate ρ_c.

The second method, on which all of our classical results are based, is a Monte Carlo evaluation[32] of ρ_c. We choose a number of random initial conditions which are uniformly distributed on the energy surface. These initial conditions must also have the same value of N. The fraction of these initial conditions which leads to chaotic trajectories is then our estimate of ρ_c.

The obvious test of whether or not a trajectory is chaotic is to calculate the maximal Lyapunov exponent,[30,32] but because of excessive computational costs we chose instead to determine whether or not the trajectory is chaotic by examination of a Poincaré section.

In Fig. 1 we show a Poincaré section representative of those which are encountered when the determination of chaotic versus regular is made. The dots in the figure all belong to a trajectory, which is labeled chaotic. The crosses, which form a nearly closed curve, belong to a quasiperiodic, i.e., regular orbit. For two energies ($\gamma E = -0.1$ and $\gamma E = -0.6$) we examined both the maximal exponents and the Poincaré sections. Good agreement on the value of ρ_c was obtained.

In roughly 95% of the sections studied, the determination of whether or not the trajectory is chaotic is quite
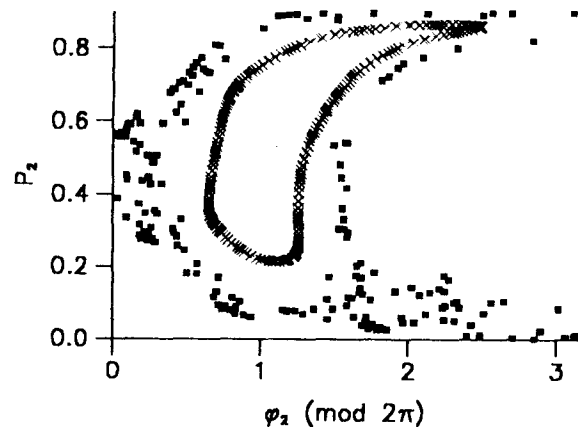

FIG. 1. Poincaré section of regular ($\times$) and chaotic ($\blacksquare$) trajectories. ($P_1 = 0.1, \gamma N = 3, \gamma E = -2.4$.)

unambiguous as in Fig. 1. Any errors introduced in this way are small in comparison with the statistical error associated with the Monte Carlo method.

Instead of working with the original variables, A_i and A_i^* (which are canonical variables with respect to the Hamiltonian $-iH$), we have made the following transformation to canonical variables:

$$A_1 = \sqrt{P_1}\, e^{-i(\phi_1+\phi_3)}, \quad 0 < P_1 < N \ ,$$

$$A_2 = \sqrt{P_2}\, e^{-i(\phi_2+\phi_3)}, \quad 0 < P_2 < N \ , \qquad (2.1)$$

$$A_3 = \sqrt{P_3 - P_1 - P_2}\, e^{-i\phi_3}, \quad 0 < P_1 + P_2 < N \ ,$$

leading to the Hamiltonian

$$H(\boldsymbol{\phi},\mathbf{P}) = -\tfrac{1}{2}\gamma[P_1^2 + P_2^2 + (N - P_1 - P_2)^2]$$

$$-2\epsilon[\sqrt{P_1 P_2}\cos(\phi_1 - \phi_2)$$

$$+\sqrt{P_1(N-P_1-P_2)}\cos\phi_1$$

$$+\sqrt{P_2(N-P_1-P_2)}\cos\phi_2] \ , \qquad (2.2)$$

where P_i is the momentum conjugate to $\phi_i, i = 1,2,3$. In this description the momentum P_3 is in fact the conserved quantity N. Hence ϕ_3 is an ignorable coordinate. Thus the equations of motion become

$$\dot{\phi}_1 = \frac{\partial H}{\partial P_1}, \quad \dot{\phi}_2 = \frac{\partial H}{\partial P_2} \ ,$$

$$\dot{P}_1 = -\frac{\partial H}{\partial \phi_1}, \quad \dot{P}_2 = -\frac{\partial H}{\partial \phi_2} \ . \qquad (2.3)$$

(The time evolution of ϕ_3, which is determined by the equation $\dot{\phi}_3 = \partial H/\partial N$ may be chaotic.) Note that Eq. (1.1) is invariant under the transformations $A_j \to \alpha A_j$, $\gamma \to \alpha^{-2}\gamma$, $N \to \alpha^2 N$, and $H \to \alpha^2 H$. Since γN and γH are unchanged under these transformations they are used to specify the number and the energy, respectively.[12]

For the purpose of computing ρ_c, the preceding transformation effectively reduces the number of degrees of freedom from three to two. The initial conditions are randomly distributed over the energy surface $H(P_1, P_2, \phi_1, \phi_2) = E$. Thus, ϕ_1 becomes a function of P_1, P_2, and ϕ_2.

The random initial conditions for P_1, P_2, and ϕ_2 are weighted by the projection of the surface element $(P_1, P_2, \phi_1, \phi_2) \to (P_1, P_2, \phi_2)$.

Thus ρ_c can be calculated from the trajectories determined by (2.3) for any fixed values of γE and γN. (The value $\gamma N = 3$ is chosen throughout.)

Figure 2 shows our results for ρ_c, based on 50–100 trajectories (vertical error bars), as well as the corresponding quantity, ρ_q (horizontal error bars), in the quantum-mechanical case considered in Sec. III. The error bars in ρ_c are determined as the 95% confidence interval of our estimate of ρ_c. In the limits of high and low γE the DST equation is integrable. As a consequence, $\rho_c \to 0$ in these limits is seen in the figure. Local minima are found at $\gamma E \sim -4.2$ and -3.8, which may be interpreted as windows of less chaotic behavior. However, the window for
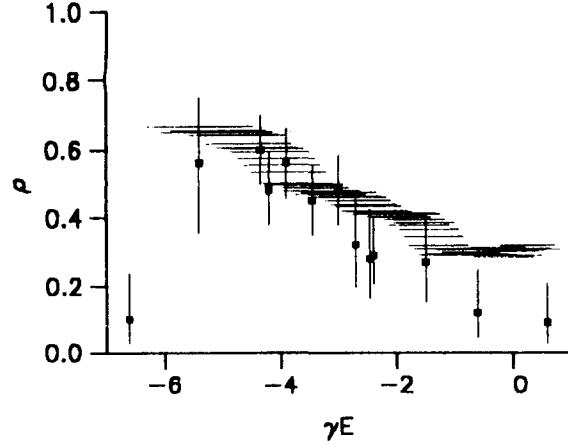

FIG. 2. $\rho_c(\blacksquare)$ and $\rho_q(-)$ as functions of energy γE for fixed $\gamma N = 3.00$. Error bounds indicated by vertical and horizontal bars. $n = 310$ in the QDST giving a total of 8164 energy levels.

$\gamma E = -10.99$ and $\gamma N = 4.5$ reported in Ref. 13 was found to give a value $\rho_c \sim 0.73 - 0.98$. Thus, although the particular initial condition considered was regular for the latter values of γN and γE, about 90% of the energy shell is actually occupied by chaotic trajectories.

III. QUANTUM ANALYSIS

In this section we study the quantum counterpart of the DST equation with three freedoms. Studies of energy spectra of quantum systems have shown that the density of spacings, S, between uncorrelated, adjacent energy levels, $p(S)$, can be used as an indicator of chaos or regularity in the corresponding classical systems.[14–18,32–38].

When the classical phase space is partitioned into regular regions and only one chaotic region the following interpolation formula has been proposed:[33]

$$p_I(S) = \exp\left[-(1-\rho_q)S - \frac{\pi}{4}\rho_q^2 S^2\right]$$

$$\times \left[(1-\rho_q)^2\exp\left[\frac{\pi}{4}\rho_q^2 S^2\right]\mathrm{erfc}\left[\frac{\sqrt{\pi}}{2}\rho_q S\right]\right.$$

$$\left.+2(1-\rho_q)\rho_q + \frac{\pi}{2}\rho_q^3 S\right] \ . \qquad (3.1)$$

Here ρ_q is the fraction of the energy shell that is chaotic.

Equation (3.1) interpolates between the Poisson distribution (for the quantum counterpart of the regular classical system[34]) and the Wigner distribution [corresponding to the chaotic classical system (Ref. 14)].

Equation (3.1) shows how the fraction of the energy shell that is chaotic in the classical system can be determined from the energy levels of the corresponding quantum system. Its use implies the assumption that all chaotic regions are connected. In the case of the DST equation with three degrees of freedom, which effectively is a system with two degrees of freedom (see Sec. II), this must be assumed in order to make a unique fitting to the

available data. Hence Eq. (3.1) is used as an approximation.[18]

Above we have specified that the spacings distribution should be done with uncorrelated energy levels. By uncorrelated we mean levels that evolve independently when parameters in the Hamiltonian (such as nonlinearity γ) are varied. In the case of the DST model this means, for instance, that states corresponding to different n values must not be mixed. Also, and generally for all Hamiltonians that possess symmetry properties, the energies must be separated according to the symmetry group in order to avoid degenerate levels.

The results shown in this article were obtained from energy sequences corresponding to the symmetric states, the number of which is $1+\text{int}[n(n+6)/12]$.[10] A final remark is that the spacings distribution should be determined from an energy sequence that possesses a large number of energy levels in a short energy range. This usually implies large quantum numbers and correspondingly large matrices to diagonalize, which is impossible in practice. Energy sequences with lower density of levels can also be used, provided they have been scaled previously into other sequences that have constant density. In this way the secular variation in the density is eliminated in order that the short range (expressed by the spacings distribution) be brought to light.[38]

Figure 2 shows the variation of ρ_q with γE (for $\gamma n = 3$). Each ρ_q value is calculated from a sequence with 2000 levels, the energy E being the average energy and the error being the corresponding standard deviation. Superimposed on them are the values of ρ_c. Our numerical calculations show that at least 1500 levels are needed for reliable statistics.

The quantum results confirm the trend of the classical ones. However, the correspondence is not as good as that found by previous authors.[15,18,36,38] One reason may be that with the value of n used, the density of levels is not

large enouch (a fact that is expressed by the horizontal error bars). A clear divergence from the classical result is observed in the low γE limit. This is due to the particularly low density of quantum levels in this region (with the correspondingly larger horizontal error bars). Our conclusion is that in the low γE region, for the values of n used, the ρ_q determined cannot be trusted. In the other regions, on the other hand, the quantum calculations correspond to an averaging over a range of classical energy shells. This leads to a loss of the more detailed structure indicated by the classical calculation.

IV. CONCLUSIONS

The fundamental aim of this paper is to study quantum and classical determinations of the chaotic fraction of the energy shell in phase space for the discrete self-trapping equation with three degrees of freedom. The classically computed fraction is called ρ_c, and the fraction determined quantum mechanically using the procedure outlined by Berry and co-workers[20,33,34] is called ρ_q.

Our results are presented in Fig. 2. In the intermediate range of energy, where $\rho_c \cong \rho_q \cong \frac{1}{2}$, the agreement seems to be within the error bars. At the extreme values of energy, however, the agreement is not good. This may be because the system is not generic[39] at the extreme values, or because the number of levels chosen (8164) is not sufficient.

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