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Nearest-neighbour level spacings for the non-periodic discrete nonlinear Schrödinger equation

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Abstract. The phase space of the classical non-periodic discrete nonlinear Schrödinger equation contains both a chaotic region and a continuous family of periodic orbits. In a bid to determine the extent to which this mixed behaviour manifests itself in the transition to quantum mechanics, we study the nearest-neighbour level-spacing distribution of the corresponding quantum energy levels. This is compared with the optimal Berry–Robnik and Brody distributions, which continuously interpolate between regular and chaotic level spacing statistics.

1. Introduction

A number of recent papers [1–5] have described an interesting, generic model for coupled, anharmonic oscillators: the discrete nonlinear Schrödinger equation (DNLSE). The DNLSE [1] may be obtained from the familiar nonlinear Schrödinger equation by replacing the continuous oscillating field by a discrete lattice, leading to the approximation of the linear dispersion in the former by a linear coupling between neighbouring sites. In the DNLSE, the interplay between the coupling and the nonlinearity leads to a range of behaviour intermediate between periodic exchange of energy between the sites when the field intensity is low, and localization for strong fields. These extremes correspond, respectively, to linear dispersive propagation and field localization in the continuum model.

Unlike the NLSE, the DNLSE is non-integrable when the lattice consists of more than two sites, and the simplest such case, the three-element lattice [2–7], has been a subject of intensive investigation in recent years. There are two standard configurations for the three-element DNLSE lattice: the periodic or triangular lattice in which all lattice sites are mutually adjacent, and therefore coupled, and the non-periodic configuration where the lattice sites are arranged as a three-element linear array. In this latter arrangement, the boundary sites are mutually uncoupled. Dynamical chaos has been found in the analysis of both cases [2–7].

The DNLSE has been found to have a wide range of application in many disparate branches of physics. In nonlinear optics, it is used as a model for systems of linearly-coupled, non-dispersive, single-mode Kerr fibres (nonlinear directional couplers) [6, 7] and in quantum chemistry it describes bond vibrations in certain molecular crystals [8, 9] and biological polymers [10]. Many properties of the DNLSE are known as a consequence of it being a particular case of a more general model, the discrete self-trapping equation [11, 12], which is not restricted to nearest-neighbour coupling.

Although motivated originally by a quantum problem, in early studies the DNLSE was considered as a classical system. In recognition of its quantum mechanical origin, the

DNLSE has more recently been given a fully quantum treatment [13]. Quantization of the DNLSE has proven to be a relatively uncomplicated matter, owing to the ease in which the standard canonical quantization procedure can be applied. Furthermore, the symmetries of the quantum DNLSE Hamiltonian imply that the corresponding time-independent Schrödinger equation can be converted into a sequence of finite matrix eigenproblems.

A number of studies of the QDNLSE [14, 15], including this one, have been motivated by the current widespread interest in quantum non-integrability; in particular, quantum manifestations of classical chaos [16, 17]. Recent years have seen considerable effort being devoted to identifying universality in the nearest-neighbour level spacing distribution for the energy levels of non-integrable Hamiltonians. The fact that the eigenvalue problem for the QDNLSE Hamiltonian can be reduced to the diagonalization of finite matrices implies that the accuracy with which energy levels can be determined is restricted only by numerical round-off errors, allowing very small level spacings to be resolved.

The nearest-neighbour level-spacing distribution has been studied for the periodic QDNLSE [14, 15]. In this paper, we carry out a similar analysis for the non-periodic case. Prior to doing so, we briefly review the main features of the classical model. The non-periodic three-element DNLSE is a conservative system and has the Hamiltonian

$$H = \gamma(|a|^4 + |b|^4 + |c|^4) + \beta(a^*b + b^*a + c^*b + b^*c) \quad (1.1)$$

where a, b and c are the complex amplitudes for the oscillators at sites 1, 2 and 3, respectively. The part of the Hamiltonian which is proportional to γ is the nonlinear self-interaction term while the remainder couples sites 1 and 3 to site 2. Hamilton's equations for the oscillator amplitudes, which for the sake of brevity we denote by a_j , are readily obtained using the prescription $\dot{a}_j = -i(\partial H/\partial a_j^*)$. We find

$$i\dot{a} = 2\gamma|a|^2a + \beta b \quad (1.2)$$

$$i\dot{b} = 2\gamma|b|^2b + \beta(a + c) \quad (1.3)$$

$$i\dot{c} = 2\gamma|c|^2c + \beta b. \quad (1.4)$$

We note that both the uncoupled ($\beta = 0$) and linear ($\gamma = 0$) limits are integrable and indeed analytically soluble. In the former case, the separate field intensities are constants of motion and the solutions are easily found to be $a_i(t) = a_i(0)e^{-2i\gamma|a_i(0)|^2t}$, corresponding to self-phase modulation when the oscillators are electromagnetic field modes. On the other hand, the linear limit can be solved with equal ease by performing a canonical transformation to the normal modes of the system.

In addition to the Hamiltonian there exists a further conserved quantity, the total field strength $N = |a|^2 + |b|^2 + |c|^2$. There are, however, no further constants of motion, implying that the system is, in general, non-integrable.

Not all solutions to (1.2)–(1.4) correspond to chaotic trajectories. Symmetric solutions ($a = c$) are fully integrable and analytical expressions for the centre-excite initial condition ($a(0) = c(0) = 0$) have been obtained in terms of Jacobi elliptic functions [7]. These solutions are periodic orbits and have been found to be unstable against antisymmetric perturbations [3, 7].

Another property of this system which has attracted a great deal of attention [2, 3] is the fact that in the linear ($\gamma = 0$) limit, the Hamiltonian is that of three *resonant* coupled oscillators. It is well known [18] that resonant and nonresonant tori undergo very different kinds of transformation upon the addition of a small perturbation to the Hamiltonian. While the KAM theorem guarantees that irrational tori will only be slightly deformed by a minor alteration of the unperturbed dynamics, resonant tori are, by contrast, completely destroyed.

This fact has important consequences for the system described by the Hamiltonian (1.1) since in the linear limit all tori are resonant.

The perturbed system can exhibit widespread dynamical chaos when the nonlinear perturbation, which gives rise to a mutual interaction among the linear canonical variables, contains terms which are resonant with the linearized system [19]. It has been observed that under such circumstances, chaos can develop even when the perturbation is arbitrarily small, owing to the fact that the linear degrees of freedom are resonantly coupled by the nonlinearity. A full discussion of this property of the DNLS is given in [3].

2. The quantum Hamiltonian

A convenient starting point for our discussion of the related quantum model is the corresponding quantum Hamiltonian

$$\hat{H} = \gamma(\hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} + \hat{b}^\dagger \hat{b}^\dagger \hat{b} \hat{b} + \hat{c}^\dagger \hat{c}^\dagger \hat{c} \hat{c}) + \beta(\hat{a}^\dagger \hat{b} + \hat{b}^\dagger \hat{a} + \hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) \quad (2.1)$$

where the pairs of operators $(\hat{a}^\dagger, \hat{a})$, $(\hat{b}^\dagger, \hat{b})$ and $(\hat{c}^\dagger, \hat{c})$ are naturally interpreted as bosonic creation and annihilation operators for the three oscillators. The following discussion is based on the treatment of the simpler two-site DNLS lattice given in [20]. Throughout this paper we shall take $\hbar = 1$. On quantization, the total field strength becomes the total boson number operator $\hat{N} = \hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b} + \hat{c}^\dagger \hat{c}$ which commutes with \hat{H} and thus remains a conserved quantity. As a consequence of the symmetry between modes 1 and 3, the parity operator \hat{P} whose three-mode number state decomposition is

$$\hat{P} = \frac{1}{2} \sum_{j,k,l=0}^{\infty} (|j, k, l\rangle \langle l, k, j| + |l, k, j\rangle \langle j, k, l|) \quad (2.2)$$

also commutes with the Hamiltonian. The Heisenberg equations of motion are readily obtained:

$$i\dot{\hat{a}} = 2\gamma\hat{a}^\dagger \hat{a} \hat{a} + \beta\hat{b} \quad (2.3)$$

$$i\dot{\hat{b}} = 2\gamma\hat{b}^\dagger \hat{b} \hat{b} + \beta(\hat{a} + \hat{c}) \quad (2.4)$$

$$i\dot{\hat{c}} = 2\gamma\hat{c}^\dagger \hat{c} \hat{c} + \beta\hat{b}. \quad (2.5)$$

In spite of the formal similarity between these equations and Hamilton's equations (1.2)–(1.4) for the classical system, operator ordering difficulties mean that an analytical solution for the quantum centre-excite initial condition cannot be found in a manner analogous to that by which the corresponding classical solution may be obtained.

Although the canonical quantization procedure does not lead to a unique prescription for ordering products of noncommuting operators, everything which will be of interest to us is insensitive to the ordering convention used in the nonlinear part of the Hamiltonian if the same convention is used for all three oscillators. If we consider two distinct quantum Hamiltonians arrived at by quantizing (1.1) according to different ordering prescriptions, they will differ at most by a linear function of the total number operator \hat{N} , and will therefore mutually commute.

The quantum problem can be solved by numerically diagonalizing the Hamiltonian. A method for doing this is suggested by the fact that total number operator \hat{N} commutes with the Hamiltonian given by equation (2.1). As a consequence, the total number of quanta in the system is a conserved quantity. One can readily verify that the Hamiltonian matrix element between two states with differing total particle number is zero

$$\langle j', k', l' | \hat{H} | j, k, l \rangle = \delta_{(j'+k'+l')(j+k+l)} H_{Njk}^{j'k'} \quad (2.6)$$

where $N = j + k + l$ and the matrix element $H_{Njk}^{j'k'}$ is given by

$$H_{Njk}^{j'k'} = \langle j', N - (j' + k'), k' | \hat{H} | j, N - (j + k), k \rangle \tag{2.7}$$

having the explicit form

$$\begin{aligned} H_{Njk}^{j'k'} = & \gamma(2(j^2 + k^2) + N^2 + 2jk + 2N(j + k) - N)\delta_{jj'}\delta_{kk'} \\ & + \beta(\delta_{k'k}(\sqrt{(j + 1)(N - j - k)}\delta_{j'j+1} + \sqrt{j(N - j - k + 1)}\delta_{j'j-1}) \\ & + \delta_{jj'}(\sqrt{(k + 1)(N - j - k)}\delta_{k'k+1} + \sqrt{k(N - j - k + 1)}\delta_{k'k-1})). \end{aligned} \tag{2.8}$$

The fact that the commutator $[\hat{N}, \hat{H}]$ is zero implies that \hat{H} and \hat{N} have a complete set of common eigenstates. Each eigenstate of \hat{H} is then a linear combination of all eigenstates of \hat{N} corresponding to a fixed degenerate eigenvalue. The m th such eigenstate of \hat{H} with N quanta has the number state expansion

$$|\psi_{Nm}\rangle = \sum_{j=0}^N \sum_{k=0}^{N-j} R_{Nm}^{jk} |j, N - (j + k), k\rangle \tag{2.9}$$

where it is easily found that m ranges from 0 to $N(N + 3)/2$, since the dimension of the subspace spanned by all three-mode number states with N quanta is equal to $1 + N(N + 3)/2$. All eigenstates of \hat{H} are orthonormal,

$$\sum_{j=0}^N \sum_{k=0}^{N-j} R_{Nm}^{jk} R_{Nm'}^{jk} = \delta_{mm'} \tag{2.10}$$

and have definite parity; that is, they are also eigenstates of the parity operator \hat{P} given by (2.2), meaning that $R_{Nm}^{jk} = \pm R_{Nm}^{kj}$ where the plus and minus signs denote positive and negative parity respectively. In order to determine the coefficients R_{Nm}^{jk} , we must solve the eigenvalue equation

$$\hat{H}|\psi_{Nm}\rangle = E_{Nm}|\psi_{Nm}\rangle. \tag{2.11}$$

Making use of (2.6), (2.7), (2.9) and (2.10), we find that in the three-mode number state basis, the Schrödinger equation (2.11) reads

$$\sum_{j=0}^N \sum_{k=0}^{N-j} H_{Njk}^{j'k'} R_{Nm}^{jk} = E_{Nm} R_{Nm}^{j'k'}. \tag{2.12}$$

All that remains to be done is to express (2.12) as an equivalent *matrix* eigenvalue problem. That is, for each N , we must rearrange the elements of $H_{Njk}^{j'k'}$ and R_{Nm}^{jk} into square matrices, so as to render the problem suitable for numerical diagonalization. We find that a standard matrix eigenvalue problem is obtained by making the following transformations of the indices j, k, j' and k' :

$$b = j(N - (j - 3)/2) + k \quad 0 \geq j \geq N \quad 0 \geq k \geq N - j \tag{2.13}$$

$$b' = j'(N - (j' - 3)/2) + k' \quad 0 \geq j' \geq N \quad 0 \geq k' \geq N - j'. \tag{2.14}$$

Although each of these transformations maps a pair of indices onto a single index, they are both invertible. Under this pair of mappings, $H_{Njk}^{j'k'}$ becomes a square matrix $h_{Nb}^{b'}$ and the number state expansion of the m th eigenvector R_{Nm}^{jk} becomes r_{Nm}^b . The matrix eigenproblem is then

$$\sum_{b=0}^{M(N)} h_{Nb}^{b'} r_{Nm}^b = E_{Nm} r_{Nm}^{b'} \tag{2.15}$$

where $M(N)$ is equal to $N(N+3)/2$. We note that, as a consequence of $H_{Njk}^{j'k'}$ being real and invariant under the transformation $(j, k, j', k') \rightarrow (j', k', j, k)$, the matrix $h_{Nb}^{b'}$ is real, symmetric and hence Hermitian. It follows from (2.10) that $r_{Nm}^{b'}$ is a real, orthogonal matrix for each N .

The eigenvalues for $N = 8$ and $N = 10$ are shown in figures 1(a) and (b) respectively. In both figures, we have taken the coupling constant β to be 10 and γ has been allowed to vary continuously from 0 to 10. When $\gamma = 0$, the energy levels form a degenerate regular ladder of levels with minimum spacing $\sqrt{2\beta}$. Both this degeneracy and the otherwise regular spacing can be readily accounted for since, in this limit, the system is simply three linearly coupled oscillators, the eigenvalues and eigenstates of which can be calculated analytically. When $\gamma = 0$, the Hamiltonian

$$\hat{H}' = \hat{H}_{\gamma=0} = \beta(\hat{a}^\dagger \hat{b} + \hat{b}^\dagger \hat{a} + \hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) \quad (2.16)$$

can be diagonalized by making a canonical transformation to the normal modes of the system, which are characterized by the operators $\hat{A}_\pm = (\hat{a} \pm \sqrt{2}\hat{b} + \hat{c})/2$ and $\hat{B} = (\hat{a} - \hat{c})/\sqrt{2}$. The only non-vanishing commutators among these three operators and their adjoints are

$$[\hat{A}_+, \hat{A}_+^\dagger] = [\hat{A}_-, \hat{A}_-^\dagger] = [\hat{B}, \hat{B}^\dagger] = 1. \quad (2.17)$$

The linear Hamiltonian may then be written as

$$\hat{H}' = \sqrt{2\beta}(\hat{A}_+^\dagger \hat{A}_+ - \hat{A}_-^\dagger \hat{A}_-) \quad (2.18)$$

and all simultaneous eigenstates of \hat{H}' and \hat{N} with eigenvalue N have the form

$$|\phi_{Njk}\rangle = \xi_{Njk} \hat{A}_+^{\dagger j} \hat{A}_-^{\dagger k} \hat{B}^{\dagger N-(j+k)} |0, 0, 0\rangle \quad (2.19)$$

where $0 \geq j + k \geq N$ and the normalization constant ξ_{Njk} is given by

$$\xi_{Njk} = (j!k!(N-j-k)!)^{-1/2}. \quad (2.20)$$

The operators \hat{A}_+ and \hat{A}_-^\dagger will transform an eigenstate of \hat{H}' with energy E into another with energy $E - \sqrt{2\beta}$, while \hat{A}_- and \hat{A}_+^\dagger act on a state with energy E to produce another with energy $E + \sqrt{2\beta}$. Although the remaining mode operators \hat{B} and \hat{B}^\dagger also change eigenstates of \hat{H}' into new ones, they do not alter the corresponding energy. We find that the energy E'_{Njk} of the state $|\phi_{Njk}\rangle$ is $\sqrt{2\beta}(j-k)$ and these eigenvalues are, in general, highly degenerate, even when we consider the fixed- N spectrum. In fact, defining

$$\mu_{Njk} = N - E'_{Njk}/\sqrt{2\beta} \quad (2.21)$$

we find that, when greater than zero, the quantities $(\mu_{Njk} + 2)/2$ and $(\mu_{Njk} + 1)/2$ are equal to the fixed- N degeneracy of the energy E'_{Njk} when μ_{Njk} is even and odd, respectively. When the appropriate degeneracy formula has a value less than 1, there is no N -boson state with energy E'_{Njk} .

The parity of the eigenstates in the linear limit is easily determined using the fact that the parity operator \hat{P} commutes with the symmetric creation operators \hat{A}_\pm^\dagger and anticommutes with the antisymmetric operator \hat{B}^\dagger . It follows from these relations that the parity of the state $|\phi_{Njk}\rangle$ is

$$\langle \phi_{Njk} | \hat{P} | \phi_{Njk} \rangle = (-1)^{N-j-k}. \quad (2.22)$$

One important consequence of (2.22) is the fact that symmetric and antisymmetric eigenstates of \hat{H}' cannot correspond to the same degenerate eigenvalue. We can show this

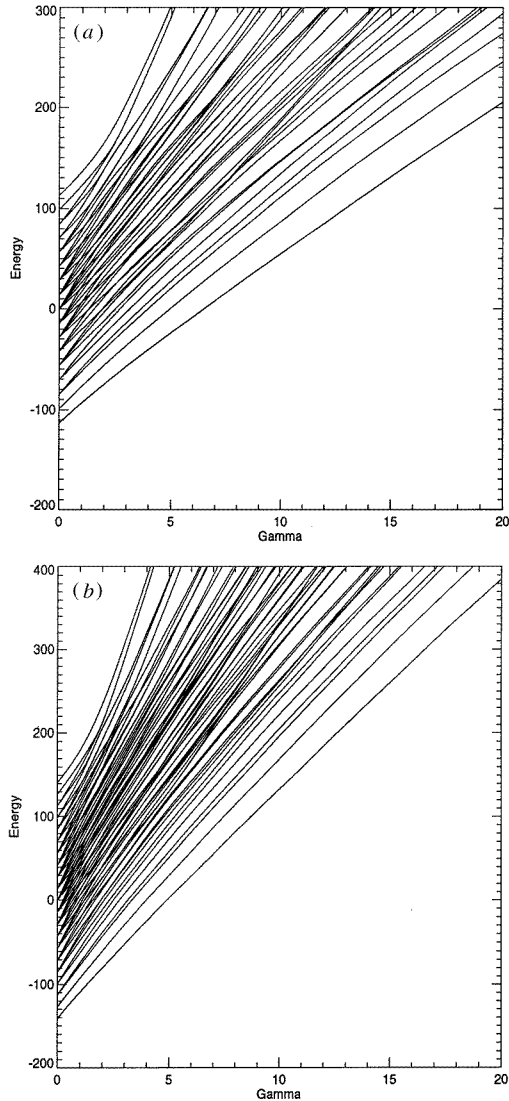


Figure 1. Energy eigenvalues for $\beta = 1$ with (a) $N = 8$ and (b) $N = 10$.

by noting that if two states, $|\phi_{Njk}\rangle$ and $|\phi_{Nj'k'}\rangle$, have the same energy, then $j - k = j' - k'$, or

$$j + k = j' + k' + 2(k - k'). \quad (2.23)$$

Since $2(k - k')$ is even, the parity of the state $|\phi_{Njk}\rangle$ as obtained from (2.22) is equal to that of $|\phi_{Nj'k'}\rangle$. That is, in the fixed- N spectrum, a degeneracy can only occur when the corresponding eigenstates have the same parity. The full significance of this result will be made clear when we come to study the nearest-neighbour level-spacing distribution in the following section.

Our numerical results indicate that these degeneracies are completely broken by the nonlinear perturbation for arbitrarily low γ , and in the vicinity of integrability adjacent

levels are seen to repel one another. As γ is increased, the system departs further from integrability and the spectra acquire the irregular character and high density of avoided level crossings commonly observed in the spectra of non-integrable Hamiltonians. The density of avoided crossings is seen to decrease for still larger values of γ as the spectra respond to the degeneracy in the nonlinear limit, at which all modes become decoupled and the system is integrable once more. As $\gamma/\beta \rightarrow \infty$, the eigenvalues of \hat{H} tend to $E = \gamma(i^2 + j^2 + k^2 - N)$, where $N = i + j + k$, which are found to be sixfold degenerate when the i , j and k are all different, threefold degenerate when two of them are equal and non-degenerate when all three are equal [14]. In this uncoupled limit, the fixed- N spectrum, clearly a quadratic function of the number of quanta in each mode, has a linear increase in level spacing. This results in the grouping of neighbouring levels and repulsion of neighbouring groups.

3. Level-spacing distribution

In both integrable limits, the spectrum of the QDNLSE Hamiltonian exhibits a high degree of degeneracy, as is typical of systems whose classical counterparts undergo regular motion. Systematic degeneracies in spectra reflect symmetries in the Hamiltonian, which in turn imply the existence of further conserved quantities. All degeneracies, except those due to the conservation of the total number operator \hat{N} , are eliminated on the transition to the non-integrable regime, and numerous avoided crossings are observed instead. This is a generic feature of the spectra of quantum systems whose classical counterparts are chaotic, and it has led to the idea that universal signatures of non-integrability may be seen in the nearest-neighbour level-spacing distribution (NNLSD) for the energy eigenvalues, $P(S)$.

For typical non-integrable Hamiltonians, $P(S)$ bears a strong resemblance to that of random matrices with the same symmetry properties. While the full extent of the similarity between non-integrable Hamiltonians and random matrices remains unelucidated, the fact that a random Hamiltonian will not possess symmetries sufficiently powerful to cause significant degeneracies gives the analogy considerable intuitive appeal.

The most fundamental result of Hermitian random matrix theory is the fact that if the elements of an Hermitian random matrix are uncorrelated and have basis-invariant probability distributions, then the matrix belongs to one of three Gaussian universality classes [21]; that is, the individual elements have Gaussian probability distributions. The universality class appropriate to the QDNLSE problem, that of real, symmetric matrices, is the Gaussian orthogonal ensemble (GOE). As is well documented [16–18, 21], Wigner's approximation $P_W(S)$ to the NNLSD for the members of the GOE is

$$P_W(S) = (\pi S/2) \exp(-\pi S^2/4). \quad (3.1)$$

This result is exact for 2×2 matrices and also holds good for $M \times M$ matrices as $M \rightarrow \infty$. At the other extreme, and with a few notable exceptions such as multidimensional resonant oscillators, the NNLSD for integrable systems typically resembles a Poisson process [22]

$$P_I(S) = \exp(-S) \quad (3.2)$$

exhibiting the widespread degeneracy expected for integrable systems ($P_I(0) = 1$) in contrast with the absence of degeneracies in the Wigner limit ($P_W(0) = 0$), corresponding to global chaos.

It is generally conceded that systems exhibiting global chaos are, like completely integrable systems, exceptional. In the generic situation for Hamiltonian systems, regular and chaotic trajectories coexist. As we have already noted, the classical non-periodic DNLS has an explicit and indeed continuous family of periodic orbit solutions for all parameter

values. We should not therefore expect the corresponding NNLS to be well approximated by Wigner's surmise. Two common choices for the NNLS in the transition region are the Brody distribution [23]

$$P_B(q, S) = \alpha(q+1)S^q \exp(-\alpha S^{q+1}) \quad (3.3)$$

where $\alpha = [\Gamma((q+2)/(q+1))]^{q+1}$ and the Berry–Robnik distribution [24]

$$P_{BR}(\rho, S) = (1-\rho)^2 \exp(-(1-\rho)S) \operatorname{erfc}(\pi^{1/2}\rho S/2) \\ + (2\rho(1-\rho) + \pi\rho^3 S/2) \exp(-(1-\rho)S - \pi\rho^2 S^2/4) \quad (3.4)$$

where erfc denotes the standard complementary error function. In the Berry–Robnik distribution, the parameter ρ is the fraction of the classical phase space filled with chaotic trajectories. The parameter q in the Brody distribution does not admit a similar physical interpretation. It is easily seen that when ρ and q take the values of 0 and 1, the Poisson and Wigner distributions are respectively reproduced. Prior to comparing these distributions with $P(S)$, the exact NNLS for the non-periodic discrete nonlinear Schrödinger equation, a few comments are in order regarding how $P(S)$ is constructed.

When forming $P(S)$ for systems, such as the one considered here, which have another constant of motion besides the Hamiltonian, care should be taken to ensure that only spacings between correlated levels are included in the NNLS. It is often the case that levels belonging to different symmetry classes, as defined by the additional constant, are uncorrelated, permitting the occurrence of level crossings. We therefore consider only spacings between levels corresponding to the same quantum number N .

Although there is, in addition to \hat{H} and \hat{N} , a further constant of motion, the parity operator \hat{P} given by (2.2), this does not give rise to additional degeneracies except in the nonlinear limit. The reader will recall that we demonstrated this for the linear limit in the previous section. As a consequence, when forming $P(S)$ it is necessary to include all spacings between adjacent levels belonging to the same symmetry class defined by \hat{N} , and not just those corresponding to either symmetric or antisymmetric states, as must be done for the periodic configuration [14]. We discuss this point more fully in the appendix.

It is also necessary to eliminate system-specific global trends in the spectrum by unfolding it to unit mean density on a scale much larger than that of microscopic level fluctuations. The spacing distribution for a given quantum number N was calculated from the levels $e_{Ni} = f(E_{Ni})$ where f is the numerical staircase function of the smoothed density of states [17].

For various values of the physical parameters, γ and β , we have determined the values of p and q for which the test distributions $P_{BR}(\rho, S)$ and $P_B(q, S)$ give the best approximation to the exact distribution $P(S)$. The best-fit criterion is as follows. For the Berry–Robnik distribution, we construct the function

$$\Delta_{BR}(\rho) = \int dS |P_{BR}(\rho, S) - P(S)| \quad (3.5)$$

and $\Delta_B(q)$ is defined analogously for the Brody distribution. The optimum values of the parameters in $P_{BR}(\rho, S)$, and $P_B(q, S)$, which we denote by $\bar{\rho}$ and \bar{q} , are taken to be those for which $\Delta_{BR}(\rho)$ and $\Delta_B(q)$ are minimized.

Our results are shown in table 1 for $\beta = 1$ and $N = 40$, which gives 860 spacings. For this choice of parameters, we have found that $P(S)$ bears the strongest resemblance to both distributions (3.3) and (3.4) when γ lies between 0.001 and 0.01.

Figures 2(a) and (b) show $P(S)$ compared with the corresponding optimal Berry–Robnik and Brody distributions with $\gamma = 0.008$ and $\gamma = 0.01$ respectively. In these figures, we see that the Berry–Robnik distribution bears a closer resemblance to $P(S)$ than

Table 1. Parameters for the optimal Berry–Robnik and Brody distributions as functions of the nonlinear coefficient γ .

γ	$\bar{\rho}$	\bar{q}	$\Delta_{\text{BR}}(\bar{\rho})$	$\Delta_{\text{B}}(\bar{q})$
0.001	0.000	0.000	0.937	1.424
0.002	0.000	0.000	0.727	0.935
0.003	0.984	0.463	0.671	0.600
0.004	0.995	1.000	0.490	0.490
0.005	0.960	0.992	0.398	0.405
0.006	0.885	0.835	0.331	0.357
0.007	0.805	0.559	0.361	0.388
0.008	0.789	0.604	0.347	0.377
0.009	0.749	0.409	0.339	0.368
0.01	0.721	0.393	0.358	0.374

the Brody distribution. Indeed, in all results reported in the table, with the exception of those given for $\gamma = 0.002$, $P_{\text{BR}}(\bar{\rho}, S)$ is closer to the exact distribution than $P_{\text{B}}(\bar{q}, S)$. A possible explanation for this is suggested by the behaviour of the energy eigenvalues shown in figures 1(a) and (b) as γ increases. With the exception of eigenvalues corresponding to states of the form $|n, n, n\rangle$, all levels tend to converge with one or more neighbours as γ/β is increased, eventually leading to widespread degeneracy as $\gamma/\beta \rightarrow \infty$. However, not all level spacings decrease with equal rapidity. As γ/β is increased, the speed at which neighbouring levels converge is seen to grow with energy, and avoided crossings become restricted to lower energies on approach to the nonlinear limit. Furthermore, in the numerically obtained NNLS, there is an inevitable blurring of the distinction between true degeneracies and minute level spacings which cannot be resolved due to the finite bin size. We also note that these spacings are no greater than the typical separation between a pair of levels at an avoided crossing, and so will not be significantly altered by the numerical unfolding procedure. Consequently, the numerically computed $P(S)$ exhibits a gradual increase in the number of degeneracies as γ/β is increased, which also occurs in the Berry–Robnik distribution as ρ is decreased but which cannot be accounted for by the Brody distribution, since $P_{\text{B}}(q, 0)$ is strictly zero for all positive, non-zero q .

4. Discussion

For some parameter choices, the nearest-neighbour level-spacing distribution for the quantum discrete nonlinear Schrödinger equation shows reasonably good agreement with the Brody and Berry–Robnik distributions. It is noteworthy that the latter generally provides a better approximation. We regard this to be partly a consequence of the inappropriate behaviour of the Brody distribution in the vicinity of $S = 0$. The value of the Berry–Robnik distribution at the origin varies continuously from one to zero between the Poisson and Wigner limits. With a suitable choice of the parameter ρ , it can resemble the numerically computed distributions $P(S)$ at $S = 0$ for reasons we outlined in the previous section. On the other hand, the Brody distribution vanishes at the origin and, moreover, its derivative with respect to S diverges as q goes to zero.

Curiously, this latter feature does give rise to some degree of similarity between the Brody distribution for small q and $P(S)$ prior to unfolding in the vicinity of the integrable linear limit. Figures 1(a) and (b) show that as γ increases from zero, all degeneracies in the linear limit are broken. As $N \rightarrow \infty$ this implies the instantaneous breaking of an infinite

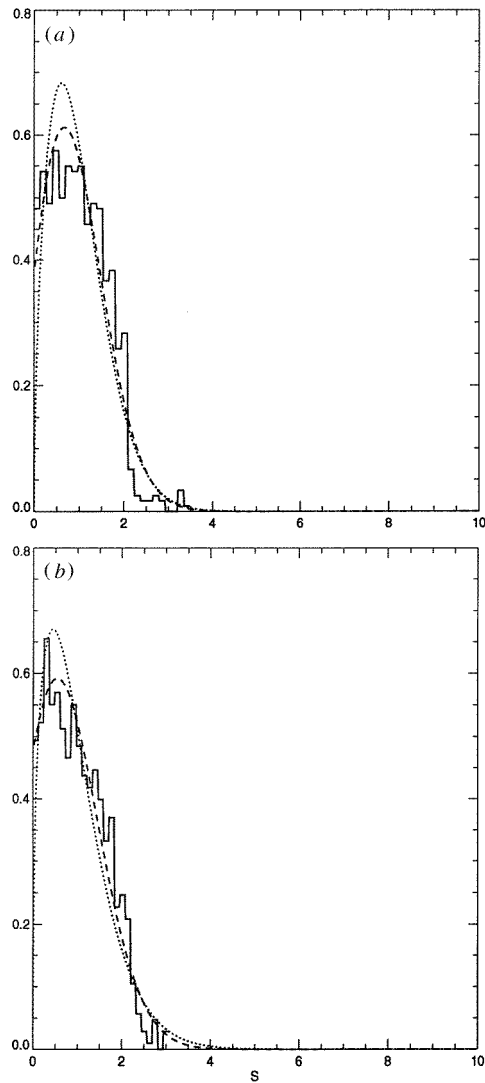


Figure 2. Nearest-neighbour level-spacing distribution (full curve) compared with the optimal Brody (dotted) and Berry–Robnik (broken) distributions, for $N = 40$, $\beta = 1$ with (a) $\gamma = 0.008$ and (b) $\gamma = 0.01$.

number of degeneracies. This will cause the nearest-neighbour spacing distribution, which in the linear limit is a pair of delta functions, with one at the origin, to broaden slightly. Furthermore, the peak at the origin is displaced to the right so as to give $P(0) = 0$. Both the broadening and this slight shift go to zero as the linear limit is approached, implying that the derivative of $P(S)$ with respect to S will become divergent as $\gamma \rightarrow 0$.

In spite of this partial similarity between $P(S)$ for minute nonlinear perturbations and the Brody distribution for infinitesimal q , the overall forms of both functions are completely different. This is essentially due to the fact that for small γ , $P(S)$ still bears a strong qualitative resemblance to that of the linear system, which is composed of three resonantly coupled oscillators. Resonant multidimensional oscillatory systems are,

as we have mentioned, highly non-generic. It is worth noting that in the nonlinear limit, $P(S)$ becomes a series of equally spaced delta functions whose strengths diminish with increasing S . This distribution is again highly atypical among level-spacing distributions for integrable systems, and consequently one cannot make use of the Berry–Robnik conjecture to illuminate the manner in which the system returns to integrability as $\gamma/\beta \rightarrow \infty$.

Appendix

Here, we show that there are no degeneracies associated with the parity symmetry of the Hamiltonian given by (2.1). The parity symmetry we are considering here has the unusual property of not having a related unitary parity-shift operator, since any operator which alters the parity of an arbitrary eigenstate of \hat{P} must necessarily annihilate symmetric product states of the form $|n, m, n\rangle$. It is, however, possible to construct parity-shift operators which are unitary on the remainder of the Hilbert space, although we must, in general, choose a different one for each fixed-parity basis. In this case, the natural basis is formed by the eigenstates of \hat{H} . As we shall see, this does not prevent us from unravelling the prerequisites for parity-degeneracy in an effectively basis-invariant manner. To this end, it will be useful to express the N -boson subspace as the direct product $\mathcal{H}_N = \mathcal{H}_{1N} \times \mathcal{H}_{2N} \times \mathcal{H}_{3N}$, where the \mathcal{H}_{iN} are defined by

$$\mathcal{H}_{1N} = \text{sp}\{|j, N - (j + k), k\rangle \quad j < k\} \tag{A.1}$$

$$\mathcal{H}_{2N} = \text{sp}\{|j, N - 2j, j\rangle\} \tag{A.2}$$

$$\mathcal{H}_{3N} = \text{sp}\{|j, N - (j + k), k\rangle \quad j > k\}. \tag{A.3}$$

Each eigenstate $|\psi_{Nm}\rangle$ may be expressed as the sum of its projections onto these subspaces in the following way:

$$|\psi_{Nm}\rangle = \sum_i \hat{P}_{iN} |\psi_{Nm}\rangle = \sum_i |\psi_{Nm}^i\rangle \tag{A.4}$$

where we have introduced \hat{P}_{iN} , the projector onto the subspace \mathcal{H}_{iN} . Each state $|\psi_{Nm}\rangle$ has definite parity, which implies the relation

$$\langle j, N - (j + k), k | \psi_{Nm}^1 \rangle = \pm \langle k, N - (j + k), j | \psi_{Nm}^3 \rangle \tag{A.5}$$

with $j < k$. The time-independent Schrödinger equation may then be written as

$$\hat{H} \sum_i |\psi_{Nm}^i\rangle = E_{Nm} \sum_i |\psi_{Nm}^i\rangle. \tag{A.6}$$

Were the parity-shift operation on $|\psi_{Nm}\rangle$ to produce another eigenstate of \hat{H} with the same eigenvalue, we would then have

$$\hat{H}(|\psi_{Nm}^1\rangle - |\psi_{Nm}^3\rangle) = E_{Nm}(|\psi_{Nm}^1\rangle - |\psi_{Nm}^3\rangle). \tag{A.7}$$

Substitution of (A.7) into (A.6) readily gives the result

$$\hat{H}|\psi_{Nm}^i\rangle = E_{Nm}|\psi_{Nm}^i\rangle. \tag{A.8}$$

We may then choose the eigenstates of \hat{H} to be localized in the subspaces \mathcal{H}_{iN} . One important consequence of the decomposition given in (A.4) is that the states $|\psi_{Nm}^i\rangle$, although unnormalized, are for each i orthogonal and complete on \mathcal{H}_{iN} . We may then expand any state $|\phi_N^i\rangle$ in \mathcal{H}_{iN} as a linear combination of the $|\psi_{Nm}^i\rangle$. As a consequence of (A.8), this state will be transformed by the Hamiltonian \hat{H} into another state in \mathcal{H}_{iN} . It follows that the matrix element of \hat{H} between states lying in different subspaces \mathcal{H}_{iN} will be zero, which

is not the case for the Hamiltonian given by (2.1), simply because this matrix element does vanish for the nonlinear part of the Hamiltonian but not for the linear interaction term, and thus not for their sum. In short, it is not possible to diagonalize the Hamiltonian separately on the subspaces \mathcal{H}_{iN} , while in contrast a further reduction to an irreducible representation of the permutation group S_3 is possible for the periodic DNLS lattice [14]. We can then see that the parity symmetry of the non-periodic lattice does not cause degeneracies.

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References

- [1] Bang O, Rasmussen J J and Christiansen P L 1993 *Physica* **68B** 169
- [2] Finlayson N and Blow K J 1994 *Chaos, Solitons, Fractals* **4** 1817
- [3] Finlayson N, Blow K J, Bernstein L J and DeLong K W 1993 *Phys. Rev. A* **48** 3863
- [4] DeLong K W, Yumoto J and Finlayson N 1991 *Physica* **54D** 36
- [5] De Filippo S, Fusco Girard M and Salerno M 1987 *Physica* **26D** 411
- [6] Finlayson N and Stegeman G I 1990 *Appl. Phys. Lett.* **56** 2276
- [7] Bernstein L J 1992 *Opt. Commun.* **94** 406
- [8] Careri G, Buontempo U, Galluzzi F, Scott A C, Gratton E and Shyamsunder Y 1984 *Phys. Rev. B* **30** 4689
- [9] Eilbeck J C, Lomdahl P S and Scott A C 1984 *Phys. Rev. B* **30** 4703
- [10] Feddersen H 1991 *Phys. Lett.* **154A** 391
- [11] Eilbeck J C, Lomdahl P S and Scott A C 1985 *Physica* **16D** 318
- [12] Carr J and Eilbeck J C 1985 *Phys. Lett.* **109A** 201
- [13] Scott A C and Eilbeck J C 1986 *Phys. Lett.* **119A** 60
- [14] De Filippo S, Fusco Girard M and Salerno M 1989 *Nonlinearity* **2** 477
- [15] Cruzeiro-Hansson L, Feddersen H, Fleisch R, Christiansen P L, Salerno M and Scott A C 1990 *Phys. Rev. B* **42** 522
- [16] Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (Berlin: Springer)
- [17] Haake F 1992 *Quantum Signatures of Chaos* (Berlin: Springer)
- [18] Ott E 1993 *Chaos in Dynamical Systems* (Cambridge: Cambridge University Press)
- [19] Ford J and Lunsford G H 1970 *Phys. Rev. A* **1** 1
- [20] Cheffes A and Barnett S M 1996 *J. Mod. Opt.* **40** 709
- [21] Mehta C L 1991 *Random Matrix Theory* 2nd edn (Boston, MA: Academic)
- [22] Berry M V and Tabor M 1977 *Proc. R. Soc. A* **356** 375
- [23] Brody T A 1973 *Lett. Nuovo Cimento* **7** 482
- [24] Berry M V and Robnik M 1984 *J. Phys. A: Math. Gen.* **17** 413