Quantum signatures of breather-breather interactions

J. Dorignac* and J. C. Eilbeck†
Department of Mathematics, Heriot-Watt University, Riccarton, Edinburgh, EH14 4AS, UK

M. Salerno‡
Dipartimento di Scienze Fisiche "E. R. Caianiello" and INFM Unitá di Salerno, via S.Allende, I-84081, Baronissi (SA), Italy

A. C. Scott§
Department of Mathematics, University of Arizona, Tucson, AZ 85721, USA
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The spectrum of the Quantum Discrete Nonlinear Schrödinger equation, or Boson Hubbard Hamiltonian, on a periodic 1D lattice shows some interesting detailed band structure which may be interpreted as the quantum signature of a two-breather interaction in the classical case. This fine structure is studied using degenerate perturbation theory. We present also a modification to this model which increases the mobility of bound states.

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The localization and transport of energy in lattices by intrinsic localized modes or discrete breathers, has recently been the subject of intense theoretical and experimental investigation (see [1] and references therein). Corresponding results on the quantum equivalent of these states are less numerous, c.f. [2, 3] for some theoretical results and [4] for some experimental work. Studies of quantum modes on small lattices are of increasing interest for quantum devices based on quantum dots (c.f. [5]), for studies of photonic crystals, and for studies of Bose-Einstein condensates in periodic optical traps [6]. In particle terms these modes can be interpreted as bound multi-boson states.

We present some novel results on breather bands in periodic one dimensional lattices with f sites containing a small number of bosons. These lattices are described by the quantum version of the discrete nonlinear Schrödinger equation (QDNLS) whose Hamiltonian

$$H_1 = -\sum_{s=1}^{f}\left[\gamma_1 a_s^\dagger a_s^\dagger a_s a_s + \epsilon a_{s+1}^\dagger a_s + \text{h.c.}\right] \qquad (1)$$

conserves the number of bosons n. According to the sign of γ_1, this model is also known as the repulsive ($\gamma_1 < 0$) or attractive ($\gamma_1 > 0$) Bose-Hubbard model. In the study of cold bosonic atoms in optical lattices, the repulsive case was already investigated in [7], but as far as we know the attractive case has only been treated classically, by the mean-field approximation (see [8] for example). We mention also that the trimer version of (1) has been studied, c.f. [9].

Assuming that the anharmonic parameter $\gamma_1 > 0$ is stronger than the intersite coupling, the eigenvalues of (1), plotted as a function of the wave number k, separate out into distinct bands [2]. The eigenstates of each band are dominated by states in which the bosons have clumped together, two or more on one site. For example, with $n = 4$, the lowest band is, to a good approximation, a linear combination of states with 4 bosons on site i and no bosons elsewhere. The next lowest band is mostly composed of states with 3 bosons on one site and another boson elsewhere. The third band essentially consists of states with 2 bosons on one site and 2 bosons on a separate site. We will refer to it as the $\{2, 2\}$ band in an obvious notation. This band is of great interest since it represents the simplest case of a band describing two "composite" particles interacting with each other. Our letter is devoted to the fine structure of this and similar bands such as the $\{4, 2\}$ and $\{3, 3\}$ bands in the $n = 6$ case.

Bands involving the interactions of single bosons with composite states, such as $\{3, 1\}$, $\{1, 1, 4\}$, etc., do not reveal such interesting structure and are more difficult to analyse. We do not considered these bands here.

The fine structure of the $\{2, 2\}$ band, see Fig. 1, shows the eigenvalues (crosses) in the $n = 4$ case. The solid lines show the results of the theoretical calculations (described below) in the asymptotic limit $f \to \infty$. We stress again that this picture shows only *one* of the bands in the $n = 4$ spectrum. Its fine detail is revealed as a "continuum" band (in the $f \to \infty$ limit), plus a single k-dependent "line band". Examination of the corresponding eigenvectors shows that the "line band" is mostly composed of states where the two sites each with two quanta lie occupy *adjacent* sites, whereas in the "continuum" band these sites are separated by one or more vacant sites.

One flaw of the standard QDNLS Hamiltonian is its thermodynamical instability (the energy per particle in the ground state goes to $-\infty$ as $n \to \infty$). Moreover, some bands are degenerate with others, for example the $\{3, 3\}$ and the $\{4, 1, 1\}$ bands in the $n = 6$ case. For these reasons, we consider also the following generalized

*Electronic address: J.Dorignac@hw.ac.uk
†Electronic address: J.C.Eilbeck@hw.ac.uk
‡Electronic address: salerno@sa.infn.it
§Electronic address: rover@theriver.com

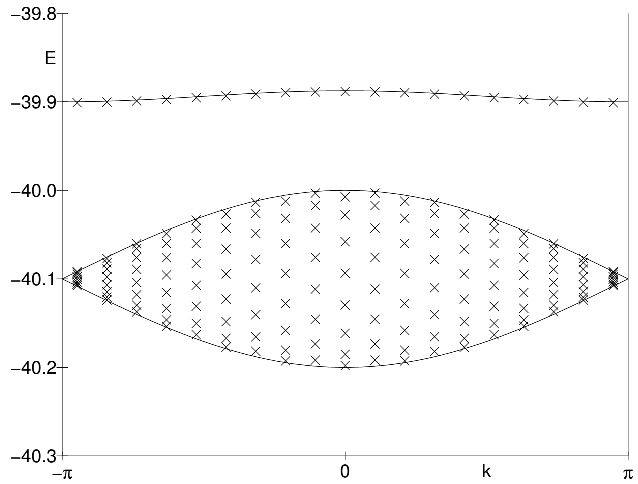

FIG. 1: Detail of the eigenvalue spectrum for the QDNLS periodic lattice (see Eq. (1)), $n = 4, f = 19, \gamma_1 = 10, \epsilon = 0.5$.

QDNLS Hamiltonian

$$H_2 = H_1 + \gamma_2 \sum_{s=1}^{f} a_s^\dagger a_s^\dagger a_s^\dagger a_s a_s a_s \,. \tag{2}$$

The $\gamma_2 > 0$ term is a saturation term which discourages too many bosons occupying the same site. It appears in nonlinear optics [10] or in cold bosonic atoms trapped in optical lattices [11] where it describes three body interactions. At zero coupling ($\epsilon = 0$), the energy of l bosons on the same site is now given by $E_l = -l(l-1)[\gamma_1 - (l-2)\gamma_2]$. Thus in the $n = 4$ case, for example, the $\{4\}$ band has energy E_4, the $\{31\}$ band has energy E_3, the $\{22\}$ band energy $2E_2$, etc. As a general result, if $3(n-2)\gamma_2 < 2\gamma_1$, the n-boson bound state is the ground state of the n-boson sector and it can be shown that its effective mass decreases as γ_2 increases. The main physical effect of the saturation term is then to increase the mobility of the ground state within this range of parameters.

Now, regarding the $n = 4$ sector, it is seen that providing $\gamma_1 < 3\gamma_2$, the bottom of the $\{2,2\}$ band is the *ground state* of the system.

To describe the components of the quantum states we use a position state representation, where for example the state $|020020\ldots\rangle$ represents a state with two boson at site 2, two boson at site 5, and no boson elsewhere. In view of the periodic nature of the lattice, we can generate an equivalence class of states by applying the translation operator (with periodic boundary condition) to one of these states. We will refer to these classes by ordering them such that the leftmost number is the largest, so for example $|3000\ldots\rangle$ is shorthand for $|3000\ldots\rangle, |0300\ldots\rangle, |0030\ldots\rangle$, etc. For further conciseness we will truncate all trailing zeros, so the above class becomes $|3\rangle$. The set of all the classes containing $|22\rangle, |202\rangle, |2002\rangle$, etc. is referred to as the $\{2,2\}$ band.

At zero coupling, all the $\{2,2\}$ states $|22\rangle$, $|202\rangle, |2002\rangle, \ldots$ are degenerate. We use degenerate perturbation theory to obtain both eigenvalues and eigenstates for $\epsilon \neq 0$. For the sake of simplicity, we consider an odd number of sites $f = 2\sigma + 1$. Bloch waves of $\{2,2\}$ states can be written (in the notation of [2, 12])

$$|\psi\rangle = \sum_{j=1}^{\sigma} c_j |\psi_j\rangle \tag{3}$$

where

$$|\psi_j\rangle = \frac{1}{\sqrt{f}} \sum_{s=1}^{f} (e^{ik\hat{T}})^{s-1} |2, \underbrace{0, \ldots, 0}_{j-1}, 2\rangle \tag{4}$$

Here $\hat{T}$ is the translation operator and $k = 2\pi l/f$ where $l \in \{-\sigma, \ldots, \sigma\}$, is the wave number.

Using (3) and standard Brillouin-Wigner perturbation theory up to second order in ϵ we obtain

$$\begin{aligned}(E - 2E_2)c_j = &\sum_{j'=1}^{\sigma} \langle\psi_j|V|\psi_{j'}\rangle c_{j'} + \\ &+ \sum_{j'=1}^{\sigma} \sum_{\tilde{\psi}} \frac{\langle\psi_j|V|\tilde{\psi}\rangle\langle\tilde{\psi}|V|\psi_{j'}\rangle}{2E_2 - \tilde{E}} c_{j'}\end{aligned} \tag{5}$$

where V is the hopping term in the Hamiltonian, and $|\tilde{\psi}\rangle$ is any state not in the $\{2,2\}$ subspace. $\tilde{E}$ is the energy corresponding to $|\tilde{\psi}\rangle$ in the uncoupled limit ($\epsilon = 0$).

It is obvious that the first sum of (5) is zero as V does not link any of the $|\psi_s\rangle$ to each other. Then, defining

$$H^{(22)}_{j,j'} = \sum_{\tilde{\psi}} \frac{\langle\psi_j|V|\tilde{\psi}\rangle\langle\tilde{\psi}|V|\psi_{j'}\rangle}{2E_2 - \tilde{E}} \,, \tag{6}$$

we obtain

$$H^{(22)} = -\frac{4\epsilon^2}{\gamma_1} I_\sigma - \frac{2\epsilon^2}{\gamma_1} \begin{pmatrix} \Gamma & \kappa^* & & & \\ \kappa & 0 & \kappa^* & & \\ & \ddots & \ddots & \ddots & \\ & & \kappa & 0 & \kappa^* \\ & & & \kappa & p \end{pmatrix} \tag{7}$$

where I_m is the $m \times m$ unity matrix and

$$\kappa = e^{i\frac{k}{2}} \cos\left(\frac{k}{2}\right) \;;\; p = \cos\sigma k \;;\; \Gamma = \frac{3\gamma_2 - 4\gamma_1}{\gamma_1 - 3\gamma_2} \,. \tag{8}$$

The structure of the matrix (7) is very similar to the two-boson case described in [2]. The first term represents a global shift of the $\{2,2\}$-band, whereas the "impurity" Γ will in general be responsible for a splitting of the states $|22\rangle$ from the rest of the band ($|202\rangle$, $|2002\rangle$, etc.). In this respect, the $|22\rangle$'s can be seen as "bound states of doublets" within the $\{2,2\}$-band. It is separated from the continuum band because in addition to linking with states such as $|211\rangle$, it also links to states such as $|31\rangle$. This explains the $\{2,2\}$-band fine structure.

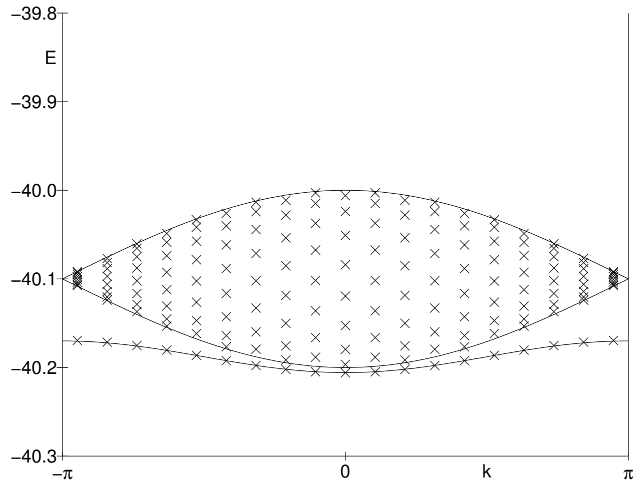

FIG. 2: Detail of the eigenvalue spectrum for the generalized QDNLS periodic lattice (2), $n = 4, f = 19, \gamma_1 = 10, \gamma_2 = 7.5, \epsilon = 0.5$.

In case the number of sites tends to infinity, (7) may be diagonalised exactly to yield

$$E = -4\gamma_1 - \begin{cases} \frac{2\epsilon^2}{\gamma_1}\left(2 + \Gamma + \frac{\cos^2(k/2)}{\Gamma}\right) \text{ iff } |\Gamma| > \cos\left(\frac{k}{2}\right) \\ \\ \frac{4\epsilon^2}{\gamma_1}\left(1 + \cos\left(\frac{k}{2}\right)\cos\theta\right) \text{ where } \theta \in (0, \pi) \end{cases} \tag{9}$$

Depending on the various values of γ_1, γ_2, and ϵ, we can get the line band completely above, below or partially merged with the continuum band. Fig 2 shows a case where the line part is below the continuum part of the $\{2,2\}$ band and represents the ground state of the $n = 4$ sector.

To provide some insight in the way the two groups of two bosons interact within a $|22\rangle$ state, we may compare its effective mass m^*_{22} with twice the effective mass m^*_2 of a single $|2\rangle$ state. From [2] and (9), we obtain $m^*_2 \simeq \gamma_1/(2\epsilon^2)$ as $\epsilon \to 0$ and $m^*_{22}/(2m^*_2) = \Gamma$ (see (8)). Depending on the ratio γ_2/γ_1, Γ and thus m^*_{22} are either positive or negative. The same phenomenon is observed for bright solitons in systems of Bose-Einstein condensates in optical lattices for which (1) may be seen as a tight-binding limit (see [13] and references therein).

As a further example we consider the $n = 6$ case. Now there are two bands describing an interaction of two anharmonic states: the $\{4,2\}$ and the $\{3,3\}$ bands. Fig 3 shows a $n = 6$, $\{4,2\}$ example, again the crosses represent numerically exact solutions in the $f = 11$ case, and the lines represent perturbation theory calculations. In this case we have a "continuum band" which shows very weak k-dependence, plus two "line bands", one above and one below. With other choices of γ_1 and γ_2 we can move one or both of the "line bands" into the continuum.

Fig 4 shows the corresponding $\{3,3\}$ case. In this case there appears to be only two "line bands", but a closer examination reveals the upper "line" is in fact a contin-

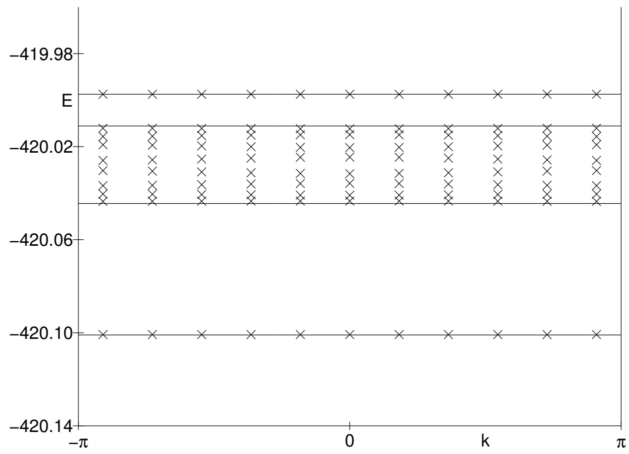

FIG. 3: Detail of the eigenvalue spectrum for the generalized QDNLS periodic lattice (2), $n = 6$, $f = 11$, $\gamma_1 = 30, \gamma_2 = 0, \epsilon = 0.5$.

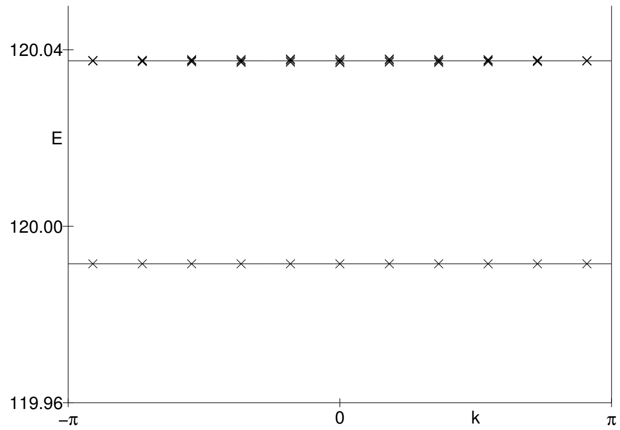

FIG. 4: Detail of the eigenvalue spectrum for (2), $n = 6$, $f = 11$, $\gamma_1 = 10$, $\gamma_2 = 20$, $\epsilon = 0.5$.

uum band with the degeneracy split at an $O(\epsilon/\gamma)^3$ level. For the $n = 6$, $\{4,2\}$ band, proceeding as in the $\{2,2\}$ case, we now obtain

$$H^{(42)} = D\epsilon^2 I_{2\sigma} - \frac{\epsilon^2}{\gamma_1}\begin{pmatrix} \Gamma & 1 & & & p \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ p^* & & & 1 & \Gamma \end{pmatrix} \tag{10}$$

where

$$D = -\frac{2}{3}\frac{5\gamma_1 - 9\gamma_2}{\gamma_1(\gamma_1 - 3\gamma_2)} \;;\; \Gamma = \frac{2}{3}\frac{4\gamma_1^2 - 27\gamma_2^2}{(\gamma_1 - 3\gamma_2)(\gamma_1 - 6\gamma_2)};$$
$$p = \frac{6\gamma_1 e^{ik}}{\gamma_1 - 6\gamma_2}\,.$$

An analysis of the eigenvalues of this matrix in the $f \to \infty$ limit is somewhat messy but explicit results can be found: details will be published elsewhere. Essentially the results depend on whether two rational functions of γ_1/γ_2 are less than or greater than 1 in modulus. This gives the two "line bands" in Fig 3. The corresponding eigenstates are essentially symmetric and antisymmetric combinations of the Bloch waves made from $|42\rangle$ and $|24\rangle$.

The "continuum band" is given by the formula

$$E_c = 24\gamma_2 - 14\gamma_1 + \frac{2\epsilon^2}{\gamma_1}\left[\frac{5\gamma_1 - 9\gamma_2}{9\gamma_2 - 3\gamma_1} - \cos\theta\right] + \mathcal{O}\left(\epsilon^3\right), \tag{11}$$

where $\theta \in (0, \pi)$. Note that, up to order 2 in ϵ, the energies of this band do not depend on the crystal momentum k, in accord with the numerical results.

In the case of the $n = 6$, $\{3, 3\}$ band, the correction to the zeroth order states is given by

$$H^{(33)} = \frac{6\epsilon^2}{3\gamma_2 - 2\gamma_1}\left(I_\sigma + M\right) \tag{12}$$

where $M_{1,1} = \Gamma = \frac{9}{2}(2\gamma_2 - \gamma_1)/(\gamma_1 - 6\gamma_2)$ and $M_{i,j} = 0$ otherwise. The diagonal matrix (12) has an "impurity" Γ responsible for a splitting of the states $|33\rangle$ from the rest of the band. In this respect, the $|33\rangle$'s can be seen as "bound states of doublets" within the $\{3, 3\}$-band. Note again that none of the elements of the matrix above contains the wave vector k. At this order of perturbation theory, the bands are then flat. Moreover, the degeneracy of the $|3 \cdots 3\rangle$'s (i.e. two 3-quanta breathers separated by one or more empty sites) has still not been lifted although it would to next order.

It is possible to generalize the above results to discuss $\{m, \ell\}$ bands when $m + \ell = n > 6$. The case $m = \ell$ is similar to the $\{3, 3\}$ case and the case $m > \ell > 1$ follows the $\{4, 2\}$ case discussed above. Details will be given elsewhere.

The results known previously for bound states representing a group of n bosons located on the same site [2] have been extended here to higher order states representing two interacting groups of bosons. This opens up the possibity of a study of the collision process between these composite particles, that is a quantum breather collision. A similar study has already been done for the *continuous* version of (1), i.e. the *integrable* quantum nonlinear Schrödinger equation (QNSE), well known in nonlinear optics and quantum field theory [14]. However, the bound states of groups of quanta which we have described here within the $\{m, \ell\}$ bands do not exist in QNSE. Their appearence in these *nonintegrable* discrete systems is thus expected to affect the collision process between two quantum breathers and to bring new features in comparison to the quantum soliton collisions described in [14]. Results of this investigation will be reported elsewhere.

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[1] L. Vázquez, R. S. MacKay, and M. P. Zorzano, eds., *Localization and Energy Transfer in Nonlinear Systems* (World Scientific, Singapore, 2003).
[2] A. C. Scott, J. C. Eilbeck, and H. Gilhøj, Physica D **78**, 194 (1994).
[3] R. S. MacKay, Physica A **288**, 174 (2000), V. Fleurov, Chaos **13**, 676 (2003).
[4] F. Fillaux, et al., Phys. Rev. B **58**, 11416 (1998), B. L. Swanson, et al., Phys. Rev. Letts. **82**, 3288 (1999), T. Asano, et al. Phys. Rev. Lett. **84**, 5880 (2000), L. Schulman, et al., Phys. Rev. Lett. **88**, 224101 (2002).
[5] X. Q. Li, et al., Science **301**, 809 (2003).
[6] G.L. Alfimov, V.V. Konotop and M. Salerno, Europhys. Lett. **58**, 7 (2002), R. Carretero-González and K. Promislow, Phys. Rev. **66**, 033610 (2002).
[7] D. Jaksch et al., Phys. Rev. Lett. **81**, 3108 (1998).
[8] P.J.Y Louis et al., Phys. Rev. A. **67**, 013602 (2003).
[9] L. Cruzeiro-Hansson et al., Phys. Rev. B **42**, 522 (1990), R. Franzosi and V. Penna, Phys. Rev. A **65**, 013601 (2001).
[10] H. Michinel, et al., Phys. Rev. E **65**, 066604 (2002).
[11] A. Gammal et al., J. Phys. B: At. Mol. Opt. Phys. **33**, 4053 (2000).
[12] A. C. Scott, *Nonlinear Science, 2nd Ed.* (OUP, 2003).
[13] M. Salerno, arXiv:cond-mat/0311630 (2003).
[14] Y. Lai and H.A. Haus, Phys. Rev. A **40**, 854 (1989).