

SOME EXACT RESULTS FOR QUANTUM LATTICE PROBLEMS

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We study the exact eigenvalue spectrum for a variety of quantum lattice models, concentrating on the Quantum Discrete Nonlinear Schrödinger (QDNLS) model. In particular we discuss eigenstates which are the quantum equivalent of the classical breather. These results extend previous work, by considering larger number of quanta and bigger lattices.

1. Introduction

Physics is increasingly moving towards nano-scale technology, and with this comes the need to understand small lattices or quasi-lattices supporting a small number of quanta. Often this gives the quantum equivalent of a classical breather, though with some interesting differences. In this short paper we review some work on quantum lattice problems, concentrating mainly on the quantum discrete nonlinear Schrödinger (QDNLS) model. The corresponding classical DNLS lattice is discussed elsewhere in this book. Our eventual aim is to understand such systems as quantum dot arrays, Bose-Einstein Condensate lattices, and even models for Quantum Computers.

We adopt here a pedagogical approach with many details omitted—see^{2,5,6} for a fuller description of the background material in our approach, and^{3,4} for some other interesting developments by other authors.

Consider the classical DNLS model¹ in one spatial dimension with nearest-neighbour interactions

$$i\frac{dA_j}{dt} + A_{j-1} + A_{j+1} + \gamma|A_j|^2 A_j = 0,$$

where $j = 1, 2, \dots, f$ are the lattice points, the A_j 's are the complex mode amplitudes at each site j , and γ is the anharmonic parameter. This

equation can be derived from the following Hamiltonian

$$H = - \sum_{j=1}^f \left[\frac{1}{2} \gamma |A_j|^4 + A_j^* (A_{j+1} + A_{j-1}) \right],$$

where the canonical variables are A_j, A_j^* , and periodic boundary conditions are assumed ($A_{j+f} = A_j$). As shown elsewhere in this volume, this model supports both stationary and mobile breathers, strongly localized solutions with an internal mode of oscillation. How do these properties carry over to the quantum case?

A corresponding Quantum DNLS Hamiltonian is

$$\hat{H} = - \sum_{j=1}^f \left[\frac{\gamma}{2} b_j^\dagger b_j^\dagger b_j b_j + b_j^\dagger (b_{j-1} + b_{j+1}) \right] \quad (1)$$

where the boson annihilation (b_j) and creation (b_j^\dagger) operators destroy or create a boson at site j according to the following rules.

$$b_j |n_j\rangle = \sqrt{n_j} |n_j - 1\rangle, \quad b_j |0\rangle = 0, \quad b_j^\dagger |n_j\rangle = \sqrt{n_j + 1} |n_j + 1\rangle$$

where $|n_j\rangle$ is the number of bosons at lattice point j . The b_j satisfy the boson commutation relations $b_j b_k^\dagger - b_k^\dagger b_j = \delta_{j,k}$

An important feature is that the Hamiltonian (1) conserves the *number* of bosons in the system

$$\hat{N} = \sum_{j=1}^f b_j^\dagger b_j.$$

The methods we discuss can be extended to a range of other number-conserving models, for example the following boson models

- The Quantum Ablowitz-Ladik (QAL) model

$$\hat{H} = - \sum_{j=1}^f \left[a_j^\dagger (a_{j+1} + a_{j-1}) \right],$$

where a_j^\dagger and a_j are operators satisfying the commutation relations

$$[a_j^\dagger, a_k^\dagger] = [a_j, a_k] = 0, \quad [a_j, a_k^\dagger] = \left(1 + \frac{1}{2} \gamma a_j^\dagger a_k \right) \delta_{jk}.$$

- The Salerno system. This is a q -deformation of the QDNLS system which interpolates between the QAL and QDNLS systems. Now $[a_j, a_k^\dagger] = \left(1 + \frac{1}{2} (\gamma - \epsilon) a_j^\dagger a_k \right) \delta_{jk}$, and the Hamiltonian is

$$\hat{H} = - \sum_{j=1}^f \left[a_j^\dagger (a_{j+1} + a_{j-1}) - \right]$$

$$- \frac{2\epsilon}{(\gamma - \epsilon)} \left(\frac{\ln \left(1 + \frac{1}{2}(\gamma - \epsilon) a_j^\dagger a_j \right)}{\ln \left(1 + \frac{1}{2}(\gamma - \epsilon) \right)} + a_j^\dagger a_j \right) \Bigg].$$

Note that the corresponding number operator will be different in all these cases, details can be found in ^{6,5}. The methods also extend to a number of fermion models such as a fermionic polaron model and the Hubbard model.

2. Eigenvalues of the QDNLS Hamiltonian

We now describe our computational method. Since the number is conserved, we can block-diagonalize the Hamiltonian matrix using states which are simultaneously eigenstates of \hat{H} and \hat{N}

$$H = \langle \Psi | \hat{H} | \Psi \rangle = \begin{pmatrix} H_0 & 0 & & & \\ 0 & H_1 & 0 & & \\ & 0 & H_2 & 0 & \\ & & & \ddots & \ddots \\ & & & & \ddots \end{pmatrix}$$

where H_n is the block describing states with a total of n bosons. Each eigenstate for a fixed value of n is formed as a linear combination of number states with a fixed n .

$$|\Psi_n\rangle = \sum_i c_i |\psi_n^{(i)}\rangle$$

The number states $|\psi_n^{(i)}\rangle$ are formed from the different ways we can distribute n bosons over the f sites on the lattice (we are assuming a finite lattice with periodic boundary conditions).

$$|\psi_n^{(i)}\rangle = |n_1^{(i)}\rangle |n_2^{(i)}\rangle \dots |n_f^{(i)}\rangle = [n_1^{(i)}, n_2^{(i)}, \dots, n_f^{(i)}], \text{ where } n = \sum_j n_j^{(i)}.$$

For example, $[2, 2, 0, 0, 0, 1]$ means a state with 2 bosons on site 1, 2 bosons on site 2, and 1 boson on site 6. For a fixed value of n and f there are $(n + f - 1)!/n!(f - 1)!$ different number states, a quantity which expands rapidly with n and f .

We can further block-diagonalize the Hamiltonian by using the fact that it is translationally invariant, and hence we can simultaneously diagonalize with respect to the momentum operator^{5,6}. As a simple example, consider a 1D periodic lattice of length $f = 3$ with $n = 2$ bosons. There are 6 possible number states $[2, 0, 0], [0, 2, 0], [0, 0, 2], [1, 1, 0], [0, 1, 1], [1, 0, 1]$, so H_2 in this case is 6×6 . But we can block-diagonalize this into three 2×2

blocks $H_{2,k}$ using the translationally invariant states

$$\begin{aligned} |\Psi_2^{(a)}\rangle &= [2, 0, 0] + t[0, 2, 0] + t^2[0, 0, 2] \\ |\Psi_2^{(b)}\rangle &= [1, 1, 0] + t[0, 1, 1] + t^2[1, 0, 1] \end{aligned}$$

with $t = 1, \exp 2\pi i/3, \exp -2\pi i/3$, so that $t^3 = 1$, with corresponding k (momentum) values $0, \pm 2\pi/3$ respectively. When f and n are large this can give a substantial saving in calculation time.

The problem of a non-translationally invariant \hat{H} , such as a lattice with a defect, is a more difficult problem and is currently under investigation.

2.1. Quantum Mechanics in Maple

We can further speed up our studies by using an algebraic manipulation package to manipulate the states and to calculate the Hamiltonian in algebraic form as a function of the parameters. In Maple, for example, we represent $[2, 2, 0, 0, 0, 1]$ as `psi(2,2,0,0,0,1)`, where `psi()` is an “undefined” function. Then the operators b_j^\dagger are defined something like

```
bd := proc(phi, j::nonnegint)
    nj:=op(j, phi);
    RETURN(sqrt(nj+1)*subsop(j=nj+1, phi))
end
```

with a corresponding definition for b , the QDNLS \hat{H} is defined along the following lines

```
H := sum('gamma/2*bd(bd(b(phi, i), i), i), i)
    +bd(b(phi, cyc(i+1)), i)+bd(b(phi, cyc(i-1)), i)', 'i'=1..f)
```

where `cyc` deals with the periodic boundary conditions, i.e. `cyc(f+1)=1`, etc. This is only a brief sketch of the codes lying behind the calculations. It has recently been found that by careful optimization of the algorithms, a speedup of almost two orders of magnitude is possible. This, combined with the continuing improvement in micro-chip speeds, means that much bigger problems can be tackled than 10 years ago.

2.2. The $n = 2$ case

In this case each $H_{2,k}$ is tridiagonal. In the case of the QDNLS equation for large odd f , the value of $H_{2,k}$ is given by

$$H_{2,k} = \begin{pmatrix} \gamma & \sqrt{2}q^* & & & \\ \sqrt{2}q & 0 & q^* & & \\ & q & 0 & q^* & \\ & & q & 0 & q^* \\ & & & \ddots & \ddots & \ddots \end{pmatrix},$$

where $q = -(1 + \exp(ik))$. Eigenvalues and eigenvectors can be calculated numerically, or analytically, and some simple formula are known in the limit $f \rightarrow \infty$. An investigation of the 1D case for various models was made in 1992 by Eilbeck and Pego, but unfortunately this work has not yet been published. The results in the limit $f \rightarrow \infty$ for the QDNLS model are shown in Fig.1. In this figure, eigenvalues are plotted vertically for each k value

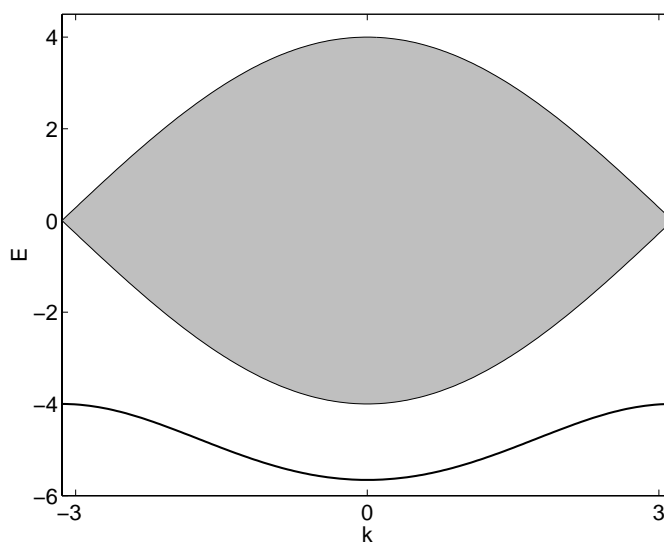


Figure 1. Eigenvalues $E(k)$ for QDNLS, $n = 2$, $\gamma = 4$. The lower band is the “breather” band.

on the horizontal axis. There is a continuum set and an isolated eigenvalue for each k . The equation for the lower band of isolated eigenvalues is, in the limit $f \rightarrow \infty$,

$$E = -\sqrt{\gamma^2 + 16 \cos^2(k/2)}$$

The isolated band corresponds to an eigenvector of $H_{2,k}$ with the following form

$$v = \left(\frac{1}{\sqrt{2}}, \mu, \mu^2, \mu^3, \dots \right)',$$

where

$$\mu = \frac{-(\gamma + E)e^{ik/2}}{4 \cos(k/2)}.$$

This eigenvalue and the corresponding eigenvector can be checked by direct calculation. It is also straightforward to check that $|\mu|^2 < 1$ for $\gamma > 0$. When $\gamma \gg \cos(k/2)$ we have

$$\mu \approx \frac{2}{\gamma} \cos(k/2) \exp(ik/2)$$

so that $\mu \rightarrow 0$ as $\gamma \rightarrow \infty$. Note also that $\mu = 0$ when $k = \pm\pi$, a result originally pointed out by S. Flach (private communication).

The ordering is such that the i th element of v multiplies the following translatory invariant states Ψ_i

$$\begin{aligned} \Psi_1 &= [2, 0, 0, \dots] + e^{ik}[0, 2, 0, \dots] + e^{2ik}[0, 0, 2, \dots] + \dots \\ \Psi_2 &= [1, 1, 0, \dots] + e^{ik}[0, 1, 1, 0, \dots] + e^{2ik}[0, 0, 1, 1, 0, \dots] + \dots \\ \Psi_3 &= [1, 0, 1, 0, \dots] + e^{ik}[0, 1, 0, 1, 0, \dots] + e^{2ik}[0, 0, 1, 0, 1, 0, \dots] + \dots \\ &\dots = \dots \end{aligned}$$

so that the (unnormalized) eigenfunction is

$$\Psi = \sum_{i=1}^{\infty} v_i \Psi_i$$

This is a localized eigenfunction in the sense that there is a high probability of finding the two bosons on the *same* site, but with an equal probability of finding these two bosons at *any* site in the system. *We claim this is a quantum analogue of the classical localized breather.*

2.3. Results for general n , γ

There are some general results for general n , but only in the large γ limit^{6,5}. In this case there is still a “breather” band with eigenfunction

$$\Psi \approx [n, 0, 0, \dots] + [0, n, 0, \dots] + \dots + [0, 0, \dots, n] + O(\gamma^{-1}) ([n-1, 1, 0, \dots] + \dots),$$

but the continuum band in the $n = 2$ case now bifurcates into a number of separate bands. These can be understood by considering the γ -dependent term in the Hamiltonian

$$-\sum_{j=1}^f \left[\frac{\gamma}{2} b_j^\dagger b_j^\dagger b_j b_j \right].$$

Any site with $n_j > 1$ will contribute a value $\frac{1}{2}\gamma n_j(n_j - 1)$ to this sum. If all the bosons are on one site this gives $\frac{1}{2}\gamma n(n - 1)$. If there are $n - 1$ bosons at one site and 1 at another site, the contribution will be $\frac{1}{2}\gamma(n - 1)(n - 2)$. If there are $n - 2$ bosons at one site and 2 at another site, the contribution will be $\frac{1}{2}\gamma[(n - 2)(n - 3) + 2]$, and so on.

For example, consider the case $n = 4$. With $\gamma = 0$ we get the spectrum shown in Fig.2. Note that now we are working with a finite size lattice, the spectrum is for discrete k values, but it is clear that in the continuum limit we will get a single continuum band. If we now increase γ to 7 we get Fig.3.

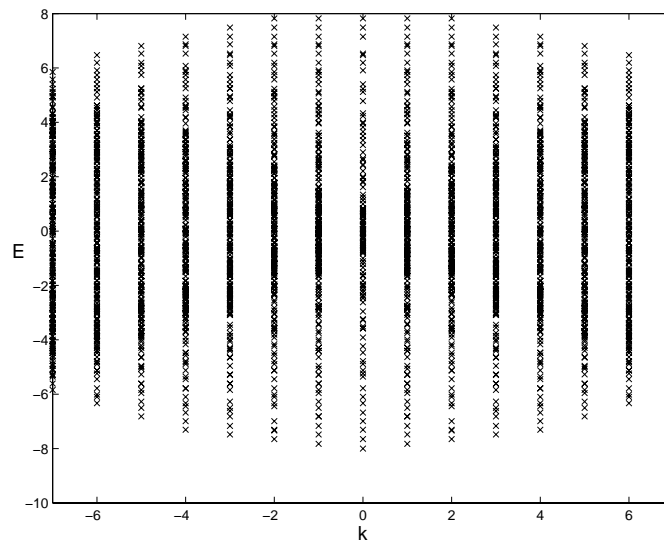


Figure 2. Example: 4 bosons, 15 sites, $\gamma = 0$

Now the single breather band has clearly split off below, and the main continuum band has started to split into two or more bands. If we increase γ to 14 we get Fig.4. Now there are 5 bands clearly visible. The lowest corresponds to the single 4-breather band, conveniently labelled (in the

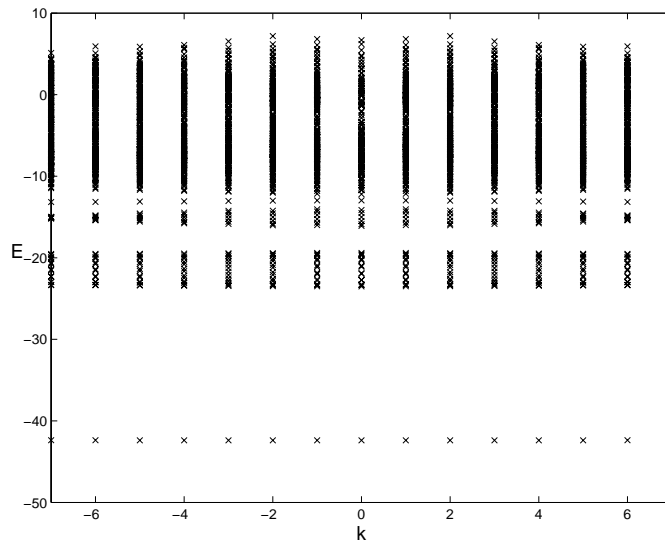


Figure 3. Example: 4 bosons, 15 sites, $\gamma = 7$

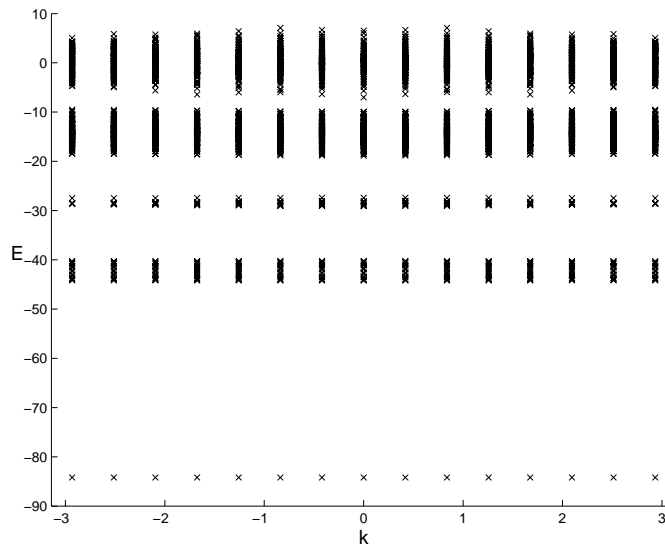


Figure 4. Example: 4 bosons, 15 sites, $\gamma = 14$

large γ limit) as $[4, 0, \dots]$ (plus cyclic permutations). The next lowest is the “3-breather band plus single boson” band $[3, 1, 0, \dots]$, plus permutations. The next narrow band is the “double 2-breather band” $[2, 2, 0, \dots]$. Interestingly, this band shows some structure at higher magnification which will be reported elsewhere. Moving up, the penultimate band is the “2-breather band plus single bosons”, $[2, 1, 1, 0, \dots]$, and the top band consists of single bosons only, $[1, 1, 1, 1, 0, \dots]$.

As a final example, we show the result of a calculation on a 2D lattice with $n = 2$. Fig.5. The “breather band” is now a 2-dimensional sheet, and

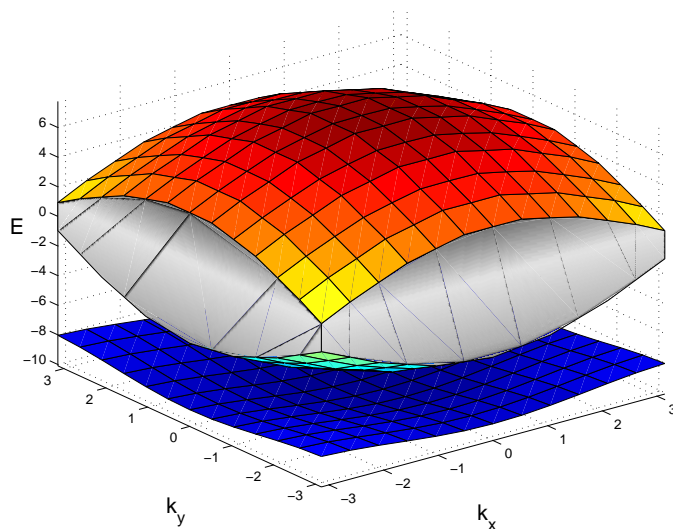


Figure 5. Example: 2 bosons, 13×13 lattice

the “continuum band” is a lens-shaped volume.

Further work is now concentrating on the fine structure of these bands in one and higher dimensions, both in QDNLS and in QAL and other models.

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