

Some quantum lattice problems

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Summary:

- Introduction
 - DNLS lattice
- Fermi resonance lattice
 - 1 site case
 - 2 site case
 - f site case
- Quasi-exactly solvable model
 - arbitrary cutoff m , monomer case
 - arbitrary cutoff m , dimer case
 - $m = 2$, arbitrary f

Introduction

Quantum DNLS (boson Hubbard) Hamiltonian in 1D, nearest neighbour interactions:

$$\hat{H} = -\frac{\gamma}{2} \sum_{j=1}^f b_j^\dagger b_j^\dagger b_j b_j - \sum_j b_j^\dagger (b_{j+1} + b_{j-1})$$

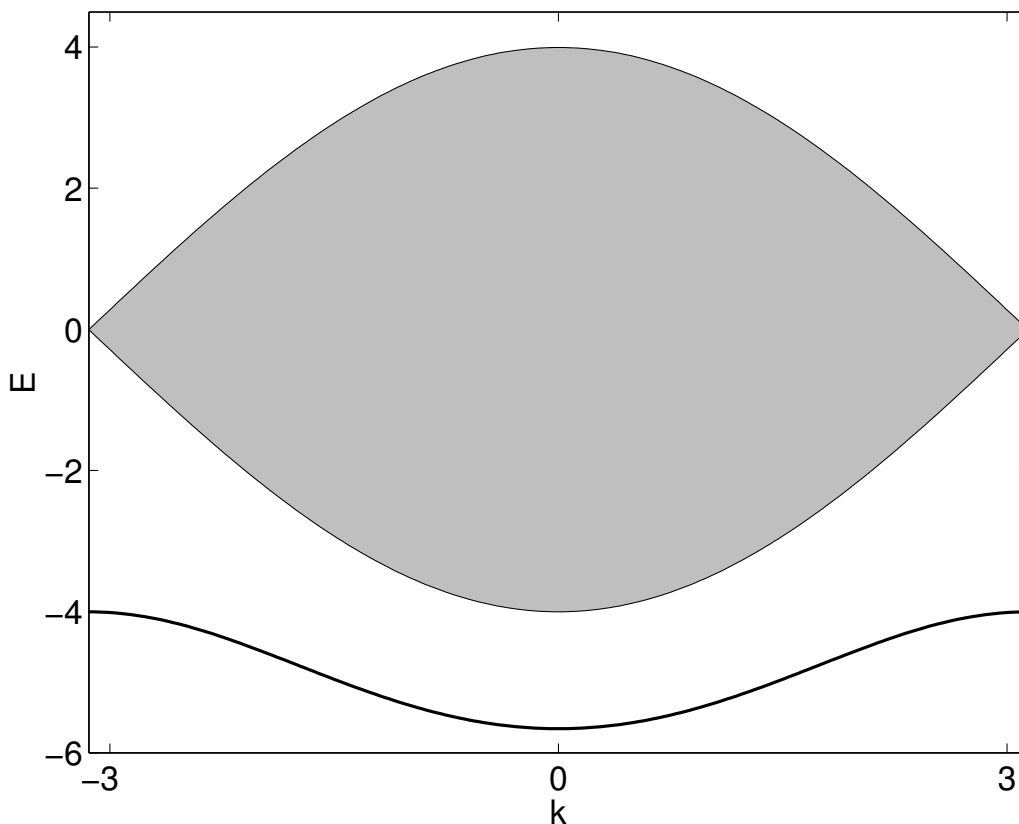
\hat{H} conserves the *number* of quanta

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

The operators b_j , (b_j^\dagger) destroy (create) a boson at site j on the lattice of size f . We assume periodic boundary conditions.

1D “Quantum Breather”

Simplest non-trivial case, lattice with only 2 bosons.



Eigenvalues $E(k)$ for QDNLS. The lower band is the “breather” band. Similar results in 2- and D- dimensions.

Modified QDNLS

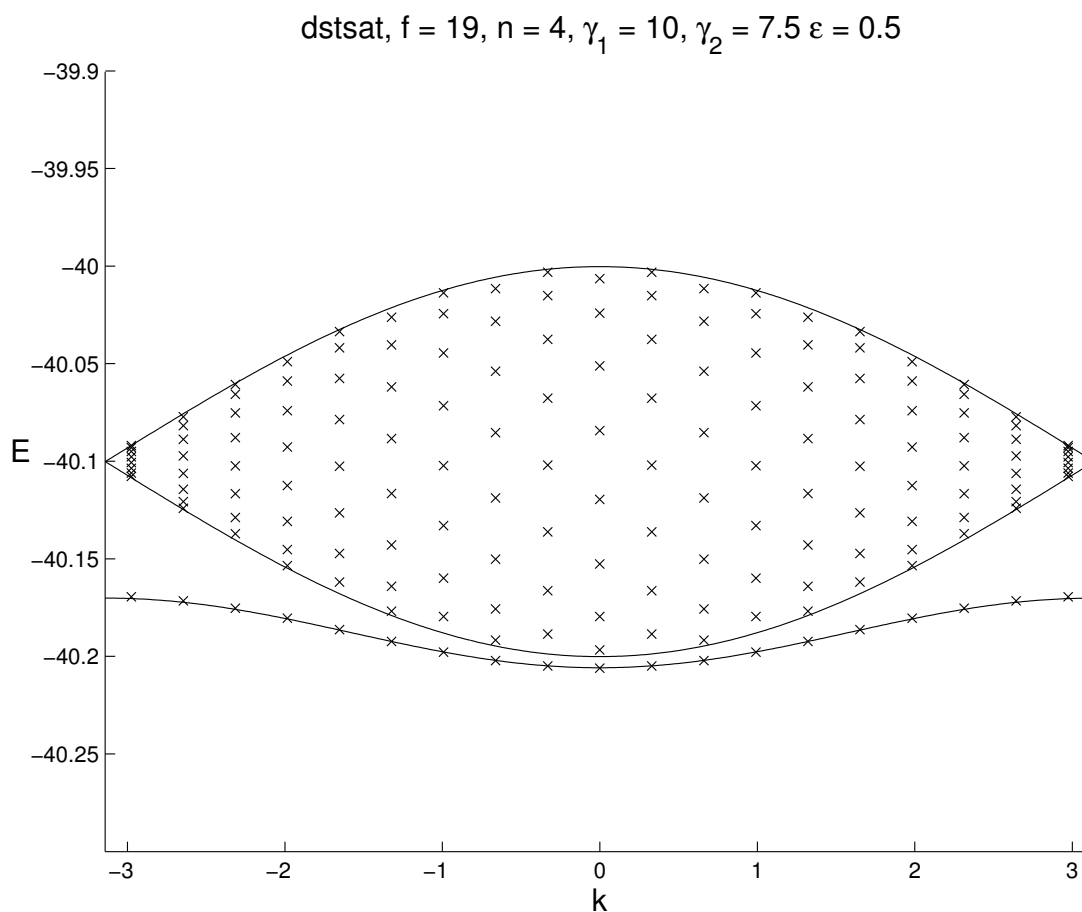
A disadvantage of the QDNLS is that the energy of the ground state $\Rightarrow -\infty$ as the number of bosons increases. To avoid this we can use the modified QDNLS Hamiltonian:

$$\hat{H} = -\frac{1}{2}\gamma_1 \sum_{j=1}^f b_j^\dagger b_j^\dagger b_j b_j + \frac{1}{2}\gamma_2 \sum_{j=1}^f b_j^\dagger b_j^\dagger b_j^\dagger b_j b_j b_j - \sum_j \left(b_j^\dagger b_{j+1} + b_j^\dagger b_{j-1} \right)$$

This is equivalent to adding a saturation term in nonlinear optics.

Modified QDNLS

We can now get some interesting detailed band structure in the 4-boson case which is reminiscent of the 2-boson case



see Dorignac et al., PRL **93** 025504, 2004.

Fermi Resonance Model

Now *two* types of bosons, a and b

$$\begin{aligned} H = & \sum_{n=1}^f \omega_a a_n^\dagger a_n + \omega_b b_n^\dagger b_n - \gamma_a a_n^\dagger a_n^\dagger a_n a_n \\ & - \gamma_b b_n^\dagger b_n^\dagger b_n b_n - (b_n^\dagger b_n^\dagger a_n + a_n^\dagger b_n b_n) \\ & - \eta a_n^\dagger (a_{n+1} + a_{n-1}) - \chi b_n^\dagger (b_{n+1} + b_{n-1}) \end{aligned}$$

The Hamiltonian commutes with the number operator

$$\hat{N} = \sum_{n=1}^f 2a_n^\dagger a_n + b_n^\dagger b_n$$

We will use m for the number of a bosons and ℓ for the number of b bosons, so

$$N = 2m + \ell$$

is conserved.

The monomer case

We write the wave function of a monomer with m type a bosons and ℓ type b bosons as

$$|_{\ell}^m\rangle \equiv [_{\ell}^m]$$

For each $N = 2m + \ell$, we have $M + 1$ different states, where M is the integer part of $N/2$

$$[_{N-2M}^M], [_{N-2(M-1)}^{M-1}], \dots, [_{N}^0]$$

for even N , we have the tridiagonal $(N/2 + 1) \times (N/2 + 1)$ Hamiltonian

$$H = \begin{bmatrix} d_1 & c_1 & 0 & & \\ c_1 & d_2 & c_2 & 0 & \\ 0 & c_2 & d_3 & c_3 & 0 \\ & 0 & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

where

$$\begin{aligned} d_i &= -(2i-2)(2i-3)\gamma_b + (M-i+1)\omega_a + \\ &\quad + 2(i-1)\omega_b - (M-i)(M-i+1)\gamma_a, \\ c_i &= -\sqrt{2i(2i-1)(M-i+1)}. \end{aligned}$$

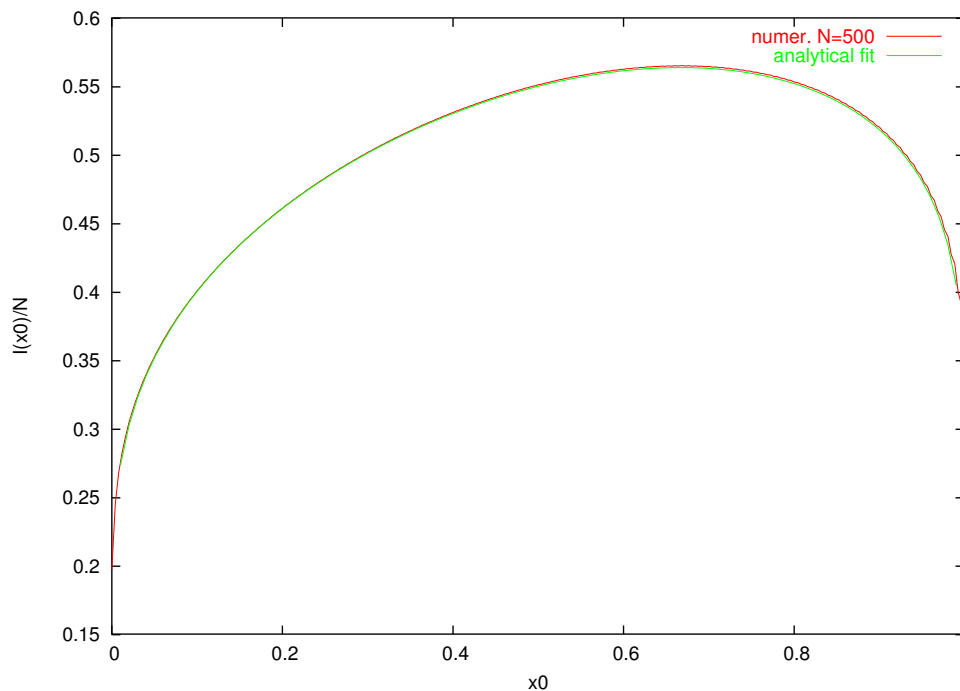
Monomer case – applications

The eigenvectors in the monomer case can be calculated numerically in a straightforward way. However the dynamics of the monomer case have an interesting application - the atomic–molecular Bose-Einstein condensate. Now a is the atomic field and b the molecular field, and the model is simplified

$$H = \frac{1}{2}\Delta a_n^\dagger a_n + \frac{\chi}{2\sqrt{V}}(b_n^\dagger b_n^\dagger a_n + a_n^\dagger b_n b_n).$$

We can integrate the time-dependent problem numerically using the eigenvalues and eigenvectors of H , but Dorignac and Gaididei et al. have used the discrete WKB approach to find some nice analytic approximations, much more accurate than the normal mean-field approximation.

Monomer case – applications

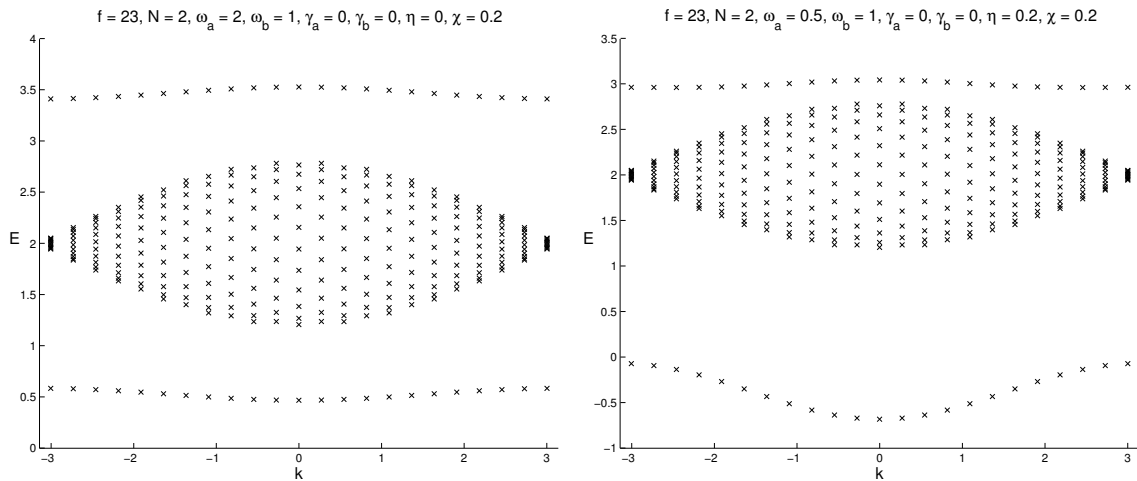


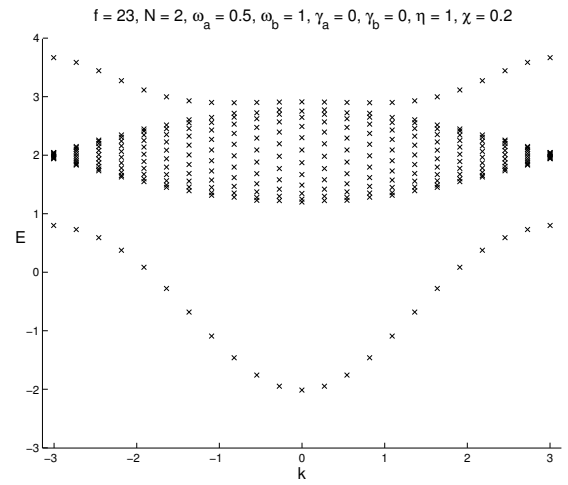
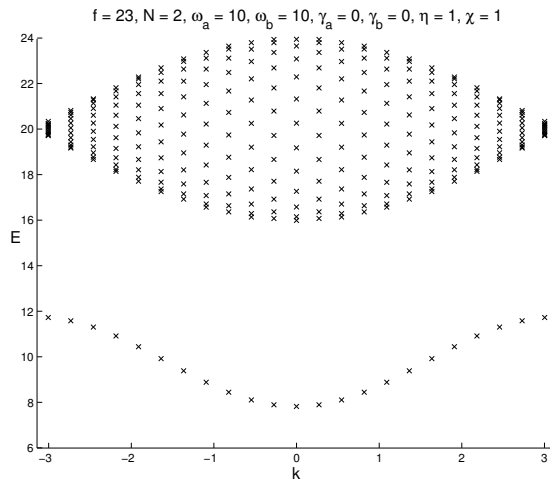
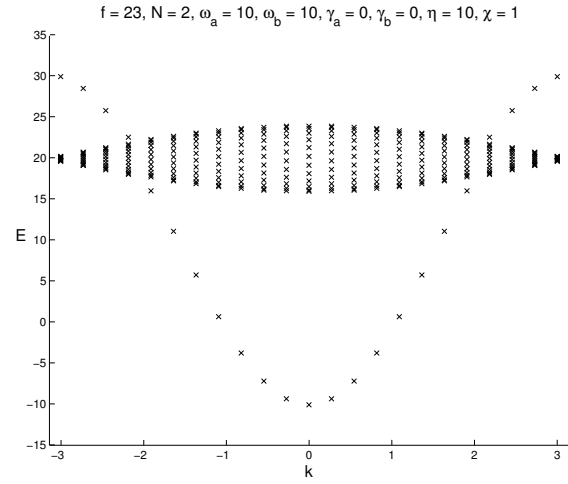
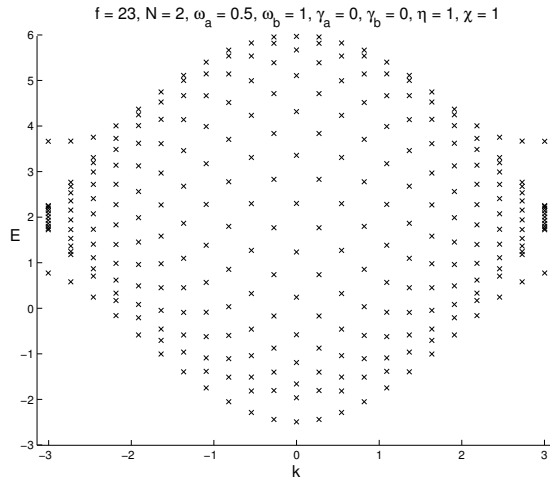
The figure shows the comparison between the “exact” numerical and the approximate values of the dc-component of the fraction of atomic states as a function of the initial number of atoms in the system.

$N = 2$, general f

We can calculate results for the dimer for small N , but if we restrict ourselves to the case $N = 2$ it is possible to get results for general f .

This corresponds to a generalization of the $n = 2$ case for the QDNLS model. We get again a tridiagonal Hamiltonian matrix, giving various band structures even when $\gamma_a = \gamma_b = 0$, i.e. the nonlinearity comes from the interaction term alone.





Caisar Katerji has also done a careful study of the dynamics in various cases.

Quasi-exactly solvable model

A major feature to the QDNLS family of models is that there is a *conserved* number of bosons. In seeking to understand models with no conserved number, we have been studying the following model

$$\begin{aligned}\hat{H} = & -\gamma_1 \sum_{j=1}^f b_j^\dagger b_j^\dagger b_j b_j + \gamma_2 \sum_{j=1}^f b_j^\dagger b_j^\dagger b_j^\dagger b_j b_j b_j + \\ & - \epsilon \sum_j \left(b_j^\dagger b_{j+1} + b_j^\dagger b_{j-1} \right) \\ & + \beta \sum_{j=1}^f \left[b_j^\dagger \left(\hat{N} - m \right) + \left(\hat{N} - m \right) b_j \right]\end{aligned}$$

The first three terms are as before, and conserve N , but the final term does not, *except* when $N = m$.

Quasi-exactly solvable model

The result of the m -dependent term is to divide the Hamiltonian matrix into two blocks, a finite size one and an infinite one

$$H = \begin{bmatrix} H^m & 0 \\ 0 & H^\infty \end{bmatrix}.$$

By adjusting the value of γ_1 and γ_2 we can make sure that some of the eigenvalues of H^m lie below all those of H^∞ .

In the *monomer* case H^m , is tridiagonal with diagonal elements

$$H_{n,n}^m = -\gamma_1 n(n-1) + \gamma_2 n(n-1)(n-2)$$

and off-diagonal

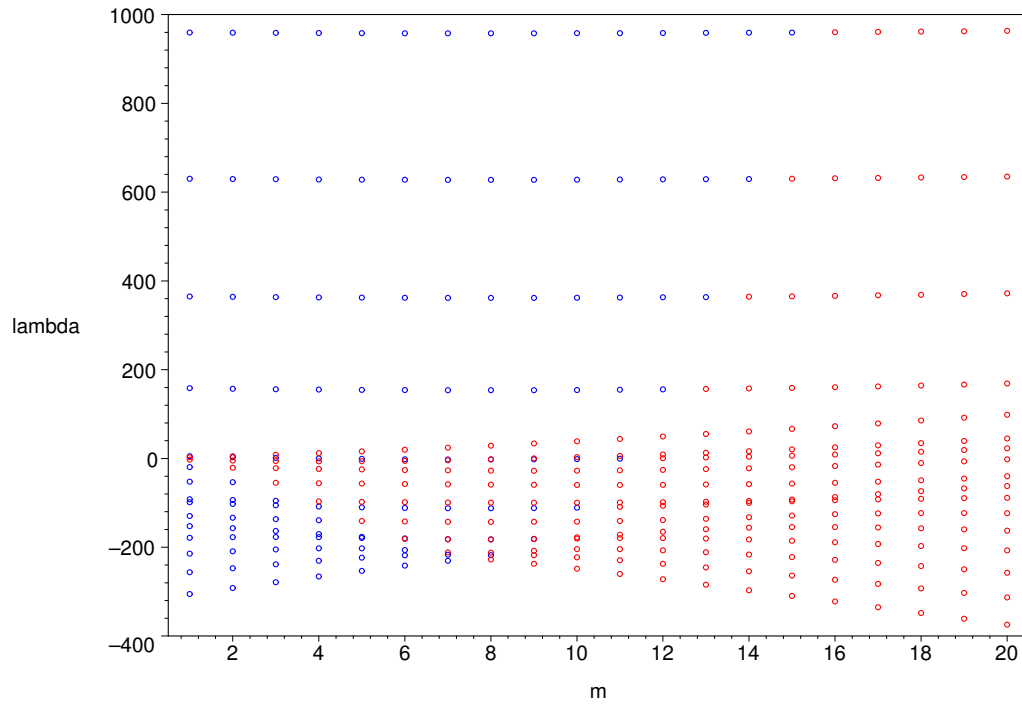
$$H_{n,n+1}^m = H_{n+1,n}^m = -\beta (m-n) \sqrt{n+1}$$

Quasi-exactly solvable model - dimer case

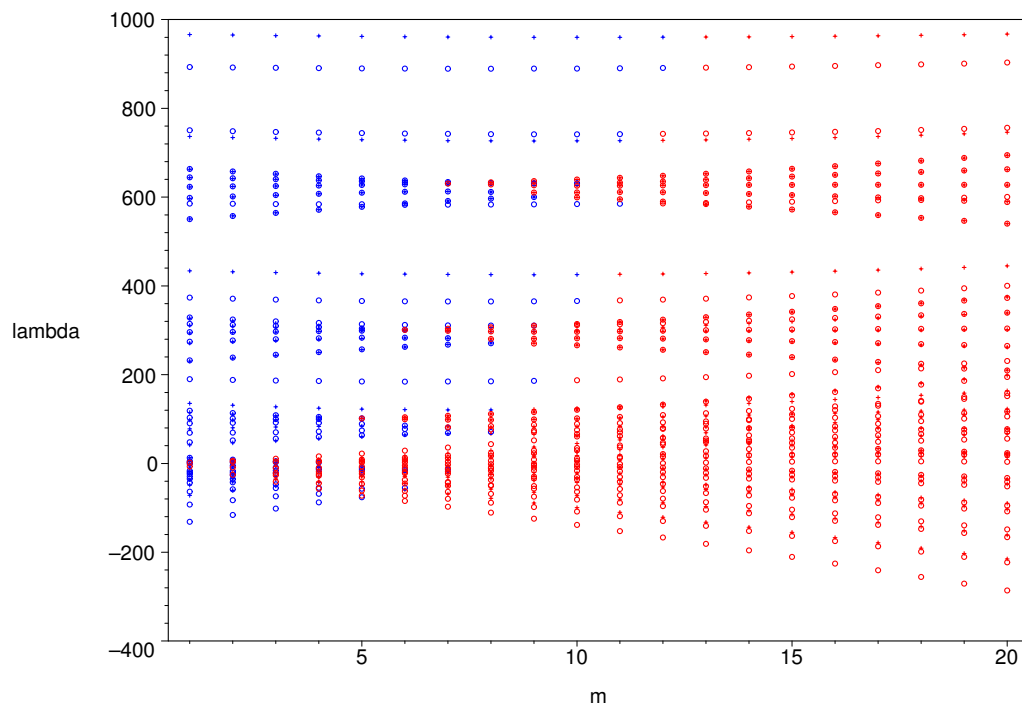
We can split the basis states into symmetric ($k = 0$) and anti-symmetric ($k = 1$) states, then H^m and H^∞ split also. Now $H^{(m,k)}$ is *block*-tridiagonal.

$$H^{(k,m)} = \begin{bmatrix} \ddots & & \ddots & & \bigcirc \\ & \ddots & H_{n,n}^{(k,m)} & H_{n,n+1}^{(k,m)} & \\ & & H_{n+1,n}^{(k,m)} & \ddots & \ddots \\ & & & \ddots & \ddots \\ \bigcirc & & & \ddots & H_{m,m}^{(k,m)} \end{bmatrix}.$$

and the formula for the elements of each block can be written down.



monomer case, infinite matrix, finite matrix,
 $\gamma_1 = 10$, $\gamma_2 = 1$, $\beta = 2.5$



dimer case, \circ symm., $+$ anti-symm., $\epsilon = 2.5$.

Quasi-exactly solvable model

$m = 2$, general f case

In this case we can also write down exact equations for the *block*-tridiagonal matrix H^m (see Brihaye, quant-ph/0412174).