QUANTUM LATTICE SOLITONS

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Abstract

The number state method is used to study soliton bands for three anharmonic quantum lattices: i) The discrete nonlinear Schrödinger equation, ii) The Ablowitz-Ladik system, and iii) A fermionic polaron model. Each of these systems is assumed to have $f$-fold translational symmetry in one spatial dimension, where $f$ is the number of freedoms (lattice points). At the second quantum level ($n = 2$) we calculate exact eigenfunctions and energies of pure quantum states, from which we determine binding energy ($E_b$), effective mass ($m^*$) and maximum group velocity ($V_m$) of the soliton bands as functions of the anharmonicity in the limit $f \to \infty$. For arbitrary values of $n$ we have asymptotic expressions for $E_b$, $m^*$, and $V_m$ as functions of the anharmonicity in the limits of large and small anharmonicity. Using these expressions we discuss and describe wave packets of pure eigenstates that correspond to classical solitons.

1 Introduction

Throughout the development of modern nonlinear dynamics the investigation of lattices has played a significant role. Often the motivation for such studies is that molecular crystals are lattices, and in these applications quantum effects cannot be ignored. Typical experiments—such as infra-red absorption, Raman scattering, and neutron diffraction—deal with line spectra, where every line corresponds to a pair of quantum states, each with a particular number of quanta. At larger quantum numbers—approaching the correspondence limit—one is often interested in knowing how quantum corrections alter the results of classical calculations. Our aim in this paper is to present some results of an exact theory of lattice solitons in the quantum regime. To this end we consider the following specific models, which are defined on one-dimensional lattices of $f$ freedoms (or lattice sites) with periodic boundary conditions and with $\gamma$ being the ratio of anharmonicity to nearest neighbor hopping energy.

(i) The quantum discrete nonlinear Schrödinger (QDNLS) equation

This system arises in the study of molecular vibrations in one-dimensional chains such as benzene and certain molecular crystals [3, 24]. With site energies scaled out through a gauge transformation the reduced Hamiltonian operator is

$$\hat{H}_1 = -\sum_{j=1}^{f} \left[ b_j^\dagger b_{j+1} + b_j^\dagger b_{j-1} + \frac{\gamma}{2} b_j^\dagger b_j^\dagger b_j b_j \right],$$  \hspace{1cm} (1.1)$$

where $b_j^\dagger$ and $b_j$ are standard bosonic raising and lowering operators satisfying the commutation relations $[b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0$, $[b_i, b_j^\dagger] = \delta_{ij}$ at each freedom.

(ii) The quantum Ablowitz-Ladik (QAL) equation

The Ablowitz-Ladik equation is of interest because the corresponding classical system is integrable via the inverse scattering method [1] and the quantum system is a simple example of a $q$-boson model [14]. The reduced Hamiltonian operator is

$$\hat{H}_2 = -\sum_{j=1}^{f} \left[ b_j^\dagger (b_{j+1} + b_{j-1}) \right],$$  \hspace{1cm} (1.2)$$
where $b_j^\dagger$ and $b_j$ are operators satisfying “$q$-deformed” commutation relations
\[
[b_j^\dagger, b_k] = [b_j, b_k] = 0, \quad [b_j, b_k^\dagger] = \left(1 + \frac{\gamma}{2} b_j^\dagger b_k^\dagger\right) \delta_{jk}.
\]

(iii) A fermionic polaron (FP) model

This model describes the dynamics of electrons in a one-dimensional crystal \[17\] and is related to the XXZ spin chain model \[20\]. The reduced Hamiltonian operator is
\[
\hat{H}_3 = -\sum_{j=1}^f \left[ a_j^\dagger a_{j+1} + a_j^\dagger a_{j-1} + \gamma a_j^\dagger a_j a_{j+1} a_{j+1}\right], \tag{1.3}
\]
where $a_j^\dagger$ and $a_j$ are standard fermion raising and lowering operators satisfying the anticommutation relations \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0, \{a_i, a_j^\dagger\} = \delta_{ij}.

These systems are chosen to exhibit three different types of fundamental quanta: i) standard bosons, ii) $q$-deformed bosons, and iii) standard fermions. A classical analog (or correspondence limit) exists only in the first two examples.

Since each of these three models is assumed to satisfy periodic boundary conditions, the Hamiltonians are invariant under the action of the translation operator with eigenvalue $\exp(ik)$, where $k$ is the crystal momentum. For a fixed number of quanta ($n$) the energy eigenstates for a particular value of $k$ are separated into bands, and the band of lowest energy is of the form \[2\]
\[
E = E_n(k), \tag{1.4}
\]
which is of particular interest for two reasons:

- Within this band there is but a single eigenstate for each value of $k$.
- The $n$ quanta of the eigenfunctions for the band are located more closely together than in the bands of higher energy.

We call this lowest band the soliton band and use Equation (1.4) to compute the binding energy, effective mass, and maximum group velocity of the corresponding quantum soliton.

In the following section we sketch our procedure for computing $E_n(k)$ as a function of the ratio of anharmonicity to nearest neighbor hopping energy ($\gamma$), and in Section 3 we give complete descriptions of the bands of our three models for the second quantum level ($n = 2$). Asymptotic expressions for $E_n(k)$ at small and large values of $\gamma$ are derived in Section 4. In Section 5 we use these results to construct wave packets—over $n$ and $k$—of pure eigenstates that correspond to classical solitons, and some conclusions are presented in Section 6. Throughout the discussion we assume units of energy and time for which $\hbar = 1$.

We have chosen to call our method of analysis the number state method, to distinguish it from the Quantum Inverse Scattering Method \[12, 13\]. The advantages and disadvantages of each of these two methods is discussed at some length in \[7\]. In all cases where both techniques have been used they give (as expected) the same results. However it is important to note that the first model we consider (QDNLS) is nonintegrable and cannot be analysed by the QISM.
2 The number state method of analysis

In our study of these three quantum lattices we take advantage of the fact that each Hamiltonian operator commutes with a number operator \( \hat{N} \), which counts the number of fundamental quanta (bosons, \( q \)-deformed bosons, or fermions) associated with each degree of freedom \([23, 7]\). Thus a general eigenfunction of \( \hat{N} \) can be written in the form

\[
|\psi_n\rangle = \sum_{l=1}^{p} c_l |\phi_l\rangle ,
\]

where \( p = p(n, f) \) is the number of different ways that \( n \) quanta can be arranged on \( f \) freedoms, \( |\phi_l\rangle \) is the number state corresponding to a particular arrangement, and the \( \{c_l\} \) are a set of \( p \) arbitrary complex constants. For example if we are placing two bosons \( (n = 2) \) on two freedoms \( (f = 2) \), there are three possible number states \( (p = 3) \):

\[
|\phi_1\rangle = |2\rangle|0\rangle, \quad |\phi_2\rangle = |1\rangle|1\rangle, \quad \text{and} \quad |\phi_3\rangle = |0\rangle|2\rangle,
\]

which for typographical convenience we write as \([20], [11], \text{and} [02]\). Requiring \( |\psi_n\rangle \) to satisfy the time independent Schrödinger equation

\[
\hat{H}|\psi_n\rangle = E|\psi_n\rangle \quad (2.2)
\]
generates a \( p \times p \) matrix equation for the \( \{c_l\} \)'s, which determines the energy eigenvalues, and the eigenvectors—upon substitution into Equation (2.1)—yield the corresponding stationary state wave functions. We refer to this technique as the “number state method” (NSM) to differentiate it from the quantum inverse scattering method (QISM) over which it has some theoretical and computational advantages \([7]\).

In effect the NSM diagonalizes the infinite Hamiltonian matrix into finite blocks of size \( p \). For the bosons of \( \hat{H}_1 \) and the \( q \)-deformed bosons of \( \hat{H}_2 \)

\[
p_1 = p_2 = \frac{(n + f - 1)!}{n!(f - 1)!} . \quad (2.3)
\]

Only one of the fermions of \( \hat{H}_3 \) can be placed on a single freedom so in this case

\[
p_3 = \frac{f!}{n!(f - n)!} . \quad (2.4)
\]

A moment’s reflection will convince the reader that \( p \) can easily become inconveniently large, but this is not a problem particular to the number state method. Exact quantum wave functions on lattices are complicated objects, and the same difficulty appears with the QISM \([7]\). Each of our three systems has translational symmetry so these \( p \times p \) blocks can be further diagonalized into smaller blocks with fixed values of crystal momentum \( k \), where \( \tau = \exp(ik) \) is an eigenvalue of the translation operator \( \hat{T} \). \( \hat{T} \) is defined by the property \( \hat{T}b_j^\dagger = b_{j+1}^\dagger \) so that

\[
\hat{T}|n_1n_2\ldots nf\rangle = |n_fn_1\ldots nf-1\rangle.
\]

In this manner we find \( E = E(k) \) for every allowed momentum state with a minimum of computational effort.

As a simple example of this method, consider the first quantum level \( (n = 1) \). The energy bands for all three models are identical because there are just \( f \) ways that a single quantum can be placed on \( f \) freedoms. Thus we find

\[
|\psi_1(k)\rangle = \frac{1}{\sqrt{f}} \sum_{j=1}^{f} (e^{ik}\hat{T})^{j-1}|100\ldots0\rangle , \quad (2.5)
\]
and
\[ E_1(k) = -2\cos k, \quad (2.6) \]
where \( k = 2\pi \nu / f \) and \( \nu = 0, \pm 1, \pm 2, \ldots, \pm (f/2-1), f/2 \) for \( f \) even and \( 0, \pm 1, \pm 2, \ldots, \pm (f-1)/2 \) for \( f \) odd.

Since the effective mass \( (m^*) \) is defined as
\[ E_1(k) = E_1(0) + \frac{k^2}{2m^*} + O(k^4), \quad (2.7) \]
we have
\[ m^* = 1/2. \quad (2.8) \]

3 The second quantum level

Here we show how to compute the exact eigenstates and energy eigenvalues of the soliton bands at the second quantum level \( (n = 2) \). To this end we display number operators, \( \hat{N}_i \), \( i = 1, 2, 3 \) that commute with each other and the Hamiltonian, and we construct the most general eigenfunctions of \( \hat{N}_i \) and the translation operator \( \hat{T} \) as a sum of products of elementary number states \([4, 10]\).

(i) QDNLS

\( \hat{H}_1 \), the Hamiltonian of Equation (1.1), commutes with the number operator
\[ \hat{N}_1 = \sum_{j=1}^{f} b_j^\dagger b_j, \quad (3.1) \]
which has eigenvalue \( n \). As discussed in the previous section, the most general eigenfunction of \( \hat{N}_1 \) is a sum of products of elementary number states of the form \([n_1 n_2 \ldots n_f]\), where \( n = n_1 + n_2 + \cdots + n_f \).

For \( n = 2 \) and \( f \) odd a general eigenfunction of both \( \hat{N}_1 \) and \( \hat{T} \) is
\[ |\psi_2\rangle = \frac{1}{\sqrt{f}} \{ c_1 \sum_{j=1}^{f} (\tau \hat{T})^{j-1} [20 \ldots 0] + c_2 \sum_{j=1}^{f} (\tau \hat{T})^{j-1} [1010 \ldots 0] + + c_3 \sum_{j=1}^{f} (\tau \hat{T})^{j-1} [1010 \ldots 0] + \ldots + + c_{(f+1)/2} \sum_{j=1}^{f} (\tau \hat{T})^{j-1} [10 \ldots 010 \ldots 00] \}, \quad (3.2) \]
where \( \tau = \exp(ik) \) is the eigenvalue of \( \hat{T} \) that corresponds to the wavenumber \( k = 2\pi \nu / f \). To ensure that \( \langle \psi_2 | \psi_2 \rangle = 1 \), it is necessary that the \( c_i \)'s be normalized as
\[ \sum_{i=1}^{(f+1)/2} |c_i|^2 = 1. \quad (3.3) \]

Requiring that \( \hat{H}_1 |\psi_2\rangle = E |\psi_2\rangle \) leads to the matrix equation \( Q_1(\tau) c = Ec \), where \( c = \text{col}(c_1, c_2, \ldots, c_{(f+1)/2}) \) and \( Q(\tau) \) is the \([ (f+1)/2 ] \times [(f+1)/2] \) matrix
\[ Q_1(\tau) = - \begin{pmatrix} \gamma & q^* \sqrt{2} \\ \sqrt{2} & 0 & q^* \\ q & 0 & q^* \\ \vdots & \ddots & \ddots & \ddots \\ q & 0 & q^* \\ 0 & q & p \end{pmatrix}, \quad (3.4) \]
and
\[ q \equiv 1 + \tau, \quad p \equiv (\tau^{(f+1)/2} + \tau^{(f-1)/2}). \tag{3.5} \]

For \( f \) even (which is a special case of the condition \( f \mod n = 0 \)), the wave function depends on whether the integer \( \nu \) in the translational eigenvalue \( \tau = \exp(2\pi i \nu/f) \) is even or odd. For \( \nu \) even

\[ |\psi_2\rangle = \frac{1}{\sqrt{f}} \left\{ c_1 \sum_{j=1}^{f} (\tau \hat{T})^{j-1}[20 \cdots 0] + c_2 \sum_{j=1}^{f} (\tau \hat{T})^{j-1}[110 \cdots 0] + \right. \]
\[ + c_3 \sum_{j=1}^{f} (\tau \hat{T})^{j-1}[1010 \cdots 0] + \cdots \]
\[ \left. + (c(f+1)/\sqrt{2}) \sum_{j=1}^{f} (\tau \hat{T})^{j-1}[10 \cdots 010 \cdots 00] \right\}, \tag{3.6} \]

whereas for \( \nu \) odd the last term in the sum is omitted.

For \( f \) and \( \nu \) both even, \( Q_1(\tau) \) is the \((f/2 + 1) \times (f/2 + 1)\) matrix

\[ Q_1(\tau) = - \begin{pmatrix} \gamma & q^* \sqrt{2} & 0 & & & 0 \\ q \sqrt{2} & 0 & q^* & & & \vdots \\ & q & 0 & q^* & & \vdots \\ & & \ddots & \ddots & \ddots & \ddots \\ & & & q & 0 & q^* \sqrt{2} \\ & & & & q \sqrt{2} & 0 \end{pmatrix}, \tag{3.7} \]

where \( q \) is defined in Equation (3.5). For odd \( \nu \), \( Q_1(\tau) \) is the \((f/2) \times (f/2)\) matrix obtained from Equation (3.7) by omitting the last row and column.

Finding the eigenvalues of tridiagonal matrices of this sort is an interesting exercise in analysis; full details are given [6]. Exact results can be obtained in the limit \( f \to \infty \); for finite but large \( f \) analytic correction factors can be found.

In the limit \( f \to \infty \) the soliton band has the energy

\[ E_2(k) = -\sqrt{\gamma^2 + 16\cos^2(k/2)}. \tag{3.8} \]

Defining the binding energy, \( E_b \), as the difference between the energy of the soliton band at \( k = 0 \) and the bottom of the continuum band, one finds that

\[ E_b = \sqrt{\gamma^2 + 16} - 4, \tag{3.9} \]

and with effective mass defined as in Equation (2.7)

\[ m^* = \frac{\sqrt{\gamma^2 + 16}}{4}, \tag{3.10} \]

and maximum group velocity

\[ V_m \equiv \left[ \frac{dE}{dk} \right]_{k=\pi/2} = \frac{4}{\sqrt{\gamma^2 + 8}}. \tag{3.11} \]

In Figure 1(i) we display the energy eigenvalues calculated from Equation (3.4) with \( \gamma = 3 \) in the limit \( f \to \infty \). The existence of a quasi-continuum and a lower discrete band is clear.

(ii) QAL

The Hamiltonian \( \hat{H}_2 \) commutes with the translation operator and with the number operator \[ 21, 22 \]

\[ \hat{N}_2 = \sum_{j=1}^{f} \frac{\ln \left( 1 + \frac{q_j}{2} b_j^\dagger b_j \right)}{\ln \left( 1 + \frac{q_j}{2} \right)}. \tag{3.12} \]
(i) QDST  
(ii) QA-L  
(iii) Fermionic model

Figure 1: Soliton bands in the three models considered in the text
Taking the eigenvalue \( n \) of \( \hat{N}_2 \) to be 2 the wave functions are as in Equations (3.2) and (3.6). For \( f \) odd the energy eigenvalues are found from the \( [(f+1)/2] \times [(f+1)/2] \) matrix

\[
Q(\tau) = -\begin{pmatrix}
0 & q^* \sqrt{2 + \gamma/2} & 0 & q^* \\
q \sqrt{2 + \gamma/2} & 0 & q & 0 \\
0 & q & 0 & q^* \\
q^* & 0 & q & p \\
\end{pmatrix},
\]

(3.13)

where \( q, p \) are as defined in (3.5).

For \( f \) and \( \nu \) both even, \( Q_2(\tau) \) is the \( (f/2 + 1) \times (f/2 + 1) \) matrix

\[
Q(\tau) = -\begin{pmatrix}
0 & q^* \sqrt{2 + \gamma/2} & 0 & q^* \\
q \sqrt{2 + \gamma/2} & 0 & q & 0 \\
0 & q & 0 & q^* \\
q^* & 0 & q & p \\
\end{pmatrix},
\]

(3.14)

whereas for \( \nu \) odd it is the \( (f/2) \times (f/2) \) matrix obtained from Equation (3.14) by omitting the final row and column.

In the QAL case we find two soliton bands, which are shown in Figure 1(ii). The top band corresponds to the classical AL soliton that alternates in sign between each lattice point.

In the limit \( f \to \infty \) the soliton band has energy \( E_2(k) = \pm \frac{2\cos (k/2)(\gamma + 4)}{\sqrt{2\gamma + 4}} \).

(3.15)

Defining the binding energy, \( E_b \), as above, one finds that

\[
E_b = \frac{2(\gamma + 4)}{\sqrt{2\gamma + 4}} - 4,
\]

(3.16)

and the effective masses are

\[
m^* = \pm \frac{2\sqrt{2\gamma + 4}}{\gamma + 4},
\]

(3.17)

where the “+” corresponds to the lower band and the “−” sign to the upper band. In this case the maximum group velocity is

\[
V_m = \left[ \frac{dE}{dk} \right]_{k=\pi} = \frac{\gamma + 4}{\sqrt{2\gamma + 4}}.
\]

(3.18)

(iii) FP

The Hamiltonian \( \hat{H}_3 \) commutes with the number operator

\[
\hat{N}_3 = \sum_{j=1}^{f} a_j^\dagger a_j.
\]

(3.19)
Because of the anti-commutation relations, the order in which one inserts the fermions into the chain is important \[3\]. We define the normal ordering to be that in which the fermions are inserted from left to right. Hence \(a_2^\dagger a_1^\dagger [00] = [11]\), but \(a_1^\dagger a_2^\dagger [00] = -[11]\). The translation operator is defined by \(T a_j^\dagger = a_j^\dagger + T\), so, for example, \(T[1001] = -[1100]\). As was pointed out by Dirac, this makes hand calculations tedious, but fortunately an algebraic manipulation system like Mathematica \[27\] can be programmed to take such sign changes into account.

Again assuming the eigenvalue of \(N_3\) to be 2 and \(f\) odd, a general eigenfunction of \(N_3\) and \(T\) is

\[
|\psi_2\rangle = \frac{1}{\sqrt{f}} \{ c_1 \sum_{j=1}^{f} (\tau T)^{j-1} [110\cdots0] + c_2 \sum_{j=1}^{f} (\tau T)^{j-1} [1010\cdots0] + \cdots + c_{(f-1)/2} \sum_{j=1}^{f} (\tau T)^{j-1} [10\cdots010\cdots0]\}.
\]

(3.20)

Note that this wavefunction has one less term than that given in Equation (3.2) because no more than one fermion can be assigned to any one freedom. Requiring \(H_3|\psi_3\rangle = E|\psi_3\rangle\) leads to the matrix equation \(Q_3(\tau)e = Ee\), where \(Q_3(\tau)\) is the \([f/2 - 1] \times [f/2 - 1]\) matrix

\[
Q_3(\tau) = -\begin{pmatrix}
\gamma & q^* & q & \cdots & q & q^* \\
q & 0 & q^* & \cdots & q & q^* \\
q & 0 & q^* & \cdots & q & q^* \\
\end{pmatrix},
\]

(3.21)

and \(q, p\) are as defined in (3.5).

If \(\gamma > 2\), the resulting eigenvalue plot appears as in Figure 1(i), but for \(0 < \gamma < 2\), the central part of the soliton band merges with the quasi-continuum as is shown in Figure (iii).

For \(f\) and \(\nu\) both even,

\[
|\psi_2\rangle = \frac{1}{\sqrt{f}} \{ c_1 \sum_{j=1}^{f} (\tau T)^{j-1} [110\cdots0] + c_2 \sum_{j=1}^{f} (\tau T)^{j-1} [1010\cdots0] + \cdots + c_{(f-1)/2} \sum_{j=1}^{f} (\tau T)^{j-1} [10\cdots010\cdots0]\}.
\]

(3.22)

and \(Q_3(\tau)\) is the \((f/2 - 1) \times (f/2 - 1)\) matrix

\[
Q_3(\tau) = -\begin{pmatrix}
\gamma & q^* & q & \cdots & q & q^* \\
q & 0 & q^* & \cdots & q & q^* \\
q & 0 & q^* & \cdots & q & q^* \\
\end{pmatrix}.
\]

(3.23)

For \(\nu\) odd \(|\psi_2\rangle\) is as in Equation (3.22) with the last term omitted, and \(Q_3(\tau)\) is as in Equation (3.23) but with the last row and column omitted.

In the limit \(f \to \infty\) the soliton band has energy \[3\]

\[
E(k) = -\left[ \gamma + \frac{4}{\gamma} \cos^2 \left( \frac{k}{2} \right) \right] \quad \text{for} \quad \gamma > 2\cos(k/2).
\]

(3.24)

For \(\gamma > 2\) the binding energy and effective mass are

\[
E_b = \gamma + \frac{4}{\gamma},
\]

(3.25)
\[ m^* = \frac{\gamma}{2}, \quad (3.26) \]

and the maximum group velocity is

\[ V_m = \left[ \frac{dE}{dk} \right]_{k = \pi/2} = \frac{2}{\gamma}. \quad (3.27) \]

## 4 Asymptotic expressions for arbitrary quantum levels

Proceeding as in the previous section it is possible—in principle—to construct block diagonalized Hamiltonian matrices for any value of the quantum number \( n \). As was noted in Section 2, however, the sizes of these blocks may grow beyond the limits of computational convenience (or even possibility) so it is of interest to consider approximate calculations that are useful in asymptotic limits. In this section we present results for arbitrary values of the quantum level that are asymptotically correct for small or large values of the anharmonicity parameter.

### 4.1 Small \( \gamma \)

Binding energy has been studied in detail for the QDNLS and QAL systems in reference [18], and with \( \gamma \ll 1 \) these results are identical for QDNLS and QAL. To calculate the binding energy in this limit it is necessary to know whether the size of the classical soliton is large or small compared with the number of freedoms. If \( 1 \gg \gamma > 24/((n + 1)f) \), the size of the classical soliton is smaller than \( f \) [19] and both the QDNLS and the QAL equations are well approximated by the continuum nonlinear Schrödinger equation for which the binding energy of a quantum soliton is [11]

\[ E_b = \frac{\gamma^2}{48} n(n^2 - 1). \quad (4.1) \]

To calculate the effective masses for QDNLS and QAL in the limit of small \( \gamma \) we refer to Equation (2.6), which gives the energy as a function of the wave number for a single quantum. Since the classical problem is linear in this limit, the energy for \( n \) quanta with wave numbers: \( k_1, k_2, \ldots, k_n \) is just the sum: \(-2\sum_j \cos k_j \). For the \( n \)-quantum wave function \( k = \sum_j k_j \), and the lowest value of energy is found for \( k_1 = k_2 = \cdots = k_n \); thus in this limit

\[ E_n(k) = -2n\cos (k/n) \quad (4.2) \]

so

\[ m^* = \frac{n}{2}, \quad (4.3) \]

and the maximum group velocity of a wave packet is

\[ V_m = \left[ \frac{dE}{dk} \right]_{k = \pi/2} = 2\sin \left( \frac{\pi}{2n} \right). \quad (4.4) \]

For the FP system the soliton band merges into the continuum at small \( \gamma \) so \( E_b \) and \( m^* \) are not defined in this limit.

### 4.2 Large \( \gamma \)

In the limit of large \( \gamma \) it is evident that for \( n = 2 \) the dominant elements of the matrices \( Q_1, Q_2, \) and \( Q_3 \), which are displayed in Equations (3.4), (3.13), and (3.21),
are the $2 \times 2$ submatrices in the upper left hand corners. For arbitrary values of $n$, perturbation theory in $\gamma^{-1}$ shows that to calculate the leading $k$-dependent terms it is only necessary to consider the sequence of interactions

$$[n] \leftrightarrow [n-1,1] \leftrightarrow [n-2,2] \leftrightarrow \cdots \leftrightarrow [2,n-2] \leftrightarrow [1,n-1] \leftrightarrow [n]. \quad (4.5)$$

For the QDNLS and QAL systems this sequence requires an approximate wave function of the form

$$|\psi_n\rangle \equiv \frac{1}{\sqrt{n}} \{ c_{1} \sum_{j=1}^{f} (\tau T)^{j-1} [n0 \cdots 0] + c_{2} \sum_{j=1}^{f} (\tau T)^{j-1} [(n-1)10 \cdots 0] +$$

$$+ c_{3} \sum_{j=1}^{f} (\tau T)^{j-1} [(n-1)00 \cdots 1] + \cdots +$$

$$+ c_{n} \sum_{j=1}^{f} (\tau T)^{j-1} [(n/2)(n/2)0 \cdots 0] \}, \quad (4.6)$$

with $n$ even, and

$$|\psi_n\rangle \equiv \frac{1}{\sqrt{n}} \{ c_{1} \sum_{j=1}^{f} (\tau T)^{j-1} [n0 \cdots 0] + c_{2} \sum_{j=1}^{f} (\tau T)^{j-1} [(n-1)10 \cdots 0] +$$

$$+ c_{3} \sum_{j=1}^{f} (\tau T)^{j-1} [(n-1)00 \cdots 1] + \cdots +$$

$$+ c_{n-1} \sum_{j=1}^{f} (\tau T)^{j-1} [(n+1)/2((n-1)/2)0 \cdots 0], +$$

$$+ c_{n} \sum_{j=1}^{f} (\tau T)^{j-1} [(n+1)/20 \cdots 0((n-1)/2)] \} \quad (4.7)$$

for $n$ odd.

(i) QDNLS

As an illustrative example, consider the QDNLS equation with $n$ even for which the $n \times n$ matrix $-\hat{Q}_{1}(\tau)$ formed from the approximate wave function in Equation (4.6) is

$$\begin{pmatrix}
\frac{\gamma n(n-1)}{2} & \sqrt{n} & \sqrt{n} \\
\sqrt{n} & \frac{\gamma(n-1)(n-2)}{2} & 0 \\
\sqrt{n} & 0 & \gamma(n-1)(n-2) \\
\cdots & \cdots & \cdots \\
0 & \gamma(n-1)(n-2) & \sqrt{3(n-2)} \\
\sqrt{\frac{n}{4}}(\frac{n}{4}+1) & \sqrt{\frac{3}{2}(\frac{3}{2}+1)} & \gamma(n-1)(n-2) \\
\end{pmatrix} \quad (4.8)$$

We have no exact results for the eigenvalues of such approximate matrices for arbitrary values of $n$. However we have done extensive investigations of the asymptotic expansions of the eigenvalues in powers of $1/\gamma$ for finite values of $n$ using Mathematica [27] and perturbation theory. Clearly the most negative eigenvalue has a leading term $-n(n-1)/2\gamma$. Higher order terms can be calculated but they are of secondary interest except for the lowest order term that depends on $k$. Perturbation theory shows that this term is of order $1/\gamma^{n-1}$. In summary, the most negative root of the determinantal equation, $\det[\hat{Q}_{1} - IE] = 0$, defines a soliton band of the form

$$E_{n}(k) \equiv -\frac{1}{2} n(n-1) \gamma - \left( \frac{2n}{(n-1)!\gamma^{n-1}} \right) \cos k, \quad (4.9)$$
where the symbol “±” indicates that the first term on the right hand side is correct to $O(\gamma^{-1})$ while the second ($k$-dependent) term is correct to $O(\gamma^{1-n})$. In other words, terms of order $O(1/\gamma)$ that do not depend on $k$ have been dropped. The second term on the right comes from the perturbation correction.

Equation (4.9) implies that for the QDNLS equation

$$E_b = \frac{1}{2} n(n-1) \gamma,$$  \hspace{1cm} (4.10)

and

$$m^* = \frac{(n-1)!}{2n} \gamma^{n-1},$$  \hspace{1cm} (4.11)

and

$$V_m = \left[ \frac{dE}{dk} \right]_{k=\pi/2} = \frac{2n}{(n-1)!} \gamma^{n-1}.$$  \hspace{1cm} (4.12)

(ii) QAL

For the QAL equation the wave functions are of the forms given in Equations (4.6) and (4.7) except that it is convenient to permute the order of terms such that

$$\{c_1, c_2, \ldots, c_n\} \rightarrow \{c_{n-3}, c_{n-5}, \ldots, c_3, c_1, c_2, c_4, \ldots, c_{n-2}, c_n, c_{n-1}\}.$$  \hspace{1cm} (4.13)

where

$$\beta(n) \equiv \left( \frac{\gamma}{2} \right)^{(n-1)/2}.$$  \hspace{1cm} (4.14)

Now define $Q_n = \det[\beta^{-1} \hat{Q}_2(\tau) - \epsilon I]$. Expanding $Q_n$ by final rows and columns gives eventually that

$$Q_n = (-1)^{n+1} 2 \cos k - 2P_{n-2} + \epsilon P_{n-1},$$

where $P_{n-1}$ is the tridiagonal determinant formed by removing the final row and column of $Q_n$.

A standard calculation shows that $P_n(\epsilon)$ is a polynomial satisfying the recursion relation

$$P_n = \epsilon P_{n-1} - P_{n-2},$$  \hspace{1cm} (4.15)

where $P_1 = \epsilon$ and $P_2 = \epsilon^2 - 2$. Thus $P_n(\epsilon) = 2U_n(\epsilon/2)$, where $U_n(x)$ is a Chebyshev polynomial of the second kind. Hence

$$Q_n = (-1)^{n+1} 2 \cos k + U_n - U_{n-2} = (-1)^{n+1} 2 \cos k + 2T_n\left( \frac{\epsilon}{2} \right)$$  \hspace{1cm} (4.16)

Where $T_n(x)$ is a Chebyshev polynomial of the first kind.

A further short calculation shows that the eigenvalues of (4.13) are

$$E_n(k) = -2\cos \left( \frac{k}{n} \right) \left( \frac{\gamma}{2} \right)^{(n-1)/2}.$$  \hspace{1cm} (4.17)
so for \( n > 1 \)
\[
E_b = 2 \left( \frac{\gamma}{2} \right)^{(n-1)/2},
\]
and
\[
m^* = \frac{n^2}{2} \left( \frac{2}{\gamma} \right)^{(n-1)/2}.
\]

The maximum group velocity on the QAL soliton band occurs at the band edge \( k = \pi \), therefore
\[
V_m \equiv \left[ \frac{dE}{dk} \right]_{k=\pi} = \frac{2}{n} \sin \left( \frac{\pi}{n} \right) \left( \frac{\gamma}{2} \right)^{(n-1)/2}.
\]

(iii) FP

For the FP model a translationally invariant wave function in the large \( \gamma \) limit is
\[
|\psi_n\rangle = \frac{1}{\sqrt{f}} \left\{ c_1 \sum_{j=1}^f (\tau \tilde{T})^{j-1} [11 \cdots 10 0] + 
          + c_2 \sum_{j=1}^f (\tau \tilde{T})^{j-1} [11 \cdots 10 1 0 \cdots 0] + 
          + c_3 \sum_{j=1}^f (\tau \tilde{T})^{j-1} [011 \cdots 10 1 \cdots 0] + 
          + \cdots + c_n \sum_{j=1}^f (\tau \tilde{T})^{j-1} [11 \cdots 0 1 \cdots 1 0 \cdots 0] \right\},
\]
for \( n \) even. For \( n \) odd there will be a corresponding expression with the last two terms given by
\[
c_{n-1} \sum_{j=1}^f (\tau \tilde{T})^{j-1} [11 \cdots 0 1 \cdots 1 0 \cdots 0] + 
\]
\[
c_n \sum_{j=1}^f (\tau \tilde{T})^{j-1} [11 \cdots 0 1 \cdots 1 0 \cdots 0] .
\]

Again it is convenient to reorder to get a periodic tridiagonal matrix. For \( n \) even, take \( \{ c_1, c_2, \ldots, c_n \} \to \{ c_1, c_3, c_5, \ldots, c_{n/2}, c_{n/2-1}, c_{n/2-3}, \ldots, c_2 \} \), with a similar permutation in the \( n \) odd case. This leads to a \( n \times n \) matrix \(-Q_3(\tau)\)
\[
\begin{pmatrix}
(n-1)\gamma & \tau^{-1} & 0 & 0 & 1 \\
\tau & (n-2)\gamma & 1 & 0 & 0 \\
0 & 1 & (n-2)\gamma & 1 & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & 1 & (n-2)\gamma \\
1 & 0 & \cdots & 0 & 1 & (n-2)\gamma 
\end{pmatrix} \quad (4.22)
\]

The characteristic equation is calculated in a similar way to the QAL case. If we define \( Q_n = \det[-Q_3(\tau) + (n-2)\gamma \cdot eI] \), then
\[
Q_n = 0 \Rightarrow (\gamma + e)U_{n-1}(e/2) - 2U_{n-2}(e/2) - (-1)^n 2 \cos k = 0
\]
To solve this polynomial equation for \( e \) by a perturbation series around \( \gamma = \infty \), put 
\[
\gamma = \epsilon^{-1}, \quad z = -e \epsilon,
\]

to get
\[
(-1)^n z^{n-1}(z-1) + (-1)^{n+1} \epsilon^n 2 \cos k + \sum_{m=1}^{M} \epsilon^{2m} z^{2(M-m)} p_m(z) = 0
\]

where \( M = \lfloor n/2 \rfloor \) and the \( p_m \) are linear functions of \( z \) with constant coefficients. A series expansion shows that one root is 
\[
z = 1 + O(\epsilon^2)
\]
and the others are \( O(\epsilon) \).

If we seek the lowest order \( k \)-dependent correction to the \( z = 1 \) root, along the lines of eqn (4.9), it is not difficult to show that this occurs at \( O(\epsilon^n) \) and is equal to \( \epsilon^n 2 \cos k \). Resubstituting this back into the original problem, we have that the soliton band is given by
\[
E_n(k) = -(n-1)\gamma - \frac{2}{\gamma^{n-1}} \cos k,
\]
where the symbol \( \sim \) has the same meaning as that discussed following (4.9). This implies that
\[
E_b = (n-1)\gamma,
\]
\[
m^* = \frac{\gamma^{n-1}}{2}, \quad \text{and}
\]
\[
V_m \equiv \left[ \frac{dE}{dk} \right]_{k=\pi/2} = \frac{2}{\gamma^{n-1}}.
\]

5 Soliton wave packets

The picture that emerges from our studies of one dimensional quantum lattices with \( f \) degrees of freedom and translational symmetry is as follows. For each value of the principle quantum number \( n \) and wave number \( k \), there is a lowest energy eigenvalue. These \( f \) lowest eigenvalues lie on a band (see Figure 1)
\[
E = E_n(k),
\]
where the wave number
\[
k = \frac{2\pi \nu}{f},
\]
and \( \nu = 0, \pm 1, \pm 2, \ldots, \pm (f/2 - 1), f/2 \) for \( f \) even and \( 0, \pm 1, \pm 2, \ldots, \pm (f-1)/2 \) for \( f \) odd. Each energy eigenvalue corresponds to a pure eigenstate \( |\psi_n(k)\rangle \), which is normalized as \( \langle \psi_n(k)|\psi_n(k)\rangle = 1 \).

For \( \hat{H} \) being one of the Hamiltonian operators in Equations (1.1), (1.2) or (1.3), solutions of the time dependent Schrödinger equation
\[
i \frac{d}{dt} |\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle
\]
can be constructed as sums over the quantum number and the wave number. Thus for QDNLS and QAL
\[
|\Psi(t)\rangle = \sum_n a_n \sum_k G_n(k)|\psi_n(k)\rangle \exp (-iE_n(k)t),
\]
where \( n = 0, 1, 2, \ldots, \infty \), and \( k \) takes the values between \(-\pi\) to \( \pi \) that are indicated in Equation (5.2). Since \( \langle \Psi(t)|\Psi(t)\rangle = 1 \), both the \( a_n \) and the \( G_n(k) \) are sets of complex numbers that satisfy the normalization conditions
\[
\sum_n |a_n|^2 = 1 \quad \text{and} \quad \sum_k |G_n(k)|^2 = 1.
\]
It should be noted that Equation (5.4) does not represent the most general wave function that satisfies Equation (5.3) because it is constructed only from eigenstates with eigenvalues on the soliton bands. It is seen from Figure 1 that the system has many other eigenstates, and these are excluded from $|\Psi(t)\rangle$ as defined in Equation (5.4), which is characterized by two interdependent properties:

- For given values of $n$, $k$, and the expansion coefficients, $|\Psi(t)\rangle$ has the lowest energy, and
- Under the same conditions, $|\Psi(t)\rangle$ has the highest probability of quanta being located near each other.

These properties are the basis for referring to $|\Psi(t)\rangle$ as a “soliton wave packet”.

An effect of dispersion in the wave packet of Equation (5.4) is to introduce uncertainties in position ($j$) and crystal momentum ($k$) that satisfy the Heisenberg relation. Such uncertainties appear in a natural way because $G_n(k)$ is a discrete Fourier transform of the soliton pulse shape so

$$\Delta k \times \Delta j \sim 1. \quad (5.6)$$

This point has been neglected at times in discussions of “Davydov’s soliton”, which has been proposed as a polaronic means for transport of energy or charge in protein.

In this section we present some properties of soliton wave packets. In addition to considering the differences between the QDNLS, QAL, and FP models, we also distinguish between spectral problems, where $n$ has a small, fixed value, and the correspondence limit for QDNLS and QAL, where values of $n$ are large compared with unity and $|\Psi(t)\rangle$ is approximated by the solution of a classical nonlinear equation.

### 5.1 Spectral problems

The ground state ($n = 0$) energy is zero for all three models, and the corresponding eigenstate is $|\psi_0\rangle = [000 \cdots 0]$. For $n = 1$ the wave function of an exact eigenstate is given in Equation (2.5), again for all three models, and the energy eigenvalues are given in Equation (2.6). For $n = 2$ exact expressions for $|\psi_2(k)\rangle$ and $E_2(k)$ are presented in Section 3, and in Section 4 we have derived approximate expressions for $|\psi_n(k)\rangle$ and $E_n(k)$ that hold in the limits $\gamma \ll 1$ and $\gamma \gg 1$.

When the expression for $|\Psi(t)\rangle$ in Equation (5.4) represents the wave function at a particular energy level (say $n = n_0$), then

$$a_n = \delta_{n, n_0}. \quad (5.7)$$

In measurements involving infra-red or Raman spectra on molecular crystals, the wave length of the interacting radiation is much larger than the dimensions of a unit cell so it is often reasonable to assume $k \approx 0$, but one can arrange experiments for which this is not the case.

The results of Section 3 permit exact calculations of features for the three transitions:

$$|\psi_0\rangle \rightarrow |\psi_1\rangle,$$
$$|\psi_0\rangle \rightarrow |\psi_2\rangle,$$
$$|\psi_1\rangle \rightarrow |\psi_2\rangle.$$

From the results of Section 4, which obtain in the limit $\gamma \gg 1$, approximate features can be calculated for the transitions:

$$|\psi_0\rangle \rightarrow |\psi_n\rangle,$$
\[ |\psi_1 \rangle \rightarrow |\psi_n \rangle , \]
\[ |\psi_2 \rangle \rightarrow |\psi_n \rangle , \]
\[ \cdots \text{etc.} \cdots \]
\[ |\psi_m \rangle \rightarrow |\psi_n \rangle . \]

5.2 Large wave packets

(i) QDNLS solitons in the Hartree approximation

In the continuum limit this problem has been studied in detail by Lai and Haus \[15\] and by Wright \[28\] as a model for the propagation of solitons on an optical fiber. The exact solution exhibits two quantum effects: phase spreading, which is caused by different values of \( n \) in the wave packet, and dispersion, caused by different values of \( k \). Lai and Haus have shown that the effects of dispersion become negligible compared with phase spreading at large values of the average number of quanta (bosons) in the soliton.

For the QDNLS equation with \( n \gg 1 \), the soliton wave function at a particular value of \( n \)
\[
|\Psi_n(t)\rangle = \sum_k G_n(k)|\psi_n(k)\rangle \exp[-iE_n(k)t] \tag{5.8}
\]
is close to the Hartree approximation \[29\]
\[
|\psi_n(t)\rangle^{(H)} = \frac{1}{\sqrt{n!}} \left[ \sum_{j=1}^{f} \Phi_{n,j}(t)b_j^\dagger \right]^n |0\rangle , \tag{5.9}
\]
where \( \Phi_{n,j}(t) \) is a solution of
\[
i\frac{d\Phi_{n,j}}{dt} + (\Phi_{n,j+1} + \Phi_{n,j-1}) + \gamma(n - 1)\Phi_{n,j}^2\Phi_{n,j} = 0 \tag{5.10}
\]
that satisfies the normalization condition
\[
\sum_{j=1}^{f} |\Phi_{n,j}(t)|^2 = 1 . \tag{5.11}
\]

Since \( \langle \psi_n(j,t)|b_j|\psi_n(j,t)\rangle^{(H)} = 0 \), it is convenient to choose the \( \{a_n\} \) in Equation (5.4) so that \( |\Psi(t)\rangle \) is the coherent wave packet
\[
|\Psi(t)\rangle = \sum_n \frac{n_0^{n/2}}{\sqrt{n!}} \exp\left( -\frac{n_0}{2} \right) |\psi_n(j,t)\rangle^{(H)} . \tag{5.12}
\]

In the correspondence limit, \( n_0 \gg 1 \),
\[
\langle \Psi(t)|b_j|\Psi(t)\rangle \rightarrow A_j(t) , \tag{5.13}
\]
where \( A_j(t) \) is a solution of the classical equation
\[
i\frac{dA_j}{dt} + (A_{j+1} + A_{j-1}) + \gamma|A_j|^2A_j = 0 \tag{5.14}
\]
with normalization
\[
\sum_{j=1}^{f} |A_j|^2 = n_0 . \tag{5.15}
\]
For \( \gamma > O(1) \) both classical solutions of Equation (5.14) and solutions of Equation (5.10) do not propagate; they are pinned to the lattice by the Peierls barrier \[8\]. The exact expression for \( |\Psi(t)\rangle \) is seen from Equation (4.12) to have a maximum wave packet velocity

\[
V_m = \frac{2n_0}{(n_0 - 1)! \gamma^{n_0 - 1}}
\]

for \( n_0 \gg 1 \). Thus the exact quantum mechanical solution also becomes pinned in the correspondence limit in the sense that \( V_m \to 0 \) strongly as \( n_0 \to \infty \).

(ii) QAL solitons

For \( \gamma \ll 1 \) the QAL equation approaches the QDNLS equation and the wave function of a QAL soliton is close to that given by Equations (5.9) and (5.12). For \( \gamma > O(1) \) there is—to our knowledge—no Hartree approximation, and the two systems are quite different. From Equations (4.6) and (4.7)

\[
|\psi_n(k)\rangle = \frac{1}{\sqrt{f}} \sum_{j=1}^{f} (e^{i k \hat{T}})^{-1} [n00 \cdots 0] + O(\gamma^{-1})
\]

and

\[
b_j \hat{T}^{-1} [n00 \cdots 0] = \beta(n) \hat{T}^{-1} [(n - 1)00 \cdots 0],
\]

where \( \beta(n) \) is defined in Equation (4.14). Thus it is possible to construct

\[
|\Psi(t)\rangle = c \sum_{j=1}^{f} |\Psi_j(t)\rangle,
\]

where \( |\Psi_j(t)\rangle \) is the coherent state

\[
|\Psi_j(t)\rangle \equiv \sum_{n=0}^{\infty} \left( \frac{2}{\gamma_j} \right)^{n(n-1)/4} \Phi^n_j(t) \hat{T}^{-1} [n00 \cdots 0],
\]

for which

\[
b_j |\Psi_j(t)\rangle = \Phi_j(t) |\Psi_j(t)\rangle
\]

and

\[
c = \left[ \sum_{n=0}^{\infty} \sum_{j=1}^{f} \left( \frac{\Phi_j(0)^2}{\beta(n)} \right)^n \right]^{-1/2}.
\]

Thus the Heisenberg operator equation

\[
i \frac{db_j}{dt} + (b_{j+1} + b_{j-1})(1 + \gamma \frac{b_j^2}{2} b_j) = 0,
\]

and Equation (5.21) imply that

\[
i \frac{d\Phi_j}{dt} + (\Phi_{j+1} + \Phi_{j-1})(1 + \frac{\gamma}{2} |\Phi_j|^2) = 0.
\]

From Equation (4.20) we see that the maximum group velocity is unbounded as \( n \to \infty \). This is consistent with the fact that Equation (5.24) supports moving solitons that do not become pinned as \( \gamma \) increases \[1\].

(iii) FP solitons

\[
\]

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Having arisen in the context of classical dynamics, the term “soliton” is essentially a classical concept, and a “quantum soliton” is often considered to be an object that becomes a classical soliton in the correspondence limit. For the fermionic polaron model, however, there is no correspondence limit because the number of fermions is at most equal to the number of freedoms. Nonetheless one can construct a wave function of the form of Equation (5.4), where \( n = 0, 1, 2, \ldots, f \). Since this wave packet shares many properties with Equation (5.4), and the FP equation can be analyzed using the quantum inverse scattering method \[20\], it is appropriate to call \(|\Psi(t)\rangle\) in Equation (5.4) a quantum soliton.

Since there is no correspondence limit for an FP soliton, it is not inappropriate to choose a particular value for \( n \) (say \( n_0 \)) for the sum in Equation (5.4). Thus \( a_n = \delta_{n,n_0} \), and for \( \gamma \gg 1 \) an approximate picture of our soliton (with velocity \( v \)) becomes

\[
\begin{align*}
[0000 \cdots 11 \cdots 1000 \cdots 0000]_{n_0} \\
v \rightarrow
\end{align*}
\]

However this diagram does not show uncertainties in position (\( j \)) and momentum (\( k \)), which are required by the Heisenberg principle and included in the structure of Equation (5.4). For \( n = n_0 \) this equation takes the form

\[
|\Psi_{n_0}(t)\rangle = \frac{1}{\sqrt{f}} \sum_{j=1}^{f} G_{n_0}(k)|\psi_{n_0}(k)\rangle \exp[-iE_{n_0}(k)t],
\]

where, from Equation (4.21),

\[
|\psi_{n_0}(k)\rangle \equiv \frac{1}{\sqrt{f}} \sum_{j=1}^{f} (e^{i\hat{T}})^{-1}[11 \cdots 100 \cdots 0],
\]

and, from Equation (4.23),

\[
E_{n_0}(k) \equiv -(n_0 - 1)\gamma - \frac{2}{\gamma_{n_0-1}} \cos k.
\]

Since \( G_{n_0}(k) \) is the probability amplitude for the FP soliton to have momentum \( k \), Equation (5.23) can be written as

\[
|\Psi_{n_0}(t)\rangle \equiv \frac{1}{\sqrt{f}} \sum_{j=1}^{f} F_{n_0}(j,t)\hat{T}^{-1}[11 \cdots 100 \cdots 0],
\]

where

\[
F_{n_0}(j,t) \equiv \sum_{k} G_{n_0}(k)\exp[i(k(j - 1) - E_{n_0}(k)t)].
\]

Thus uncertainties in position and momentum are related by Equation (5.6). If \( k \) lies within the range

\[
k = k_0 \pm \Delta k,
\]

then the soliton speed is in the range

\[
v = \pm \frac{\Delta v}{2} = \frac{2}{\gamma_{n_0-1}} \left[ \sin k \cos \frac{\Delta k}{2} \pm \cos k \sin \frac{\Delta k}{2} \right].
\]

Since wave functions of an FP soliton are dominated by components of the form

\[
[\cdots 00 11 \cdots 11 00 \cdots]\text{ times } n,
\]

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it becomes more extended as the number of fermions increases. For an infinite number of freedoms on the lattice, one could allow the number of fermions in Equation (5.4) to grow without bound, but the size of the soliton would also become infinite.

For \( n = f \), \( |\psi_f\rangle = [111 \ldots 1] \) with energy \( E_f = -\gamma f \), while for \( f = 0 \), \( |\psi_0\rangle = [000 \ldots 0] \) with energy \( E_0 = 0 \). In general the exact eigenfunctions for \( n = f - m \) will have the same structure as those for \( n = m \), but with the 1’s and 0’s interchanged. Thus for \( n = f - m \), where \( m = 0, 1, \ldots, f \), the corresponding energy will be

\[
E_{f-m}(k) = -\gamma(f - 2m) + E_m(k),
\]

(5.32)

where \( E_m(k) \) is the soliton energy band in the case \( n = m \).

6 Conclusions

The primary aim of this work is to make clear the concept of a quantum soliton by presenting several specific examples. Lattice solitons are of particular interest in this effort because it is possible—in certain cases—to examine details of the corresponding wave functions and to appreciate their complex character. The properties of quantum solitons are found to depend strongly upon the level of anharmonicity and the commutation relations that characterize the fundamental quanta.

The number state method of analysis, which has been somewhat obscured by the quantum inverse scattering method, is found to be a useful computational tool for such problems as well as a helpful theoretical perspective.

Whereas previous publications have concentrated on solving the quantum problem with only a few quanta using the number state method, we have shown that an approximate version of this method, valid in the limit of large nonlinearity, is also useful for larger values of \( n \). In particular, we have found general expressions for the binding energy, the effective mass and the maximum group velocity in this limit for arbitrary \( n > 1 \).

| model | \( E_b \) | \( m^* \) | \( V_m \) |
|-------|---------|---------|---------|
| QDNLS | \( \frac{1}{2} n(n-1)\gamma \) | \( \frac{(n-1)!\gamma^{n-1}}{2n} \) | \( \frac{2n}{(n-1)!\gamma^{n-1}} \) |
| QAL   | \( 2 \left( \frac{\gamma}{2} \right)^{(n-1)/2} \) | \( \frac{\gamma^{(n-1)/2}}{2n} \) | \( \frac{2\sin \left( \frac{\pi}{n} \right) \left( \frac{\gamma}{2} \right)^{(n-1)/2}}{\gamma^{n-1}} \) |
| FP    | \( (n-1)\gamma \) | \( \frac{\gamma^{n-1}}{2} \) | \( \frac{2}{\gamma^{n-1}} \) |

We note that the results for the group velocities confirm that the QDNLS and the FP solitons get pinned for large \( \gamma \) whereas this is not the case for QAL solitons, in agreement with the findings of classical soliton theory.

This method can also be applied to Hubbard models [18], which are of interest as theories of superconductivity and ferromagnetism. This application will be discussed elsewhere.

Finally we note that the band structures shown in Figure 1 may be somewhat misleading because they are for two fundamental quanta \( (n = 2) \). With \( n \geq 3 \), exploratory numerical and theoretical studies show that additional bands reside in the gap between the lowest (soliton) band and the principal continuum band. The significance of these bands will be the subject of future research.
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