

Lattice Formulation of the Non-Relativistic Scalar Field

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1. Motivation

The motivation behind this brief study is the wish to make well defined the notion of particle states at specified points. Thus, we wish to talk consistently about, say, a two-particle state which consists of one particle at position x and the other at position y . In a continuum formulation there is a difficulty with this because such states cannot be normalised. Consequently, we consider a lattice formulation to make the concept well defined. The price that is paid for this is that, in discrete space, it becomes mathematically inconsistent to also introduce a canonically conjugate momentum such that $[p, x] = i\hbar$ (at least, if we expect the momentum eigenvalues to be discrete, as explained in Part 4 of these QM Notes, QM4). So we shall avoid any mention of momentum in our discrete space formulation.

2. The Problem with Position States in the Continuum

In the continuum, creation and annihilation operators for momentum states can be defined, such that $a_{\vec{k}}^+|0\rangle = |\vec{k}\rangle$, and these momentum states are sensible, normalisable, states. Corresponding creation and annihilation operators for position states are defined by the Fourier transform: $a_{\vec{r},t} = \int_{-\infty}^{\infty} a_{\vec{k}} \exp\{i(\vec{k} \cdot \vec{r} - \omega t)\} \frac{d^3k}{\sqrt{2\omega}}$. The commutator between the momentum space operators, $[a_{\vec{k}}^+, a_{\vec{k}'}] = \delta^3(\vec{k} - \vec{k}')$, induces the following commutator between the configuration spacetime operators:

$$[a_{\vec{r},t}, a_{\vec{r}',t'}^+] = \int_{-\infty}^{\infty} a_{\vec{k}} \exp\{i(\vec{k} \cdot (\vec{r} - \vec{r}') - \omega(t - t'))\} \frac{d^3k}{2\omega} \quad (\text{QM14.1})$$

This is, of course, the usual propagator of a free scalar field (modulo conventional constant factors). The reason is that the field in quantum field theory is essentially synonymous with what we have called the configuration spacetime creation and annihilation operators. Specifically, $\phi(x) \equiv a_{\vec{r},t}^+ + a_{\vec{r},t}$. But (QM14.1) blows up when $x' = x$. This means that the position states, which we would define via $a_x^+|0\rangle = |x\rangle$ and $a_x|0\rangle = 0$ are not normalisable since $\langle x|x\rangle = \langle 0|a_x a_x^+|0\rangle = \langle 0|[a_x, a_x^+]0\rangle = \text{QM14.1} = \infty$. Admittedly we have used a relativistic formulation here, in which the position states are actually instantons (i.e. the particle exists only for an instant). But the same problem exists in the non-relativistic formulation.

In the continuum the usual way around this (other than avoiding the use of position based states, which is the most common strategy) is to make the position states 'fuzzy'. Thus the creation operator creates a Gaussian wavepacket state rather than a state of unique \vec{r} . Here, however, we will insist on an exact, point-like, state. So we are forced to consider a discrete lattice.

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3. Non-Relativistic Lattice Scalar Field

The Schrodinger equation for the energy eigenstates is,

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \Phi(\vec{r}) = -i\hbar \frac{\partial \Phi}{\partial t} \rightarrow E\Phi(\vec{r}) \quad (\text{QM14.2})$$

The Schrodinger equation can be derived from a Lagrangian density,

$$\mathcal{L} = i\hbar \psi^* \dot{\psi} - \frac{\hbar^2}{2m} \bar{\nabla} \psi^* \cdot \bar{\nabla} \psi - V(\vec{r}) \psi^* \psi \quad (\text{QM14.3})$$

The Hamiltonian turns out to be just (minus) the second pair of terms (integrated over all space),

$$\mathcal{H} = \int d^3r \left[\frac{\hbar^2}{2m} \bar{\nabla} \psi^* \cdot \bar{\nabla} \psi + V(\vec{r}) \psi^* \psi \right] \quad (\text{QM14.4})$$

(see Schiff §55 for the derivation). For simplicity we shall consider only the 1D case here. On a lattice this becomes,

$$\mathcal{H} = \sum_x \left[\frac{\hbar^2}{2m} \left(\frac{\psi^*(x+s) - \psi^*(x)}{s} \right) \left(\frac{\psi(x+s) - \psi(x)}{s} \right) + V(x) \psi^*(x) \psi(x) \right] \quad (\text{QM14.5})$$

where s is the lattice spacing. Strictly, of course, there is not a unique correspondence between the continuum and the lattice formulation. However, (QM14.5) is the simplest and most obvious which has (QM14.4) as the correct continuum limit.

The single particle Schrodinger equation is turned into a field theory by 'second quantisation', i.e. by replacing the field function by a field operator, which in turn is interpreted in terms of creation and annihilation operators,

$$\psi(x) \rightarrow a_j; \quad \psi^*(x) \rightarrow a_j^+; \quad \psi(x+s) \rightarrow a_{j+1}; \quad \psi^*(x+s) \rightarrow a_{j+1}^+ \quad (\text{QM14.6})$$

Hence, the lattice Hamiltonian is,

$$\hat{\mathcal{H}} = \sum_{j=0}^N \left[\frac{\hbar^2}{2m} \left(\frac{a_{j+1}^+ - a_j^+}{s} \right) \left(\frac{a_{j+1} - a_j}{s} \right) + V(j) a_j^+ a_j \right] \quad (\text{QM14.7})$$

where the lattice sites are labelled 1 to N corresponding to field degrees of freedom, and sites 0 and $N+1$ have specified boundary conditions. The Fock space of position states is such that $[a_i, a_j^+] = \delta_{ij}$ which leads to a single particle position state being defined as

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$|j\rangle \equiv a_j^\dagger |0\rangle$, where the notation $|j\rangle$ means a single particle occupying lattice site j . We also have $a_j |i\rangle = \delta_{ij} |0\rangle$.

A more general notation, in which there are n_1 particles occupying site 1, n_2 particles occupying site 2, etc, is $|n_1, n_2, \dots\rangle$. In this latter notation the n_1, n_2 , etc represent the numbers of particles, and all the lattice sites are listed in order. Hence this notation is a field notation. In this field notation, the objects whose states are being specified are the lattice sites, and their states are labelled by the occupation number at that site. This contrasts with the first ('particle') notation, in which the objects whose states are being specified are the particles, and their states are labelled by the lattice site which they occupy. In the field notation, the creation and annihilation operators act in general as follows,

$$a_j |n_1, n_2, \dots, n_j, \dots\rangle = \sqrt{n_j} |n_1, n_2, \dots, (n_j - 1), \dots\rangle \quad (\text{QM14.8a})$$

$$a_j^\dagger |n_1, n_2, \dots, n_j, \dots\rangle = \sqrt{n_j + 1} |n_1, n_2, \dots, (n_j + 1), \dots\rangle \quad (\text{QM14.8b})$$

Note that this field notation has assumed that the particles must be identical, since the notation does not distinguish which particle is where. Moreover, if any of the n_i are > 1 then the particles must be bosons.

In the particle notation, a state of two identical bosons is written,

$$|2 \text{ bosons}\rangle = \frac{1}{\sqrt{2}} [|i\rangle |j\rangle + |j\rangle |i\rangle] \quad (\text{QM14.9})$$

where the first state represents the first particle, and the second state represents the second particle. Symmetrisation of the state under particle interchange is essential for a bosonic state. Hence the correspondence between the two notations, for a 2-particle state, is,

$$|2 \text{ bosons}\rangle = \frac{1}{\sqrt{2}} [|i\rangle |j\rangle + |j\rangle |i\rangle] \equiv |0, 0, \dots, 1, 0, \dots, 1, 0, \dots, 0\rangle \equiv |i, j\rangle \quad (\text{QM14.10})$$

where the non-zero entries in the field state occur in the i^{th} and j^{th} sites.

We have introduced an obvious compact notation for the 2-particle field state. In this field notation the states are automatically symmetrised, in that $|i, j\rangle \equiv |j, i\rangle$, where i and j are the occupied sites. If there is any potential confusion as to whether we are referring to a 'particle' or a 'field' state, the subscripts $_p$ and $_f$ will be used. In the case $i = j$ the two particles are in the same state and the field notation can be written, $|0, 0, \dots, 2, 0, \dots, 0\rangle \equiv |2i\rangle_f$, which equals $|i\rangle_p |i\rangle_p$.

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Similarly,

$$\begin{aligned} |3 \text{ bosons}\rangle &= \frac{1}{\sqrt{6}} \left[|i\rangle|j\rangle|k\rangle + |j\rangle|i\rangle|k\rangle + |i\rangle|k\rangle|j\rangle + |k\rangle|i\rangle|j\rangle + |j\rangle|k\rangle|i\rangle + |k\rangle|j\rangle|i\rangle \right] \\ &\equiv |0,0,\dots,1,0,\dots,1,0,\dots,1,0,\dots,0\rangle \equiv |i, j, k\rangle \end{aligned} \tag{QM14.11}$$

where the non-zero entries in the field state occur in the i^{th} , j^{th} and k^{th} sites. Again we have re-written the field state in a more compact and transparent manner. Again the field state is already fully symmetrised, in that $|i, j, k\rangle$ means the same thing regardless of the order of i, j, k . If particles occupy the same site then the notation becomes, for example, $|0,0,\dots,2,0,\dots,1,0,\dots,0\rangle \equiv |2i, j\rangle_f \equiv \frac{1}{\sqrt{3}} \left[|i\rangle_p |i\rangle_p |j\rangle_p + |i\rangle_p |j\rangle_p |i\rangle_p + |j\rangle_p |i\rangle_p |i\rangle_p \right]$, etc.

The reason that we have laboured these notational issues so much is because of potential confusion over the requirement to symmetrise the state. For 'particle' states, symmetrisation is required for identical particles. For 'field' states, explicit symmetrisation is *not* required – contrast the LHS and RHS of (QM14.11). For the field states symmetrisation is already implicit in that $|i, j, k\rangle \equiv |i, k, j\rangle$, etc.. Note that, whereas the particles are indistinguishable, the lattice sites are distinguishable. But in the field notation, only the number of particles at each site is stated. Since we do not state which particle is at which site, the particles are implicitly indistinguishable.

4. One-Particle Energy Eigenstates of the Lattice Scalar Field

We seek solutions to $\hat{H}|\psi\rangle = E|\psi\rangle$, where \hat{H} is given by (QM14.7) and the states are one-particle states, which may be written in 'particle' or 'field' notation (which become identical for a single particle). The one particle energy eigenstate can therefore be written,

$$|\psi\rangle = \sum_{i=1}^N A_i |i\rangle \tag{QM14.12}$$

We assume that the field vanishes at $j = 0$ and $j = N+1$. We have,

$$(a_{j+1}^+ - a_j^+)(a_{j+1} - a_j)|j\rangle = -|j+1\rangle + |j\rangle \text{ and } (a_{j+1}^+ - a_j^+)(a_{j+1} - a_j)|j+1\rangle = |j+1\rangle - |j\rangle \tag{QM14.12b}$$

but the action of this operator on all other states gives zero. Hence, we find,

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(QM14.13)

$$\begin{aligned}
 \hat{H}|\psi\rangle &= \sum_{j=0}^N \left[\frac{\hbar^2}{2m} \left(\frac{a_{j+1}^+ - a_j^+}{s} \right) \left(\frac{a_{j+1} - a_j}{s} \right) + V(j)a_j^+ a_j \right] \sum_{i=1}^N A_i |i\rangle \\
 &= \sum_{j=0}^N \left[\frac{\hbar^2}{2ms^2} \{A_j(-|j+1\rangle + |j\rangle) + A_{j+1}(|j+1\rangle - |j\rangle)\} + V(j)A_j |j\rangle \right] \\
 &= \sum_{j=0}^N \left[\frac{\hbar^2}{2ms^2} \{A_j(-|j+1\rangle + |j\rangle)\} + V(j)A_j |j\rangle \right] + \sum_{j=1}^N \left[\frac{\hbar^2}{2ms^2} \{A_j(|j\rangle - |j-1\rangle)\} \right] \\
 &= \sum_{j=1}^N \left[\frac{\hbar^2}{2ms^2} \{(-|j+1\rangle + 2|j\rangle - |j-1\rangle)\} + V(j)|j\rangle \right] A_j \\
 &= \sum_{j=1}^N \left[\frac{\hbar^2}{2ms^2} \{(-A_{j-1} + 2A_j - A_{j+1})\} + A_j V(j) \right] |j\rangle
 \end{aligned}$$

(where $A_0 = 0$). But this must equal $E \sum_{j=1}^N A_j |j\rangle$ for an energy eigenstate, and so the eigenvalue condition becomes,

$$EA_j = \frac{\hbar^2}{2ms^2} \{(-A_{j-1} + 2A_j - A_{j+1})\} + A_j V(j) \quad (\text{QM14.14})$$

(QM14.14) defines the matrix,

$$(\mathbf{H}) = \frac{\hbar^2}{2ms^2} \begin{pmatrix} 2 + v_1 & -1 & 0 & 0 \\ -1 & 2 + v_2 & -1 & 0 \\ 0 & -1 & 2 + v_3 & -1 \\ 0 & 0 & -1 & \text{etc.} \end{pmatrix} \quad (\text{QM14.15})$$

where, $\frac{\hbar^2 v_1}{2ms^2} = V(1)$, etc. The energy eigenvalues and eigenvectors are thus given by,

$$(\mathbf{H})\bar{A} = E\bar{A} \quad (\text{QM14.16})$$

Since we have imposed the condition that the wavefunction vanish on the boundaries ($j = 0$ and $j = N+1$), when the potential is zero we should regain the usual particle-in-a-box energy levels in the continuum limit of large N . This has been investigated (using MATLAB) as follows:-

We set the box side to unity, in which case the continuum energy levels are

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m}. \text{ Normalising by } \frac{\hbar^2}{2m} \text{ we express energies in the form } \tilde{E}_n = \frac{2mE_n}{\hbar^2} = n^2 \pi^2.$$

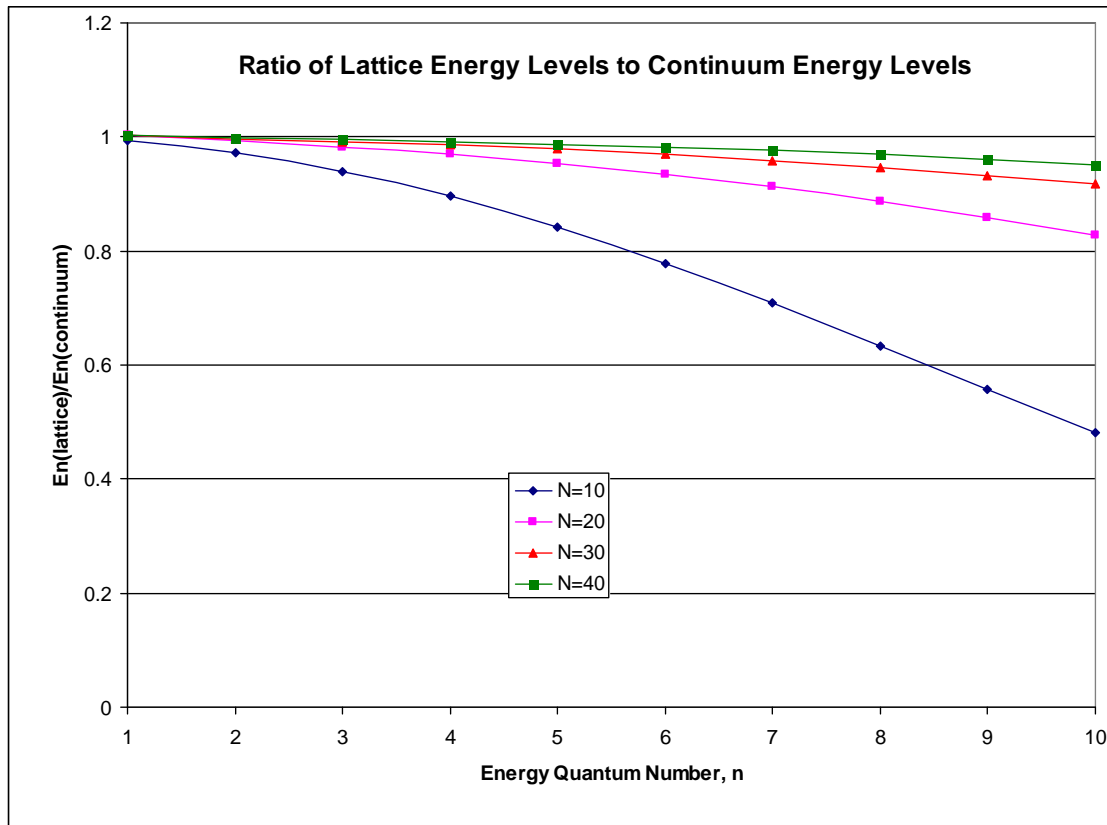
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The coefficient in front of the matrix in (QM14.15) thus becomes just $1/s^2 = (N+1)^2$.

The corresponding eigenvectors are $\sin\left(\frac{n\pi x}{L}\right)$, so that, $A_j \propto \sin\left(\frac{n\pi j}{(N+1)}\right)$, the latter becoming exact in the limit $N \rightarrow \infty$. The results are illustrated as follows:-

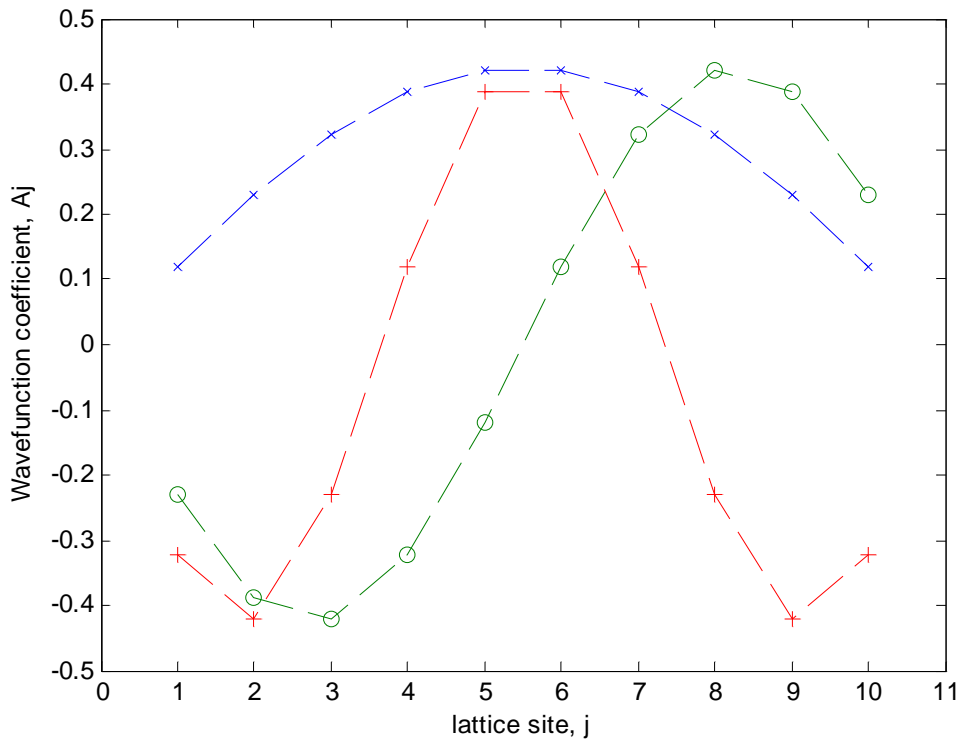
First 10 Energy Levels: Lattices With Various N and Continuum Compared

Mode	N=10	N=20	N=30	N=40	Exact (continuum)
1	9.8027	9.9	9.9	9.9	9.869604
2	38.4166	39.2	39.3	39.4	39.47842
3	83.5237	87.3	88.1	88.4	88.82644
4	141.4696	153.3	155.8	156.7	157.9137
5	207.5598	235.4	241.5	243.7	246.7401
6	276.4402	332.1	344.5	349.1	355.3058
7	342.5304	441	463.7	472.1	483.6106
8	400.4763	559.8	597.8	612.1	631.6547
9	445.5834	685.7	745.5	768.3	799.438
10	474.1973	816.1	905.3	939.6	986.9604

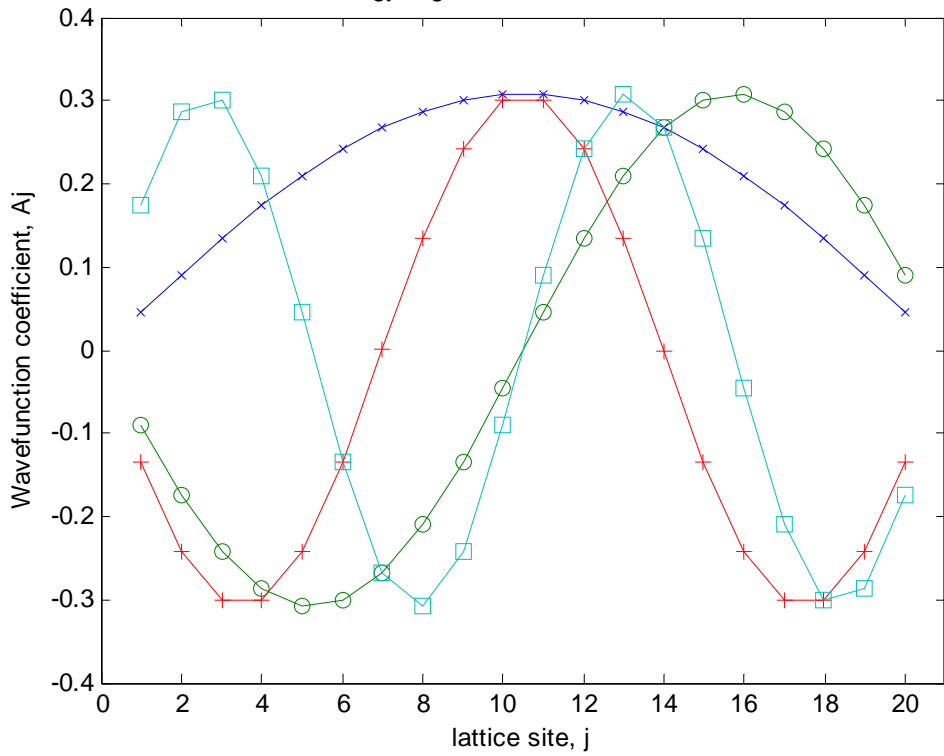


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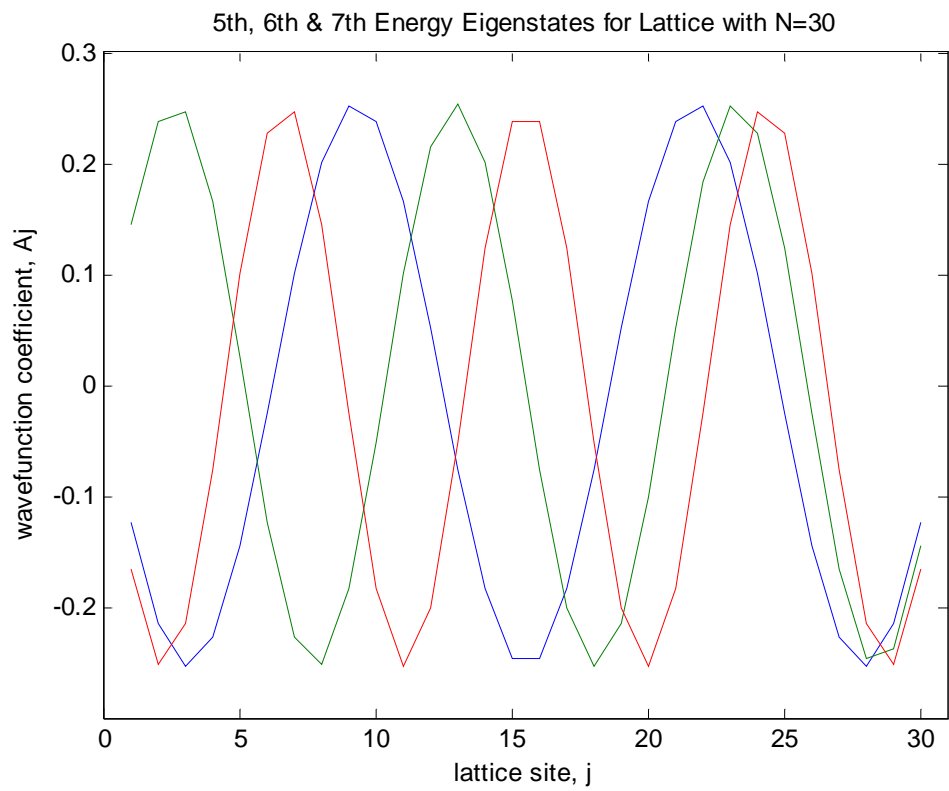
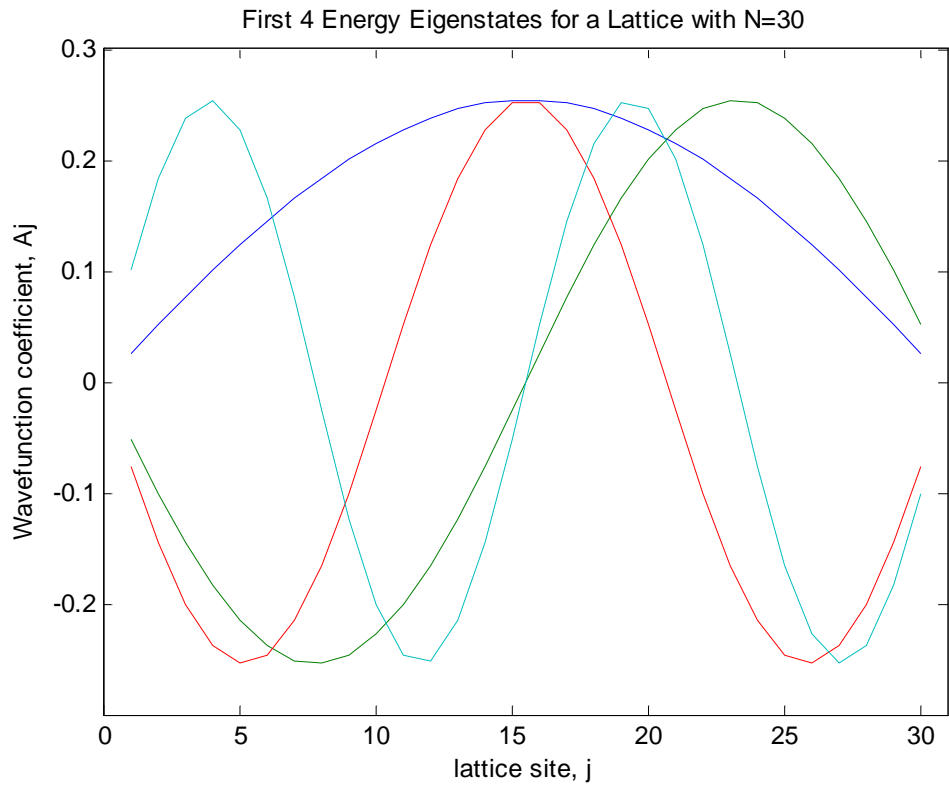
First 3 Energy Eigenstates for a Lattice with
N=10



First 4 Energy Eigenstates for a Lattice with N=20



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Hence, the lattice approximation is not bad for the lowest lying energy states even for $N=10$, and rapidly improves as N is increased.

5. Multi-Particle Energy Eigenstates of the Lattice Scalar Field

Because we are dealing with non-interacting particles, it is reasonable to suppose that the energy states of N_p particles comprise simply of all the possible direct products of one particle energy eigenstates. Write the one particle energy eigenstates as,

$$|\phi_n^1\rangle = \sum_{i=1}^N A_{ni} |i\rangle \quad (\text{QM14.17})$$

where n is the energy quantum number (and N is the number of lattice sites). The state of three bosons, for example, in states with energy quantum numbers n, m, q , is,

$$|\phi_{nmq}^3\rangle = \frac{1}{\sqrt{6}} \left[|\phi_n^1\rangle |\phi_m^1\rangle |\phi_q^1\rangle + |\phi_m^1\rangle |\phi_n^1\rangle |\phi_q^1\rangle + |\phi_n^1\rangle |\phi_q^1\rangle |\phi_m^1\rangle + |\phi_q^1\rangle |\phi_n^1\rangle |\phi_m^1\rangle + |\phi_m^1\rangle |\phi_q^1\rangle |\phi_n^1\rangle + |\phi_q^1\rangle |\phi_m^1\rangle |\phi_n^1\rangle \right] \quad (\text{QM14.18})$$

where each of the six terms is of the form,

$$|\phi_n^1\rangle |\phi_m^1\rangle |\phi_q^1\rangle = \sum_{i,j,k=1}^N A_{ni} A_{mj} A_{qk} |i\rangle |j\rangle |k\rangle \quad (\text{QM14.19})$$

Each of the six terms is obtained by permuting the order of the three states on the RHS of (QM14.19). Hence, we can write the symmetrised state, (QM14.18), more simply in terms of the 'field' state, (QM14.11), than the 'particle' states. This gives simply,

$$|\phi_{nmq}^3\rangle = \sum_{i,j,k=1}^N A_{ni} A_{mj} A_{qk} |i, j, k\rangle \quad (\text{QM14.20})$$

The extension to N_p particles is obvious. Recall that N is the number of lattice sites and is not to be confused with the number of particles, N_p . Note that in (QM14.20) the same state occurs several times in the sum, since $|i, j, k\rangle \equiv |i, k, j\rangle \equiv |k, i, j\rangle$, etc. Hence, it is implicit in (QM14.20) that the product of A-terms is symmetrised. For example, the coefficient of the state $|1,2,3\rangle$ is,

$$[A_{n1} A_{m2} A_{q3}] = A_{n1} A_{m2} A_{q3} + A_{n1} A_{m3} A_{q2} + A_{n2} A_{m1} A_{q3} + A_{n2} A_{m3} A_{q1} + A_{n3} A_{m2} A_{q1} + A_{n3} A_{m1} A_{q2} \quad (\text{QM14.21})$$

Where the square-bracket notation denotes the symmetrisation indicated by (QM14.21). Note that no factor of $1/\sqrt{6}$ appears in (QM14.21) since this factor has been absorbed in the definition of the $|i, j, k\rangle$ states, which are normalised. Hence (QM14.20) may be re-written as,

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$$|\phi_{nmq}^3\rangle = \sum_{\substack{i=1 \\ j \geq i \\ k \geq j}}^N [A_{ni} A_{mj} A_{qk}] |i, j, k\rangle \quad (\text{QM14.22})$$

6. Entanglement of States in the Particle and Field Bases

We may make the following observations regarding the entanglement of multi-particle states,

- [1] There is particle-particle entanglement in any multi-particle pure energy eigenstate, *except* if all the particles are in the same energy state;
- [2] Particle-particle entanglement clearly does not arise for a single particle state, since a single particle state has no product structure in the particle basis.
- [3] There is site-site entanglement in any multi-particle pure energy eigenstate *including* the case that all the particles are in the same energy state.
- [4] There is also site-site entanglement in any pure energy eigenstate of a single particle.

The first of these observations follows simply from symmetrisation in the particle basis, like Equ.(QM14.18). This ensures entanglement except when $n=m=q$, i.e. the particles are all in the same energy state.

To understand site-site entanglement we must recall that the field basis is really a product representation for every site. For example, the state of a single particle in the field basis is,

$$|1 \text{ bosons}\rangle = |0,0,..1,0...0\rangle \equiv |i\rangle \quad (\text{QM14.23})$$

This is actually a product state for all the lattice sites, which written explicitly is,

$$|0,0,..1,0...0\rangle \equiv |0\rangle|0\rangle...|1\rangle|0\rangle...|0\rangle \quad (\text{QM14.24})$$

where it is understood that the first ket refers to lattice site 1, the second ket to lattice site 2, etc. Suppose we wish to investigate the entanglement between the I^{th} and J^{th} sites for the single particle energy eigenstate,

$$|\phi_n^1\rangle = \sum_{i=1}^N A_{ni} |i\rangle \quad (\text{QM14.17})$$

With this in mind we can identify separately the site-basis states,

$$|site - I\rangle = |1\rangle_I |0\rangle_J |0\rangle_{\text{othersites}} \quad (\text{QM14.25a})$$

$$|site - J\rangle = |0\rangle_I |1\rangle_J |0\rangle_{\text{othersites}} \quad (\text{QM14.25b})$$

$$|\text{othersites}\rangle = |0\rangle_I |0\rangle_J |1\rangle_{\text{othersites}} \quad (\text{QM14.25c})$$

(QM15.25a) is the state of the particle being at site I, and hence not at the other sites.

(QM15.25b) is the state of the particle being at site J, and hence not at the other sites.

(QM15.25c) is the state of the particle being at neither site I nor site J, and hence at one

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of the other sites.

The energy eigenstate is thus,

$$|\phi_n^1\rangle = A_{nI} |1\rangle_I |0\rangle_J |0\rangle_{\text{othersites}} + A_{nJ} |0\rangle_I |1\rangle_J |0\rangle_{\text{othersites}} + |0\rangle_I |0\rangle_J \sum_{\substack{i \neq I \\ i \neq J}}^N A_{ni} |i\rangle \quad (\text{QM14.26})$$

This displays explicitly the entanglement between the Ith and Jth sites. To evaluate the degree of entanglement would require the 'other' sites to be traced out. This is treated in detailed in another Note.

Since a single particle has entangled sites, it is clear that multi-particle states will also have entangled sites. The difference is that there is a greater number of contributing product states, even after tracing out the 'other' sites. These are: two particles at site I and none at site J; two particles at site J and none at site I; one particle at each of sites I and J; one particle at site I but none at site J; one particle at site J but none at site I; and finally, no particle at either of sites I and J. Thus, the two particle case has 6 possible product states, compared with just 3 for the single particle. This will be developed further in another Note.

7. Extremely High Particle Number Density

We note that the assumption that energy eigenstates are direct products of one particle states is not strictly correct. This is because it is not quite true that the particles do not interact. The Hamiltonian, (QM14.7), imposes an interaction between nearest and next-nearest neighbour sites, and also for particles on the same site. If two particles in a multi-particle state are coincident, adjacent, or separated by only one lattice site, then (QM14.12b) no longer holds for each particle separately. For example, if the two particles occupy the same site we get,

$$(a_{j+1}^+ - a_j^+) (a_{j+1} - a_j) |2j\rangle_f = -\sqrt{2} |j, j+1\rangle_f + 2 |2j\rangle_f \quad (\text{QM14.27a})$$

and,
$$(a_{j+1}^+ - a_j^+) (a_{j+1} - a_j) |2(j+1)\rangle_f = 2 |2(j+1)\rangle_f - \sqrt{2} |j, j+1\rangle_f \quad (\text{QM14.27b})$$

Similarly, an effective interaction occurs between nearest and next-nearest neighbour sites. We may surmise that this is the origin of the pathology in the continuum formulation as $x' \rightarrow x$.

However, we can safely ignore this complication in normal situations. The reason is that we are free to make the number of lattice sites, N, as large as we wish. Provided that we choose $N \gg N_p$, then the probability that two particles will be close enough to interact can be made arbitrarily small. Presumably the ultimate physical limit is the Planck scale. But the Planck length is so tiny that this does not detract from this perspective for most situations. Hence, multi-particle energy states of the form (QM14.20) can be safely adopted.

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One may speculate, however, that at the big crunch, when particle number densities become comparable with unity on a Planck length scale, that such effects may become dominant. What effect do terms like (QM14.27) have on the contraction of the universe? Could they cause a bounce, as is claimed for loop quantum cosmology?

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