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QUANTUM LATTICE GASES AND THEIR INVARIANTS

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ABSTRACT

The one particle sector of the simplest one dimensional quantum lattice gas automaton has been observed to simulate both the (relativistic) Dirac and (nonrelativistic) Schrödinger equations, in different continuum limits. By analyzing the discrete analogues of plane waves in this sector we find conserved quantities corresponding to energy and momentum. We show that the Klein paradox obtains so that in some regimes the model must be considered to be relativistic and the negative energy modes interpreted as positive energy modes of antiparticles. With a formally similar approach—the Bethe *ansatz*—we find the evolution eigenfunctions in the *two* particle sector of the quantum lattice gas automaton and conclude by discussing consequences of these calculations and their extension to more particles, additional velocities, and higher dimensions.

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1. Introduction

The recent interest in quantum lattice gas automata (QLGA) is at least partly stimulated by the prospect of quantum computation. Quantum computers are (as yet hypothetical) physical systems designed and programmed to take advantage of the quantum mechanical phenomena of superposition and interference in order to perform calculations more efficiently than is possible with a classical computer [1]. As the size of semiconductor devices decreases, useful quantum coherence first seems possible at the nanoscale [2] where the most plausible computer architecture is that of a cellular automaton [3]. Thus it is natural to consider quantum computation with lattice gas automata (LGA).

Just as classical LGA are more efficiently deployed to simulate physical processes like diffusion and fluid flow than for universal computation [4], it seems likely that, as anticipated already by Feynman [5], the first useful quantum computation will be a QLGA simulation of some quantum mechanical process. Thus it is important to understand the physics of QLGA: their symmetries, their conserved quantities, and their macroscopic/continuum limits.

In the next section we begin by reviewing the one particle sector of the simplest QLGA in one dimension. Determining the discrete analogue of plane waves, we find a complete set of invariants. These conserved quantities bear interpretation as energy and momentum, and enable the exact computation of the evolution.

This model has been observed to simulate both the (nonrelativistic) Schrödinger equation [6,7] and the (relativistic) Dirac equation [8,9,10]. Although perhaps surprising at first, this is not inconsistent as the Dirac equation is well known to have a nonrelativistic limit [11] and, as Benzi and Succi have emphasized, numerical evolution of parabolic equations can be stabilized and localized by the use of artificially hyperbolic equations [6]. In Section 3 we use the physical interpretation of the conserved quantities in the model to distinguish relativistic and nonrelativistic regimes of the QLGA. Specifically, we show that the Klein paradox obtains [12]: a sufficiently discontinuous geometry/potential precludes interpretation of the QLGA as simulating a single nonrelativistic particle, compelling recognition of antiparticles in the model as well.

In Section 4 we extend the one particle model to a multiparticle QLGA. Introduction of all the two particle and antiparticle scattering amplitudes makes the QLGA formally (almost) equivalent to the six vertex model [13]. The exact solvability of the six vertex model leads us to expect a *computable* complete set of invariants for the multiparticle QLGA. Concentrating on the two particle sector of the model, we find these invariants explicitly and explain their physical meaning.

In Section 5 we conclude with a brief discussion of our results and their extension to more particles, additional velocities, and higher dimensions.

2. The one particle sector

A LGA should be envisioned as a collection of particles moving synchronously from vertex to vertex on a fixed graph (lattice) L: At the beginning of each timestep each particle is located at some vertex and is labelled with a 'velocity' indicating along which edge incident to that vertex it will move during the 'advection' half of the timestep. After moving along the designated edge to the next vertex, in the 'scattering' half of the timestep the particles at each vertex interact according to some rule which assigns new 'velocity' labels to each. Here we will consider only the one dimensional lattice isomorphic to the integer lattice $\mathbb{Z}$.

A QLGA is a LGA for which the time evolution is unitary. To make this precise we must first identify the Hilbert space of the theory. An orthonormal basis for the one particle sector H_1 of the Hilbert space H of the one dimensional QLGA is given by $\{|x,\alpha\rangle\}$ (in the standard Dirac notation [14]), where $x \in L$ denotes position and $\alpha \in \{\pm 1\}$ denotes 'velocity'. At each time the state of the QLGA is described by a *state vector* in H_1:

$$\Psi(t) = \sum_{x,\alpha} \psi_\alpha(t,x)|x,\alpha\rangle,$$

where the *amplitudes* $\psi_\alpha(t,x) \in \mathbb{C}$ and the norm of $\Psi(t)$, as measured by the inner product on H, is:

$$1 = \sum_{x,\alpha} \overline{\psi_\alpha(t,x)}\psi_\alpha(t,x). \tag{2.1}$$

The state vector evolves unitarily, *i.e.*, $\Psi(t+1) = U\Psi(t)$, where U is a unitary operator on H. Since the evolution is unitary, the inner product is preserved and (2.1) holds for all times if it holds for one; this allows the interpretation of $\overline{\psi_\alpha(t,x)}\psi_\alpha(t,x)$ as the *probability* that the particle be in the state $|x,\alpha\rangle$ at time t [14,15]. The total probability is the most fundamental conserved quantity of a QLGA.

The 'advection' followed by 'scattering' evolution of the quantum particle is implemented by having the basis vectors evolve as

$$U|x,\alpha\rangle = a|x+\alpha,\alpha\rangle + b|x+\alpha,-\alpha\rangle. \tag{2.2}$$

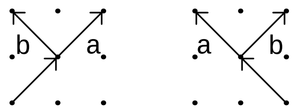

Figure 1. Spacetime diagrams of the one particle scattering amplitudes. Time runs upward.

That is, an initially right (left) moving quantum particle moves one lattice point to the right (left) and then continues in the same direction with amplitude a or changes direction with amplitude b as shown in Figure 1. We showed in [10] that the most general unitary evolution for a one dimensional QLGA with parity invariance* and particle speed 1 is described in the one particle sector by a unitary *scattering matrix*

$$S := \begin{pmatrix} b & a \\ a & b \end{pmatrix}. \tag{2.3}$$

* *I.e.*, invariance under $x \to -x$; also called *reflection* invariance.

S may be parameterized by $a = \cos\theta$, $b = i\sin\theta$. The model is then equivalent to Feynman's path integral for a Dirac particle of mass θ [8], but one might ask for the origin of the evolution rule (2.2) and (2.3)—from what does the particle scatter? One answer to this question will emerge at the end of the next section.

It is convenient to introduce the parity transformed scattering matrix $\check{S} := PS$, where

$$P := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Then (2.2) becomes

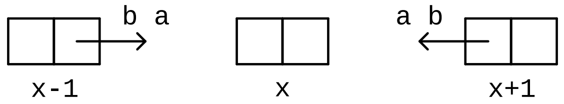

Figure 2. Schematic diagram of a subspace of H_1. Each box represents one dimension of the Hilbert space. The arrows indicate the amplitude flow into the two components at x; the labels a and b are the multiplicative factors to the corresponding boxes.

$$U|x,\alpha\rangle = \sum_{\alpha'} \check{S}_{\alpha'\alpha}|x+\alpha,\alpha'\rangle. \tag{2.4}$$

This is equivalent to a condition on the amplitudes:

$$U\psi_{\alpha'}(x) = \sum_{\alpha} \check{S}_{\alpha'\alpha}\psi_\alpha(x-\alpha), \tag{2.5}$$

where the time argument is omitted. Figure 2 illustrates the amplitude flow in H_1 described by (2.5). The discrete analogues of *plane waves* are *wave functions* $\psi_\alpha : L \to \mathbb{C}$ which evolve by phase multiplication. Since U is unitary, these are exactly its eigenvectors; they evolve by multiplication by the corresponding norm 1 eigenvalues $e^{-i\omega}$. For plane waves, therefore, (2.5) becomes

$$e^{-i\omega}\psi_{\alpha'}(x) = \sum_{\alpha} \check{S}_{\alpha'\alpha}\psi_\alpha(x-\alpha). \tag{2.6}$$

Solving an equation like (2.6) is a problem we will face three times in this paper. In each case we proceed the same way, by making an appropriate *ansatz* for the form of a solution and then constraining the parameters in the *ansatz* by imposing additional (matching) conditions.

As we explain in some detail in [16] for a QLGA which generalizes the one defined by (2.2) and (2.3), the appropriate *ansatz* for (2.6) is

$$\psi_\alpha^{(k)}(x-\alpha) = e^{-i\alpha k}\psi_\alpha^{(k)}(x), \tag{2.7}$$

just as we would expect for a plane wave. Plugging (2.7) into (2.6) gives

$$e^{-i\omega}\psi_{\alpha'}(x) = \sum_{\alpha} \check{S}_{\alpha'\alpha}e^{-i\alpha k}\psi_\alpha(x). \tag{2.8}$$

As the notation suggests, the $\psi_\alpha(x)$ are the components of a vector $\psi(x) \in \mathbb{C}^2$ (in this notation the state vector is $\Psi = \sum_x \psi(x)|x\rangle$); thus (2.8) can be rewritten as an eigenvalue problem:

$$e^{-i\omega}\psi^{(k)}(x) = D(k)\psi^{(k)}(x),$$

where

$$D(k) := \begin{pmatrix} ae^{ik} & be^{-ik} \\ be^{ik} & ae^{-ik} \end{pmatrix}$$

is unitary since S is. $D(k)$ summarizes the amplitude flow into the central pair of blocks in Figure 2.

The characteristic equation for $D(k)$ is the *dispersion relation*:

$$\cos\omega = \cos\theta\cos k. \tag{2.9}$$

For pairs (ω, k) satisfying the dispersion relation, the plane wave *ansatz* satisfies (2.6). The dispersion relation (2.9) has two solutions $\pm\omega_k$ for each k, as shown in Figure 3. The eigenvalues $e^{\mp i\omega_k}$ have eigenvectors

$$\psi^{(k,\pm)}(0) := \begin{pmatrix} -be^{-ik} \\ ae^{ik} - e^{\mp i\omega_k} \end{pmatrix}. \tag{2.10}$$

The plane wave solutions to (2.6) are thus

$$\psi^{(k,\pm)}(x) = e^{ikx}\psi^{(k,\pm)}(0), \tag{2.11}$$

where for positive ω_k, positive (negative) k gives a right (left) moving plane wave. That the wave functions (2.11) are the discrete analogues of continuum plane waves is visible in Figures 4 and 5 which show, respectively, the evolution of right moving $k = \pi/16$ and $k = \pi/8$ plane waves for $0 \le x \le 31$.

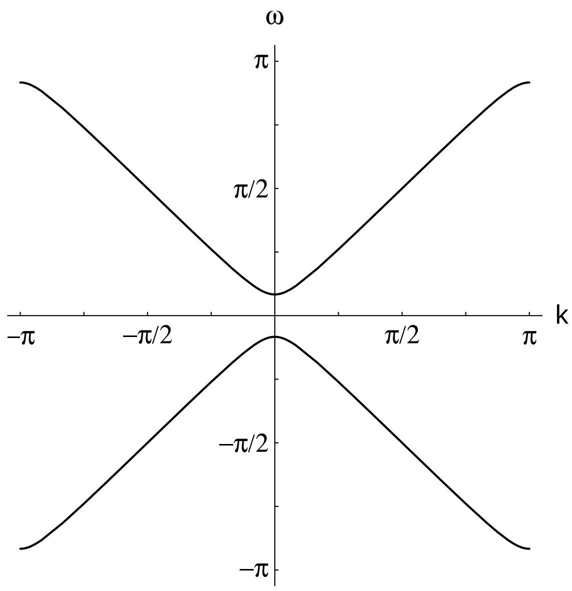

Figure 3. The dispersion relation for $\theta = \pi/12$. There are two branches and a frequency gap between θ and $-\theta$.

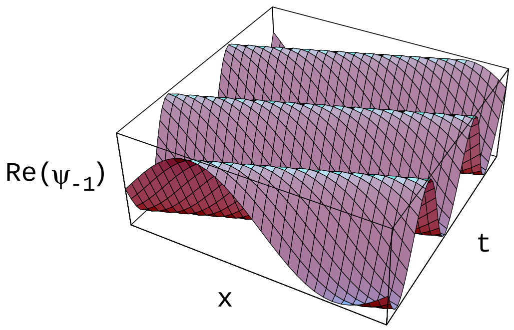

Figure 4. Evolution of the $k = \pi/16$ right moving plane wave for the interval $0 \le x \le 31$ when $\theta = \pi/12$.

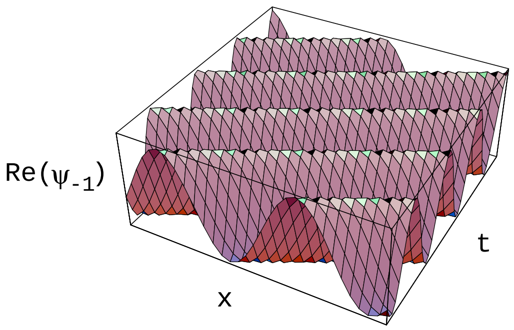

Figure 5. The same simulation for the $k = \pi/8$ right moving plane wave. This wave has a higher frequency.

Just as in the continuum situation, therefore, ω and k bear interpretation as being proportional to energy and momentum, respectively [16]. Furthermore, they label a complete set of conserved quantities in terms of which the evolution can be exactly computed: Let

$$|k,\epsilon\rangle := \sum_x \psi^{(k,\epsilon)}(0)e^{ikx}|x\rangle$$

denote the plane wave state vectors in H_1. Then (dealing with normalization in the usual way [8]) the set $\{|k,\epsilon\rangle\}$ is an orthonormal basis for H_1 [16]. Consider any state vector $\Psi \in H_1$:

$$\begin{aligned}
\Psi &= \sum_x \psi(x)|x\rangle \\
&= \sum_x \psi(x) \sum_{k,\epsilon} |k,\epsilon\rangle\langle k,\epsilon|x\rangle \\
&= \sum_{k,\epsilon} \Big(\sum_x \langle k,\epsilon|x\rangle\psi(x)\Big)|k,\epsilon\rangle
\end{aligned}$$

The parenthesized expression gives the components in the new $|k,\epsilon\rangle$ basis:

$$\begin{aligned}
\hat{\psi}_\epsilon(k) &:= \sum_x \langle k,\epsilon|x\rangle\psi(x) \\
&= \sum_x \Big(\sum_y \psi^{(k,\epsilon)}(0)e^{iky}|y\rangle\Big)^\dagger |x\rangle\psi(x) \\
&= \big(\psi^{(k,\epsilon)}(0)\big)^\dagger \sum_x \psi(x)e^{-ikx} \\
&=: \big(\psi^{(k,\epsilon)}(0)\big)^\dagger \hat{\psi}(k),
\end{aligned}$$

where $\hat{\psi}(k)$ is the *discrete Fourier transform* of $\psi(x)$. The plane waves $|k,\epsilon\rangle$ evolve by phase multiplication so the probabilities $\overline{\hat{\psi}_\epsilon(k)}\hat{\psi}_\epsilon(k)$ are left invariant by the evolution. Since any initial state vector $\Psi(0)$ can be expressed in the plane wave basis this way, the existence of these conserved quantities is equivalent to exact solvability for the one particle sector of the QLGA.

There is, however, a familiar problem with the physical interpretation of these conserved quantities. We have identified ω as being proportional to energy, so for each k there are plane waves with either positive or negative energy. We could restrict our state vectors to have nonzero amplitudes only in the directions $|k,+\rangle$, *i.e.*, not allow any negative energy states; the conservation laws would preserve this condition. This would, however, preclude highly localized states: $\Psi = |x_0,+1\rangle$, to take an extreme example, has nonzero amplitudes in *all* the negative energy directions $|k,-\rangle$. Furthermore, introducing any interaction into the model risks disturbing this symmetry and allowing the system access to the (apparently) unphysical negative energy states. In the next section we will see exactly how this can happen and how we should reinterpret the model as a consequence.

3. The Klein paradox

A single electron moving ballistically in a nanoscale semiconducting device is a conceivable implementation of a QLGA. Alternatively, simulation of such a physical situation is a possible application of a QLGA implemented in some other way. In either case, inhomogeneous potentials must be included in the model. As explained in [17,8,7,16], modifying the evolution rule by an inhomogeneous phase factor has the desired effect. For a time independent potential, (2.5) is modified as

$$U\psi_{\alpha'}(x) = \sum_{\alpha} \check{S}_{\alpha'\alpha} e^{-i\phi(x-\alpha)} \psi_\alpha(x-\alpha), \tag{3.1}$$

where $\phi(x)$ is the potential.

Consider a simple potential step:

$$\phi(x) = \begin{cases} 0 & \text{if } x \leq 0; \\ \phi & \text{if } x > 0, \end{cases} \tag{3.2}$$

and let us study right moving plane waves scattering off the step. Using (3.1), the equation analogous to (2.6) is

$$e^{-i\omega}\psi_{\alpha'}(x) = \sum_{\alpha} \check{S}_{\alpha'\alpha} e^{-i\phi(x-\alpha)} \psi_\alpha(x-\alpha). \tag{3.3}$$

For $x < 0$, inserting the potential (3.2) into (3.3) gives exactly equation (2.6). With an incident right moving plane wave we expect a reflected left moving plane wave, so an appropriate *ansatz* is

$$\psi^{(\omega)}(x) = \psi^{(k,+)}(x) + A\psi^{(-k,+)}(x) \qquad \text{if} \quad x \leq 0, \tag{3.4}$$

where $(\omega, \pm k)$ satisfy the dispersion relation (2.9).

For $x > 1$, inserting the potential (3.2) into (3.3) gives

$$e^{-i\omega}\psi_{\alpha'}(x) = \sum_{\alpha} \check{S}_{\alpha'\alpha} e^{-i\phi} \psi_\alpha(x-a)$$

which is equivalent to

$$e^{-i(\omega-\phi)}\psi_{\alpha'}(x) = \sum_{\alpha} \check{S}_{\alpha'\alpha} \psi_\alpha(x-a). \tag{3.5}$$

Again (3.5) has the same form as (2.6) so we make the *ansatz*

$$\psi^{(\omega)}(x) = B\psi^{(k',+)}(x) \qquad \text{if} \quad x \geq 1, \tag{3.6}$$

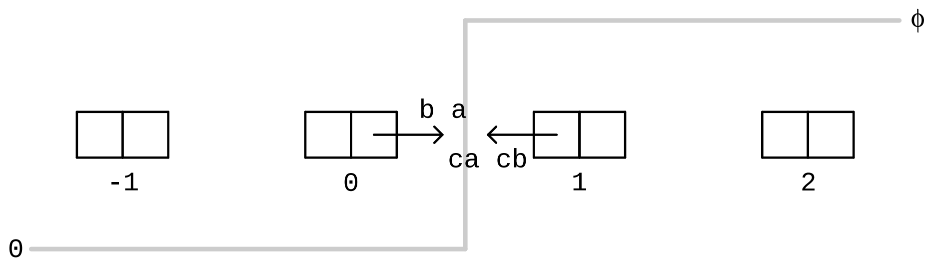

Figure 6. Schematic diagram of a subspace of H_1 when there is a potential step of height ϕ between $x = 0$ and $x = 1$. As in Figure 2, the boxes represent dimensions of the Hilbert space and the labelled arrows indicate the amplitude flow (here $c := e^{-i\phi}$). Equations (3.8) correspond to the statements that the left moving amplitude flow from $x = 1$ equals what it would be were the *ansatz* for $x \le 0$ continued to $x = 1$, and that the right moving amplitude flow from $x = 0$ equals what it would be were the *ansatz* for $x \ge 1$ continued to $x = 0$, respectively.

for the transmitted amplitudes, where

$$\cos(\omega - \phi) = \cos\theta\cos k'. \tag{3.7}$$

As illustrated in Figure 6, at $x = 0$ and $x = 1$ (3.3) gives a pair of boundary conditions which constrain the two parameters A and B:

$$\begin{aligned} e^{-i\omega}\psi^{(\omega)}_{\alpha'}(0) &= \check{S}_{\alpha',-1}e^{-i\phi}\psi^{(\omega)}_{-1}(1) + \check{S}_{\alpha',+1}\psi^{(\omega)}_{+1}(-1) \\ e^{-i\omega}\psi^{(\omega)}_{\alpha'}(1) &= \check{S}_{\alpha',-1}e^{-i\phi}\psi^{(\omega)}_{-1}(2) + \check{S}_{\alpha',+1}\psi^{(\omega)}_{+1}(0). \end{aligned}$$

These constraints imply that

$$\begin{aligned} Be^{-i\phi}\psi^{(k',+)}_{-1}(1) &= \psi^{(k,+)}_{-1}(1) + A\psi^{(-k,+)}_{-1}(1) \\ \psi^{(k,+)}_{+1}(0) + A\psi^{(-k,+)}_{+1}(0) &= Be^{-i\phi}\psi^{(k',+)}_{+1}(0), \end{aligned} \tag{3.8}$$

after inserting the *ansatz* (3.4) and (3.6). Using the formulae (2.10) and (2.11) for the plane waves and simplifying, the pair of equations (3.8) becomes

$$\begin{aligned} A - Be^{-i\phi} &= -1 \\ Ae^{-ik} - Be^{-i(\phi-k')} &= -e^{ik}. \end{aligned}$$

These equations can be solved for A and B to give

$$\begin{aligned} A &= -\frac{e^{ik'} - e^{ik}}{e^{ik'} - e^{-ik}} \\ B &= e^{i\phi}\frac{e^{ik} - e^{-ik}}{e^{ik'} - e^{-ik}}. \end{aligned}$$

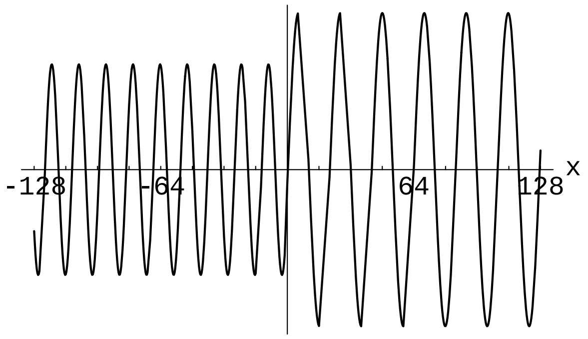

Figure 7. The real part of the $\alpha = -1$ component of an eigenfunction of U with frequency $\omega = \pi/6$ for a step of height $\pi/24$ with $\theta = \pi/12$ on the interval $-128 \le x \le 128$. This wave function has wave numbers aproximately 0.459 to the left of, and 0.296 to the right of the step.

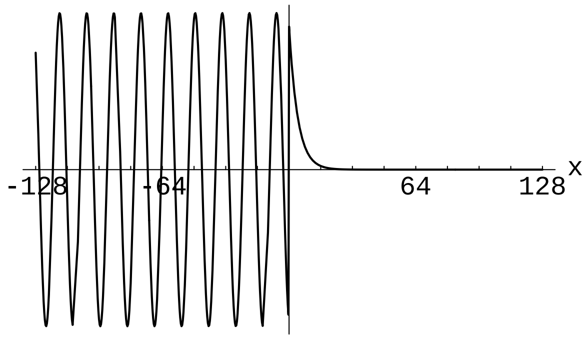

Figure 8. The eigenfunction of U in the same situation as in Figure 7 except that in this case the step is taller—it has height $\pi/8$. The incident right moving wave still has wave number approximately 0.459. To the left of the step the wave function decays exponentially.

This justifies the *ansatz* of (3.4) and (3.6) as a solution to (3.3).

Notice that the solution k' to (3.7) will not always be real, so (3.6) and (3.7) will not always describe a plane wave. For example, given $0 < \theta < \omega$, when the step is small, *i.e.*, $0 < \phi < \omega - \theta$, the transmitted amplitudes form a plane wave of lower frequency $\omega - \phi$ (and smaller wave number k') than the incident plane wave, but still lying on the upper branch of the dispersion relation shown in Figure 3. When the step is larger, *i.e.*, $\omega - \theta < \phi < \omega + \theta$, $\omega - \phi$ lies in the gap between the branches of the dispersion relation so (3.7) has purely imaginary solutions k' and the only physical solution of the form (3.6) decays exponentially past the step.

Figures 7 and 8 illustrate these situations on the interval $-128 \le x \le 128$ with $\theta = \pi/12$ for an incident right moving plane wave with $\omega = \pi/6$ and $k = \arccos(\cos\omega/\cos\theta) \approx 0.459$. In Figure 7 the step has height $\pi/24$ and we have plotted the real part of $\psi^{(\omega)}_{-1}$. This is the case $0 < \phi = \pi/24 < \omega - \theta = \pi/12$ so there is a transmitted plane wave with $k = \arccos(\cos(\omega - \phi)/\cos\theta) \approx 0.296$. In Figure 8 the step has height $\pi/8$; this is the case $\omega - \theta = \pi/12 < \phi = \pi/8 < \omega + \theta = \pi/4$ so there is no transmitted plane wave and the amplitude decays exponentially in x.

This much is exactly what we would expect in the nonrelativistic situation; and we would expect the transmitted amplitudes to simply decay exponentially faster as the height of the step is increased. Instead, we find that when the step is even larger, *i.e.*, $\omega+\theta < \phi$, the transmitted amplitudes again form a plane wave, but now with frequency $\omega - \phi < -\theta < 0$. Figure 9 illustrates this situation—the Klein paradox [12]—with a square well of depth $\phi = 7\pi/24$ and $\omega = \pi/6$ again, so that $\omega + \theta = \pi/4 < \phi = 7\pi/24$. Here the transmitted plane wave has frequency $\omega - \phi = -\pi/8 < 0$ and hence negative energy. This situation is out of the nonrelativistic regime; the large potential step localizes the particle too strongly, exciting negative energy states.

Just as in the continuum model for a relativistic quantum particle, therefore, since we take negative energies to be unphysical, we are forced to recognize the existence of *anti*particles in the model, *i.e.*, particles which are the time reverse T (or charge conjugate C) of the particles with which we started. The tokens representing the antiparticles must be the 'empty' (lattice point, direction) pairs; that is, the single particle state $|x,\alpha\rangle$ should now be interpreted as a particle at (x,α) and antiparticles at all $(y,\beta) \neq (x,\alpha)$. Since the antiparticles are the time reverse of particles, a negative frequency corresponds to a *positive* energy state for them; thus there are no unphysical negative energy states. In this relativistic interpretation, the amplitude for the single particle to change direction is identified with the amplitude for it to scatter back from an oppositely moving antiparticle—answering the question asked in the previous section. A complete reinterpretation of the model requires definition of the two antiparticle, and hence two particle, scattering amplitudes. We do so, completing the definition of the QLGA, in the next section.

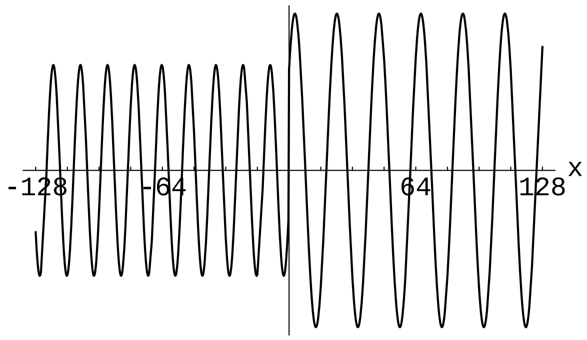

Figure 9. The eigenfunction of U in the same situation as in Figures 7 and 8, but now for an even taller step, of height $7\pi/24$. Rather than decaying even faster than in Figure 8, the amplitude of the wave function oscillates to the right of the step, with wave number approximately 0.296.

4. The two particle sector

In Section 2 we defined only the one particle sector of the model; in [10] we showed that the most general parity invariant local evolution rule which preserves particle number and has an exclusion principle is defined by the unitary scattering matrix

$$R = \begin{array}{cc} & \begin{array}{cccc} & \nwarrow & \nearrow & \nearrow\nwarrow \end{array} \\ \begin{array}{c} \\ \nearrow \\ \nwarrow \\ \nwarrow\nearrow \end{array} & \begin{pmatrix} d & & & \\ & b & a & \\ & a & b & \\ & & & f \end{pmatrix} \end{array}, \tag{4.1}$$

where the central block is the scattering matrix S (2.3) and unitarity requires $\bar{d}d = 1 = \bar{f}f$. The phase f is the amplitude for a pair of particles to scatter off one another, while the phase d is the amplitude for either a pair of empty states to evolve to a pair of empty states or a pair of antiparticles to evolve to a pair of antiparticles, depending on our interpretation of the model. Figure 10 shows all the scattering rules implied by R; as in Figure 1 time runs upward so we indicate the presence of antiparticles by *downward* pointing arrows. This notation displays the (formal) equivalence of our one dimensional QLGA with two copies of the six vertex model [13]. The fact that two copies of the six vertex model are required stems from the usual $\mathbb{Z}_2$ symmetry in one dimensional LGA: particles an even distance apart initially cannot interact on the integer lattice [18,19].

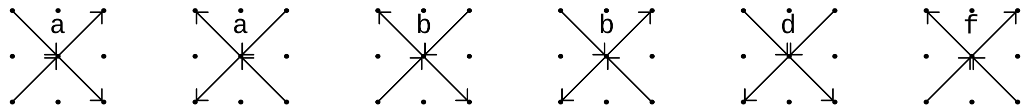

Figure 10. Spacetime diagrams of all the QLGA scattering amplitudes. Time runs upward so antiparticles are represented by downward pointing arrows.

In the nonrelativistic interpretation it is most natural to set $d = 1$, while in the relativistic interpretation we must set $d = \bar{f}$ to maintain CT invariance [20,19]. In either case, the evolution rule (2.2) for the basis vectors of the one particle sector of the Hilbert space gets multiplied by a factor of d for each antiparticle/hole. Since an overall phase is unobservable, we can always multiply R by $\bar{d}$ to set $R_{11} = 1$ and avoid the normalization problem associated with an infinite number of factors of d. The one particle sector of the model is now completely defined and so supports the particle/antiparticle relativistic interpretation introduced at the end of the last section.

Furthermore, since particle number is preserved, only the relative phase between S and f has observable consequences, so the parameterization of S in the previous sections can be maintained in each of the multiparticle sectors of the QLGA. Since the inhomogeneous potentials considered in Section 3 are also implemented by a relative phase, this form for the scattering matrix R suggests that similar calculations will determine the eigenfunctions of the evolution matrix for interacting particles. In this section we demonstrate this explicitly for the two particle sector of the QLGA.

An orthonormal basis for the two particle sector $H_2 \subset H$ is given by the set $\big\{|x_1, \alpha_1\rangle \otimes |x_2, \alpha_2\rangle \bigm| (x_1, \alpha_1) \neq (x_2, \alpha_2)\big\}$; this reflects an exclusion principle in the model—the two particles cannot occupy the same state—but not necessarily fermionic statistics. A state vector for a pair of particles has the form

$$\Psi(t) = \sum_{(x_1,\alpha_1)\neq(x_2,\alpha_2)} \psi_{\alpha_1\alpha_2}(t, x_1, x_2)|x_1, \alpha_1\rangle \otimes |x_2, \alpha_2\rangle$$

and just as in the one particle sector $\Psi(t)$ must have norm 1:

$$1 = \sum_{(x_1,\alpha_1)\neq(x_2,\alpha_2)} \overline{\psi_{\alpha_1\alpha_2}(t, x_1, x_2)}\psi_{\alpha_1\alpha_2}(t, x_1, x_2).$$

The evolution of the two particle basis vectors implied by the scattering matrix R (4.1) divides into two cases. For $x_1 + \alpha_1 \neq x_2 + \alpha_2$ the evolution rule (2.4) is simply applied to the two particles independently:

$$U|x_1, \alpha_1\rangle \otimes |x_2, \alpha_2\rangle = \sum_{\alpha_1',\alpha_2'} \check{S}_{\alpha_1'\alpha_1}\check{S}_{\alpha_2'\alpha_2}|x_1 + \alpha_1, \alpha_1'\rangle \otimes |x_2 + \alpha_2, \alpha_2'\rangle, \tag{4.2}$$

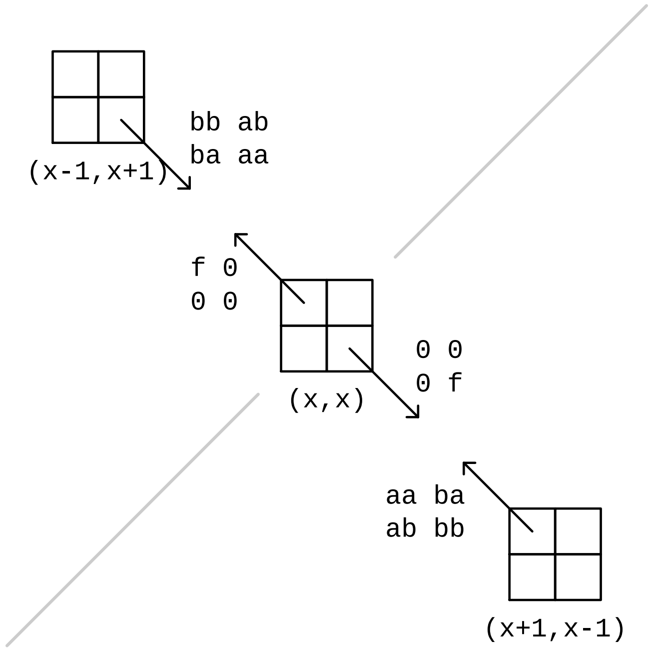

Figure 11. Schematic diagram of a subspace of $H_{2,\mathrm{int}}$. The coordinates x_1 and x_2 of the two particles label the sets of four boxes, each of which corresponds to a pair of 'velocities'. The evolution rule (4.4) gives the amplitude flows shown pointing toward the diagonal (where the particles coincide), while (4.5) gives the amplitude flows shown pointing away from it. In order for the *ansatz* (4.9) to satisfy (4.7) for $x_1 \neq x_2$, the amplitude flows away from the diagonal must satisfy (4.10); in order for it to satisfy (4.11) the amplitude flows toward the diagonal must satisfy (4.12).

while for $x_1 + \alpha_1 = x_2 + \alpha_2 = x$, there are two possible scattering events:

$$U|x-1,+1\rangle \otimes |x+1,-1\rangle = f|x,+1\rangle \otimes |x,-1\rangle$$
$$U|x+1,-1\rangle \otimes |x-1,+1\rangle = f|x,-1\rangle \otimes |x,+1\rangle$$

which can be summarized as

$$U|x-\alpha,\alpha\rangle \otimes |x+\alpha,-\alpha\rangle = f|x,\alpha\rangle \otimes |x,-\alpha\rangle. \tag{4.3}$$

The evolution rules (4.2) and (4.3) can be rewritten in terms of the amplitudes: For $x_1 \neq x_2$,

$$U\psi_{\alpha'_1\alpha'_2}(x_1,x_2) = \sum_{\alpha_1,\alpha_2} \check{S}_{\alpha'_1\alpha_1}\check{S}_{\alpha'_2\alpha_2}\psi_{\alpha_1\alpha_2}(x_1-\alpha_1,x_2-\alpha_2) \tag{4.4}$$

and for $x_1 = x_2 = x$,

$$U\psi_{\alpha,-\alpha}(x,x) = f\psi_{\alpha,-\alpha}(x-\alpha,x+\alpha). \tag{4.5}$$

Just as Figures 2 and 6 illustrate the evolution rules (2.5) and (3.1), respectively, Figure 11 illustrates the amplitude flow on H_2 described by (4.4) and (4.5).

Notice that we have implicitly assumed that the two particles are distinguishable, as would be the case classically, and have interpreted the scattering events with amplitude f to involve neither particle changing direction. One might be concerned that (4.3) and (4.5) would have to be changed for indistinguishable quantum particle scattering. This is not the case when the particles have fermionic statistics, for example: if the initial wave function is antisymmetric under the exchange of two particles, *i.e.*,

$$\psi_{\alpha_1\alpha_2}(x_1,x_2) = -\psi_{\alpha_2\alpha_1}(x_2,x_1), \tag{4.6}$$

then the evolution rules (4.4) and (4.5) preserve this property. We will consider this case in more detail at the end of this section.

At the beginning of this section we noted the close relation of our one dimensional QLGA with the six vertex model. The six vertex model is exactly solvable [21,13], which suggests that we should be able to find the analogue of plane waves in the two particle sector, namely the two particle eigenfunctions of U. The associated conserved quantities will describe the physics of this sector. For an eigenfunction, (4.4) becomes

$$e^{-i\omega}\psi_{\alpha'_1\alpha'_2}(x_1,x_2) = \sum_{\alpha_1,\alpha_2} \check{S}_{\alpha'_1\alpha_1}\check{S}_{\alpha'_2\alpha_2}\psi_{\alpha_1\alpha_2}(x_1-\alpha_1,x_2-\alpha_2). \tag{4.7}$$

A straightforward *ansatz* for a solution to (4.7) is:

$$\psi_{\alpha_1\alpha_2}(x_1,x_2) = \psi^{(k_1,\epsilon_1)}_{\alpha_1}(x_1)\psi^{(k_2,\epsilon_2)}_{\alpha_2}(x_2), \tag{4.8}$$

where $\psi^{(k_i,\epsilon_i)} =: \psi^{(i)}$ are the one particle plane waves we found in Section 2. It is easy to verify that (4.8) solves (4.7):

$$\begin{aligned}
U\psi_{\alpha'_1\alpha'_2}(x_1,x_2) &= \sum_{\alpha_1,\alpha_2} \check{S}_{\alpha'_1\alpha_1}\check{S}_{\alpha'_2\alpha_2} e^{-i\alpha_1 k_1}\psi^{(1)}_{\alpha_1}(x_1)e^{-i\alpha_2 k_2}\psi^{(2)}_{\alpha_2}(x_2) \\
&= \sum_{\alpha_1} \check{S}_{\alpha'_1\alpha_1} e^{-i\alpha_1 k_1}\psi^{(1)}_{\alpha_1}(x_1) \sum_{\alpha_2} \check{S}_{\alpha'_2\alpha_2} e^{-i\alpha_2 k_2}\psi^{(2)}_{\alpha_2}(x_2) \\
&= e^{-i\epsilon_1\omega_1}\psi^{(1)}_{\alpha'_1}(x_1)e^{-i\epsilon_2\omega_2}\psi^{(2)}_{\alpha'_2}(x_2) \\
&= e^{-i(\epsilon_1\omega_1+\epsilon_2\omega_2)}\psi_{\alpha'_1\alpha'_2}(x_1,x_2),
\end{aligned}$$

where the third equality follows from (2.8) since the pairs $(\epsilon_i\omega_i, k_i)$ satisfy the dispersion relation (2.9). Thus the *ansatz* (4.8) solves (4.7) for $\omega = \epsilon_1\omega_1 + \epsilon_2\omega_2$.

Now observe that the $\mathbb{Z}_2$ symmetry of the one dimensional QLGA partitions H_2 into two orthogonal subspaces: $H_2 = H_{2,\mathrm{int}} \oplus H_{2,\mathrm{free}}$, where

$$\begin{aligned}
H_{2,\mathrm{int}} &:= \mathrm{span}\{\, |x_1,\alpha_1\rangle \otimes |x_2,\alpha_2\rangle \bigm| x_1 - x_2 \equiv 0 \pmod 2 \text{ and } (x_1,\alpha_1) \neq (x_2,\alpha_2) \,\} \\
H_{2,\mathrm{free}} &:= \mathrm{span}\{\, |x_1,\alpha_1\rangle \otimes |x_2,\alpha_2\rangle \bigm| x_1 - x_2 \equiv 1 \pmod 2 \,\}.
\end{aligned}$$

These subspaces evolve independently since $H_{2,\mathrm{int}}$ consists of states in which the two particles can eventually interact while $H_{2,\mathrm{free}}$ consists of states in which they cannot, as is implied by the form of (4.2) and (4.3). In fact, the evolution of $H_{2,\mathrm{free}}$ is completely specified by (4.2) (or (4.4)) and depends only on the one particle scattering matrix S. On this subspace, therefore, (4.8) provides a complete solution for the eigenfunctions of U.

To find a solution for the interacting particles subspace $H_{2,\mathrm{int}}$, consider the two particle plane wave (4.8) 'incident' from the $x_1 < x_2$ subspace of $H_{2,\mathrm{int}}$. This two particle plane wave 'scatters' off the $x_1 = x_2$ subspace of $H_{2,\mathrm{int}}$ just as the right moving plane waves we considered in Section 3 scattered off the potential step, producing both a 'reflected' and a 'transmitted' two particle plane wave, in the $x_1 < x_2$ and $x_1 > x_2$ subspaces, respectively. Thus we make the *Bethe ansatz* [22,21,13]:

$$\psi^{(\omega)}_{\alpha_1\alpha_2}(x_1,x_2) = \begin{cases} \psi^{(1)}_{\alpha_1}(x_1)\psi^{(2)}_{\alpha_2}(x_2) + A\psi^{(1)}_{\alpha_2}(x_2)\psi^{(2)}_{\alpha_1}(x_1) & \text{if } x_1 < x_2; \\ B\psi^{(1)}_{\alpha_1}(x_1)\psi^{(2)}_{\alpha_2}(x_2) & \text{if } x_1 > x_2, \end{cases} \tag{4.9}$$

where $\omega := \epsilon_1\omega_1 + \epsilon_2\omega_2$, since all three two particle plane waves on the right hand side of (4.9) have the same two wave numbers k_1 and k_2 and the same frequency ω. For $|x_1 - x_2| \neq 2$, the free particle subspace computation together with linearity imply that (4.7) is satisfied by (4.9). For $|x_1 - x_2| = 2$, (4.7) implies conditions on the extension of this *ansatz* to $x_1 = x_2 = x$:

$$\begin{aligned} e^{-i\omega}\psi^{(\omega)}_{\alpha'_1\alpha'_2}(x-1,x+1) = &\sum_{(\alpha_1,\alpha_2)\neq(-1,+1)} \check{S}_{\alpha'_1\alpha_1}\check{S}_{\alpha'_2\alpha_2}\psi^{(\omega)}_{\alpha_1\alpha_2}(x-1-\alpha_1,x+1-\alpha_2) \\ &\qquad + \check{S}_{\alpha'_1,-1}\check{S}_{\alpha'_2,+1}\psi^{(\omega)}_{-1,+1}(x,x) \\ e^{-i\omega}\psi^{(\omega)}_{\alpha'_1\alpha'_2}(x+1,x-1) = &\sum_{(\alpha_1,\alpha_2)\neq(+1,-1)} \check{S}_{\alpha'_1\alpha_1}\check{S}_{\alpha'_2\alpha_2}\psi^{(\omega)}_{\alpha_1\alpha_2}(x+1-\alpha_1,x-1-\alpha_2) \\ &\qquad + \check{S}_{\alpha'_1,+1}\check{S}_{\alpha'_2,-1}\psi^{(\omega)}_{+1,-1}(x,x). \end{aligned}$$

These conditions will be satisfied provided

$$\begin{aligned} \psi^{(\omega)}_{-1,+1}(x,x) &= \psi^{(1)}_{-1}(x)\psi^{(2)}_{+1}(x) + A\psi^{(1)}_{+1}(x)\psi^{(2)}_{-1}(x) \\ \psi^{(\omega)}_{+1,-1}(x,x) &= B\psi^{(1)}_{+1}(x)\psi^{(2)}_{-1}(x), \end{aligned} \tag{4.10}$$

i.e., provided the form of the *ansatz* (4.9) extends to the two nonzero components of $\psi^{(\omega)}_{\alpha_1\alpha_2}(x,x)$ in this way.

Now the problem is to find $A, B \in \mathbb{C}$ such that (4.9) and (4.10) define an eigenfunction of (4.5); that is, $\psi^{(\omega)}$ must also satisfy

$$e^{-i\omega}\psi^{(\omega)}_{\alpha,-\alpha}(x,x) = f\psi^{(\omega)}_{\alpha,-\alpha}(x-\alpha,x+\alpha). \tag{4.11}$$

This gives two constraints on A and B:

$$
\begin{aligned}
e^{-i\omega}\big[\psi^{(1)}_{-1}(x)\psi^{(2)}_{+1}(x) + A\psi^{(1)}_{+1}(x)\psi^{(2)}_{-1}(x)\big] &= fB\psi^{(1)}_{-1}(x+1)\psi^{(2)}_{+1}(x-1) \\
e^{-i\omega}B\psi^{(1)}_{+1}(x)\psi^{(2)}_{-1}(x) &= f\big[\psi^{(1)}_{+1}(x-1)\psi^{(2)}_{-1}(x+1) + A\psi^{(1)}_{-1}(x+1)\psi^{(2)}_{+1}(x-1)\big].
\end{aligned}
\tag{4.12}
$$

Inserting the form (2.11) of the one particle plane waves into (4.12) and rearranging gives

$$
\begin{aligned}
Ae^{-i\omega}\psi_{+-} - Be^{i(k_1-k_2)}f\psi_{-+} &= -e^{-i\omega}\psi_{-+} \\
Ae^{i(k_1-k_2)}f\psi_{-+} - Be^{-i\omega}\psi_{+-} &= -e^{-i(k_1-k_2)}f\psi_{+-}
\end{aligned}
\tag{4.13}
$$

where $\psi_{\epsilon_1\epsilon_2} := \psi^{(1)}_{\epsilon_1}(0)\psi^{(2)}_{\epsilon_2}(0)$. Solving (4.13) for A and B gives

$$
\begin{aligned}
A &= \frac{\psi_{-+}\psi_{+-}(f^2 - e^{-2i\omega})}{(e^{-i\omega}\psi_{+-})^2 - (e^{i(k_1-k_2)}f\psi_{-+})^2} \\
B &= \frac{e^{-i\omega}f\big[e^{-i(k_1-k_2)}\psi^2_{+-} - e^{i(k_1-k_2)}\psi^2_{-+}\big]}{(e^{-i\omega}\psi_{+-})^2 - (e^{i(k_1-k_2)}f\psi_{-+})^2}.
\end{aligned}
\tag{4.14}
$$

Thus (4.9) and (4.10), with the coefficients A and B given by (4.14), define a set of eigenfunctions for the two interacting particles subspace $H_{2,\mathrm{int}}$. Each is described by a pair of wave numbers k_1 and k_2, and a frequency $\omega = \epsilon_1\omega_1 + \epsilon_2\omega_2$, where the pairs $(\epsilon_i\omega_i, k_i)$ satisfy the dispersion relation (2.9). When the two particles are apart, *i.e.*, not at the same lattice point, these eigenfunctions each put the particles into a superposition of two particle plane waves, with momenta proportional to k_1 and k_2. Thus we should interpret these two particle eigenstates as describing pairs of particles with distinct momenta before they interact (*i.e.*, arrive at the same lattice point), and the same distinct, but possibly permuted, momenta after they interact. The relative amplitudes of the permutations are A and B in (4.14). To understand their physical meaning, notice that $|A|^2 + |B|^2 = 1$. Since A and B generically have both nonzero norms and phase angles, one may interpret B, for example, as describing the relative probability of transmission $|B|^2$ as well as a phase angle shift $\Theta(k_1, k_2)$ between the incoming and scattered (transmitted) two particle plane waves.

When $A \neq 0$, a necessarily independent set of eigenfunctions for the two interacting *distinguishable* particles subspace $H_{2,\mathrm{int}}$ is obtained by the same calculation, only starting with an 'incident' two particle plane wave in the $x_1 > x_2$ subspace:

$$
\psi^{(\omega)}_{\alpha_1\alpha_2}(x_1,x_2) = \begin{cases} B'\psi^{(1)}_{\alpha_1}(x_1)\psi^{(2)}_{\alpha_2}(x_2) & \text{if } (x_1,\alpha_1) < (x_2,\alpha_2); \\ \psi^{(1)}_{\alpha_1}(x_1)\psi^{(2)}_{\alpha_2}(x_2) + A'\psi^{(1)}_{\alpha_2}(x_2)\psi^{(2)}_{\alpha_1}(x_1) & \text{if } (x_1,\alpha_1) > (x_2,\alpha_2), \end{cases}
\tag{4.15}
$$

where the ordering on pairs (x_i, α_i) is lexicographic and A' and B' are given by the formulae (4.14) for A and B, but with k_1 and k_2 exchanged (including the k_1 and k_2 in ψ_{-+} and ψ_{+-}).

These eigenfunctions (4.15), together with our first set (4.9), form a basis in terms of which antisymmetric wave functions (4.6) (and symmetric ones) can be expanded. Since indistinguishable fermionic particles with a necessarily antisymmetric wave function are the most plausible components of a QLGA quantum computer, however, it is perhaps more natural to work in the antisymmetric subspace of H_2 from the beginning. Then the natural eigenfunction *ansatz* is antisymmetric:

$$\psi^{(\omega)}_{\alpha_1\alpha_2}(x_1,x_2) = \begin{cases} \psi^{(1)}_{\alpha_1}(x_1)\psi^{(2)}_{\alpha_2}(x_2) + A\psi^{(1)}_{\alpha_2}(x_2)\psi^{(2)}_{\alpha_1}(x_1) & \text{if } (x_1,\alpha_1) < (x_2,\alpha_2); \\ -\psi^{(1)}_{\alpha_1}(x_1)\psi^{(2)}_{\alpha_2}(x_2) - A\psi^{(1)}_{\alpha_2}(x_2)\psi^{(2)}_{\alpha_1}(x_1) & \text{if } (x_1,\alpha_1) > (x_2,\alpha_2). \end{cases} \tag{4.16}$$

The *ansatz* (4.16) satisfies (4.7); the interaction condition (4.11) imposes only a single constraint in this case:

$$e^{-i\omega}\big[\psi^{(1)}_{-1}(x)\psi^{(2)}_{+1}(x) + A\psi^{(1)}_{+1}(x)\psi^{(2)}_{-1}(x)\big] = f\big[-\psi^{(1)}_{-1}(x)\psi^{(2)}_{+1}(x) - A\psi^{(1)}_{+1}(x)\psi^{(2)}_{-1}(x)\big].$$

Inserting the form (2.11) of the one particle plane waves and solving for A gives

$$A = -\frac{e^{-i\omega}\psi_{-+} + fe^{-i(k_1-k_2)}\psi_{+-}}{e^{-i\omega}\psi_{+-} + fe^{i(k_1-k_2)}\psi_{-+}}. \tag{4.17}$$

Thus (4.16) with the coefficient A given by (4.17) defines a set of antisymmetric eigenfunctions in the two interacting particles subspace; the eigenfunctions in the two free particles subspace are simply obtained by antisymmetrizing (4.8).

5. Discussion

We began our analysis in Section 2 by determining the eigenvalues and eigenfunctions—the phases $e^{-i\omega}$ and the plane waves $\psi^{(k,\epsilon)} \equiv |k,\epsilon\rangle$—of the evolution operator U on the one particle sector of the QLGA. We found that the probability that a single particle with initial wave function $\Psi(0)$ has wave number k_0 and frequency $\omega_0 = \epsilon_0 \arccos(\cos\theta\cos k_0)$ at time t is an invariant: $|\langle\Psi(0)|k_0,\epsilon_0\rangle|^2$. It is constant in time since each plane wave $|k,\epsilon\rangle$ evolves by phase multiplication $e^{-i\omega t}$ over t timesteps. Consequently, the expectation value of the wave number

$$\langle k\rangle := \sum_{k,\epsilon} k|\langle\Psi(0)|k,\epsilon\rangle|^2$$

and of the frequency

$$\langle\omega\rangle := \sum_{k,\epsilon} \epsilon\omega_k|\langle\Psi(0)|k,\epsilon\rangle|^2$$

are also invariants of the evolution. Physically, of course, this means that momentum and energy are conserved.

Identification of k and ω as proportional to momentum and energy, respectively, led to our interpretation in Section 3 of the eigenfunctions of U in the presence of a large step potential not as negative energy modes of the particle but rather as positive energy modes of antiparticles in the model. Since there are no antiparticles in the (nonrelativistic) Schrödinger equation continuum limit of this model, our analysis of invariants in the one particle sector of the QLGA enables us to identify this as a parameter regime whose continuum limit must be described by the (relativistic) Dirac equation.

The eigenfunction *ansatz* and matching conditions we used for the step potential forshadowed the Bethe *ansatz* approach we applied in Section 4 to find the eigenvalues and eigenfunctions of U in the two particle sector of the QLGA. Just as the one particle plane waves determine evolution invariants in the one particle sector, the two particle eigenfunctions $|k_1, \epsilon_1; k_2, \epsilon_2\rangle := \psi^{(\omega)}$ defined by (4.9) and (4.10), or (4.15), and (4.14) (or by (4.16) and (4.17)) define invariants in the two particle sector: The probability that a pair of particles with initial wave function $\Psi(0)$ have wave numbers k_i and frequencies $\omega_i = \epsilon_i \arccos(\cos\theta \cos k_i)$ at time t is an invariant: $|\langle\Psi(0)|k_1, \epsilon_1; k_2, \epsilon_2\rangle|^2$. Again, this is simply because the two particle eigenfunction evolves by phase multiplication by $e^{-i\omega}$, where $\omega = \epsilon_1\omega_1 + \epsilon_2\omega_2$.

In fact, the Bethe *ansatz* extends to each of the multiparticle sectors of the QLGA [22,21,13] so the evolution of an arbitrary initial wave function can be computed exactly. Of course, it had to be the case that the *unitary* evolution operator U has eigenfunctions which evolve by phase multiplication; what is remarkable, and what is meant by 'exactly solvable', is that these eigenfunctions and eigenvalues can be effectively computed, just as we have done in the one and two particle sectors of the QLGA.

The most general, no less local, QLGA in one dimension includes particles with 'velocity' 0 [10]. We have determined the one particle plane waves for this model in [16] and it is natural to ask if the Bethe *ansatz* also solves this model exactly. One expects this calculation to be possible, but more difficult: H_2, for example, does not decompose into a direct sum of 'interacting' and 'free' subspaces as it does in the single speed case analyzed here. Similarly, Boghosian and Taylor have simulated the evolution of one particle plane waves in a two dimensional QLGA [7]. One would like to extend the Bethe *ansatz* to find multiparticle eigenfunctions in such a higher dimensional model, but should expect it to be even more difficult—there are very few higher dimensional lattice models known to be exactly solvable [13,23].

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