Spontaneous orientation of a quantum lattice string.

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Using exact diagonalization and quantum Monte-Carlo techniques we study a quantum lattice string model introduced as a model for a single cuprate stripe. We focus on the ground state properties of the string. Our result shows that in the physically relevant region of the parameter space a zero-temperature spontaneous symmetry breaking occurs. The string spontaneously orients itself along one direction in space and becomes directed. We introduce an order parameter for the directedness and show that at zero temperature this order parameter reaches its saturation value.

Since the experimental discovery of the stripe phase [1], interest in this field has grown rapidly. Many issues concerning stripes are discussed, ranging from their origin to their relation to high-temperature superconductivity, including the dynamical properties of the stripes. In this contribution we are concerned with the last subject. We focus on the problem of a single stripe/ single charged domain wall. We consider the domain wall to be a connected trajectory (string) of particles, communicating with the lattice, while the precise nature of these particles is not further specified: the quantum lattice string (QLS) model [2].

Studying this model numerically, we discovered a zero-temperature symmetry breaking: although the string can be quantum delocalized, it picks spontaneously a direction in space. This symmetry breaking happens always in the part of parameter space which is of physical relevance. At first sight, one might expect that the quantum fluctuations (kinetic energy) would tend to disorder the string, i.e., to decrease the tendency for the string to be directed. That the opposite effect happens, can be seen as follows. A first intuition can be obtained by considering the analogy with surface statistical mechanics. The quantum string problem can be formulated as a classical problem of a two-dimensional surface (worldsheet) in 2+1 dimension, where the third direction is the imaginary time direction. The larger the kinetic term, or the smaller the temperature, the further the worldsheet stretches out in the time direction. At zero temperature, the worldsheet becomes infinite in this direction as well. The statistical physics of a string is then equivalent to that of a fluctuating sheet in three dimensions. Now, it is well known from studies of classical interfaces [3] that while a one-dimensional classical interface in two dimensions does not stay directed due to the strong fluctuations, for a two-dimensional sheet the entropic fluctuations are so small that interfaces can stay macroscopically flat in the presence of a lattice [4]. In other words, even if microscopic configurations with overhangs are allowed, a classical interface on a lattice in three dimensions can stay macroscopically flat or “directed”. In the present context, we will show that the directedness is a caused by an order-out-of disorder mechanism: in order to maximize the fluctuations transversal to the local string directions, overhangs should be avoided on the worldsheet. It remains to be seen if this mechanism is of a more general application.

In the QLS model the string configurations are specified by the position of the particles \( \mathbf{r}_l = (x_l, y_l) \). Two consecutive particles \( l \) and \( l + 1 \) should either be nearest or next-nearest neighbors, i.e. \( | \mathbf{r}_{l+1} - \mathbf{r}_l | = 1 \) or \( \sqrt{2} \). The set of all such configurations is the string Hilbert space.

The Hamiltonian consists of a classical energy term and a quantum (hopping) term. The classical energy is a sum of local interactions between nearest and next-nearest particles in the string.

\[
\mathcal{H}_C = \sum_{l} [K \delta(|x_{l+1} - x_l| - 1) \delta(|y_{l+1} - y_l| - 1) \\
+ \sum_{i,j=1}^2 \mathcal{L}_{ij} \delta(|x_{l+1} - x_{l-1} - i) \delta(|y_{l+1} - y_{l-1} - j|)] .
\]  

(1)

with \( \mathcal{L}_{ij} = \mathcal{L}_{ji} \) (see Fig. 1). The quantum term allows the particles to hop to nearest-neighbor lattice positions, giving rise to the meandering of the whole string. These hops should respect the string constraint. To enforce the constraint a projection operator \( P_{Str}(\mathbf{r}) = \delta(|\mathbf{r} - \mathbf{r}_l|) + \delta(|\mathbf{r} - \sqrt{2} \mathbf{r}_l|) \) is introduced which insures that the motion of particle \( l \) keeps the string intact. The string is quantized by introducing conjugate momenta \( \pi^a_l, [\pi^a_l, \pi^b_m] = i \delta_{l,m} \delta_{a,b} \) and the hopping is described by \( e^{i \pi} | \mathbf{x}_l \rangle = | \mathbf{x}_{l+1} \rangle \). The kinetic energy becomes, (Fig. 1)

\[
\mathcal{H}_Q = 2T \sum_{l,a} P^{\alpha}_{Str}(\mathbf{r}_{l+1} - \mathbf{r}_l) P^{\alpha}_{Str}(\mathbf{r}_l - \mathbf{r}_{l-1}) \cos(\pi^a_l). 
\]

(2)

FIG. 1. (a) The set of local configurations and their classical energies. (b) The two allowed hoppings. We take \( l = l' \).

The above string model is invariant under rotation of the string in space. As will be discussed below, we find that for physical choices of the parameters the invariance under symmetry operations of the lattice is broken. The
string acquires a sense of direction in space. This occurs even when the string is critical (delocalized in space). The string’s trajectories, on average, are such that they move forward in one direction while the string might delocalize in the other direction.

The relation of the string problem to surface models is established by using the Suzuki-Trotter mapping which maps a 2D quantum problem to a 2+1 D classical problem. A classical model of two coupled RSOS (restricted solid-on-solid) surfaces results. These are classical models for surface roughening where overhangs are not allowed. For the quantum string case, the two RSOS surfaces describe the motion of the string in the $x$ and $y$ spatial directions.

Skipping detailed calculation, the partition function of the quantum string can be mapped to the following classical problem:

$$Z = \lim_{n \to \infty} Tr e^{H_{eff}}$$

$$H_{eff} = \sum_{l,k} \left[ \frac{\epsilon}{n} \delta(|x_{l+1,k} - x_{l,k}| - 1) \delta(|y_{l+1,k} - y_{l,k}| - 1) \right] + \sum_{i,j=1}^{2} L_{ij} \delta(|x_{l+1,k} - x_{l-1,k}| - i) \delta(|y_{l+1,k} - y_{l-1,k}| - j)$$

$$+ \ln \left( \frac{T}{n} \right) \delta(|x_{l,k+1} - x_{l,k}| - 1) + \delta(|y_{l,k+1} - y_{l,k}| - 1) \right].$$

where $k$ is the trotter index and with the constraint $|x_{l,k+1} - x_{l,k}| \leq 1$ and $|y_{l,k+1} - y_{l,k}| \leq 1$. The above classical model can be viewed as two coupled RSOS surfaces, $x_{l,k}$ and $y_{l,k}$. The $x$ coordinate of particle $l$ at the trotter height $k$ is the height at position $(l,k)$ in the first surface and similarly the $y$ coordinates define a second RSOS surface, coupled strongly to the first by the above classical interactions.

Let us first discuss the numerical results. It is clear that the directedness property is a global quantity. For a string living in 2D lattice with open boundary conditions, directedness means that if it start at, say, the left boundary it has to end at the right boundary and will never end at the top or the bottom boundaries of the lattice. Although in the above model one can introduce a local order parameter to measure the directedness of a string, a more general quantitative measure for this global property can be constructed. This measure is not easily evaluated analytically but it can easily be calculated numerically; most importantly it illustrates clearly and effectively the directedness phenomenon. Every string configuration $s$ defines a curve in the 2D space $[x(t), y(t)]$, where $t$ could for instance be the discrete label of the successive particles along the string. When this curve can be parametrized by a single-valued function $x(y)$ or $y(x)$, we call the string configuration directed. The quantum string vacuum is a linear superposition of many string configurations. When all configurations in the vacuum correspond to single valued functions $x(y)$ or $y(x)$, the string vacuum is directed. At zero temperature, the ground state wave function of the string is $|\Psi_0\rangle = \sum_{\{x_l,y_l\}} |\alpha_0(\{x_l,y_l\})\rangle |\{x_l,y_l\}\rangle$, where every state in string configuration space ($|\{x_l,y_l\}\rangle$) corresponds to a trajectory $[x(t), y(t)]$. Consider first the case of a continuous string. For every configuration, the total string arclength is given by

$$L(\{x_l,y_l\})_{tot} = \int dt \sqrt{dx^2 + dy^2}.$$
results, as it will give a clear indication for the symmetry breaking directly at zero temperature. Here we consider an \(N \times N\) lattice. We think of a string living in such a finite lattice as part of an infinite one and therefore the ends of the string should live on the boundaries of the cluster. To fix the length of the string inside the cluster, we take as a criterion that the energy per particle be minimum. We plot the energy per particle versus the number of particles in the string. The minimum defines the optimal length of a string in the cluster. Upon setting the parameter \(L_{11}\) to zero and investigating different points in the parameter space, we found that the optimal length one should consider is the linear dimension of the lattice. Therefore in an \(N \times N\) lattice we will consider a string of length \(N\). Such a string can be directed along the \(x\) (horizontal) or \(y\) (vertical) direction. If the directedness assumption is fulfilled, the Hilbert space will effectively split into two subspaces: strings directed along the \(x\) direction and those along the \(y\). If nondirected strings are present there should be a non-zero tunnelling probability between the two sectors. By measuring the probability to tunnel from the \(x\)- to the \(y\)-sectors as a function of the linear dimension of the system, it should be possible to see the tendency towards spontaneous directedness symmetry breaking in the thermodynamic limit. Table 1 gives this tunnelling probability for different points in the parameter space. For all cases we set \(L_{11} = 0\). The choice of these points was motivated by the directed string problem \([2]\). The data are shown for lattices up to \(7 \times 7\). For a \(9 \times 9\) lattice the tunnelling probability turns out to be less than the accuracy of our numerical technique.

![Image](image-url)

**FIG. 3.** Monte-Carlo results for the directedness measure \(N_{\text{dir}}(T)\) at 4 points in parameter space. (see the text).

The classical string \((T = 0)\) would be flat at zero temperature, directed along (say) a \((1,0)\) direction. A local ‘corner’ (Fig. 3(a)) would be an excitation with energy \(L_{11}\) (alternatively, one could consider two kinks). Clearly, a single corner suffices to destroy the directedness of the classical ground state. At any finite temperature, the probability of the occurrence of at least one corner is finite: \(P = N \exp(-\beta L_{11})\). Hence, directedness order cannot exist at any non-zero temperature, for the same reason that any long range order is destroyed at any finite temperature in one dimension. In the simulations the string is of finite length, and the infinite temperature limit of \(N_{\text{dir}}(T)\) is therefore not zero but rather a small but nonzero value \(\approx 0.03\) for a domain wall of length 50). \(N_{\text{dir}}(T)\) is already close to this value for all temperatures of order \(L_{11}\) and larger. For an infinitely long domain wall \(N_{\text{dir}}(T)\) drops very fast to zero with increasing temperature. For low \(T\) where \(T \ll L_{11}\), \(N_{\text{dir}}(T)\) grows rapidly to 1. Again, because the string is of finite length, it becomes directed already at a finite temperature: For all temperatures such that \(L \exp(-\beta L_{11}) < 1\) the string configurations in our simulations are typically
completely directed. An infinitely long classical string becomes directed only at $T = 0$, of course, since at any nonzero temperature always some corners will occur in a sufficiently long string.

The results for the quantum string look always similar to the classical one. For temperatures higher than the kinetic scale, $T \gg \mathcal{T}$, all curves approach each other and the classical limit is reached. At low $T$, $T \ll \mathcal{T}$, $N_{\text{dir}}(T)$ grows rapidly to 1. As in the classical case, it reaches this value at a finite temperature for a finite length string. This is even valid for the pure quantum string, where all classical energies are zero (dashed line in Fig. 3(a)). Again this can be understood in terms of an effective corner or bend energy $\mathcal{L}$ that is produced by the quantum fluctuations. In analogy to the classical case, the probability for the occurrence of a bend is proportional to $\sim \exp(-\beta \mathcal{L})$. At zero temperature no bend is present and the string becomes directed. A finite length string effectively becomes directed already at a temperature such that $L \exp(-\beta \mathcal{L}) < 1$. At intermediate temperatures, where the temperature is of the order of the kinetic term, the situation is less clear. Especially in this region, all the various energies may play a role, and the interplay of these on the directedness is rather complicated. Nevertheless, as is clear from the data of Fig. 3(a), this region connects the high and low temperature limits smoothly. Finally, by comparing the results for the three quantum strings in this figure it is also clear that when the string is more quantum mechanical $N_{\text{dir}}(T)$ is higher.

The spontaneous directedness of the quantum string for $\mathcal{L}_{11} \geq 0$ can be understood by the following argument. The $\pi/2$ bends in strings block the propagation of links along the chain. Close to the bend itself the particles in the chain cannot move as freely as in the rest of the chain. This effect is shown in Fig. 4.

FIG. 4. Bends blocks the propagation of links along the string. Note holes 1 and 2 cannot move.

In space-time the $\pi/2$ bend is like a straight rod in time. Therefore the presence of such kinks increase the kinetic energy. For the argument it makes little difference whether the bend consists of a single $\pi/2$ corner or two $\pi/4$ corners. This confirms that it is the kinetic energy which keeps the strings oriented along one particular direction. In terms of a directedness order parameter this result implies that such a quantity is always finite, except when $\mathcal{L}_{11} \ll 0$ or when the hopping term vanishes (it is easy to see that in the classical case, $\mathcal{T} = 0$, in many regions of parameter space the problem becomes that of a self-avoiding walk on a lattice in the limit $T \to 0$). For the two equivalent RSOS surfaces this means that one of the two surfaces spontaneously orders while the other RSOS sheet can be either ordered or disordered.

Our general conclusion, based also on Monte-Carlo studies of the behavior in many other points in the parameter space, is that apart from some extreme classical limits, the general lattice string model at zero temperatures is a directed string. The qualitative picture of $\pi/2$ corners blocking the propagation of kinks appears to be a natural explanation for these numerical findings.

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