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LETTER TO THE EDITOR

Confinement in vertex models

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Abstract. An example is given of a vertex model that exhibits confinement of quasi-particles in the sense that the force required to separate the particles by a distance Δx is independent of the separation x for large x. The particular vertex model given here has two basic types of confined quasi-particle excitation, a mesonic type involving pairs of quasi-particles and a baryonic type involving triplets. Vertex models in general are derived from modeling hydrogen bonded crystals and confinement explains the result of a recent experiment on ammonia hemihydrate.

It may be interesting to consider an abstract model that exhibits confinement of quasi-particle excitations. The model is a discrete, graph theoretical, cooperative model for which the ground state is shown in figure 1. For convenience, only two spatial dimensions will be shown in the figures; extension to three or more dimensions is straightforward. There are two intrinsically different kinds of vertices, designated A and B in figure 1. Each A (B) type is connected by an edge to three vertices of B (A, respectively) type. Notice that there is no requirement that the vertices be arranged on a spatially regularly lattice, although they will be so drawn in the figures for convenience. Each edge joining an AB pair of vertices has an arrow associated with it. In the ground state each arrow points from an A vertex to a B vertex. The energy E_s of any state s, consisting of any configuration of arrows, is given as a sum of the energies $E_{si}(v_{si})$ of each individual vertex, designated as v_{si} for the ith vertex in the sth state,

$$E_s = \sum_i E_{si}(v_{si}), \tag{1}$$

where the different kinds of vertex arrow configurations v that may occur at a given site i are shown in figure 2 along with their energies $E(v)$. The 'Hamiltonian' in (1) is purely classical, like the Ising model. This vertex model may be made into a dynamical model in several ways. One could simply introduce a stochastical arrow reversing dynamics, similarly to the stochastic Ising model (Glauber 1963). One could also introduce a quantum tunnelling term along the lines of models for ice (Chen *et al* 1974). This aspect of the model will not be developed further in this paper, even though mention will be made of rearrangements from state to state in the basically classical model.

The regime of interest for the vertex energies $E(v)$ in figure 2 is $y > \delta \gg \varepsilon > 0$. An excitation from the ground state may be obtained by reversing one arrow. This creates two δ vertices which will be described as a pair of quasi-particles of δ type. To separate the two δ particles further one may reverse any arrow adjacent to the already reversed

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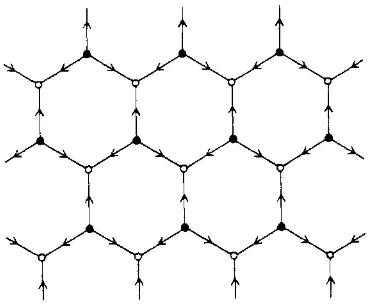

Figure 1. The ground state of an abstract vertex model. Vertices of A (B) type are represented by full (open, respectively) circles.

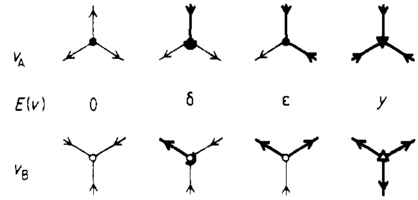

Figure 2. The vertex configurations and the vertex energies. In the first (third, respectively) row are the different kinds v_A (v_B, respectively) of arrow arrangements that may occur at any A (B, respectively) vertex. In the second row are the vertex energies $E(v)$ corresponding to the vertex configurations above and below. Each δ and ε type of vertex configuration has two additional symmetrical equivalents under $2\pi/3$ rotations, yielding a total of eight vertex configurations possible at each vertex. Those arrows that are reversed with respect to the ground state and the associated edges are drawn with bold lines.

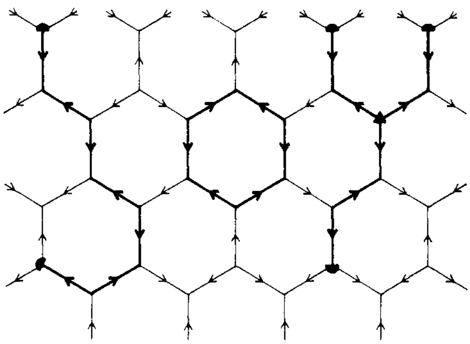

Figure 3. Some selected higher energy states. Towards the left of the figure is shown a pair of δ vertices and the connecting string of ε vertices. In the centre is shown the smallest example of an ε cycle. Towards the right of the figure is shown a Y particle consisting of a y vertex joined by three ε strings to three δ vertices. Those arrows that are reversed with respect to the ground state and the associated edges are drawn with bold lines.

arrow; this results in the retention of two δ vertices and converts a 0 vertex to an ε vertex. Further separation of the two δ vertices creates a string of ε vertices between them as shown in figure 3. Since $\varepsilon > 0$, the force required to separate the δ particles is independent of the distance of separation between them and has a magnitude that is roughly $4\varepsilon/3d$ where d is the mean distance between nearest-neighbouring vertices.

As shown in figure 3, there are other low lying excitations in this vertex model; in particular there are cycles (i.e. loops or rings) of ε vertices which, unlike the strings described in the last paragraph, do not end at two δ vertices. Such cycles of ε vertices can be formed by creation of a δ pair followed by stretching the string around one of the topological cycles in the lattice graph, culminating in annihilation of the δ pair. Clearly, the vacuum state for embedding a pair of δ particles is not the ground state, but is a renormalised state containing ε cycles. The degree of renormalisation can be determined by introducing an effective temperature T in the model and finding the renormalised vacuum state corresponding to the partition function

$$Z' = \sum_s{}' \exp(-\beta E_s), \tag{2}$$

where $\beta = 1/kT$ and the prime means that the sum is constrained to states s with vertices only of 0 type or ε type in figure 2. Similarly, the states with one pair of quasi-particle δ vertices will be dressed with ε cycles in addition to the string of ε vertices between the two δ vertices. If T is small, then there are few ε cycles in the renormalised vacuum state and the δ pair is clearly still confined, though the average statistical force for separation is smaller because a fraction of the string stretching, arrow-reversing, steps will involve changing existing ε vertices in ε cycles into 0 vertices of ground state type. For larger T a better criterion for confinement involves consideration of

$$\langle r_{12}^2 \rangle = \sum_s{}'' (r_{\delta_1} - r_{\delta_2})^2 \exp(-\beta E_s)/Z''. \tag{3}$$

where $''$ indicates that the sums are over states consisting of only two δ vertices and r_{δ_1} and r_{δ_2} are the locations of the δ vertices in the sth state. For small T, $\langle r_{12}^2 \rangle$ is expected to be finite, meaning that the δ pair is confined, because the 'entropy' factor corresponding to the multiplicities of longer strings of n ε vertices goes roughly as 2^n whereas the energy factor goes as $\exp(-n\beta\varepsilon)$. This rough argument also suggests that $\langle r_{12}^2 \rangle$ will become infinite at a critical temperature T_c.

In the case of a regular two-dimensional honeycomb lattice shown in the figures the critical temperature is given by $kT_c = 2\varepsilon/\ln 3$. This follows from the isomorphism of the states in (2) to the graphs for the high-temperature series expansion (Domb 1960) for the Ising model on the honeycomb lattice with interaction strength J, the corresponding relation for the weights in the respective partition functions,

$$\tanh(J/kT) = \exp(-\varepsilon/kT), \tag{4}$$

and the exact result for T_c (Domb 1960). Furthermore, the states containing a δ pair are isomorphic to the dominant graphs for the spin–spin correlation functions in the hyperbolic tangent expansion for the Ising model; the isomorphism is not complete because tadpole and dumbbell graphs (Domb 1960) are included in the spin–spin correlation functions, but these do not correspond to δ pair states. Nevertheless, the sum in (3) can be approximated as a sum over all distances of the spin–spin correlation functions times $(r_{\delta_1} - r_{\delta_2})^2$. For large ε/T, which corresponds to small J/T in (4), these correlations decay to zero exponentially (McCoy and Wu 1973) with distance $r_{\delta_1} - r_{\delta_2}$, so the sum in (3) is finite strongly suggesting that the δ pair is confined. However, for small ε/T, which corresponds to large J/T, the Ising model correlations decay to a non-zero value related to the spontaneous magnetisation, so the sum in (3) diverges corresponding to the δ pair not being confined. Incidentally, the vertex model in figures 1–3 could also be described in terms of monomers and dimers on a more complicated lattice graph, following Kasteleyn's method of solving the Ising model (Kastelyn 1963), but the y vertex is then not seen so clearly as a distinct entity, so that description will not be pursued.

With the introduction of an arrow reversing dynamic, confined pairs of δ vertices are mobile *as a pair.* Movement of the pair can proceed by reptation wherein one δ vertex advances to increase the length of the string and the other δ vertex follows the first δ vertex along the string, thereby restoring its original length and advancing the δ pair by one edge length. This mobility only involves simple sequences of arrow reversal, one edge at a time.

A different sort of elementary excitation is also shown in figure 3. This involves three δ vertices, each connected by a string of ε vertices, to a central y vertex. This trio of quasi-particles will be called a Y quasi-particle. The constituent parts of the Y particle will also be confined at low T. Unlike the δ pair, the Y particle is not mobile by simple reptation. To obtain mobility, a means must be derived to move the y vertex. This may be accomplished by momentary annihilation of the y vertex with one of the δ vertices followed by reformation of the y vertex and the δ vertex elsewhere on the string of ε vertices connecting the remaining two δ vertices. A final feature of the Y particle as presented is that two of its δ vertices may annihilate each other leaving a loop of ε vertices connected to the y vertex.

Let us now consider a modification of the above model that prohibits the feature in the last sentence of the last paragraph. Instead of one arrow on each edge of the lattice, let there be three arrows, coloured red, green and blue, respectively. There are now $8^3 = 512$ vertex configurations, most of which will be prohibited by assigning them infinite energy. Vertices will have non-zero finite energies $\varepsilon(\delta)$ if and only if the arrows of one and only one colour have the configurations shown as ε vertices (δ vertices, respectively) in figure 2 *and* if and only if the arrows with the other two colours are in the ground 0 energy configuration in figure 2. In addition, vertices will have energy y if and only if there are precisely three reversed arrows, each of *different* colour, and each along a different edge adjacent to the y vertex. Other vertex configurations are prohibited except for the zero energy configurations with arrows of all three colours in the ground state in figure 2. The quasi-particles now consist of (1) three different colours of δ pairs connected by a coloured ε string and (2) Y particles consisting of a y vertex and three δ vertices, each having a different colour and each connected to the y vertex by an ε string of the same colour.

The genesis of this kind of model is the vertex models in statistical mechanics (Baxter 1982). In turn, the vertex models have their origins in hydrogen bonded crystals, such as ice (Onsager and Dupuis 1960), KH_2PO_4, (Slater 1941), $SnCl_22H_2O$ (Salinas and Nagle 1974), $Cu(HCOO)_24H_2O$ (Youngblood *et al* 1980) and many others. The arrows on the edges in the vertex models simply correspond to the bimodal, non-symmetric, but reversible hydrogen bonds in the crystal. The vertex models for which the statistical mechanics has been solved exactly (Baxter 1982) correspond to hydrogen bonded crystals with no mechanism for dynamic equilibration. The analogy to the model presented is $\delta = \infty = y$ in (2). Dynamic mechanisms for thermal equilibration in real hydrogen bonded crystals involve charged defect vertices which are either of ionic type or Bjerrum type (Onsager 1973) and are aptly thought of as quasi-particle excitations. The high energy δ vertices in the model presented here play the same role as the ionic type excitation in hydrogen bonded crystals, even though the electric charge analogy is not obligatory.

Confinement of ionic defects provides an interpretation of a recent experiment on a hydrogen bonded crystal, ammonia hemihydrate (Bertie and Devlin 1983). It was observed that a small concentration of D_2O codeposited in ice results, upon warming the sample, in the decay of D_2O vibrational modes into HOD modes. This corresponds to the passage of ionic defects through the D_2O molecules (Onsager 1973). A similarly prepared sample of D_2O in $2(NH_3)H_2O$ shows little decay of the D_2O modes. One explanation (Bertie and Devlin 1983) is that the basic energy difference between NH···O and N···HO hydrogen bonds prevents proton hopping necessary for ionic defect transport. However, this does not prevent concerted hopping such as NH···OD···N going to N···HO···DN. Another difference between ice and ammonia hemihydrate is that the H_2O locations in ice are highly symmetric so that an H_2O dipole has six orientations with very nearly equal energy and the corresponding state of arrows is disordered. In contrast, in $2(NH_3)H_2O$ the crystal symmetry (Siemons and Templeton 1954) is much lower. Assuming that only one orientation is preferred (Siemons and

Templeton 1954) and the others cost a higher energy ε leads to an ordered state of arrows. This in turn leads to confinement of the ionic defects and to little decay of the D_2O modes. More generally, confinement of pairs of defects would account for the much slower thermal and electrical relaxation times in low-temperature ordered phases, including ferroelectric phases, of hydrogen bonded crystals. However, the interplay between the ionic defects and the Bjerrum defects that gives rise to the DC current must be remembered when interpreting data.

The particular model presented here was chosen because of its local symmetry and the possibility of the additional Y quasi-particle. It does not have any known direct hydrogen bonded crystal analogy. It may be emphasised that this model depends crucially upon the topological discreteness of the underlying space, although no length scale or geometrical regularity need be specified. In view of developments in discrete mechanics (Friedberg and Lee 1983) and lattice field theories (Wilson 1974, McCoy and Wu 1978, Baker and Kincaid 1981) and in view of some analogies between the δ pair with the current view of mesons consisting of two bound quarks and of the Y particle with baryons consisting of three quarks, perhaps such models, suitably modified to be acceptable field theories, would also be of some interest outside the area of condensed matter physics of hydrogen bonded crystals. In any case, the confinement of quasi-particles is a natural feature in ordered phases of vertex models and hydrogen bonded crystals.

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