

Resonating Valence Bond Liquid Physics on the Triangular Lattice

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We give an account of the short-range RVB liquid phase on the triangular lattice, starting from an elementary introduction to quantum dimer models, including details of the overlap expansion used to generate them. The fate of its topological degeneracy under duality is discussed, as well as recent developments and its possible relevance for quantum computing.

§1. Short-range RVB physics — some history

The question posed by high-temperature superconductors is what happens to an antiferromagnetic Mott insulator upon doping with mobile charge carriers. The basic problem arises from the fact that a hole hopping through an ordered Néel background is frustrated: in the absence of spin flips, the hole leaves behind a trail of broken bonds; optimising kinetic and exchange energy at the same time appears impossible.

Early on, Anderson¹⁾ suggested that one way of resolving this dilemma would be for the magnet to enter a state which has no long-range order but is nonetheless energetically competitive. Such a quantum state could be based on singlet bonds (valence bonds), as, for a given pair of spins, these optimise the exchange energy. However, this is again a frustrated problem as each spin can only form a singlet bond with one of its neighbours. Hence, a product of singlet wavefunctions has a hard time competing against the Néel state, where each site gains energy from its four neighbours.

This energy can be retrieved, at least in part, by resonance processes between different pairings of the spins into singlet bonds, as quantum mechanically a spin can after all be in a superposition of singlet bonds with different neighbours. One would then hope that such a sea of singlet pairs would present less of an obstacle to hole motion than the Néel state.

Following this route, Kivelson, Rokhsar and Sethna developed what has become known as short-range resonating valence bond (SR-RVB) physics.²⁾ In particular, the Rokhsar-Kivelson (RK) quantum dimer model (QDM),³⁾ which this account is in large part devoted to, restricts the wavefunctions to contain products of valence bonds between nearest neighbours only, as opposed to the longer-range valence bonds included in more general approaches. Somewhat disappointingly, they found that such a model would again lead to a ground state with broken translational symmetry,^{3),4)} except at an isolated critical point, with order not in the spin-spin but rather in a correlation function of singlets. The resulting crystalline order again impedes

hole motion in a manner completely analogous to the situation in the Néel state (see Fig. 1).

The short-range RVB liquid was thus a phase in search of a Hamiltonian. In the following, we show that the RK quantum dimer model on the *triangular* lattice, has an RVB liquid phase for a finite region of parameter space, flanked by a number of crystalline phases. Unlike those, the liquid is topologically ordered and exhibits fractionalised deconfined excitations. We show how the topological degeneracy gets lost under the duality transformation to an Ising model, and close by mentioning recent developments. We have tried not to duplicate any technical content, which can be found in Ref. 5) (RVB liquid), Ref. 6) (with Premi Chandra on transverse field Ising models) and Ref. 7) (with E. Fradkin on gauge theories).

§2. The Rokhsar-Kivelson quantum dimer model

In this section, we give a description of the RK-QDM on the triangular lattice, following the original formulation for the square lattice.^{3),8)} The basic starting point is the restriction of the Hilbert space of the spins with $S = 1/2$ residing on the sites of the lattice to those states which can be written as a product of singlet pairs between spins on neighbouring sites. Such singlet pairs are conveniently denoted by dimers, and the requirement that each spin be in a singlet pair with exactly one of its neighbours implies that the restricted Hilbert space can be labelled by *hardcore* dimer coverings of the lattice that the spins reside on.

The first issue to worry about is whether such states are linearly independent. The answer to the first question on the square lattice is yes.⁹⁾ This appears to be the case as well for a sufficiently large triangular lattice.¹⁰⁾ For increasingly highly-connected lattices, this will certainly cease to be the case, as can easily be seen for a quadruplet of mutually interconnected spins, which have two global singlet states but allow three dimer coverings.

Quite generally, different dimer coverings are not orthogonal. In fact, the overlap between two dimer coverings can be determined as follows. One can form what is known as a transition graph by superimposing two dimer configurations. Where the locations of a pair of dimers coincides in the two coverings, one obtains a doubly occupied bond. The other dimers give rise to closed loops, of varying length L_i , in the transition graph. The overlap between the two wavefunctions is the product over such loops of $2x^{L_i}$, where $x = 1/\sqrt{2}$.

2.1. The overlap expansion

Let us label the dimer coverings by $|i\rangle$, so that their overlap matrix (which is real and symmetric: $S = S^T$) is given by $S_{ij} = \langle i | j \rangle$. Let us now assume that $S^{-\frac{1}{2}}$, the inverse square root of S , exists.^{*}) We define an orthonormal basis set $\{|\alpha\rangle\}$ via $|\alpha\rangle = \sum_i S_{\alpha,i}^{-\frac{1}{2}} |i\rangle$, so that $\langle \alpha | \beta \rangle = S^{-\frac{1}{2}} S S^{-\frac{1}{2}T}$, the unit matrix. The matrix elements of the antiferromagnetic nearest neighbour Heisenberg $S = 1/2$

^{*}) Since S is symmetric, so is $S^{-1T} = ((SS^{-1})^T S^{-1})^T = (SS^{-1})^T S^{-1}$, and hence also $S^{-\frac{1}{2}} = S^{-\frac{1}{2}} S S^{-\frac{1}{2}T} S^{-\frac{1}{2}T} = S^{-\frac{1}{2}} S^{-\frac{1}{2}} S S^{-\frac{1}{2}T} = S^{-\frac{1}{2}T}$.

Hamiltonian $H = J \sum_{\langle ab \rangle} \mathbf{S}_a \cdot \mathbf{S}_b$ are hence $\langle \alpha | H | \beta \rangle = \sum_{ij} S_{i\alpha}^{-\frac{1}{2}} \langle i | H | j \rangle S_{j\beta}^{-\frac{1}{2}}$. The trick devised by RK is to use the parameter x defined above to obtain an expansion of this expression which is then truncated.¹¹⁾ One finds $S^{-\frac{1}{2}} = 1 - x^4 \square + O(x^6)$, where \square equals one for the matrix element of two dimer configurations differing only by a single loop of length four in the transition graph, and vanishes otherwise. Note that each orthogonal state can still be labelled by the dimer covering, of which it contains an amplitude of $O(1)$. Similarly, $\langle i | H | j \rangle = -\frac{3}{4} J \hat{n}_d - (\eta - \zeta - 2)x^4 \square + O(x^6)$. Here, η (ζ) are the number of bonds linking sites separated by an odd (even) number of steps along the loop in the transition graph.

To obtain the lowest order contributions to the QDM Hamiltonian, H_{RK} , we first note that we are free to subtract a constant from H as this only changes H_{RK} by the same constant. We thus subtract the zeroth order term involving the number of dimers, $-\frac{3}{4} J \hat{n}_d$, so that the effective Hamiltonian is given by $H_{\text{RK}} = [1 - x^4 \square + O(x^6)] [-(\eta - \zeta - 2)x^4 \square + O(x^6)] [1 - x^4 \square + O(x^6)]$, so that the lowest order term is a kinetic (off-diagonal) one, namely $-(\eta - \zeta - 2)x^4 \square \equiv -t \square$. Its strength is thus given by $t = 2x^4$ for the square and $t = x^4$ for the triangular lattice.

We have so far ignored the issue of the sign of t . For the square lattice, RK noted that the sign of t is a matter of convention, and we can show that this remains the case for the triangular lattice. We do this in two steps. First, one can show by explicit computation that the Sutherland phase convention for the square lattice can be extended to the triangular lattice by choosing the sign of a singlet bond involving sites a, b such that $(a, b) = [\uparrow_a \downarrow_b - \uparrow_b \downarrow_a] / \sqrt{2}$ if site a is below site b or directly to its left. In this case, one finds $t < 0$.

To change the sign of t , one multiplies all basis states by a factor of $i^{s_r + s_{l,g} - s_{l,u}}$. Here s_r counts the number of dimers in that state on links pointing upwards and right, and $s_{l,g}$ ($s_{l,u}$) count the number of dimers on links pointing upwards and left

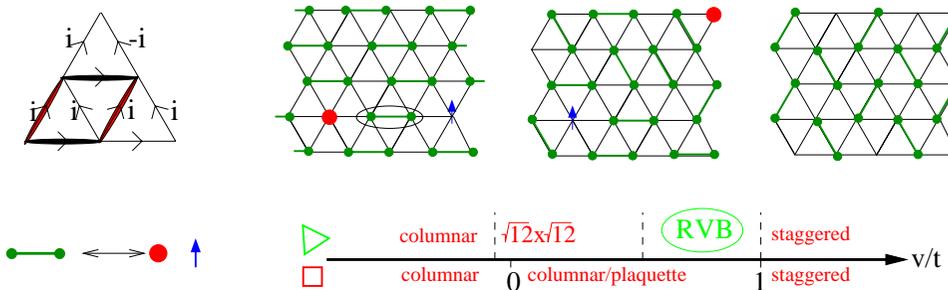


Fig. 1. Top left: The basic dimer resonances consist of replacing the horizontal pair of dimers by the slanted pair, and the symmetry equivalent moves. This process has kinetic energy t , and the presence of such a flippable pair costs potential energy v . The Sutherland singlet sign convention for the triangular lattice is indicated by arrows. Multiplying dimers on links by the phase factors $\pm i$ changes the sign of t . Bottom left: Knocking out an electron leaves behind a hole and an unpaired spin. Top right: Cartoons of columnar, RVB and staggered phases. Whereas a hole hopping through the columnar state generates a domain wall (encircled dimer), no such impediment to hopping exists in the liquid phase. Bottom right: phase diagram of square and triangular RK-QDM at zero temperature.

from a site with an even (odd) vertical coordinate (see Fig. 1). By this operation, every resonance move picks up an overall minus sign, and hence $t \rightarrow -t$.

In the perturbation expansion, one generates a non-trivial diagonal (potential) term at $O(x^8)$. This potential term (which is not affected by the factors introduced above) counts the number of dimer pairs which can participate in resonance moves, and has an amplitude of $v = 2(\eta - \zeta - 2)x^8$. In the RK model, however, one treats the ratio v/t as an adjustable parameter.

§3. The phase diagram — the RVB liquid phase

Two phases which occur as v/t is varied are easily identified. For $v/t > 1$, one finds that the ground state is one of twelve symmetry-equivalent staggered states, which are annihilated by the action of H_{RK} . For $v/t = -\infty$, there are $O(e^L)$ degenerate states, but fluctuations appearing for finite v/t select one (of six) columnar states at a high order in degenerate perturbation theory. Whether any other crystalline phases, as indicated in the phase diagram, are present as v/t is increased further is not settled.

The most interesting phase is a liquid anchored at the RK point $v = t$,⁵⁾ where the diagonal correlations³⁾ of the QDM are identical to the correlations of the *classical* dimer model. We have shown analytically that at the RK point, *all* dimer correlations are short ranged. We have also argued that this disordered point in fact terminates a gapped, liquidlike phase which exists for a nonzero range of values $v/t < 1$, and have provided evidence from Monte Carlo simulations on large systems at low temperature backing up this claim.⁵⁾

This phase finally realises one important aspect of the short-range RVB scenario: we have discovered a model, albeit an effective one, that has an RVB liquid ground state. One can verify that this phase bears all the important hallmarks, most crucially spin-charge separation and holon deconfinement. If one knocks out one electron, what is left behind is a hole on the site of the missing electron and an unpaired spin on the site of its partner; in this model, both are represented by monomers. An easy way to see that these entities are deconfined is provided by the following heuristic argument. Consider the energy of two static monomers a distance l apart. If l is much bigger than the correlation length, ξ , of the liquid, then separating the monomers even further will not change this energy significantly, as the effect of one monomer felt at the location of the other is exponentially suppressed. The monomer potential thus levels out and there is no confinement.

§4. Topological order — its fate under duality, and its relevance to quantum computation

Although the liquid phase breaks no symmetries, there turn out to be degenerate states of the QDM on a surface of nontrivial topology, for example a torus. The origin of this degeneracy can be seen by forming a transition graph of any state with some arbitrarily chosen reference state. One then finds that the transition graphs can contain noncontractible loops winding all the way around the torus; their number is

known as the winding number. Under any local dynamics, it becomes impossible in the thermodynamic limit to have matrix elements between dimer configurations with winding numbers differing by an odd number. One thus obtains degenerate sectors, labelled ‘even’ and ‘odd’. This degeneracy in the absence of symmetry breaking is a consequence of what Wen has termed ‘topological order’,¹²⁾ a concept we have discussed in this context in Ref. 7).

Duality: We have given a simple geometric demonstration of a duality between generalised dimer models (formulated as an ‘odd’ Ising gauge theory,⁷⁾ a topic of considerable current interest following a recently proposed experiment by Senthil and Fisher for the detection of fractionalisation¹³⁾ in the underdoped cuprates¹⁴⁾ and fully frustrated Ising models in a transverse field on the dual lattice. The basic idea is that each frustrated bond in the fully frustrated Ising model (on the dual hexagonal lattice) is denoted by a dimer; the frustration of the Ising model implies that the number of dimers per site is odd. The condition of only one dimer per site translates into considering only ground states of the Ising model in zero field. One may now ask what happens to the topological degeneracy under duality.

First, note that the mapping of spins onto dimers loses the Ising symmetry: a globally Ising reversed state produces the same dimer configuration. The Ising states can be paired into symmetric and antisymmetric combinations of Ising reversed states, which form disconnected sectors. The Hamiltonian in the former sector, which contains the system’s ground state, is identical to that of the dimer model, whereas in the latter sector, where the lowest excited state may reside, some matrix elements have the ‘wrong’ sign.⁶⁾ However, a gap in the symmetric sector (dimer model) will generally imply a gap for the Ising system.

In the reverse direction, note that the number of dimers crossed by a noncontractible loop on the torus encodes the number of spin flips encountered. For one (the other) sector, this number will be even (odd). For a consistent assignment of Ising spins, (anti-)periodic boundary conditions are thus required. Hence, the topologically degenerate sectors of the QDM map onto Ising models with different boundary conditions and *without* topological order.

So the question arises whether there can nonetheless be topological order in a ‘real’ spin system, rather than dimer systems. One possible path is to think of the dimers not of valence bonds but rather as spin 1/2 degrees of freedom, in terms of which the dimer model Hamiltonian has a different interpretation.

Reference 15) analyses an Ising spin model on the kagome lattice with ring-exchange dynamics, the ground states of which map onto a dimer model on the triangular lattice with three nonoverlapping dimers per site, rather than just a single one. Here, the above RK arguments and numerics yield the presence of a deconfined phase, in which a flipped spin will decay into two deconfined spin-1/2 excitations.

Quantum computing: Developing ideas by Kitaev,¹⁶⁾ Nayak and Shtengel¹⁷⁾ propose to use the degenerate liquid states of the kind we find in the triangular RVB liquid to construct q -bits. These are hoped to be especially stable as tunneling events are suppressed because the necessary matrix elements are absent for topological reasons.

A concrete realisation of such a q -bit, using the triangular RVB liquid, was very

recently proposed via a realisation of the triangular QDM in a Josephson junction array.¹⁸⁾ This proposal includes an idea of how to tune the tunneling rate between the topologically degenerate states, essentially by considering a system on an annulus near the inner, small circumference of which links can be weakened so as to lower the energy cost for the formation of a defect. On moving around the inner circumference, this defect induces tunnelling, the rate being exponentially sensitive to the energy cost of the defect.

§5. Conclusion

The QDM on the triangular lattice realises a bona fide RVB liquid phase. This demonstrates, as a point of principle, the possibility of constructing fractionalised phases via the SR-RVB scenario, as well as providing a route between a microscopic model and an effective Ising gauge theory. Its relation to other fractionalised triangular phases is at this point unclear.^{19), 20)} Finally, the liquid phase discovered by us may prove to be of substantial use in the context of quantum computing by virtue of its topologically stabilised degeneracy.

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