Spin Hamiltonians with resonating-valence-bond ground states

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Quantum dimer models exhibit quantum critical points and liquid states when the ground state is the resonating-valence-bond (RVB) state. We construct SU(2)-invariant spin-1/2 Hamiltonians with the same RVB ground state. The main technical obstacle overcome is the fact that different “dimer” configurations in the spin model are not orthogonal to each other. We show that the physics depends on how dimers are related to the spins, and find a Hamiltonian that may be quantum critical.

Quantum dimer models were designed to model antiferromagnets with a strong tendency to form short-range spin-singlet valence bonds [1]. They can be obtained in certain large-N limits from antiferromagnets with SU(N) or Sp(N) symmetry [2]. An important question is if the interesting physics found in quantum dimer models – e.g. quantum critical points with exactly computable exponents, and resonating-valence-bond (RVB) liquids [1, 3] – can be realized in spin-1/2 systems with an unbroken SU(2) symmetry. A “dimer” in the spin model is a nearest-neighbor singlet state, and a “dimer configuration” is a state where each spin is paired into a singlet with one of its neighbors. The RVB state is the equal-amplitude sum over all dimer configurations [4].

A crucial distinction between a quantum dimer model and the spin systems it models is that in the former, different dimer configurations are orthogonal, whereas in the latter they are not. This difference can dramatically change the physics [3]. There have been a variety of attempts to find quantum dimer physics in spin models (or vice versa). One can decorate the lattice so that different dimer states become more orthogonal as the amount of decorating is increased [3]. One also can define a spin model that resembles the quantum dimer model, and study it numerically [2]. Another method is to expand around the orthogonal limit, and develop a renormalization scheme to map the Heisenberg model onto a generalized dimer model [5].

Here we take a different tack. We construct a SU(2)-invariant spin Hamiltonian with an exact RVB ground state. This is similar in spirit to Refs. [9] and [10], but differs in detail. Because of the non-orthogonality, there are two distinct ways of defining spin models associated with a given quantum dimer model. When the Hamiltonian includes a nearest-neighbor antiferromagnetic Heisenberg term, the spin-spin correlation is exponentially decaying [5]. Changing the sign of this term causes competing ferromagnetic and antiferromagnetic interactions, likely resulting in very different physics.

We start by recalling some results for quantum dimer models with Rokhsar-Kivelson (RK) Hamiltonians [1, 3]. The Hilbert space in a quantum dimer model is spanned by configurations of nearest-neighbor dimers on some two-dimensional lattice, such that each site has a single dimer touching it. Each dimer configuration is orthogonal to all the others. Given a particular dimer configuration, a plaquette is flippable when each of its sites belongs to a dimer with an adjacent site on the plaquette. There are thus two possible ways a plaquette can be flippable, which we denote as $|h_a⟩$ and $|v_a⟩$. The RK Hamiltonian is comprised of a sum of projectors, each of which acts only on the dimers on a single plaquette. It includes a “flip” interchanging $|h_a⟩$ and $|v_a⟩$, the simplest off-diagonal term possible in the quantum dimer model. Letting $Φ_a ≡ |h_a⟩ − |v_a⟩$ and $P^Φ_a = |Φ_a⟩⟨Φ_a|/2$ be the projector onto this state, we have

$$H_{RK} = ∑_a P^Φ_a . \quad (1)$$

Each term annihilates the sum $χ_a ≡ |h_a⟩ + |v_a⟩$, as well as all states non-flippable on $a$. Since each term in $H_{RK}$ is positive semi-definite, any state annihilated by all the terms is a zero-energy ground state. The RVB state, the equal-amplitude sum over all dimer states, is indeed such a ground state. The lattice and the boundary conditions determine whether this ground state is unique.

One remarkable consequence of having a RVB ground state in a quantum dimer model is that exact computations are possible, because equal-time correlators in this ground state are the same as those in the classical dimer model. The classical dimer model on any planar lattice can be solved by a mapping onto free fermions [11–13]. The resulting physics depends on the lattice. The classical dimer model on a bipartite lattice has a critical point where correlators decay algebraically. The RK Hamiltonian at this point therefore must be gapless and quantum critical [14]. When the lattice is not bipartite, the classical dimer model is not critical, and the quantum model has topological order: the model is gapped, and the excitations are fractionalized [3].

We turn to spin models, whose Hilbert space is comprised of a spin-1/2 particle at each site of a two-dimensional lattice. Our aim is to find an SU(2)-invariant Hamiltonian with the RVB state as its ground state. By RVB state, we always mean the equal-amplitude sum over all dimer configurations. To define this uniquely in the spin model, we must specify the convention for the sign of each dimer, i.e. which spin state in the singlet has a plus sign in front of it, and which
a minus sign. For our purposes, we need to distinguish only between two different kinds of RVB states, which we dub the positive-overlap and negative-overlap RVB states, or PRVB and NRVB respectively. In the PRVB state, the inner product between the two flippable configurations on a single plaquette obeys \( \langle h_a | v_a \rangle > 0 \), while in the NRVB state, \( \langle h_a | v_a \rangle < 0 \).

The Hamiltonians we construct contain two types of terms: “Klein” terms and “flip” terms. Klein terms (at least attempt to) give an energy to all non-dimer states \( \Phi \), whereas flip terms work analogously to \( H_{RR} \). All terms are written as products of various \( P^s(\Lambda) \), the \( SU(2) \)-invariant projector of the spin-1/2 particles at sites in the set \( \Lambda \) on to overall spin \( s \), i.e.

\[
P^s(\Lambda) = \prod_{j=r,f \neq s} \left( \hat{S}^s_\Lambda - j(j+1) \right),
\]

where \( \hat{S}^s_\Lambda = \sum_{\lambda \in \Lambda} \hat{S}^s_\lambda \) and \( r = (1 - (-1)^{2s}) / 4 \). Since a projector is positive semi-definite, a zero-energy ground state is annihilated by each term individually.

A Klein term acts on spins at site \( i \) and its nearest neighbors, a set we denote as \( N(i) \). In a dimer state, the spin \( i \) and one of the neighbors are in a singlet, so the spin of these \( |N(i)\rangle \) spins is less than \(|N(i)\rangle/2\). The Klein Hamiltonian

\[
H_K = \sum_i P^{\left| N(i) \right|/2}(N(i))
\]

then annihilates all dimer states, and sometimes certain non-dimer states as well. We say that the Klein term is perfect if the null space of \( H_K \) is exactly the dimer subspace. It was proved in \([10]\) that on dimerizable subsets of the honeycomb lattice, the square ladder, and the octagon-square lattice, the Klein term is perfect with open boundary conditions. (A dimerizable lattice is defined as a lattice that can be completely covered in dimers.) It also appears to be perfect for subsets of the square lattice with open boundary conditions.

Once a sign convention for the dimers is specified, the two flippable plaquettes \( |h_a\rangle \) and \( |v_a\rangle \) are defined in the spin model as in the dimer model, but these states are no longer orthogonal. While \( |\Phi_a\rangle \) and \( |\chi_a\rangle \) remain orthogonal, \( |\chi_a\rangle \) is no longer orthogonal to non-flippable plaquettes, so \( P^s \) no longer annihilates it. Therefore using \( H_{RR} \) in the spin model does not result in the RVB state as a ground state. We thus must find a projection operator that does not annihilate \( |\Phi_a\rangle \), and that annihilates all other dimer configurations on this plaquette, including \( |\chi_a\rangle \). It does not matter whether it annihilates non-dimer configurations, as long as these are given an energy by the Klein term.

We construct each flip term as a product \( A_a F_a \) of projectors obeying \( [F_a, A_a] = 0 \). The projector \( A_a \) annihilates all dimer states on a plaquette \( a \) that are not flippable, while \( F_a \) annihilates \( |\chi_a\rangle \) but not \( |\Phi_a\rangle \). Because \( F_a \) and \( A_a \) commute, such a flip term satisfies the desired properties. It is then straightforward to show that the ground states of the Hamiltonian

\[
H = H_K + \sum_a [F_a A_a + P_a \mathcal{P}_a]
\]

are the same as those of the quantum dimer model on the same lattice, if the Klein term is perfect. We will show that we always can find such pairs of projectors annihilating a NRVB state. For positive overlap, we can sometimes find such pairs, and sometimes not.

Before presenting the general result, we discuss the square lattice. The flip terms act on the eight spins illustrated in figure 1 the four spins comprising the plaquette \( a \), and the four nearest neighbors of two opposite corners. Any dimer configuration must contain exactly two dimers on the links connecting these eight spins, one dimer touching \( u_2 \) and the other \( l_2 \). If the plaquette is flippable, then these two are on the plaquette; if not, there must be at least one dimer on the links outside \( a \). Denoting by \( U_a \) the set of sites \( \{u_1, u_2, u_3\} \), and likewise for \( L_a \) and \( D_a \), the operator \( A_a = P_1^{3/2}(U_a)P_3^{1/2}(L_a) \) therefore annihilates any dimer configuration non-flippable on \( a \). (When the plaquette \( a \) is at the boundary of the lattice, this operator is modified to \( P_1^{1/2}(U_a)P_3^{1/2}(L_a) \).)

To find \( F_a \) for the square lattice, we exploit the fact that here, \( |\chi_a\rangle \) and \( |\Phi_a\rangle \) are each proportional to either the product of singlets or triplets on the diagonals. It is easy to check by writing out the states explicitly that for positive overlap \( P_0(D_a)|\chi_a\rangle = 0 \) and \( P_0(D_a)|\Phi_a\rangle = 0 \), while for negative overlap we have \( P_1(D_a)|\chi_a\rangle = 0 \) and \( P_1(D_a)|\Phi_a\rangle = 0 \). Since \( A_a \) does not act on the spins \( d_1 \) and \( d_3 \), it commutes with both \( P_0(D_a) \) and \( P_1(D_a) \). Thus \( A_a P_0(D_a) \) annihilates PRVB states, and \( A_a P_1(D_a) \) annihilates NRVB states. Thus for each overlap, we have explicitly constructed a Hamiltonian of the form (3) with a square-lattice RVB state as its ground state. The second term in (3) acts on the four spins of \( a \) and the four spins adjacent to the other two corners (i.e. the 90-degree rotation of fig. 1). Each term in \( H_K \) involves five spins, while each term \( F_a A_a \) or \( P_a \mathcal{P}_a \) involves 8 spins. We note that the square-lattice Hamiltonian proposed in Ref. [1] has extraneous ground states, because it annihilates the state \( |\Phi_a\rangle \) as well as \( |\chi_a\rangle \).

The projectors \( A_a \) and \( \mathcal{P}_a \) are easily generalized to other lattices. The plaquette \( a \) must be a polygon with
an even number $2n$ of sides, each connecting adjacent sites on the lattice. For each site $i$ on the polygon, let $\sigma(i)$ be the set consisting of $i$ and its nearest neighbors that are not adjacent on the polygon. The operator $P^{\sigma(i)/2}(\alpha(i))$ then annihilates any configuration with an "external" dimer connecting $i$ to a site not adjacent on the polygon. Labeling the sites on the polygon consecutively, the operators

$$A_a = \prod_{i \text{ odd}} P^{\sigma(i)/2}(\alpha(i)), \quad \overline{A}_a = \prod_{i \text{ even}} P^{\sigma(i)/2}(\alpha(i))$$

each annihilate all dimer configurations not flippable on $a$. Both work because all non-flippable dimer configurations on $a$ must have the same number of external dimers touching odd sites on $a$ as there are touching even sites.

For negative overlap between the flippable plaquettes, flip operators with the desired properties are

$$F_a = P^{n/2}(E_a), \quad \overline{F}_a = P^{n/2}(O_a), \quad (4)$$

where $E_a$ and $O_a$ are the sets of the even sides and the odd sides on the polygon respectively. Since $F_a$ acts only on the even spins, it commutes with $A_a$, and likewise $[F_a, \overline{A}_a] = 0$. Let $|h_a\rangle$ be the flippable plaquette where the dimers connect sites $(2j-1, 2j)$, while $|v_a\rangle$ has dimers on sites $(2j-1, (2j-2)\text{mod } n)$. This determines these states up to an overall sign. Up to this sign, the state $|h_a\rangle$ can be obtained from the state $|v_a\rangle$ by shifting just the even spins by 2 mod $n$. Since $F_a$ acting on the $n$ even spins is the projector of maximal spin, it produces a state completely symmetric in these spins. We therefore have $F_a|h_a\rangle = \pm F_a|v_a\rangle$, with the plus sign and minus signs occurring respectively for positive and negative overlaps between $|h_a\rangle$ and $|v_a\rangle$. Thus indeed $F_a|\chi_a\rangle = 0$ for negative overlap.

We thus have found a Hamiltonian of the form with the NRVB state as its ground state. This construction works for any lattice where the sign convention can be chosen so that $\langle h_a|v_a\rangle < 0$ for all $a$. The problem of constructing a Hamiltonian with the PRVB state for an arbitrary lattice is still open. Although our method works for the square lattice, it will not work for lattices such as the honeycomb where the plaquette has $4j + 2$ sites (such as the honeycomb): no $SU(2)$-invariant operator $F_a$ with the desired properties exists. However, in the honeycomb case, the Hamiltonian of Ref. 10 works. Moreover, for some non-bipartite lattices like the "pentagonal" lattice, there is no way to have positive overlap for all plaquettes, only negative $\overline{O}_a$.

One way to make a Klein term perfect is to "decorate" the lattice by adding two spins on every link 6. On such a decorated lattice, the RVB state is annihilated by a Hamiltonian whose terms involve only the spins on a given (decorated) plaquette $a$. As before, the flipping operator must annihilate all dimer states save the difference of the flippable configurations $|\chi_a\rangle$. For an even number $2p$ of sites on the undecorated lattice, we define

$$B_a = \prod_{j=1}^{p}(2 - P^{0}(a_{6j-2}, a_{6j-1}) - P^{0}(a_{6j+1}, a_{6j+2})), \quad \overline{B}_a = \prod_{j=1}^{p}(2 - P^{0}(a_{6j+1}, a_{6j+2}) - P^{0}(a_{6j+4}, a_{6j+5})), \quad (4)$$

where the site labels 0, 1, . . . , 6$p$−1 are interpreted mod 6$p$.

It is straightforward to check that both $B_a$ and $\overline{B}_a$ indeed annihilate all configurations not flippable on $a$, and that the operators $F_a = B_a F^P_a B_a$ and $\overline{F}_a = \overline{B}_a F^P_a \overline{B}_a$ have all the desired properties. Thus the Hamiltonian $H = H_K + \sum_a |F_a + \overline{F}_a|$ has the RVB state as a ground state.

We turn to the physics of the spin models with these RVB ground states. First, we note that the physics of the PRVB and NRVB states is likely to be quite different. One reason we expect this is that when $\langle h_a|v_a\rangle < 0$, then the two Néel states of alternating values of $S_z$ around the plaquette (i.e. + + + . . . ) are absent from $|h_a\rangle + |v_a\rangle$. Thus one does not expect an RVB state with this choice of overlap to be the ground state of a Hamiltonian with purely antiferromagnetic interactions. This assertion is straightforward to check by explicitly rewriting Heisenberg Hamiltonians in the dimer basis 8. For the quantum dimer model, the model is simply the classical dimer model. This follows from the fact that different dimer configurations are orthogonal. Letting $O(D)$ be the value of the operator $O$ in the dimer configuration $D$, we have

$$\langle \text{RVB}|O|\text{RVB}\rangle = N_D^{-1} \sum_D O(D),$$

where $N_D$ is the number of different dimer configurations, the partition function of the classical dimer model.

To generalize this to the spin model, we need to take into account the non-orthogonality of the inner product in the dimer basis. The inner product of two dimer configurations $D, D'$ has a nice geometric description 13. If we place both configurations on the same lattice, we then can form loops by gluing the dimers from $D$ and $D'$ together at each site. These are dense loops with exactly one loop touching each site. Then $\langle D|D'\rangle = \pm 2^{n_{z}+n_{x}−n_{D}}$, where $n_{D}$ is the number of loops of length 2 formed by this gluing (i.e. the number of links covered by a dimer in both $D$ and $D'$), $n_{z}$ is the number of closed loops of length greater than 2, and $n_{D}$ is the number of
The singlet state, while the factor of 2 for each loop arises because there are two non-vanishing terms in the inner product coming from alternating values of $S_z$ around the loop. Thus in the spin model \[17\],

$$\langle \text{PRVB}|O|\text{PRVB} \rangle = \frac{\sum \epsilon^{2n_c} n_2 O(\mathcal{L})}{\sum \epsilon^{2n_c} n_2}, \quad (5)$$

where each sum is over all closed loop configurations $\mathcal{L}$ formed by gluing two dimer configurations together. The extra factor of 2 for loops of length longer than 2 arises because there are two dimer configurations corresponding to each such loop. Equal-time correlators in the spin model with PRVB ground state thus identical to those in a classical dense loop model with weight 4 per loop (the effect of the length-2 loops can be absorbed in a weight per unit length of the longer loops \[8\]). The only terms contributing to the spin-spin correlator are those where both spins are on the same loop: when the two spins are on different loops, the sum over the two alternating-$S_z$ values on each loop makes this contribution vanishing.

Classical loop models, often known as the $O(N)$ loop models for weight per loop $N$, have been studied extensively. When the loops are on a two-dimensional bipartite lattice, the model can be mapped onto a Coulomb gas, and when $|N| \leq 2$, it has a critical phase \[19\]. For $N > 2$, correlators decay exponentially: heuristically, the energy from creating more loops always beats the entropy gain from creating long loops. For the PRVB state, $N=4$, and numerics for the square lattice indicate that the spin-spin correlator in the PRVB state indeed decays exponentially with a small correlation length \[2\]. This seems very different from the quantum dimer model, which on the square lattice with RK Hamiltonian is critical \[3\]. However, one can gradually go from spins to dimers by using decorated lattices \[4\], and there is no particular indication that the physics changes dramatically as the amount of decoration is increased. One way of reconciling these observations is if some quantities (e.g. dimer-dimer correlations) behave as they do in the dimer model, even though the spin-spin correlations decay exponentially.

We expect that the physics of the PRVB and NRVB states is very different, even though they correspond to the same quantum dimer model. Different inner products results in different physics for quantum dimer models on the Kagome lattice \[20\], and for quantum loop models \[21\]. For the NRVB state, the expression for correlators is the same as \[5\], except for important relative signs. For the square lattice with open boundary conditions, each plaquette flip changes the total number of loops by $\pm 1$. Therefore on the square lattice, each loop gets a negative weight:

$$\langle \text{NRVB}|O|\text{NRVB} \rangle = \frac{\sum \epsilon (-4)^{n_c} (-2)^{n_2} O(\mathcal{L})}{\sum \epsilon (-4)^{n_c} (-2)^{n_2}}, \quad (6)$$

Negative weights can cause cancellations between different configurations. For example, as we saw, the Néel state around a plaquette does not appear in $|\chi_0\rangle$ with negative overlap. Classical loop models with $N < -2$ do not seem to have been studied. Given that the classical dimer model is critical, and that size of the critical phase of the loop model gets larger as $N$ is decreased \[9\], it is possible that even spin-spin correlators in the NRVB state will be critical. Thus even though the NRVB state does not arise from purely antiferromagnetic interactions, the possibility that it could yield an $SU(2)$-invariant quantum critical point makes it a worthy subject for further study.

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