Resonating valence bond wavefunctions and classical interacting dimer models

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We relate properties of nearest-neighbour resonating valence bond (nnRVB) wavefunctions for SU(2) spin systems on two dimensional bipartite lattices to those of fully-packed classical dimer models with potential energy $V$ on the same lattice. We define a cluster expansion of $V$ in terms of $n$-body potentials $V_n$, which are recursively determined from the nnRVB wavefunction on finite subgraphs of the original lattice. The magnitude of the $n$-body interaction $V_n (n>1)$ is of order $O(g^{-(n-1)})$ for small $g^{-1}$, while $V_1$ reduces to a constant due to the fully-packed nature of the model. At leading non-trivial order on the square lattice, the interacting dimer model only has two-body interactions $V_2(g)$ that favour two parallel dimers on elementary plaquettes. Setting $g=2$ and using the results of earlier work on this interacting dimer model, we find that the long-distance behaviour of the bond-energy correlation function is dominated by an oscillatory term that decays as $1/|\vec{r}|^\alpha$ with $\alpha \approx 1.22$ for SU(2) spins. This result is in remarkable quantitative agreement with earlier direct numerical studies of the corresponding wavefunction, which give $\alpha \approx 1.20$.

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Spin liquid states of low dimensional insulating magnets, in which the constituent spins fail to develop any kind of long range order down to $T=0$ in spite of strong magnetic exchange interactions, are an interesting consequence of competition between the different magnetic interactions in the system. Explicit variational wavefunctions that encode such behaviours have played a very important role in our understanding of such states of matter [1]. Perhaps the best known examples of such wavefunctions are the resonating valence bond (RVB) wavefunctions introduced by Anderson and collaborators [2,3].

The simplest of these is the nearest neighbour RVB (nnRVB) wavefunction $|\Psi(g)\rangle$ for SU(2) spins on a two dimensional bipartite lattice. It is written as a uniform amplitude superposition of all possible product states in which each $A$-sublattice spin forms a SU(2) singlet state with one of its $B$-sublattice neighbours [4]. Although the $g=2$ wavefunction has been studied on the square lattice for over twenty years now [5], we owe a detailed understanding of its properties to much more recent work [6, 7]: In Ref [6, 7], spin and bond-energy correlations were measured in the square lattice case using Monte-Carlo methods to establish that this state has an exponentially decaying spin correlation function, $|C_S(\vec{r})| \sim \exp(-|\vec{r}|/\xi)$, but power-law bond-energy correlation functions at large $|\vec{r}|$: $|C_E(\vec{r})| \sim 1/|\vec{r}|^\alpha$, with $\alpha \approx 1.20$. While such a short-ranged spin correlation function is a characteristic property of spin-liquids, the power law form of the bond-energy correlation functions strongly suggests that the nnRVB wavefunction for SU(2) spins on the square lattice actually describes a critical state on the verge of a transition to an ordered phase in which the bond-energies order.

Here, we develop a precise non-perturbative mapping that connects properties of $|\Psi(g)\rangle$ on a two-dimensional bipartite lattice to those of a classical fully-packed dimer model on the same lattice, which has a non-trivial interaction potential $V$ for the dimers in addition to the usual non-overlapping constraint. We define a cluster expansion of $V$ in terms of $n$-body potentials $V_n$, which are recursively determined from the nnRVB wavefunction on finite subgraphs of the original lattice. $V_1$ reduces to a constant due to the fully-packed nature of the dimer model, while the $n$-body interaction $V_n (n>1)$ is of order $O(g^{-(n-1)})$ for small $g^{-1}$, and thus decreases with $n$. The rate of decrease is controlled by the smallness of $g^{-1}$, which also controls, via this mapping, the exponential decay of spin correlation functions in $|\Psi(g)\rangle$. To leading non-trivial order on the square lattice, the interacting dimer model only has two-body interactions $V_2(g)$ that favour two parallel dimers on elementary plaquettes. Setting $g=2$ and using the results of earlier work [6, 10] on this interacting dimer model, we find that the long-distance behaviour of the bond-energy correlation function in $|\Psi(g=2)\rangle$ is dominated by an oscillatory term that decays as $1/|\vec{r}|^\alpha$ with

$$\alpha \approx 1.22.$$  \hspace{1cm} (1)

This result is in remarkable agreement with recent studies of the SU(2) nnRVB wavefunction [3, 4], and provides a quantitative resolution of the surprising coexistence of short-ranged spin correlations and power-law bond-energy correlations in $|\Psi(g=2)\rangle$. Our non-perturbative mapping to an interacting fully-packed classical dimer model explains the success of the phenomenological approach of Tang et. al. [4], who were motivated by the connection between fully-packed dimer configurations and ground states of certain large-N SU(N) square lattice antiferromagnets to develop a phenomenological height model description of the critical aspects of $|\Psi(g=2)\rangle$, similar to that used for the long-wavelength properties of classical fully-packed dimer models [12, 13].
We begin our analysis by writing

\[ |\Psi(g)\rangle = \sum_{\mathcal{D}} |\mathcal{D}\rangle_g , \text{ where} \]

\[ |\mathcal{D}\rangle_g = \prod_{e \in \mathcal{D}} |\Phi_0(g)\rangle_e . \tag{2} \]

Here, the summation is over all fully-packed dimer configurations \( \mathcal{D} \), the product is over all edges \( e \) covered by a dimer in \( \mathcal{D} \), and \( |\Phi_0(g)\rangle_e \) is the \( SU(g) \) singlet state of the two spins connected by edge \( e \). The norm

\[ \langle \Psi(g) | \Psi(g) \rangle = \sum_{\mathcal{D}, \mathcal{D}'} \langle \mathcal{D}' | \mathcal{D} \rangle_g \]

(3)

can be readily expressed as the partition function \( \mathcal{Z}(g) \) of a classical fully-packed loop model in which each site belongs to exactly one non-intersecting loop, which can either be a doubled edge (consisting of a single edge traversed in both directions) or a non-trivial loop (consisting of four or more distinct edges which are each traversed once). For the case of \( SU(g) \) spins, one obtains \[ \mathcal{Z}_{\text{loop}}(g) = \sum_{\mathcal{L}} w_{\text{loop}}(g, \mathcal{L}) , \tag{4} \]

with \( w_{\text{loop}}(g, \mathcal{L}) = (g)^{n_d(\mathcal{L})} (2g)^{n_l(\mathcal{L})} \), where \( n_d(\mathcal{L}) \) is the number of doubled edges and \( n_l(\mathcal{L}) \) the number of non-trivial loops in the loop configuration \( \mathcal{L} \) (Fig 1). Expectation values and correlators of various physical quantities can also be represented in terms of estimators that measure probabilities for various loop-gas configurations. In the \( SU(2) \) case, the spin correlation function \( C_S(\vec{r}) = \langle S(0) \cdot S(\vec{r}) \rangle \) is proportional to the probability that points \( 0 \) and \( \vec{r} \) both lie on the same loop. On the other hand, the connected bond-energy correlation function \( C_{E,\mu}(\vec{r}) = \langle B_{\mu}(0) B_{\mu}(\vec{r}) \rangle - \langle B_{\mu}(0) \rangle \langle B_{\mu}(\vec{r}) \rangle \) can be related to the probabilities for the four points \( 0, \hat{\mu}, \vec{r}, \) and \( \vec{r} + \hat{\mu} \) to lie on the same loop or at most on two different loops \[ \tag{16} \]. Here, \( B_{\mu}(\vec{r}) = \langle \hat{S}(\vec{r}) \cdot \hat{S}(\vec{r} + \hat{\mu}) \rangle \) with \( \hat{\mu} = \hat{x}, \hat{y} \) representing an elementary lattice translation in the \( x \) or \( y \) direction. Since \( C_s(\vec{r}) \) is proportional to the probability of points \( 0 \) and \( \vec{r} \) being on the same loop, the short range nature of \( C_s \) implies that the \( g = 2 \) loop model is in a “gapped” phase with predominantly short loops. Indeed, since \( \mathcal{Z}_{\text{loop}} \) defines a conformally invariant loop model with a power law distribution of loop sizes for \( g = 1 \) \[ \tag{17} \], we expect that this distribution becomes exponential for \( g > 1 \). The most natural scenario is then that the entire \( g > 1 \) short-loop phase of \( \mathcal{Z}_{\text{loop}} \) is controlled (from a renormalization group standpoint) by the \( g = \infty \) fixed point.

Our approach to the existence of power law bond-energy correlation functions in this short loop phase starts with the elementary observation that a loop gas with extremely short loops can still have long-ranged correlations in the position and orientation of loops. More precisely, at \( g = \infty \), all loops are trivial in that they have length 2, and correspond to doubled-edges. The weight of any such loop configuration made up entirely of doubled edges is always \( g^{N_s/2} \) (where \( N_s \) is the number of lattice sites). We now represent all these doubled-edges by dimers to map such a loop configuration to a fully-packed dimer configuration \( \mathcal{D} \) on the same lattice. Thus, loop configurations that survive the \( g \to \infty \) limit all have equal weight and define the partition function of a fully-packed dimer model in which each dimer contributes a factor of \( g \) to the weight of \( \mathcal{D} \): \( w_{\text{dimer}}(g, \mathcal{D}) = g^{N_s/2} \) independent of \( \mathcal{D} \).

For \( g < \infty \), \( \mathcal{Z}_{\text{loop}} \) also gets contributions from more general configurations \( \mathcal{L} \) consisting of both doubled-edges and non-trivial loops (with 4 or more edges). Each non-trivial loop in such a finite-\( g \) configuration \( \mathcal{L} \) can be replaced in exactly two ways by a sequence of doubled-edges on alternating edges of this non-trivial loop. Thus, a general loop configuration \( \mathcal{L} \) with \( n_l \) non-trivial loops and \( n_d \) doubled edges maps to \( 2^{n_l(\mathcal{L})} \) different loop configurations made up purely of doubled edges, which we represent by dimers. Each finite-\( g \) configuration \( \mathcal{L} \) of the original loop model thus maps to \( 2^{n_l(\mathcal{L})} \) dimer configurations \( \mathcal{D}_\alpha \) (\( \alpha = 1, 2, \ldots 2^{n_l(\mathcal{L})} \)). Next, we distribute \( w_{\text{loop}}(g, \mathcal{L}) \), the original weight of \( \mathcal{L} \), equally among these \( \mathcal{D}_\alpha \). As a result, each of these \( 2^{n_l(\mathcal{L})} \) different configurations \( \mathcal{D}_\alpha \) acquire an additional weight \( w(g, \mathcal{L})/2^{n_l(\mathcal{L})} \).

This maps the original loop model to a dimer model...
with weights
\[ w_{\text{dimer}}(g, D) = \sum_{\mathcal{L} \subset D} \frac{w_{\text{loop}}(g, \mathcal{L})}{2^{n(\mathcal{L})}} = \langle \Psi(g) | D \rangle_g, \]
where \( \mathcal{L} \subset D \) denotes all loop configurations \( \mathcal{L} \) compatible with the fully-packed dimer cover \( D \), i.e. obtainable by superposing some fully-packed dimer cover \( D' \) on the given \( D \), and we have used Eqn (3) and (11) to obtain the second equality. The original loop partition function \( Z_{\text{loop}} \) is then equal to the partition sum over all fully-packed dimer configurations \( D \) with weights \( w_{\text{dimer}}(g, D) \):
\[ Z_{\text{loop}} = Z_{\text{dimer}} = \sum_D w_{\text{dimer}}(g, D). \]

As \( w_{\text{dimer}}(g, D) \) depends on the structure of \( D \), we have provided a precise non-perturbative mapping of the original loop model to an interacting, classical, fully-packed dimer model with potential energy \( V(g, D) \) given as
\[ V(g, D) = -\log(w_{\text{dimer}}(g, D)). \]

We now define a decomposition of the potential energy \( V(g, D) \) of a fully packed dimer configuration \( D \) into a sum of \( n \)-body potential energies \( V_n(D_n) \) of subconfigurations \( D_n \) consisting of \( n \) distinct dimers from \( D \):
\[ V(g, D) = \sum_n \sum_{D_n \in D} V_n(D_n) \]

The \( V_n \) are determined recursively from computation of the weight \( w_{\text{dimer}}^n(g, D_n) \) of \( D_n \) in the interacting dimer model on the finite subgraph \( \mathcal{G}_n(D_n) \) of the square lattice. Here, this weight is calculated via Eqn (3) from the loop model defined on \( \mathcal{G}_n(D_n) \), and the subgraph \( \mathcal{G}_n(D_n) \) consists of the \( 2n \) vertices covered by dimers of the subconfiguration \( D_n \), along with all allowed edges between these vertices.

In the first step of this recursive construction, we consider any particular \( D_1 \) and determine the weight \( w_{\text{dimer}}^1(g, D_1) \). The original loop model on \( \mathcal{G}_1(D_1) \) has only one valid configuration, which is a doubled edge on the only edge of \( \mathcal{G}_1(D_1) \). Using Eqn (11), we therefore have \( w_{\text{dimer}}^1(g, D_1) = g \). The logarithm of this weight defines the one-body potential
\[ V_1(\square) = V_1(\mathbb{I}) = -\log(g). \]

With this in hand, \( V_n \) for arbitrary \( n \) can be obtained recursively from the equation
\[ -\log\left[w_{\text{dimer}}^n(g, D_n)\right] = V_n(D_n) + \sum_{m=1}^{n-1} \sum_{D_m \in D_n} V_m(D_m), \]
where \( D_m \in D_n \) denotes all \( m \)-dimer subconfigurations \( D_m \) of \( D_n \), and \( \mathcal{G}_m(D_m) \) the corresponding subgraphs of \( \mathcal{G}_n(D_n) \).

For instance, to obtain \( V_2 \), we consider any particular \( D_2 \) and determine \( w_{\text{dimer}}^2(g, D_2) \) as follows: If \( \mathcal{G}_2(D_2) \) does not form a plaquette of the square lattice, there is only one valid configuration of the loop model on \( \mathcal{G}_2(D_2) \) (consisting of doubled edges that take the place of the dimers in \( D_2 \)). From Eqn (3), this gives \( w_{\text{dimer}}^2(g, D_2) = g^2 \). On the other hand, when \( \mathcal{G}_2(D_2) \) does form a plaquette of the square lattice, \( w_{\text{dimer}}^2(g, D_2) \) gets contributions from two of the three valid configurations of the loop model on \( \mathcal{G}_2(D_2) \). One of these consists of two doubled edges that take the place of the dimers in \( D_2 \), while the other is a non-trivial loop on the boundary of the plaquette. Eqn (3) then gives \( w_{\text{dimer}}^2(g, D_2) = g^2 + g \). Knowing \( w_{\text{dimer}}^2(g, D_2) \), \( V_2 \) can be obtained from the recursion relation Eqn (11) with \( n = 2 \). Clearly, \( V_2 \) is non-zero only if the two dimers live on the same plaquette of the square lattice, and in this non-trivial case we obtain
\[ V_2(\square) = V_2(\mathbb{I}) = -\log(1 + g^{-1}). \]

Similarly, \( V_3 \) is seen to be zero unless the three dimers live on a pair of adjacent plaquettes, and in this non-trivial case we obtain
\[ V_3(\square) = -\log\left[(1 + g^{-1} + g^{-2})(1 + g^{-1})^{-1}\right], \]
\[ V_3(\mathbb{I}) = -\log\left[(1 + 2g^{-1})(1 + g^{-1})^{-2}\right], \]
and the symmetry-related counterparts of Eqn (12) obtained by using lattice reflection and rotation symmetries.

It is clear that each \( V_n \) for \( n > 1 \) is of order \( O(g^{-n-1}) \) when the \( n \) dimers live on a contiguous set of plaquettes of the square lattice (sharing edges with each other), and zero otherwise. Our procedure thus expands \( V \) in the size of clusters, and is controlled by the smallness of \( g^{-1} \). It may be viewed as a classical version of the “Schrieffer-Wolff” canonical transformation approach familiar in the context of strongly interacting electronic systems; in the usual Schrieffer-Wolff transformation, the effects of higher energy states in a larger Hilbert space are encoded in modifications to the effective Hamiltonian that acts in the subspace of low-energy states, while in our classical version of this approach, the effects of lower weight configurations of the full loop model are encoded in the effective weights of a restricted subclass of high-weight dimer model configurations \( D \).

Expectation values of any operator \( \hat{O} \) can be calculated using the modified estimator \( \tilde{\mathcal{P}}_{\hat{O}}(D) \) constructed from the original loop gas estimator \( \mathcal{P}_{\hat{O}}(D) \) to correctly encode the effects of the low-weight configurations that are not contained in the dimer model:
\[ \tilde{\mathcal{P}}_{\hat{O}}(D) = \frac{1}{w_{\text{dimer}}(g, D)} \sum_{\mathcal{L} \subset D} \frac{w_{\text{loop}}(g, \mathcal{L})}{2^{n(\mathcal{L})}} \mathcal{P}_{\hat{O}}(\mathcal{L}). \]
Consider for instance the spin correlation function. To zeroth order in $g^{-1}$, the corresponding modified estimator is non-zero only if 0 and $\vec{r}$ are connected by a dimer in $\mathcal{D}$, while the $O(g^{-1})$ correction gives a non-zero result if 0 and $\vec{r}$ belong to the same flippable plaquette of $\mathcal{D}$ without being connected by a dimer, and similarly for higher order corrections. Thus the spin correlation function is expected to decay exponentially as a function of spatial separation. In the case of the bond-energy correlation function $C_{E_n}(\vec{r})$ defined earlier, it is readily seen that the leading large $|\vec{r}|$ behaviour is dominated by the first $O(g^0)$ term in the modified estimator, which is obtained by replacing each $B_n(\vec{r})$ by the dimer occupation number $n_\mu(\vec{r})$ of the corresponding edge in the dimer model:

$$C_{E_n}(\vec{r}) \sim \langle n_\mu(0)n_\mu(\vec{r}) \rangle_V - \langle n_\mu(0) \rangle_V \langle n_\mu(\vec{r}) \rangle_V , \quad (14)$$

where $\langle \ldots \rangle_V$ denotes averages computed in the dimer model with energy $V$.

As is well-known, such fully-packed interacting dimer models admit a microscopic height representation \[12, 13\], which upon coarse-graining leads to a coarse-grained height action that takes the form

$$S = \pi \rho \int d^2 r (\nabla h)^2 + \sum_{p=4,8,12\ldots} y_p \int d^2 r \cos(2\pi p h) + \ldots \quad (15)$$

where the ellipses denote higher gradient terms and higher powers of gradients consistent with symmetries \[12\], and the bare coefficients $\rho$ and $y_p$ are functions of $g$. The renormalization group theory for this height action is standard \[12, 13\]. In the present variables, it tells us that there is a line of fixed points $\rho^* = \kappa, y_p^* = 0$ with $0 < \kappa \leq 4$. As long as the bare values of $\rho, y_p$ and the coefficients of the omitted higher derivative and nonlinear terms are not too large, the system flows to an attractive fixed point $\kappa(g)$ on this fixed line.

As mentioned earlier, the $g \to \infty$ limit maps to a non-interacting dimer model since all interactions ($V_n$ with $n > 1$) vanish and $V_1$ simply represents the fugacity $g$ of each dimer. Therefore expect $\kappa(g \to \infty) = 1/2$ since this is the known value of the stiffness for a non-interacting dimer model on the square lattice \[12\]. As $g$ is reduced from $g = \infty$, the leading effect is an interaction $V_2$ that favours flippable plaquettes. The interacting dimer model with only $V_2$ present has been studied in detail in Ref \[8, 10\], which established that the renormalized stiffness $\kappa$ increases monotonically with the magnitude of $V_2$ until it reaches $\kappa = 4$, at which point the system undergoes a Kosterlitz-Thouless like transition to a columnar ordered state.

To access the physics of the nRVB wavefunction of $SU(2)$ spins, we therefore identify the magnitude of $V_2$ with the inverse temperature $\beta$ of Ref \[4\], and set $g = 2$ to obtain $\beta = \log(1 + g^{-1}) \approx 0.405 \quad (20)$. This places us deep in the high-temperature phase well above the transition to columnar order, and from Fig. 31 of Ref \[3\], we obtain the estimate $\kappa(g = 2) \approx 0.82$. Calculating the required dimer correlation function from the fixed point height action with this value of $\kappa$ using the standard correspondence between dimer occupation numbers and the height-field \[12, 13\], we obtain the leading, large $|\vec{r}|$ form of the bond-energy correlation functions:

$$C_{E_x}(\vec{r}) \sim \frac{(-1)^x}{|\vec{r}|^{1/\kappa(g)}} ; \quad C_{E_y}(\vec{r}) \sim \frac{(-1)^y}{|\vec{r}|^{1/\kappa(g)}} \quad (16)$$

which gives, upon setting $g = 2$, the result advertised earlier. In addition, both these correlation functions have a subdominant piece which goes as $(-1)^x y / |\vec{r}|^2$ independent of $\kappa(g)$.

We conclude by noting that our approach generalizes in an obvious way to include singlets between $A$ and $B$-sublattice sites that are further apart on the square lattice, as well as to the $SU(g)$ mRVB wavefunction on the honeycomb lattice. Again, we expect the corresponding loop models to be in a short-loop phase for all $g > 1$, and this allows us to access the physics of these wavefunctions for $g \geq 2$ by mapping to an interacting dimer model; on the honeycomb lattice, the leading interaction terms will favour flippable hexagons, while the presence of longer range singlets will introduce additional interactions on the square lattice. Possible generalizations to various three-dimensional bipartite lattices are more intriguing, since it is not obvious that the loop model will be in a short-loop phase for all $g > 1$ on any of these lattices.

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