Entanglement in doped Resonating Valence Bond states

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We investigate the entanglement properties of resonating valence bond states on a two dimensional lattice in the presence of dopants that remove electrons from the lattice creating holes. The movement of the holes generated by the Hubbard Hamiltonian in the regime of strong Coloumb repulsion in this setting could be responsible for the phenomenon of high temperature superconductivity as hypothesised by Anderson in Science 235, 1196, (1987). We argue that there is a particular density of dopants (holes) where the entanglement contained in the lattice attains its maximal value for the nearest-neighbour RVB liquid state.

INTRODUCTION.

In quantum many-body physics, resonating-valence-bond (RVB) states have received a lot of attention due to their importance in the description of different phenomena. They are used to describe the resonance of covalent bonds in organic molecules, behavior of Mott insulators without long-range antiferromagnetic order [1], superconductivity in organic solids [2], and the recently discovered insulator-superconductor transition in boron-doped diamond [3]. There are many other applications of RVB states (see e.g. [4]). Moreover, RVB states have been suggested as a basis for fault-tolerant topological quantum computation [5].

It was postulated by Anderson in Ref. [1] that the short range nearest-neighbour RVB state (also called RVB liquid) might be responsible for the phenomenon of high temperature superconductivity. The cuprate superconductors are recognized as doped Mott insulators as in the case of Strontium doped Lanthanum cuprate LSCO. The copper oxide planes are described by the one-band Hubbard model with a strong, on-site repulsion U. The RVB state on a square lattice for the Hubbard Hamiltonian with strong Coloumb repulsion was proposed by Anderson to be the Mott insulator phase of the system, i.e., the pure Lanthanum cuprate is in an RVB state [6].

Indeed, the ground state of the 2D Hubbard model with doping is still unknown. Numerical simulations indicate that the RVB scenario is the right one for coupled plaquettes and ladders [6], and recently experiments have been proposed to test the RVB scenario in fermionic atoms in 2D optical lattices [7]. These experiments propose methods to increase the inter-ladder coupling to check if the RVB state on ladders is adiabatically connected to the Hubbard model ground state on the square lattice, which would provide an experimental test of the RVB theory. In this paper, we investigate the entanglement properties of the RVB states in small-sized ladders and plaquettes and speculate on the behavior in the thermodynamic limit.

The entanglement properties of RVB states without dopants on many dimensional lattices has been investigated in [8]. The main conclusion of the Ref. [8] is that such states can only have (if any) a very small amount of bipartite entanglement between any two sites on the lattice but they are always genuinely multi-partite entangled.

In view of this, it is interesting to see how multipartite entanglement of RVB states depends on the density of holes. In particular, we are interested if changes in the amount of entanglement correspond to the experimental observation of the maximal Tc superconductivity in the hole density window 0.1 < µ < 0.15. Intuitively, one would expect entanglement to be larger in this window as well. This is because entanglement and supercurrent are both related to the existence of correlations and therefore their peaks should be related i.e. a larger entanglement would be more robust to increase in temperature.

To address these questions we first define the RVB states on a 2L site lattice with 2n holes and an appropriate entanglement measure. Subsequently, we investigate analytically lattices up to 24 sites with open boundary conditions. Based on the obtained results we conjecture that in the thermodynamic limit of L → ∞ the amount of entanglement reaches its maximum for some critical density of holes µcr, where 0 < µcr < 1.
FORMULATION OF THE PROBLEM

Let us consider a two dimensional lattice with open boundary conditions consisting of 2L sites, which is a union of two sub-lattices A and B in such a way that any site belonging to the sub-lattice A(B) has all its nearest neighbours belonging to the sub-lattice B(A). We define a dimer between sites \( a \in A \) and \( b \in B \) as a singlet state \( |\delta_{ab}\rangle = \frac{1}{\sqrt{2}}(|0\rangle_a|1\rangle_b - |1\rangle_a|0\rangle_b) \). A dimer covering is defined as a tensor product of dimers \( |\Delta_i\rangle = \otimes_{L=1}^{L=2}(|\delta_{ab}\rangle) \). Here the set of pairs \( [(a_1b_1), (a_2b_2), \ldots, (a_Lb_L)] \) represents a particular way of joining neighbouring sites of the two sub-lattices with singlets. The number of such sets for the case of square lattices with open boundary conditions is, from [9], [10], given by \( \frac{(2L)^{2L}}{2^{L}} \), where the probability distribution of the holes \( p(a_{i_1}, b_{j_1}, \ldots, a_{i_n}, b_{j_n}) \) depends on their detailed dynamics.

We would like to be very clear about the meaning of \( |\Delta_{2n}\rangle \), namely that, it may not be an accurate description of the state of the lattice of a real doped superconductor. First of all, the RVB theory is one of many theories of the discussed phenomenon [12]. Secondly, even within the RVB theory itself it is not clear how the state with 2n holes looks like [13]. For instance, one cannot exclude the possibility that long-range dimers will appear in \( |\Delta_{2n}\rangle \). However, it seems reasonable to assume that for a small amount of holes \( |\Delta_{2n}\rangle \) is an acceptable choice.

It is not clear how to quantify multiparty entanglement in the \( |\Delta_{2n}\rangle \) state. The problem arises from the fact that a commonly accepted definition of multiparty entanglement is that any bipartition of the considered many particle quantum state must be entangled. However, in our case any bipartition of the lattice (equivalently the bipartition of the state \( |\Delta_{2n}\rangle \)) leads to a state with a variable number of particles on each site of the bipartition. According to super-selection rules one cannot observe a superposition of states with different number of particles [14], which considerably complicates the task of quantifying entanglement in RVB states with holes.

As a measure of the amount of non-classical correlations in the lattice we take the geometric measure of entanglement [15], which is generalized to the multi-partite case in a straight-forward manner [16]. For pure states, the measure is given by the \( \frac{1}{2} \)-based logarithm of the squared modulo of the overlap between the state, and the separable state closest to it

\[
E(|\psi\rangle) = -\max_{|\psi_{sep}\rangle} \log_2 (|\langle\psi|\psi_{sep}\rangle|^2),
\]

where \( |\psi_{sep}\rangle \) is a separable state. In the case of our lattice, however, we deal with the subtle matter of super-selection rules, because the closest product state to the RVB state could involve forbidden local superpositions of a hole and an electron. For this reason, we use the average geometric measure. The averaging is done over all possible locations of the holes.

More precisely, we define an average geometric measure of entanglement on the state \( |\Delta_{2n}\rangle \) as

\[
E(2n) = \sum_{(a_{i_1}, b_{j_1}, \ldots, a_{i_n}, b_{j_n})} p(a_{i_1}, b_{j_1}, \ldots, a_{i_n}, b_{j_n}) E(|\Delta_{(a_1b_1), \ldots, (a_nb_n)}\rangle),
\]
where
\[
E(\{\Delta[(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)]\}) = -2 \log_2 \max_{|\psi_{sep}\rangle} \langle \psi_{sep}| \Delta[(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)] | \psi_{sep}\rangle. \quad (5)
\]

The maximum is taken over all fully separable states on the part of the lattice without holes and the physical meaning of \(E(2n)\) is clear; it is the average amount of entanglement one gets after locating the position of the holes on the lattice.

**RVB state without holes:** \(\tilde{E}(0)\).

First we consider the RVB state without holes. We already know from the Ref. [8] that it contains negligible two-site entanglement but it is genuinely multi-party entangled. Here we calculate \(\tilde{E}(0)\) that will serve us later as a basis for comparison with \(\tilde{E}(2n)\). Additionally, the same method of calculation will be used for \(n > 0\).

We have
\[
\tilde{E}(0) = -2 \max_{|\psi_{sep}\rangle} \log_2 |\psi_{sep}\rangle |\Delta| = -2 \log_2 \frac{C}{R}, \quad (6)
\]

where \(C\) is the number of dimer coverings for \(|\Delta|\), i.e.,
\[
C = \prod_{j=1}^{\sqrt{2}} \prod_{k=1}^{\sqrt{2}} (4 \cos^2(\frac{\pi j}{2n+1}) + 4 \cos^2(\frac{\pi k}{2n+1})) \text{ for open boundary conditions and } C = (\exp(\frac{2\pi}{\sqrt{2}}))^k \text{ for periodic boundary conditions in the square lattice. This result can be argued as follows. The state } |\Delta| \text{ always has an "anti-ferromagnetic" term of the form } |0101\ldots01\rangle \text{ or } |0101\ldots10\rangle \text{ with its coefficient equal to } \pm \frac{C}{R}. \text{ Naturally every other term has smaller coefficient, because in the superposition of all coverings only the antiferromagnetic terms add up. Thus, there is a fully separable state } |\psi_{sep}^{(0)}\rangle = |0101\ldots01\rangle \text{ for which the modulus of the scalar product with } |\Delta| \text{ equals } \frac{C}{\sqrt{R}}. \text{ However, the only fully separable state with equal number of zeros and ones is of the form } |x_1 x_2 \ldots x_n\rangle \text{ with } x_1 + x_2 + \cdots + x_n = L, \text{ which means that } |\psi_{sep}^{(0)}\rangle = |\psi_{sep}^{(max)}\rangle.
\]

**RVB with 2n holes:** \(\tilde{E}(2n)\).

To compute entanglement in this case it suffices to find the maximal overlap between \(|\Delta[(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)]\rangle\) and a fully separable state for every possible set of pairs \((a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)\). From the previous considerations we know that the maximum is reached for an anti-ferromagnetic separable state and it reads
\[
\frac{C[(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)]}{R[(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)]}, \text{ where } C[(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)] \text{ is the number of the coverings of the initial lattice with the sites } (a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n) \text{ removed and } R[(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)] \text{ is the normalization of the state.}
\]

**RESULTS**

In this section we present the main results of the paper.

We have analytically computed entanglement \(\tilde{E}(2n)\) using the method described above for ladders and plaquettes up to size 6x4 (ladder lattices of size \(3 \times 2, 4 \times 2, \ldots, 10 \times 2\) and rectangular lattices \(4 \times 3, 4 \times 4, 5 \times 4\) and \(6 \times 4\)). The results, shown in the Fig. [1] for ladders and Fig[2] for rectangular lattices, clearly show that \(\tilde{E}(2n)\) reaches the maximum at a certain hole density as the size of the lattice increases. Moreover, the maximum occurs at a low concentration of holes.
We now elucidate certain significant points in the calculations leading to the graphs in Figs 1 and 2. As an illustrative example, let us consider the lattice of size 6x4 with four holes, at which point the peak occurs in this structure. It is clear that the 4 holes can be in one of $C_{12}^2 \times C_{12}^2$ positions, where $C_m^n$ denotes the binomial coefficient. Hence, one has to average over the entanglement found in each of these cases to find $\bar{E}(4)$ for this lattice. However, in this calculation we omit the pathological positions of the holes in which a single site is surrounded on all sides by holes as in Fig. 3, in which case the rest of the lattice is unable to form a short-range RVB structure. Long-range dimers between sites belonging to the same sublattice would be needed to fill the lattice in such a situation and we omit the corrections accruing due to these. In any case, neglecting these situations cannot substantially alter the behaviour of entanglement because they occur with the probability of $4(C_{2}^{(ab/2)+1} - 1)/(C_{2}^{(ab/2)})^2$ for four holes in an $a \times b$ lattice. Note that the probability of occurrence of these situations is zero for two holes so that the positive gradient at the beginning of the curve is maintained and the existence of the peak is assured. Thus, we conclude that the peak in the graph is maintained even when these situations involving long-range dimers are taken into consideration.

It is seen from Fig. 2 that the initial gradient of the curve increases with the size of the lattice. If the trend continues for larger lattices, one might expect the peak to shift to the right and converge to a particular concentration in the thermodynamic limit.
and singlets are represented as lines between sites. The sublattice B. Shaded circles indicate holes in the lattice, and blue circles indicate those belonging to holes. In Fig[4] 1(A), the red circles indicate sublattice A sites and blue circles indicate those belonging to sublattice B. Shaded circles indicate holes in the lattice, and singlets are represented as lines between sites. The bipartite graph corresponding to the state is shown to its right in 1 (B). The graph has bipartition (A,B) with $A = \{1, 3, 5, 7, 9, 11, 13\}$ and $B = \{2, 4, 6, 8, 10, 12, 14\}$. Since, $|A| = |B| = L$, the graph is balanced. Edges of the graph connect vertex set A to B such that an edge connects a vertex to only one of its nearest neighbouring vertices on the lattice. Since there are L such edges, the size of the maximum matching of the graph is equal to L. The adjacency matrix for this graph is shown alongside in 1(C). To find R, we would need to superimpose the two coverings on each other as shown in Fig [5]. The resulting graph and its adjacency matrix (the sum of the two adjacency matrices in Fig [4]) are shown alongside. The number of degenerate and non-degenerate loops can then be calculated from the number of cycles in the graph.

It is hoped that with these methods and by experimental observations as suggested in [7], the entanglement vs hole density curve can be constructed in the thermodynamic limit. This might throw more light on the question of whether multipartite entanglement, defined in this average geometric sense could indicate the occurrence of the quantum phase transition.

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