Doping quantum dimer models on the square lattice

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A family of models is proposed to describe the motion of holes in a fluctuating quantum dimer background on the square lattice. Following Castelnovo et al. [Ann. Phys. (NY) 318, 316 (2005)], a generalized Rokhsar-Kivelson Hamiltonian at finite doping which can be mapped on a doped interacting classical dimer model is constructed. A simple physical extension of this model is also considered. Using numerical computations and simple considerations based on the above exact mapping, we determine the phase diagram of the model showing a number of quantum phases typical of a doped Mott insulator. The two-hole correlation function generically exhibits short-range or long-range algebraic correlations in the solid (columnar) and liquid (critical) phases of the model, respectively. Evidence for an extended region of a doped VBS phase exhibiting holon pairing but no phase separation is given. In contrast, we show that hole deconfinement occurs in the staggered dimer phase.

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Soon after the discovery of cuprate superconductors with high critical temperatures, Anderson suggested that the Resonating Valence Bond (RVB) state is the relevant insulating parent state that becomes superconducting under (arbitrary small) hole doping [1]. Such a state can alternatively be viewed as a spin liquid (SL), as it has no magnetic order and it does not break any lattice symmetry. Since then, the search for exotic SL in microscopic or effective models has been very active.

In quantum spin models, where magnetic frustration suppresses long-range magnetic order, spin liquids often compete with quantum disordered states named “Valence bond solids” (VBS) which break translation symmetry [2]. This is e.g. the case in the frustrated Heisenberg model with extended-range antiferromagnetic (AF) interactions [3]. In a VBS, nearest-neighbor spins pair up in bond singlets which order e.g. along columns or in a staggered arrangement. Hole doping has also been extensively studied in Mott insulators [4] and AF fluctuations have been identified as the glue for pairing. Unconventional pairing upon doping models exhibiting a VBS ground state has also been found [5].

In a pioneering work Rokhsar and Kivelson introduced a quantum dimer model (QDM), a Hamiltonian acting in the space of two-dimensional fully packed dimer configurations |c⟩ (generically called |c⟩). The dimer interaction V and the dimer-flip process J are schematically depicted in Fig. 1(a). As discussed in Ref. [6], the QDM can be considered as the simplest effective model to describe quantum disordered phases similar to the pseudo-gap phase of the cuprate superconductors. In that respect, one might think of the dimer flip term as originated directly from super-exchange between copper spins. At the special point V/J = 1, named Rokhsar-Kivelson (RK) point, the ground state (GS) is exactly known and can be mapped onto the partition function of a classical dimer model [6].

On the square lattice, the dimer-dimer correlations are algebraic, decaying as 1/r^2. This “algebraic SL” at the RK point is believed to be rather singular on the V/J axis since, as shown e.g. by numerical calculations [7], the GS is a VBS on both sides of it, a staggered phase for V/J > 1, a columnar phase at attractive V (i.e. V < 0), separated from the RK point by a small region of plaquette phase. The case of non-bipartite lattices, where the RK point has a gapped GS that shows fractional excita-
A generalized RK Hamiltonian is introduced in Ref. 6 and studied further later by Syljuåsen [9].

Doping was introduced at...
Fig. 3. Schematic picture of the parameter space of the models considered here: (a) J-β model (undoped) and (b) t-J-β model (doped). The RK axes (thick lines parametrized by β) are defined by J = 1 (undoped case) and by J = t = V_{hd} = 1 (doped case). The points P and R correspond to the origins at β = 0 on these axes.

In the β → 0 limit, the expression of ε_c^{\text{flip}} reduces to ε_0 and the significance of V becomes clear. Hereafter, V = 1 sets the energy scale. V_{hd} corresponds to a classical dimer-dimer interaction. We restrict ourselves to the attractive case and use units for β such that V_{cl} = -1. A cartoon of the Hamiltonian manifold parametrized by (J, β) is shown in Fig. 3(a). For J = 1 it is easy to check that the GS is simply given by \frac{1}{Z} \sum_c \exp \left( -\frac{1}{2} \beta V_{cl} |N_c| \right) |c⟩ with energy E_0 = 0, where the normalization factor Z = \sum_c \exp ( -\beta V_{cl} |N_c| ) can be considered as a partition function of a classical interacting dimer model. We have checked by ED data of a 8 \times 8 cluster within its fully symmetric space-group irreducible representation, that the specific heat [defined as β^2⟨N^2⟩ - ⟨N⟩^2] is very close to the MC results obtained for a very large cluster (not shown). The model displays a Kosterlitz-Thouless (KT) transition at β_{KT} ≃ 1.536 between a critical phase at β < β_{KT} (with β varying exponents) and a columnar dimer phase. Independently from our investigation, a similar mapping was derived and the properties of this critical phase were investigated by transfer-matrix techniques.

To investigate the expected confinement-deconfinement transition for holes at the KT transition, let us now generalize the construction by Castelnovo et al. to finite doping. We define the t-J-β Hamiltonian by adding a second diagonal term to the one of the J-β Hamiltonian, ε_c = ε_c^{\text{flip}} + ε_c^{\text{hop}},
\begin{equation}
ε_c^{\text{hop}} = V_{hd} \sum_{c' \in \mathcal{C}(c)} \exp \left\{ -\frac{1}{2} \beta V_{cl} (N_{c'} - N_c) \right\}
\end{equation}
where the sum now extends on the doped dimer coverings |c'⟩ connected to |c⟩ by a t-process [see again Fig. 1(b)]. Note that this new term, as the t-term ofIssue 1, scales like the hole concentration. V_{hd} is a new energy scale which naturally makes sense in the β → 0 limit discussed below. The term as for t = V_{hd} and J = 1 the GS can again be written as \frac{1}{Z} \sum_c \exp ( -\frac{1}{2} \beta V_{cl} |N_c| ) |c⟩. In analogy with the undoped case, we can again define a RK axis which runs along an orthogonal direction to the three-dimensional parameter space spanned by J, t, and V_{hd}. This RK axis is given by J = 1, t = V_{hd} and parametrized by β. A cartoon picture of this set of Hamiltonians is shown in Fig. 3(b). Since the hopping term (for t ≠ 0) couples all topological symmetry sectors the GS with energy E_0 = 0 becomes unique. Interestingly, the procedure followed here can be generalized to more complicated dimer or hole kinetic off-diagonal processes.

The β → 0 limit is of special interest. As seen above, the diagonal term reduces to a dimer-dimer repulsion of magnitude V (set to 1) and the undoped RK point is recovered for J = 1 (when holes are not present). Similarly, the second diagonal contribution reduces to a dimer-hole interaction on a plaquette [with definition given pictorially in Fig. 1(b)] of magnitude V_{hd}. The β = 0 limit therefore gives rise to a large class of physical Hamiltonians parametrized by arbitrary magnitudes of J, t and V_{hd} (measured in units of V = 1). A complete investigation of this model is left for a future study and, in the following, we restrict ourselves to J = V (= 1 for convenience) so that the “distance” from the RK-axis will be controlled by the deviation of t from V_{hd}.

We start first with the case of two holes in the t-J-β model. The hole-hole correlations have been computed by ED of a 6 \times 6 cluster for arbitrary t and, for convenience, for V_{hd} = 1. Results are shown in Fig. 4. The ED results show a rather smooth variation of R_{hh} across the transition at β_{KT}. However, the finite size scaling at t = 1 obtained by classical MC in Fig. 1(a) shows a clear qualitative change of behavior at the KT transi-
Conjectured phase diagram for two holes in the thermodynamic limit for $J = V (= 1)$ for $V_{\text{hd}} = V (= 1)$. Size dependence of $R_{hh}$ by (a) classical MC at $t = 1$ for various values of $\beta$ (log-log scale), (b) GFMC at $\beta = 0.8$ and $t = 0.5$ (linear scale). (c) Conjectured phase diagram for two holes in the thermodynamic limit for $J = V = V_{\text{hd}} (= 1)$ vs $\beta$ and $t$. The dashed region corresponds to the confined phase for $\beta > \beta_{\text{KT}}$.}

In conclusion, we have introduced a class of simple doped QDM on the square lattice which, we believe, provide insights on the physical quantum disordered phases of real materials. An exact mapping onto a doped classical dimer model (characterized by an inverse temperature $\beta$) can be realized along a one-dimensional manifold of this multi-dimensional space. Using numerical computations and simple considerations based on the above exact mapping, we determine the complete phase diagram of the model (at $V = J$) showing a number of interesting physical phenomena that, we believe, could be generic in the vicinity of a Mott insulator, beyond the framework of QDM. It is found that two doped holons are confined in the columnar VBS phase. At finite doping, evidence for an extended region of a metallic VBS phase exhibiting holon pairing without phase separation is given. In contrast, we find that the algebraic dimer-dimer correlations of the (undoped) critical (quasi-ordered) phase do not provide the confinement of two injected holons. Furthermore, as shown in the case of the staggered dimer phase, we point out that holon deconfinement can even occur in a VBS.

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