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Doping quantum dimer models on the square lattice

Didier Poilblanc,^{1,2} Fabien Alet,¹ Federico Becca,^{1,3} Arnaud Ralko,² Fabien Trouselet,¹ and Frédéric Mila²

¹ *Laboratoire de Physique Théorique, CNRS & Université Paul Sabatier, F-31062 Toulouse, France*

² *Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne, BSP 720, CH-1015 Lausanne, Switzerland*

³ *CNR-INFM Democritos Simulation Centre and International School for Advanced Studies (SISSA), I-34014 Trieste, Italy*

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A family of models is proposed to describe the motion of holes injected 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. More general models are also considered with arbitrary values of dimer-flip and hole hopping amplitudes, as well as dimer-dimer repulsion. Hole-hole correlations are investigated by Exact Diagonalization, Green's function and classical Monte Carlo methods. Upon increasing dimer repulsion, deconfinement abruptly appears in the staggered phase. In the generalized Rokhsar-Kivelson doped quantum dimer model derived here deconfinement occurs in the critical spin-liquid phase. We also conjecture the existence of two-hole bound states in some region of this deconfined 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 discrete (lattice) symmetry. Since then, the search for exotic SL in various type of 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. The role of hole doping in AF Mott insulators has also been extensively studied [4] and AF fluctuations have been identified as a possible source of hole pair binding. Unconventional pairing under doping frustrated spin models exhibiting VBS ground states 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 [6]. The dimer interaction V and the dimer-flip process J are schematically depicted in Fig. 1(a). In contrast to $SU(2)$ singlets, the dimer configurations (generically called $|c\rangle$) are defined *per se* to be orthogonal w.r.t. each others. 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,

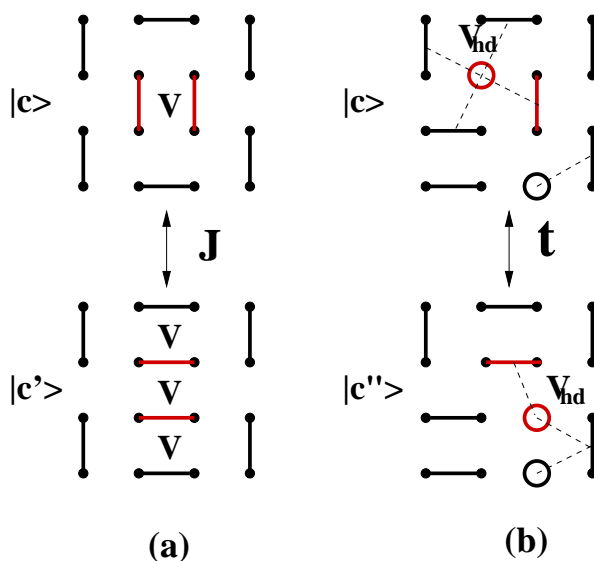


FIG. 1: (Color online) Pictures of the two quantum processes considered in this paper. (a) Dimer flip J within a plaquette. A dimer repulsion V is defined for all flippable plaquettes. (b) Hole hopping along a plaquette diagonal. In this process a dimer “rotates” from a vertical (horizontal) to a horizontal (vertical) bond. The hole-dimer repulsion V_{hd} is defined on all the dashed lines.

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 excitations [8], is also of great interest.

In this Rapid Communication we construct and study

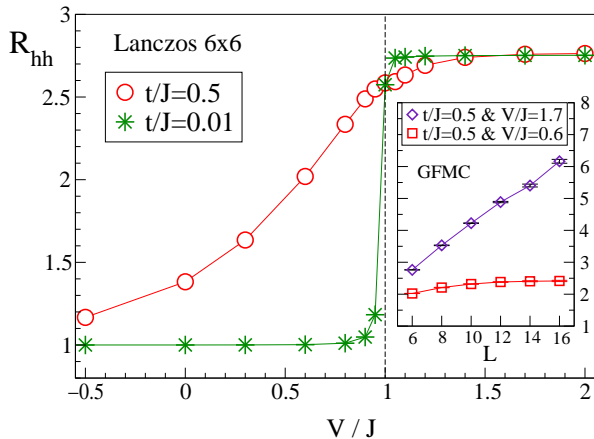


FIG. 2: (Color online) Mean-squared separation R_{hh} between two holes in the t-J-V model as a function of the ratio V/J . Calculations are done on a periodic 6×6 cluster for two values of the hopping t/J . Inset: Size dependence of R_{hh} obtained from GFMC on $L \times L$ clusters for two typical values of V/J and $t/J = 0.5$.

numerically various models of doped quantum dimers. A generalized RK Hamiltonian is introduced at *finite doping*. This model can be mapped onto a *doped* interacting classical dimer model enabling an efficient use of classical Monte Carlo (MC) [9]. We also extend this model to an enlarged physical space away from this so-called RK axis, where such a mapping is no longer valid [10] and where full quantum computations such as Lanczos Exact Diagonalisation (ED) and Green’s function Monte Carlo (GFMC) (restricted to two holes) are required. We provide evidence in favor of hole deconfinement in the algebraic dimer phase found in the extended model. However, we suggest that a two-hole bound state form in some region of this phase.

Let us first assume that holes are introduced by pairs on some of the dimer bonds. Next, the simplest way to account for the motion of these doped holes is to consider processes like the one depicted in Fig. 1(b) where a hole hops along a plaquette diagonal with some amplitude t [11]. Note that here holes are really thought of as new charge degrees of freedom originating e.g. from doping a Mott insulator by mobile carriers. A general form of doped QDM which operates in a Hilbert space with a fixed hole number can then be written as

$$H = \sum_c \epsilon_c |c\rangle \langle c| - J \sum_{(c,c')} |c'\rangle \langle c| - t \sum_{(c,c'')} |c''\rangle \langle c|, \quad (1)$$

where the sum over $|c\rangle$ includes all configurations with arbitrary hole positions. The sum over $|c\rangle$ and $|c'\rangle$ extends on all pairs of doped dimer coverings (only) differing by a single plaquette-flip [shown on Fig. 1(a)]. Similarly, the sum over $|c\rangle$ and $|c''\rangle$ extends to all pairs of doped dimer coverings differing (only) by a single hole hopping along a diagonal of a plaquette and a single dimer “hop” from a

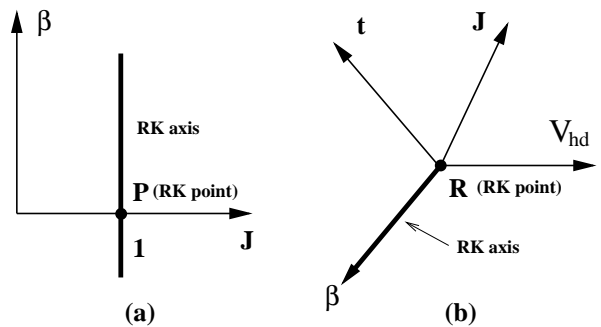


FIG. 3: Schematic picture of the parameter space of the models considered here; (a) J- β model (undoped) and (b) t-J- β model (doped). The RK axes (thick lines parametrized by β) are defined by $J = 1$ (undoped case) and by $J = t = V_{hd} = 1$ (doped case). The points P and R correspond to the origins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

vertical (horizontal) bond to a horizontal (vertical) bond. Such a process between two configurations $|c\rangle$ and $|c''\rangle$ is depicted in Fig. 1(b). As shown below, the role of the diagonal energies ϵ_c is crucial and various choices will be discussed. Whether mobile holes remain confined or not (or whether they form bound states) is the central issue of this study.

Following Ref. [6], we first start with the simple dimer interaction introduced above, namely $\epsilon_c = \epsilon_c^0 = VN_c$ where N_c corresponds to the number of flippable plaquettes in configuration $|c\rangle$. The properties of two holes [12] in such a t-J-V model [11] are studied here by ED and GFMC on finite clusters and the mean-squared hole-hole distance $R_{hh} = \sqrt{\langle r^2 \rangle}$ is shown in Fig. 2 as a function of the dimer repulsion V/J for fixed ratios t/J . A very abrupt variation is observed at $V/J = 1$ (especially at small t) showing a clear confinement at $V/J < 1$, as expected in a VBS, and a large value of the hole-hole separation for $V/J > 1$, which scales linearly with system size (see inset of Fig 2). In this case, the undoped system is also a VBS, but a pure staggered dimer state with no quantum fluctuations. It is therefore easy to see that the two holes can freely move away from each other in opposite directions along the same diagonal creating a string of dimers at 90° from the background at no energy cost [13]. On the contrary, in a plaquette or columnar VBS the energy cost grows linearly with the string length leading to confinement. Note that it was argued that confinement is lost for a sufficiently high fraction of holes (monomers) [11].

In order to construct more general doped QDM, we briefly re-examine the undoped case (i.e. zero doping for which the t term of Eq. (1) is irrelevant) and introduce a simple construction that extends the undoped RK point to an infinite axis. Following Castelnovo *et al.* [14], we define the J- β Hamiltonian by introducing new diagonal

energies as,

$$\epsilon_c = \epsilon_c^{\text{flip}} = V \sum_{c'(c)} \exp \left\{ -\frac{1}{2} \beta V_{\text{cl}} (N_{c'} - N_c) \right\} \quad (2)$$

where the sum extends on the dimer covering $|c'\rangle$ differing from $|c\rangle$ by a single plaquette-flip [shown on Fig. 1(a)]. In the $\beta \rightarrow 0$ limit, the expression of ϵ_c^{flip} reduces to ϵ_c^0 and the significance of V becomes clear. Hereafter, $V = 1$ sets the energy scale. V_{cl} corresponds to a *classical* dimer-dimer interaction. We restrict ourselves to the attractive case and use units for β such that $V_{\text{cl}} = -1$. 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 $\frac{1}{\sqrt{Z}} \sum_c \exp(-\frac{1}{2} \beta V_{\text{cl}} N_c) |c\rangle$ with energy $E_0 = 0$, where the normalization factor $Z = \sum_c \exp(-\beta V_{\text{cl}} N_c)$ can be considered as a partition function of a classical interacting dimer model [15]. Note that the above GS is in fact degenerate since this construction is valid in all topological symmetry sectors. Thermodynamic quantities can then be obtained from the corresponding GS expectation values. We have checked by ED data of a 8×8 cluster within its fully symmetric space-group irreducible representation and the $(0, 0)$ topological sector, that the specific heat [defined as $\beta^2 (\langle N_c^2 \rangle - \langle N_c \rangle^2)$] is indeed very close to the MC results obtained for a very large cluster (not shown). The model displays a Kosterlitz-Thouless (KT) transition [16] at $\beta = \beta_{\text{KT}} \simeq 1.536$ between a critical phase at $\beta < \beta_{\text{KT}}$ (with β varying exponents) and a columnar dimer phase [15]. Independently from our own investigation, a similar mapping was derived and the properties of this critical phase were investigated with transfer-matrix techniques [17].

To investigate the expected confinement-deconfinement transition for holes at the KT transition, let us now generalize the construction by Castelnovo *et al.* [14] to finite doping. We define the t - J - β Hamiltonian by adding a second diagonal term to the one (2) of the J - β Hamiltonian, $\epsilon_c = \epsilon_c^{\text{flip}} + \epsilon_c^{\text{hop}}$,

$$\epsilon_c^{\text{hop}} = V_{\text{hd}} \sum_{c''(c)} \exp \left\{ -\frac{1}{2} \beta V_{\text{cl}} (N_{c''} - N_c) \right\} \quad (3)$$

where the sum now extends on the doped dimer coverings $|c''\rangle$ connected to $|c\rangle$ by a t -process [see again Fig. 1(b)]. Note that this new term, as the t -term of (1), scales like the hole concentration. V_{hd} is a new energy scale which naturally makes sense in the $\beta \rightarrow 0$ limit discussed below. The term (3) is of central importance as for $t = V_{\text{hd}}$ and $J = 1$ the GS can again be written as $\frac{1}{\sqrt{Z}} \sum_c \exp(-\frac{1}{2} \beta V_{\text{cl}} N_c) |c\rangle$. 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 $J = 1$, $t = V_{\text{hd}}$ and parametrized by β . A

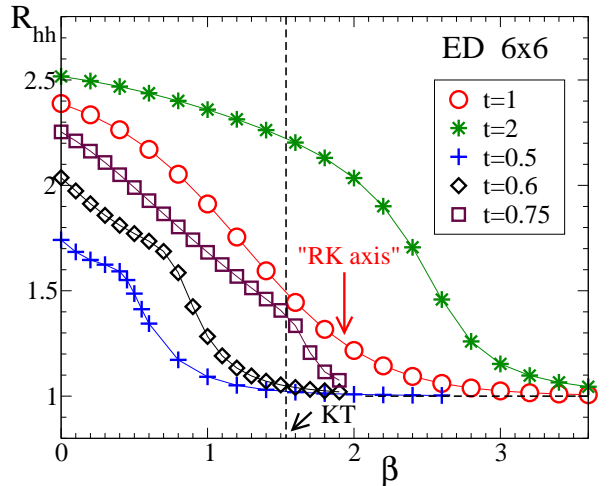


FIG. 4: (Color online) Mean-squared separation between two holes in the t - J - β model as a function of β . ED data obtained on a 6×6 periodic cluster are shown for several values of the hopping t and $J = 1$. The dashed line denotes the location of the KT transition at $\beta_{\text{KT}} \sim 1.536$. For $t = 0.5$ and $t = 0.6$ the “kinks” signal the appearance of a two-hole bound state.

cartoon picture of this set of Hamiltonians is shown in Fig. 3(b). Since the hopping term (for $t \neq 0$) couples all topological symmetry sectors the GS with energy $E_0 = 0$ becomes unique. Note also that the GS belongs to the most symmetric sector (*s*-wave, zero total momentum) since all its components have the same sign. Interestingly, the procedure followed here can be generalized to more complicated dimer or hole kinetic off-diagonal processes. Indeed, given any Hamiltonian H with *non-positive* off-diagonal matrix elements $H_{cc'}$ and a wave function $|\Psi\rangle$ with *positive* weights Ψ_c , one can always add the diagonal part $\sum_{(c,c')} (-H_{cc'}) \frac{\Psi_{c'}}{\Psi_c} |c\rangle \langle c|$ to H to get a new Hamiltonian for which $|\Psi\rangle$ is the GS with zero energy.

The $\beta \rightarrow 0$ limit is of special interest. As seen above, the diagonal term (2) 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 (3) reduces to a dimer-hole interaction on a plaquette [with definition given pictorially in Fig. 1(b)] of magnitude V_{hd} . The $\beta = 0$ 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 $J = V_{\text{hd}} = 1$ so that the “distance” from the RK-axis will be controlled by the deviation of t from 1. Note that the t - J - V model, defined above and corresponding to $\beta = 0$ and $V_{\text{hd}} = 0$, is disconnected from the restricted t - J - β model.

The hole-hole correlations in the t - J - β model have been computed by ED of a 6×6 cluster for arbitrary t and results are shown in Fig. 4. The ED results show a

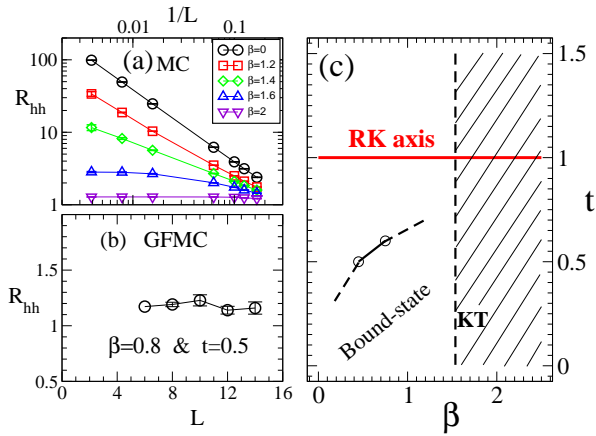


FIG. 5: (Color online) Results for the t - J - β model. Size dependence of R_{hh} by (a) classical MC at $t = 1$ for various values of β (log-log scale), (b) GFMC at $\beta = 0.8$ and $t = 0.5$ (linear scale). (c) Conjectured phase diagram for two holes in the thermodynamic limit for $J = V_{hd} = 1$. The dashed region corresponds to the confined phase for $\beta > \beta_{KT}$.

rather smooth variation of the mean-squared hole-hole distance across the transition at β_{KT} . However, the finite size scaling at $t = 1$ obtained by classical MC in Fig. 5(a) shows a clear qualitative change of behavior at the KT transition: while R_{hh} remains finite in the confined phase, it diverges as a power law in the critical phase in agreement with Ref. 15. For $t = 0.5$ and $t = 0.6$ we observe a kink in the ED data of Fig. 4. Moreover, for $t \leq 0.25$ R_{hh} remains always very close to 1, even when $\beta \rightarrow 0$ (not shown). We believe that this signals the appearance of a two-hole bound state within the critical SL phase in some range of β below β_{KT} . This scenario is supported by the GFMC data shown in Fig. 5(b). These results are summarized in a tentative phase diagram in Fig. 5(c).

In conclusion, we have introduced a class of simple doped QDM on the square lattice. An exact mapping onto a doped classical dimer model (characterized by an inverse temperature β) can be realized along a one-dimensional manifold of this multi-dimensional space. It is found that two doped holes are confined in the columnar VBS phase while bound states can appear in some region of the critical SL phase. In the original QDM Hamiltonian, by varying the dimer-dimer repulsion, we also observe a deconfinement transition of two doped holes correlated to the abrupt change of the host dimer background from a plaquette phase to a staggered dimer phase. Note that the numerical results presented here have been obtained at fixed hole *number* for which

the kinetic term of (1) is expected to have no effect on the bulk dimer-dimer correlations in the thermodynamic limit. The stability of the various phases under *finite* hole doping still remains to be investigated.

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