

Generic mixed columnar-plaquette phases in Rokhsar-Kivelson models

A. Ralko,¹ D. Poilblanc,¹ and R. Moessner²

¹ Laboratoire de Physique Théorique, CNRS and Université de Toulouse, F-31062 France
² Rudolf Peierls Centre for Theoretical Physics, Oxford University, 1 Keble Road, Oxford OX1 3NP, UK

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We revisit the phase diagram of Rokhsar-Kivelson models, which are used in fields such as superconductivity, frustrated magnetism, cold bosons, and the physics of Josephson junction arrays. From an extended height effective theory, we show that one of two simple generic phase diagrams contains a mixed phase that interpolates continuously between columnar and plaquette states. For the square lattice quantum dimer model we present evidence from exact diagonalization and Green's function Monte Carlo techniques that this scenario is realised, by combining an analysis of the excitation gaps of different symmetry sectors with information on plaquette structure factors. This presents a natural framework for resolving the disagreement between previous studies.

The Rokhsar-Kivelson Quantum Dimer model (RK-QDM) [1] on the square lattice, originally proposed in the context of high-temperature superconductivity, and its descendants have taken on a central role in the study of quantum systems incorporating a hard local constraint. They have thus been prominent in the context of hardcore bosons hopping [2] on frustrated lattices, Josephson junction arrays [3], frustrated Ising models in a transverse field or with small XY exchange [4], gauge theories in unusual sectors [5], spin orbital models [6] and cold atoms [7]. Studies of this model and its extensions have unearthed a wealth of phenomena, including instances of deconfined quantum criticality and a new route to deconfinement[8].

As many RK models belong to the rare class of models of correlated quantum matter without a sign problem, they are in principle amenable to efficient numerical study; they also tend to have well-studied effective field theories formulated in terms of height/gauge degrees of freedom [5]. This makes it all the more surprising that there is still substantial disagreement about the phase structure of the original RK model, the QDM on the square lattice. Indeed, a pioneering study by Leung et al.[12] suggested a transition out of a columnar phase (Fig. 1) to occur as v/t increases from $-\infty$ at $v/t \sim -0.2$ (see Eq. 1); however, a careful detailed recent investigation by Syljuasen[9] argued that in fact the columnar phase persists until $v/t \sim +0.6$.

A direct columnar-plaquette transition *en route* to the RK point at $v = t$ is in fact not unusual – it appears to exist in the closely related quantum six-vertex model on the square [10] and the hexagonal QDM [11]. Here, we show that there exists a second generic phase diagram where this first-order transition is replaced by a continuous interpolation via a mixed phase (Fig. 1). Based on Exact Diagonalisations (ED) and Green's Function Quantum Monte Carlo (GFMC) numerics we identify the square lattice QDM as the first candidate for realising this scenario: around $v/t = 0$, we find evidence of a mixed columnar-plaquette phase, which breaks translational symmetry in two perpendicular directions like

the plaquette, but also $\pi/2$ rotational symmetry like the columnar phase. The strongest evidence for such a phase is provided by a symmetry-based finite-size scaling analysis of the low energy spectrum.

The remainder of this paper provides the analysis backing up these assertions: first we present the pertinent numerical results on the QDM, followed by a more general analysis of RK models in $d = 2$ whose effective theory can be described by a height model.

The square lattice QDM Hamiltonian reads:[1]

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

where the sum over c runs on all configurations in the Hilbert space, $N_f(c)$ is the number of flippable plaquettes contained in $|c\rangle$, *i.e.* number of plaquettes with two parallel dimers, and the sum over (c,c') runs on all configurations $|c\rangle$ and $|c'\rangle$ that differ on a single dimer flip.

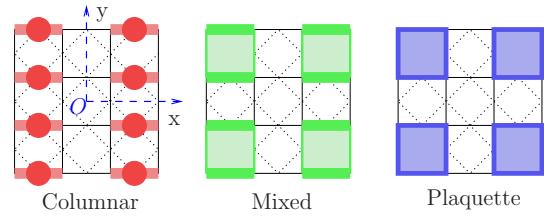


FIG. 1: Schematic representation of the different ordered states considered, the columnar, the mixed columnar-plaquette and the plaquette states. Dashed lines show the extra bonds of the checkerboard lattice of the equivalent hardcore boson model (see Ref. [2]). On the left, dimers (thick bonds) map to bosons (red circles).

Symmetry and first excitation spectrum: To compute excitation gaps we combine ED with GFMC calculations of dynamical correlations in imaginary time. In the latter case, the choice of an operator is crucial in order to “construct” an excitation with well-defined symmetry properties (*i.e.* quantum numbers). Starting with the elementary symmetry-breaking patterns of Fig. 1, degenerate ground states with different quantum numbers can

be constructed as listed in Table I. On general grounds, symmetry breaking involving any of these states is signaled on finite clusters of increasing size by the collapse of the quasi-degenerate GS and the opening of a robust gap above them to higher energy excitations. Clearly columnar and plaquette phases differ in two states with different quantum numbers (defined by a momentum and a point group quantum number), (Γ, B_1) (point $q = (0, 0)$) in the BZ depicted in the inset of Fig. 3, with symmetry B_1) for the first one and (K, A_1) ($q = (\pi, \pi)$) for the second. As shown in [10], a level crossing between two such energy levels was the signature of a first order phase transition. In contrast, as we show further down, no such level crossing is observed here, suggesting a more complex scenario.

Order	Γ, A_1	Γ, B_1	M, A_1	K, A_1	K, B_1	$M, A_1(*)$
Columnar	✓	✓	✓			
Plaquette	✓		✓	✓		
Mixed	✓	✓	✓	✓	✓	✓

TABLE I: Quantum numbers of the degenerate GS characterizing the ordered phases considered in this paper. We used the standard notation of irreducible representation of the C_{4v} and C_{2v} point group symmetries, acting around the site O as depicted in Fig. 1. Definition of the momentum points is given in the Brillouin zone of the inset of Fig. 3. Note that a state at momentum $(0, \pi)$, not shown, is degenerate with $(\pi, 0)$. (*) denotes the first excited level in the (M, A_1) sector.

Since ED are limited to 8×8 clusters we also used GFMC on clusters of size up to 22×22 to calculate gaps in different symmetry sectors by considering dynamical correlations as defined in [13]:

$$D(q, \tau) = \frac{\langle \Psi_G | P_\alpha(-q) e^{-H\tau} P_\alpha(q) | \Psi_0 \rangle}{\langle \Psi_G | e^{-H\tau} | \Psi_0 \rangle} \quad (2)$$

with $|\Psi_G\rangle$ a guiding function. To improve the quality of $|\Psi_G\rangle$ we explicitly work in the boson representation (see Fig. 1 and Ref. [2]) which enables to minimize a Jastrow wave-function with the help of a variational Monte-Carlo method. $P_\alpha(q)$ is a (diagonal) operator with the same symmetry as the excited state that we intend to target and is defined as the Fourier transform of plaquette operators

$$\begin{aligned} & \boxed{\begin{matrix} j \\ k \end{matrix} \begin{matrix} l \\ i \end{matrix}} \\ P_+ &= d(i)d(j) + d(k)d(l) \\ P_- &= d(i)d(j) - d(k)d(l) \end{aligned} \quad (3)$$

where $d(i)$ is the dimer operator acting on link i . Note that the point group symmetry of P_α depends on the momentum q . For P_+ , it always corresponds to the most symmetric A_1 irreducible representation (IR). For P_- , it

corresponds to the B_1 IR for the high-symmetry points, *e.g.* Γ and K , and to the A_1 IR at point M . Note also that the expectation value of $P_+(K)$ ($P_-(\Gamma)$) is finite in a generic plaquette (columnar) state.

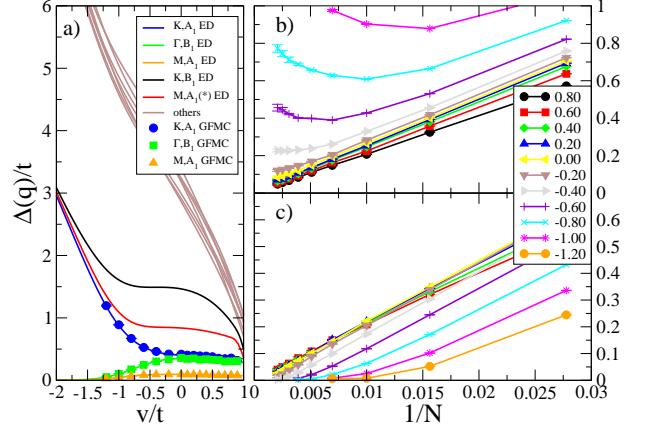


FIG. 2: First gap excitations. a) Comparison between ED and GFMC for the 8x8 site cluster for the interesting q -points. Size-scaling of the gaps for the (K, A_1) (b) and (Γ, B_1) (c) symmetries.

Our results for the excitation gaps are given in Fig. 2, with q -points defined through the Brillouin zone displayed in Fig. 3. Panel (a) shows the full exact spectrum on a 8x8-size cluster and a comparison with the GFMC estimates for the lowest levels. We find an excellent agreement which validates the GFMC method on larger clusters. Interestingly, our data distinguish three regimes: (i) for $v/t \lesssim -0.5$, the (Γ, B_1) and (M, A_1) levels have very small excitation energy and are well-separated from the rest of the spectrum by a sizable gap; (ii) for roughly $v/t > -0.5$, a second group of states of (K, A_1) , (M, A_1) and (K, B_1) quantum numbers joins the previous low energy states while remaining well separated from other higher energy states; (iii) the critical regime near the RK point $v \lesssim t$. A comparison with Table I immediately suggests a mixed phase and a columnar phase, respectively, for $v/t > -0.5$ and $v/t \lesssim -0.5$. These data seem already to be inconsistent with a pure plaquette state for which the $\Delta_{B_1}(\Gamma)$ ($\Delta_{A_1}(K)$) gap is finite (vanishing), which would imply a crossing of the (Γ, B_1) and (K, A_1) levels, in contradiction to what is seen numerically. To back up the above, we have performed finite size scalings of $\Delta_{A_1}(K)$ and $\Delta_{B_1}(\Gamma)$ shown in Fig. 2(b) and (c), respectively. $\Delta_{A_1}(K)$ clearly extrapolates to zero in the thermodynamic limit for $v/t > 0.1$ (compatible with both plaquette and mixed states) and opens up near $v/t \simeq 0.0 \pm 0.1$. Surprisingly, $\Delta_{B_1}(\Gamma)$ vanishes in the thermodynamic limit in the whole range of parameters studied (within an accuracy of 10^{-3}) with a clear exponential behavior for $v/t \lesssim -0.4$. Note that the fact that $\Delta_{B_1}(\Gamma)$ always remains smaller than $\Delta_{A_1}(K)$ for all sizes *itself* rules out a pure plaquette state.

Structure factors: Next we check that the above scenario obtained from the spectrum analysis (believed to be the most accurate criterium) is compatible with the behavior of the related structure factors,

$$I(q) = \frac{\langle \Psi_0 | P_\alpha(-q) P_\alpha(q) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}. \quad (4)$$

Results are displayed in Fig. 3 where the left panel shows the behaviors of the P_+ and P_- correlations along a given path of the Brillouin zone (on a 8x8-size cluster) and the right panel the size-scalings of their respective order parameters $M(q) = \sqrt{I(q)/L}$, L being the linear size of the system. These data correspond to $v/t = 0.2$, *i.e.* far from the proposed plaquette-columnar transition in [9], deep in the previously-supposed columnar phase. However, our results reveal a Bragg peak at point K which is found to survive upon extrapolation to the thermodynamic limit. On the right panel of Fig. 3, size-scalings suggest that columnar order only develops for $v/t \lesssim 0.6$ while a finite plaquette order is present in the range $0.0 \lesssim v/t \lesssim 0.8$.

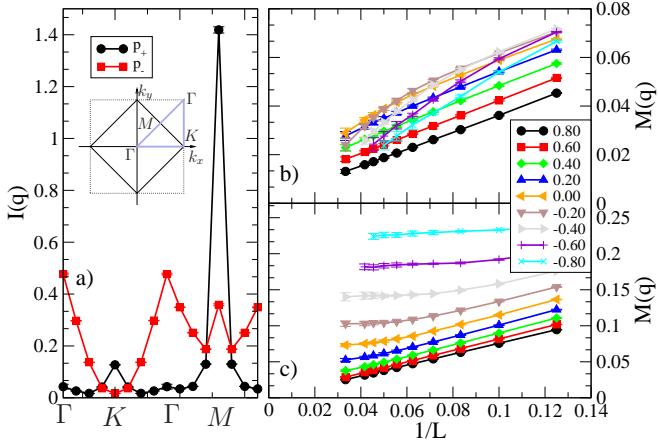


FIG. 3: a) Behaviour of the structure factor for the 8x8-site cluster at $v/t = 0.2$, along the path of the Brillouin zone depicted in the inset. A clear peak appears at point K . Size-scaling of the order parameters in the two symmetry sectors are given, for (K, A_1) (b) and (Γ, B_1) (c).

Discussion and interpretation of the numerics: Our extrapolated results as a function of v/t for the relevant gap and structure factors are summarized in Fig. 4. The results for the gaps provide clear evidence for lattice-rotation symmetry breaking for all parameters ($\Delta_{B_1}(\Gamma) = 0$) up to $v/t = 0.6$ (for $v/t > 0.6$ a tiny (Γ, B_1) gap cannot be excluded). We find two regimes: (i) For $v/t \lesssim 0.0$, $\Delta_{A_1}(K)$ is finite, indicating a pure columnar phase; (ii) for $0.0 \lesssim v/t \lesssim 1$, $\Delta_{A_1}(K)$ vanishes, implying an additional translation-symmetry breaking compatible with the mixed phase. The behavior of the structure factors is consistent with such a picture in this range of parameters. However, (i) error bars for $-0.1 < v/t < 0.1$ are still too large for *simultaneous* accurate extrapolations of *both* gaps and order parameters and (ii) upon

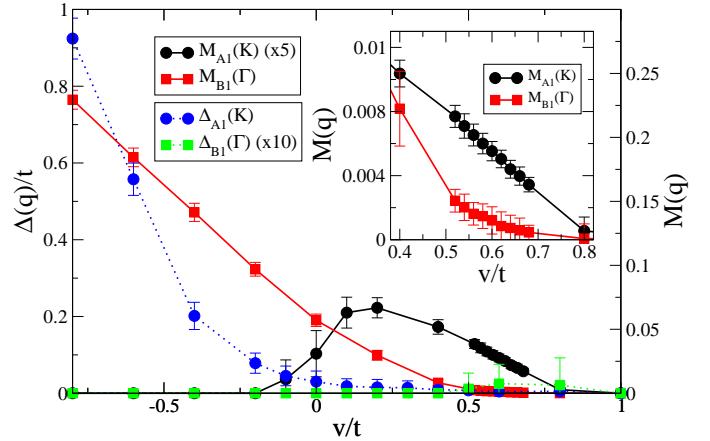


FIG. 4: Thermodynamic limit of the order parameters (black and red curves) and of the first excitation gaps (blue and green dashed curves) in function of v/t . $M_{A_1}(K)$ is multiplied by a factor 5 for clarity. A zoom around $v/t = 0.6$ is shown in the inset. $M_{A_1}(K)$ is not multiplied here.

approaching the continuous transition at the RK point, both structure factors become so small (inset in Fig. 4), that we are unable to distinguish them from zero within the accuracy of our simulations for $v/t \gtrsim 0.8$.

Syljuasen argued that rotation symmetry is restored when $v/t > 0.6$ signaling the transition to a pure plaquette phase, at least up to $v/t \simeq 0.9$ [9]. This claim is consistent with our results in that a small (Γ, B_1) gap cannot be ruled out for $v/t > 0.6$ and that it is plausible that our *diagonal* P_+ plaquette operator, although of the correct symmetry to "pick up" plaquette order, only gives a very small weight to the dynamical correlations when approaching the RK point. Also, note that the transition at $v/t = 0.0 \pm 0.1$ that we evidence here from the columnar state to the novel mixed columnar-plaquette state seems to be smooth and might be compatible with a second order phase transition. We believe our scenario of an intermediate mixed state reconciles the *a priori* conflicting results, (i) the ED data by Leung *et al.* suggesting the existence of an intermediate phase for roughly $v/t > -0.2$ [12] and (ii) Syljuasen's claim of a transition at $v/t = 0.6$ [9]. However, Syljuasen's analysis suggested that a mixed phase, if present at all, exists in a narrower range of parameters. At the same time, he pointed out that there was no sign of a discontinuous transition.

Effective height theory: We next show that the generic alternative to a first-order plaquette-columnar transition is a continuous interpolation between them *via a mixed phase*, in agreement with the scenario obtained above. This we do by reformulating the dimer model in terms of a height variable, h , living on the plaquettes of the square lattice. *Mutatis mutandis*, such a mapping applies to $d = 2$ RK models incorporating constraints which can be cast as local U(1) conservation laws [10, 11, 14].

The mapping from dimers to heights proceeds as fol-

lows. Label the two sublattices of the square lattice as red and green. When going from the centre of one plaquette to another in an (anti-)clockwise direction around a (red) green site, (add) subtract 1 from the value of the height if no dimer is crossed; and (subtract) add 3 if a dimer is crossed. An effective field theory starting from the microscopic heights can then be obtained for a *coarse-grained* height field h . This procedure is described in detail in a nice paper by Zeng and Henley [15], and the corresponding quantum theory is given in Ref. 5.

For our purposes, the following facts are important. Firstly, a ‘flat surface’, i.e. long-range order in h , corresponds to a dimer crystal. In particular, a (half-) integer valued $\langle h \rangle$ corresponds to a (columnar) plaquette phase, whereas intermediate values of $\langle h \rangle$ correspond to mixed phases like the one discussed above. Secondly, $h \rightarrow h + 1$ amounts to a $\pi/2$ rotation of the dimer configuration, so that $h \rightarrow h + 4$ leaves the dimer configuration unchanged. Finally, the leading terms in an effective action incorporating all terms not ruled out by symmetry or microscopic considerations of the model in $d = 2 + 1$ dimension are

$$\mathcal{S} = \int d^2x d\tau \quad [(\partial_\tau h)^2 + \rho_2(\nabla h)^2 \\ + \lambda \cos(2\pi h) + \mu \cos(4\pi h)], \quad (5)$$

where τ denotes Euclidean time. This action differs from that in Ref. 8 in two ways: (i) a term $(\nabla^2 h)^2$ is missing because it plays an important role only at the RK point where ρ_2 vanishes, whereas we are interested in what happens elsewhere; (ii) the term $\mu \cos(4\pi h)$ has been added as its presence is necessary for the analysis of the transition out of the columnar phase. To see this, let us minimise \mathcal{S} for uniform configurations. For $\mu = 0$, the sign of λ determines if one has a columnar ($\lambda > 0$) or plaquette state. At the transition point between the two, $\lambda = 0$, implying a continuous degeneracy ($\langle h \rangle$ can take any value $\in [0, 4]$), which has so far not been observed.

For $\mu \neq 0$, the fate of this transition depends on the sign of μ . For $\mu < 0$, the minima of the λ term coincide with those of the μ term, independently of the sign of λ . This destroys the continuous degeneracy at $\lambda = 0$, and leads to a simple first order transition between columnar and plaquette states. By contrast, for $\mu > 0$, the μ and λ terms compete: the minima of the latter coincide with the maxima of the former. Up to symmetries, one obtains $\langle h \rangle$ changing continuously between 0 at $\lambda = -4\mu$ and 1/2 at $\lambda = 4\mu$ as

$$2\pi\langle h \rangle = \begin{cases} 0, & \text{if } \lambda < -4\mu, \\ \arccos(-\lambda/4\mu), & \text{if } |\lambda| < 4\mu, \\ \pi, & \text{if } \lambda > 4\mu. \end{cases} \quad (6)$$

In the region $|\lambda| < 4\mu$ we therefore find a low-symmetry mixed state which continuously crosses over from primarily columnar to plaquette character. If $-\lambda/4\mu$ reaches

1 before v/t does, the mixed phase terminates before the RK point; otherwise, it will be terminated by the RK transition. We note that other ‘non-generic’ scenarios (e.g. for particularly small values of μ , or for non-monotonic dependence of λ/μ on v/t) are also possible.

Concluding remarks: The analysis of low energy spectra offers a powerful method to investigate spontaneous symmetry breaking, in particular eliminating the bias that the choice of an order parameter entails. While our system sizes – up to 30×30 sites with GFMC – are much bigger than those usually accessible to ED, they are still subject to the uncertainties of extrapolating delicate ordering phenomena to the thermodynamic limit.

However, our analytics support the numerics by showing that the phase diagram incorporating an intermediate mixed phase is one of two generic possibilities for such RK models, the other being a direct first order columnar-plaquette transition. The square lattice QDM is the first strong candidate for realising this new scenario.

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