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Correlations and order parameter at a Coulomb-crystal phase transition in a three-dimensional dimer model

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The three-dimensional classical dimer model with interactions shows an unexpected continuous phase transition between an ordered dimer crystal and a Coulomb liquid. A detailed analysis of the critical dimer and monomer correlation functions points to a subtle interplay between the fluctuations of the crystal order parameter and the “magnetic” degrees of freedom present in the Coulomb phase. The distribution probability of the crystal order parameter suggests an emerging continuous $O(3)$ symmetry at the critical point.

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I. INTRODUCTION

The Berezinskii-Kosterlitz-Thouless transition¹ is an example of critical phenomenon which cannot be understood from the conventional Landau-Ginzburg-Wilson (LGW) point of view, based on spontaneously broken symmetries and critical fluctuations of the associated order parameter.² Many quantum systems in one-dimension and classical systems in two-dimension (2D) exhibit such type of continuous phase transition, which is understood as a proliferation of topological defects. The recent suggestion³ that some phase transitions in $D > 2$ could also be outside the LGW framework triggered an important activity, both on the field-theoretical⁴ and numerical⁵⁻⁷ sides.

The classical dimer model on the cubic lattice^{8,9} is one of the simplest three-dimensional (3D) models with a transition which does not seem to fit in the LGW picture,⁹ although the field theory of the critical point has not yet been elucidated. Configurations of the model are hard-core dimer coverings of a cubic lattice.⁸ Each dimer occupies two sites and each site belongs exclusively to one dimer. In addition, each configuration has an energy equal to -1 times the number of square plaquettes with two parallel dimers.⁹ At low temperature T , this interaction favors the sixfold degenerate regular (crystalline) arrangements of dimers. At high T , the lattice symmetries are restored (dimer liquid), but dimer-dimer correlations decay algebraically with distance (with the same r^{-3} dependence as the interaction energy of two magnetic dipoles).⁸ This so-called *Coulomb phase* has also been found in other 3D models¹⁰ and is relevant to some pyrochlore compounds (see for instance Ref. 11).

The most intriguing properties of this dimer model concern the phase transition between the low- T crystal and the Coulomb phase. Previous simulations⁹ indicated that the transition is *continuous* (second order). This is already in contradiction with the LGW approach, which generically predicts a *first-order* transition in the present case. The main question, still open at present, is to understand what are the fields needed for a description of the long-distance properties at the critical point, and what is the associated field theory. In this Rapid Communication, we report on numerical investigations of correlation functions and order parameters in the vicinity of the critical temperature T_c . We show that the di-

polar character of the dimer correlations is gradually lost when approaching the transition, and find an unexpected probability distribution of the order parameter, with a possible emerging *continuous* symmetry. Related to rotations of a three-component order parameter, this $O(3)$ symmetry is not present at the microscopic level. Terms which make the symmetry group discrete at the lattice scale (a dimer can only take six orientations) may be irrelevant in the renormalization group (RG) sense at the critical point, but clearly relevant in the ordered phase. This finding is a step toward a description of the transition in the continuum limit, and establishes a tight connection with previous models (quantum⁶ and classical⁵) discussed in the context of non-LGW transitions.

II. DIMER CORRELATIONS: FROM DIPOLAR TO SPIN-SPIN FORM

In Coulomb phases, it is useful to introduce a magnetic field⁸ defined on each bond by $B_{ij} = -B_{ji} = 1$ if a dimer exists between sites $i \in A$ and $j \in B$ (A and B are the two sublattices) and $B_{ij} = 0$ otherwise. When considered as a vector field \mathbf{B} , its lattice divergence satisfies $\nabla \cdot \mathbf{B} = (-)^f = \pm 1$, as each site is occupied by exactly one dimer. Coarse graining over a large number of sites, the contributions of both sublattices cancel out to give $\nabla \cdot \mathbf{B} = 0$. In the continuum limit, \mathbf{B} is thus written using a vector potential: $\mathbf{B} = \nabla \times \mathbf{A}$. At high T and long distances, this zero-divergence constraint captures the essential aspects of the dimer hardcoreness.⁸ The Coulomb phase is then described by the simplest action compatible with the gauge invariance $\mathbf{A} \rightarrow \mathbf{A} + \nabla \Lambda$ (Λ is an arbitrary function), that is $S = \frac{K}{2} \int d^2 \mathbf{r} (\nabla \times \mathbf{A})^2(\mathbf{r})$. Here the rigidity K^{-1} depends on T . This effective action leads to dipolar long-distance correlations:⁸

$$\langle B^\alpha(0) B^\beta(\mathbf{r}) \rangle^c \sim \frac{1}{K(T)} \frac{3r^\alpha r^\beta - \delta^{\alpha\beta} r^2}{r^5}. \quad (1)$$

K^{-1} can be measured numerically through $LK^{-1} = \langle (\phi^z)^2 \rangle$; the fluctuations of the total flux $\phi^z = \int dx dy B^z(\mathbf{r} = [x, y, z_0])$ going through the sample (independent of z_0). Reference 9 showed that K^{-1} vanishes continuously when approaching the transition at $T_c \approx 1.675$, as magnetic-field fluctuations are costly

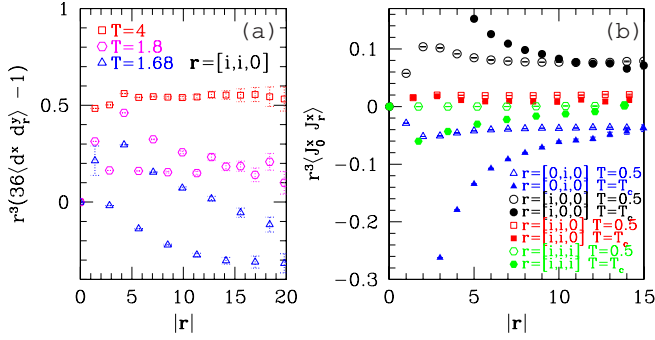


FIG. 1. (Color online) (a) Dimer correlations $\langle d_0^x d_r^x \rangle$ as a function of $|\mathbf{r}|$ and multiplied by $|\mathbf{r}|^3$ for a few selected T above T_c (system size $L=64$). For this orientation, the *spin* contribution vanishes. (b) Current correlations $\langle J_0^x J_r^x \rangle$ of the ICLM as a function of $|\mathbf{r}|$ and multiplied by $|\mathbf{r}|^3$ at $T=0.5$ (in the Coulomb phase) and $T_c=0.33305$ (system size $L=64$). Correlators at T_c have been multiplied by 50. Simulations of the dimer model (ICLM) were performed with the algorithm of Ref. 12 (Ref. 14).

when approaching the crystal. Although the dipolar form dominates at high T , we find that this contribution to the dimer-dimer correlations (Eq. (1)) progressively disappears when approaching T_c . In Fig. 1(a), the correlations $\langle d_0^x d_r^x \rangle^c$ for $\mathbf{r}=[i, i, 0]$ are multiplied by $|\mathbf{r}|^3$ to highlight the dipolar contribution and its strong reduction when going from $T=4$ to $T=1.68$ (just above T_c). This is expected since K^{-1} vanishes when approaching T_c . However, the magnetic action does not account for an important qualitative feature. Setting $\alpha=\beta=x$ in Eq. (1), the prefactor a of the dipolar contribution a/r^3 depends on the lattice direction (for instance $a=0$ for $\mathbf{r}=[i, i, i]$ and $a=1/2$ for $\mathbf{r}=[i, i, 0]$), whereas the actual correlations close to T_c appear to be almost *isotropic* [see Fig. 2(a)].

Equation (1) misses an important physical ingredient: the crystal-like dimer correlations associated to the order parameter of the symmetry-breaking phase. At each site, we define a three-component vector \vec{n} by $n^\alpha(\mathbf{r}) = \pm (-1)^{r^\alpha}$ if the dimer sitting in \mathbf{r} points in the direction $\pm \alpha$, and 0 otherwise. This ensures that \vec{n} is “ferromagnetically” correlated in the crystal phase ($\langle \vec{n} \rangle = \pm \vec{e}_x, \pm \vec{e}_y, \pm \vec{e}_z$ in the six ground states). Mak-

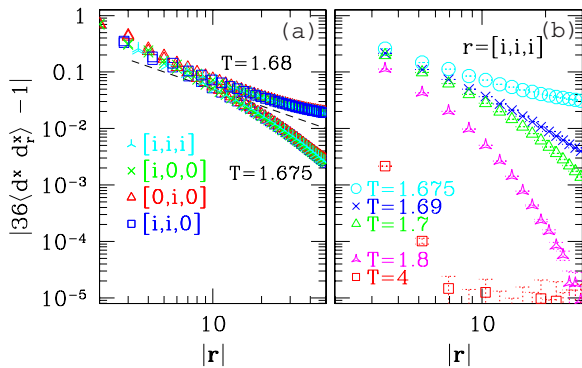


FIG. 2. (Color online) Dimer correlations $\langle d_0^x d_r^x \rangle^c$. (a) $T \approx T_c$ and just above, for different orientations of \mathbf{r} ($L=128$). (b) A few selected T above T_c ($L=64$). The lattice direction $\mathbf{r}=[i, i, i]$ is such that the *dipolar* contribution vanishes.

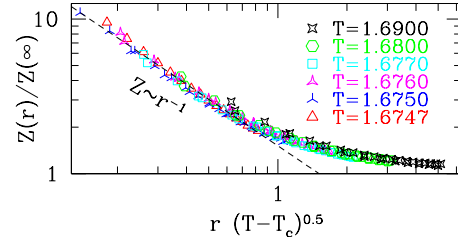


FIG. 3. (Color online) Monomer correlation as a function of r/ξ in log-log scale for a few T just above T_c , assuming $\xi = (T - T_c)^{-1/2}$ and $T_c \approx 1.6743$ ($L=128$).

ing the assumption that long-distance fluctuations of \vec{n} are described by a three-component “spin” model [i.e., absence of coupling between real space r^α and internal spin n^i indices, as in $O(n)$ models], the angular dependence of the correlations become $\langle n^\alpha(0) n^\beta(\mathbf{r}) \rangle^c \sim \delta^{\alpha\beta}$. It turns out that in a wide temperature range around T_c , the connected dimer-dimer correlations $\langle d^\alpha(0) d^\beta(\mathbf{r}) \rangle^c$ are well approximated by a dipolar contribution, plus a “spinlike” contribution:

$$\frac{(-1)^r 3r^\alpha r^\beta - \delta^{\alpha\beta} r^2}{K r^5} + (-1)^{r^\alpha} g(|\mathbf{r}|) \delta^{\alpha\beta}. \quad (2)$$

Taking $\alpha=x, \beta=y$, and $\mathbf{r}=[i, i, 0]$ [Fig. 1(a)], the “spin” term vanishes and only the dipolar part remains, whereas for $\alpha=\beta=x$ and $\mathbf{r}=[i, i, i]$ the dipolar part vanishes and one is left with $g(r)$. The latter is displayed in Fig. 2(b), where strong and slowly decaying correlations are found close to T_c . At T_c , $g(r)$ is very likely algebraic and compatible with $\sim 1/r$, although it is difficult to give an error bar on the exponent.

A more quantitative analysis can be done on the monomer correlator $Z(r, T)$, defined as the ratio of the partition function with two fixed test monomers at distance r , by the bare partition function. In the Coulomb phase, $Z(r, T)$ converges to a finite value when $r \rightarrow \infty$.⁹ As shown in Fig. 3, $Z(r, T)/Z(\infty, T)$ is well fitted by a function $F(x)$ of the single parameter $x = r\sqrt{T - T_c}$, suggesting the existence of a length $\xi(T) \approx (T - T_c)^{-1/2}$, diverging at T_c with an exponent ν compatible with 0.5. By construction $F(x \rightarrow \infty) = 1$, and we observe $F(x) \sim 1/x$ for $x \leq 1$, indicating that for distances $r \lesssim \xi(T)$, $Z(r, T)$ decays in a way consistent with $\sim 1/r$. At distances large compared to the lattice spacing, but small compared to some (diverging) correlation length $\xi(T)$, the correlations are thus qualitatively *not* of Coulomb type, although $T > T_c$. Below ξ , the correlations (of both dimers and monomers) are compatible with an exponent η close to zero. Noteworthy, these values are those obtained from independent thermodynamic measurements.⁹

It is instructive to compare these results with the correlations of a simpler model: the integer current loop model (ICLM).^{13,14} There, the allowed configurations are integer-valued currents $J_{ij} = -J_{ji} \in \mathbb{Z}$ defined on each bond (ij) of the cubic lattice (analogous to the dimer magnetic field \mathbf{B}), with the constraint that the net current arriving at each site is zero: $\text{div } \vec{J} = 0$. The energy of each configuration is $E = \frac{1}{2} \sum_{\langle ij \rangle} (J_{ij})^2$. This model also has a Coulomb phase at high T , with large

current fluctuations and dipolar $\langle J^\alpha J^\beta \rangle$ correlations. At low T , small current loops dominate and eventually $J_{ij}=0$ everywhere at $T=0$ (a state which does *not* have a dimer analog). Through a standard duality transformation,¹⁵ the ICLM maps exactly onto an $O(2)$ spin model with Villain interaction.¹⁶ In contrast to the dimer model, the phase transition of the ICLM $[T_c^{\text{ICLM}} \approx 0.333\ 05$ (Ref. 14)] is known to belong to the 3D-XY universality class. The Coulomb phase of the ICLM corresponds to the ordered phase in the angular variables θ_r , and the dipolar correlations are a direct consequence of the Goldstone mode for these dual spins. At high T , this dictionary works also well for the dimer model: K^{-1} is the *stiffness* of a dual $O(2)$ ferromagnet. The monomer correlation $Z(r)$ corresponds to the spin-spin correlation $\langle \exp(i\theta_0 - i\theta_r) \rangle$, and $Z(\infty)$ (finite in the Coulomb phase and vanishing at T_c) to the square of the order parameter (magnetization) $|\langle e^{i\theta_0} \rangle|^2$. The crucial difference with the dimer model is the absence of spontaneously broken symmetry in the low- T phase of the ICLM, and thus the absence of an order parameter similar to \vec{n} . This does not only make the critical exponents of the dimer model different from that of 3D XY,⁹ but marks a *qualitative* difference concerning the correlation in the Coulomb phase close to T_c [for $r \lesssim \xi(T)$]. The current correlations of the ICLM remain dipolar down to T_c . Both in the Coulomb phase and at T_c , they decay as $\sim 1/r^3$ with a geometric prefactor which does depend on the direction of \mathbf{r} [see the large- $|\mathbf{r}|$ behavior in Fig. 1(b)]. The ICLM obeys Eq. (1) without the need for an additional spinlike contribution. Only the overall amplitude is reduced close to T_c , with $1/K(T_c) \sim 1/L$ [see renormalization factor in Fig. 1(b)]. The fact that dimer correlations are dominated by nondipolar contributions close to T_c gives additional support for this transition not being of 3D XY nature, as naively expected from the high- T side.

III. SYMMETRY IN THE CRYSTAL ORDER PARAMETER AT T_c

The results above point to the importance of fluctuations of the crystal order parameter \vec{n} at the transition. We therefore looked at the distribution probability of $\vec{N} = L^{-3} \sum_{\mathbf{r}} \vec{n}(\mathbf{r})$ close to T_c . For large systems, the probability distribution of $(N^x, N^y, N^z \approx 0)$ is almost circular [see the distribution for $L=128$ and $T=1.673$ in Fig. 4(b)]. Some small squarelike anisotropy is still detectable but we argue below that it could be a finite-size effect and the asymptotic form of the distribution spherically symmetric in the thermodynamic limit. To quantify this, we define

$$C_4 = \frac{1}{2} \langle \cos(4 \arg[N^x + iN^y]) + \cos(4 \arg[N^y + iN^z]) + \cos(4 \arg[N^z + iN^x]) \rangle, \quad (3)$$

which measures the $O(3)$ character of the angular distribution of \vec{N} . If \vec{N} is distributed isotropically, C_4 vanishes in the thermodynamic limit. If \vec{N} preferentially points along the axis directions, one expects $C_4 > 0$. In the crystal phase $C_4 \rightarrow 1$ when $L \rightarrow \infty$, signaling that the direction of the order

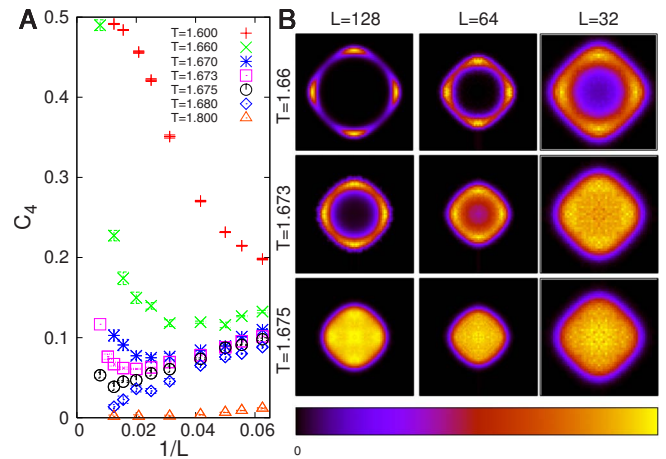


FIG. 4. (Color online) (a) Spherical character of the order parameter \vec{N} distribution (C_4) as a function of $1/L$ for different T . The data for $T=1.6$ have been divided by 2. (b) Probability distribution $P(N^x, N^y, |N^z| \leq 0.03)$ as a function of N^x and N^y for several temperature and system sizes. The range is $N^{x,y} \in [-0.3, 0.3]$ for $L < 128$ and $[-0.2, 0.2]$ for $L = 128$.

parameter \vec{N} is locked along one crystal axis [see the C_4 ($T=1.66$) and the associated distributions in Figs. 4(a) and 4(b)]. In the Coulomb phase, \vec{N} is typically very small ($\langle N^2 \rangle \sim L^{-3}$) and distributed in a Gaussian way, thus with spherical symmetry. The nontrivial result is the behavior of C_4 at T_c . Figure 4(a) suggests that $C_4(T=T_c, L) \rightarrow 0$ when $L \rightarrow \infty$, and thus indicate an $O(3)$ symmetric distribution of the order parameter.¹⁷

For T slightly below T_c , Fig. 4(a) reveals that $C_4(T, L)$ has a minimum for a system size $L_0(T)$. This minimum shifts to larger size when approaching T_c from below. $L_0(T < T_c)$ thus defines a length scale, diverging at T_c , up to which the discrete symmetry breaking becomes weaker at long distances.

This is similar to the 3D XY model with $Z_{q \geq 4}$ anisotropy,^{15,18} where the q -fold anisotropy is dangerously irrelevant and makes the (two-component) order parameter apparently $U(1)$ symmetric in the ordered phase, up to some length scale diverging at T_c . A crucial difference here is that the order parameter \vec{n} has three components, and a RG analysis of the $O(3)$ model predicts that cubic anisotropies, such as $(n^x)^4 + (n^y)^4 + (n^z)^4$, should be *relevant*.¹⁹ The latter anisotropic $O(3)$ model is however qualitatively different from the model studied here, as its high- T phase is a featureless paramagnet. From this point of view, the classical spin model of Ref. 5 (where a constraint equivalent to $\text{div } \mathbf{B} = 0$ is enforced on spin configurations) may be closer to our study since it also possesses a high- T Coulomb phase. Discrete anisotropies seeming irrelevant for the dimer critical point, both models would be predicted from the symmetry point of view to share the same universality class. However, based on the values of the critical exponents, this is not the case.

IV. DISCUSSION

The numerical observations of this Rapid Communication emphasize the unconventional nature of the Coulomb-crystal

phase transition. On one side, the presence of a diverging length scale below which correlations are not Coulomb-like cannot be interpreted by the sole high- T magnetic point of view. From the ordered side, we exhibited a length scale below which the crystal order parameter seems to fluctuate in an unexpected $O(3)$ symmetric way. Besides the difficulty to build a LGW theory from the corresponding order parameters,⁹ those are clear qualitative indications that individual (magnetic or crystalline) descriptions cannot capture the physics involved at the transition. This points to the existence of a critical regime where the interaction between the magnetic degrees of freedom at play in the Coulomb phase and the spin degrees of freedom which order in the crystal dominates the long-distance physics. This phenomenology is similar to that of a non-compact CP^1 (NCCPI) model,^{3,5} which precisely couples spin and gauge degrees of freedom. The NCCPI theory is characterized by two continuous symmetries: $SU(2)$ for spin rotations and $U(1)$ associated to the magnetic-flux conservation. In our case, the flux conservation is implemented at the lattice level and we argued that

continuous spin rotations emerge at the critical point. This is similar to the 2D quantum spin system studied in Ref. 6, but there the spin rotation symmetry is explicit and a gauge flux conservation is argued to emerge dynamically at the critical point. Despite all these common ingredients between NCCPI theories and our dimer model, there is a clear mismatch between our critical exponents and those attributed so far to NCCPI critical points.^{5,6} So, the actual field theory describing the dimer model transition remains to be uncovered. Besides its theoretical importance, the issue of the universality class of this transition will also become experimentally relevant if a Coulomb-crystal phase transition was observed in nature, as in a frustrated (icelike) magnet for instance.

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