Unconventional Continuous Phase Transition in a Three-Dimensional Dimer Model

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Phase transitions occupy a central role in physics, due both to their experimental ubiquity and their fundamental conceptual importance. The explanation of universality at phase transitions was the great success of the theory formulated by Ginzburg and Landau, and extended through the renormalization group by Wilson. However, recent theoretical suggestions have challenged this point of view in certain situations. In this Letter we report the first large-scale simulations of a three-dimensional model proposed to be a candidate for requiring a description beyond the Landau-Ginzburg-Wilson framework: we study the phase transition from the dimer crystal to the Coulomb phase in the cubic dimer model. Our numerical results strongly indicate that the transition is continuous and is compatible with a *tricritical* universality class, at variance with previous proposals.

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The Landau-Ginzburg-Wilson (LGW) theory of phase transitions [1] has been a remarkably powerful approach to study critical phenomena, both in classical and quantum systems. The basic assumption is that each phase is characterized by its symmetries and a local order parameter for the broken symmetries (in case of an ordered phase). To describe a phase transition, this approach amounts to expanding the free energy of the system in powers of the order parameter(s) describing the ordered phase(s). Exceptions are, however, known in 2D classical or equivalently 1D quantum systems where stable *critical phases* (with power-law correlations but *no* broken symmetry) exist, the low-temperature phase of the 2D XY model being one of the most famous examples. The associated Kosterlitz-Thouless (KT) phase transition [2] and the role of topological defects have become very fruitful concepts in the statistical physics of 2D phases not described by a simple order parameter in the LGW sense.

The stimulating idea that ''non-LGW'' continuous phase transitions could also occur in higher dimensions has recently been proposed in the context of quantum magnetism [3]. There, the possibility of a generic (i.e., not requiring fine tuning) continuous transition between two phases with different symmetry breakings (Néel and valence bond solid states) was pointed out, in contrast to the LGW prediction of either an intermediate phase with none of the two orders, or a coexistence region, or a direct first-order transition. So far, simulations on all candidate quantum models [4] rather see a first-order phase transition, a possibility which can never be discarded for a given microscopic model (see, however, recent claim of a continuous transition [5]).

From these perspectives, *classical* dimers at close packing on simple hypercubic lattices are particularly interesting as they are too constrained to form a liquid with a finite correlation length, even at infinite temperature: instead of decaying exponentially, the dimer-dimer correlations are algebraic, both in 2D [6] and 3D [7]. In 2D, the transition from such a critical state to a broken-symmetry phase (dimer crystal) has been studied in Ref. [6]. In this Letter we study the analogous transition in a three-dimensional classical dimer model. Both in 2D and 3D, a naive LGW expansion in terms of the low-temperature order parameter completely misses the critical nature of the high-temperature phase and thus cannot describe correctly the transition. Whereas in 2D the situation is well understood in terms of a KT transition [6], our numerical simulations on the 3D model show the existence of a single continuous *second-order* phase transition between the algebraic liquid at high temperature (so-called Coulomb phase) and a crystal with broken lattice symmetries. Our high-precision Monte Carlo (MC) data allow us to locate independently the transition starting from both phases. We determine the critical exponents and find that they are surprisingly close to those of a tricritical point. In a related recent work, Bergman *et al.* [8] further argue that the very existence of the Coulomb phase guarantees that this transition lies outside the standard LGW framework (see also Ref. [9]). The Coulomb phase in turn owes its presence to the absence of unpaired sites (monomers) [7]. In this spirit, it is the suppression of such topological defects which opens the way to new types of critical behavior. Indeed, such ''topological engineering'' has previously been used in the context of liquid crystals [10], and more recently for a nonlinear σ model [11]; as we discuss before concluding, the numerical values of the critical exponents obtained in Ref. [11] are not consistent with the ones reported here.

The model is a 3D extension of the one studied in Ref. [6] on the square lattice. Configurations are dimer coverings of the simple cubic lattice of volume $N = L^3$ sites, with L the linear dimension. Dimers are hard core

and close packed, i.e., every lattice site is part of one and only one dimer. Interactions favor aligment of nearest neighbors (n.n.) dimers on plaquettes of the lattice:

$$E = -\sum_{\text{plaquettes}} n_{||} + n_{=} + n_{//}, \qquad (1)$$

with $n_{||}$, $n_{=}$ and $n_{//}$ denoting the number of plaquettes with parallel n.n. dimers in the x, y, and z directions. Simulations (up to $N = 96^3$) are performed with a recent MC directed-loop algorithm [12].

At $T = 0$, the dimers order in columns to minimize the energy, resulting in a sixfold degenerate ground state. The associated order parameter is a three-component vector $m^{\alpha}(\mathbf{r}) = (-)^{r_\alpha} n_\alpha(\mathbf{r})$, with $n_\alpha(\mathbf{r}) = 1$ for a dimer pointing in direction $\alpha \in x, y, z$ at site $\mathbf{r}$, and 0 otherwise. Naively, one would expect a high-T phase with $\langle \vec{m} \rangle = 0$ and exponentially decaying dimer correlations. However, as shown by Huse *et al.* [7], at $T = \infty$ the system is in a "Coulomb phase", with no true long-range order but with dipolar dimer-dimer correlations. To see this, the appropriate variable is the "electric field" [7] $E_\alpha(\mathbf{r}) = (-)^{\mathbf{r}} n_\alpha(\mathbf{r})$. This field satisfies $\nabla \cdot \mathbf{E} = (-)^{\mathbf{r}} = \pm 1$, as the dimers are close packed. The Coulomb phase can be characterized [7] in the continuum by an effective "electrostatic" action $S = \frac{K}{2} \int d\mathbf{r} \mathbf{E}^2(\mathbf{r})$ which generates the dipolar correlations. Dimer fluxes $\phi = \int_\Sigma \mathbf{E} \cdot d\mathbf{S}$ through the planes perpendicular to the units vectors are conserved quantities and vanish on average. One easily shows that flux fluctuations allow the calculation of K,

$$\langle \phi^2 \rangle / L = \frac{1}{3L} (\langle \phi_x^2 \rangle + \langle \phi_y^2 \rangle + \langle \phi_z^2 \rangle) = 1/K. \qquad (2)$$

A close similarity with a 3D XY model can be seen through a duality transformation [13] in which $\nabla \cdot \mathbf{E} = (-)^{\mathbf{r}}$ is enforced by an angular Lagrange multiplier θ at each site. The discrete sums on E_α are then performed by a Poisson formula, resulting in an XY interaction (Villain form) between the θ variables. In this language, the Coulomb phase corresponds to an ordered phase with broken $O(2)$ symmetry for θ, and $1/K$ is the associated spin stiffness.

We first present thermodynamic results. Figure 1 (left panel) shows the behavior of the specific heat per site C_v/N as a function of T. Two close-by peaks are observed around $T \sim 1.52$ and $T \sim 1.67$. The first peak is much broader and *does not* diverge with system size: since it is already present and almost converged on small lattices $L < 16$ (not shown), it cannot be associated to any long distance or critical behavior. The second peak is much more characteristic of a phase transition: it diverges with L, with a power-law-like envelope typical of second-order phase transitions (see top right panel). Note that this peak is extremely hard to detect since it is absent on small systems ($L \leq 16$) and also very sharp. We interpret this peak as the signature of the direct transition (see below) between the Coulomb and columnar phase. Our best estimate for the temperature of its divergence is $T_c^{C_v} = 1.676(1)$. To determine the nature of the transition, we also considered energy histograms and the energy cumulant [14] defined as $1 - \langle E^4 \rangle / 3 \langle E^2 \rangle^2$. No sign of a double peak is detected in histograms and the energy cumulant is found to saturate to $2/3$ at the transition point: this indicates that the transition is not first order.

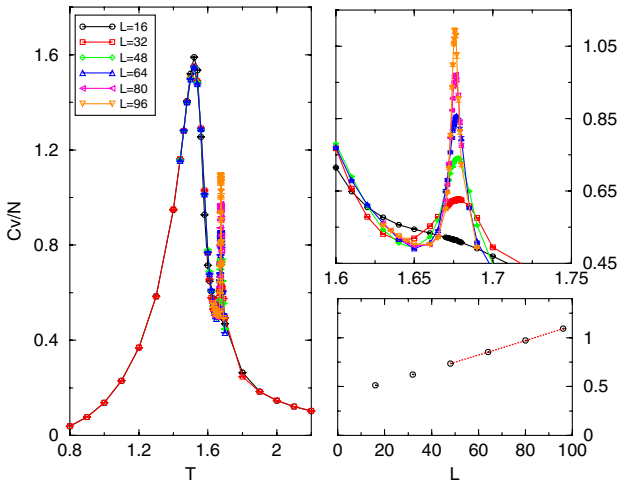

FIG. 1 (color online). Left panel: Specific heat per site C_v/N as function of temperature T for different system sizes L. Top right panel: Zoom on the second peak. Bottom right panel: Scaling of the specific heat at $T_c^{C_v} = 1.676$ as a function of system size L. The dotted line denotes a power-law fit for the 4 largest systems $L = 48, 64, 80, 96$ (see text).

Let us now consider the high-T phase. The left inset of Fig. 2 displays typical data for K^{-1} for a sample $L = 32$. K is finite in the whole high-T range [with a value $K(T = \infty) = 5.12(1)$ in agreement with Ref. [7]] and diverges below $T \simeq 1.6$ (rough estimate from the plot, and inset of Fig. 3). We expect for a second-order phase transition a scaling form of the type

$$K^{-1} = \langle \phi^2 \rangle / L = L^{-z} f[L^{1/\nu}(T - T_c)], \qquad (3)$$

where z is a scale exponent, ν the correlation length exponent, f a scaling function and T_c the critical temperature. Dimensional analysis of the Coulombian action gives $z = 1$ and therefore, at T_c, the curves of LK^{-1} intersect for all L and the derivative $L \frac{dK^{-1}}{dT}$ scales as $L^{1/\nu}$. Numerically, an accurate crossing point (see main panel of Fig. 2) is indeed obtained for $z = 1$, which is also a good check of the second-order nature of the transition. An estimate $T_c^K = 1.6745(5)$ can be obtained from the crossing of the curves for the largest L. In the Coulomb phase, dimer-dimer correlations are expected to be dipolar [7], and this is found to be indeed true all along the high-T phase. The prefactor in the dipolar form of the correlation functions varies as $1/K$, and we have checked with high precision that the value of K obtained from flux fluctuations perfectly coincides with that from correlations. *Monomer-monomer* correlators are also available in the simulations [6,12] and

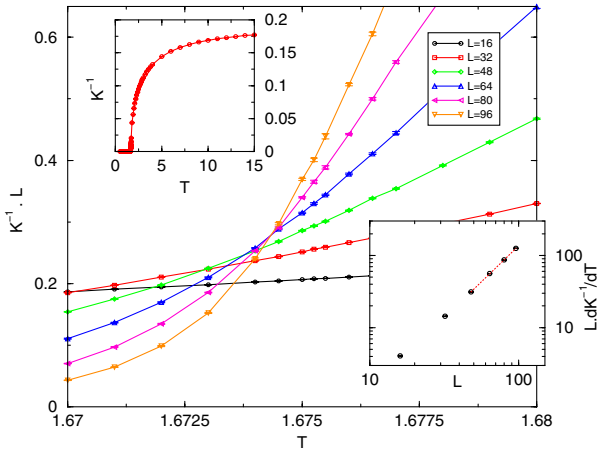

FIG. 2 (color online). Stiffness K^{-1} multiplied by L [obtained from $\langle\phi^2\rangle$, see Eq. (2)] versus T near the transition, for different system sizes L. Left inset: Stiffness K^{-1} for the whole high-T range for $L = 32$. Right inset: Scaling of the derivative LdK^{-1}/dT versus L in log-log scale for the estimated critical temperature $T_c^K = 1.6745$. The dotted line denotes a power-law fit for the 4 largest systems.

we find that test monomers are deconfined from $T = \infty$ down to T_c, confirming the Coulombian nature of the phase.

To probe the nature of the low-T phase, we calculate the columnar order parameter

$$m = \frac{2}{N} \left|\left| \sum_{\mathbf{r}} \vec{m}(\mathbf{r}) \right|\right| \tag{4}$$

and its Binder cumulant [15] $B = 1 - \langle m^4\rangle/3\langle m^2\rangle^2$. The left inset of Fig. 3 shows the expectation value $\langle m\rangle$ for a

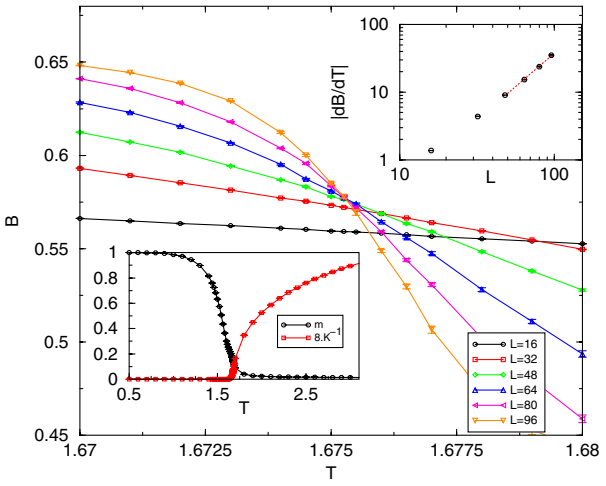

FIG. 3 (color online). Crossing of the columnar Binder cumulant B as a function of T near the transition point for different system sizes L. The sample $L = 16$ is again out of scaling. Left inset: Columnar order parameter m and stiffness K^{-1} (multiplied by 8) in the whole T range for $L = 32$. Right inset: Cumulant derivative $|dB/dT|$ at $T_c^{\rm col} = 1.67\,525$ versus L in log-log scale. The dotted line is a power-law fit for the 4 largest L.

sample $L = 32$ (for illustration, K^{-1} is again shown). Columnar order is observed to set in at low T. Binder cumulants in the main panel admit a crossing point for systems with different L, leading to an estimate $T_c^{\rm col} = 1.67525(50)$. Assuming the standard scaling form $B = f[L^{1/\nu}(T - T_c)]$, the derivative dB/dT should scale as $L^{1/\nu}$ at T_c.

The previous findings and the agreement between the various estimates of T_c clearly indicate that the model displays a *single second-order phase transition between Coulomb and columnar phases*. A straightforward choice for a LGW theory would be to use m as an order parameter. However, this fails as the Coulomb phase is not just a simple liquid where all correlations decay exponentially. Rather, it retains algebraic dimer correlations whose dipolar nature, crucially, does not lead to a peak in the structure factor anywhere in Fourier space (unlike the analogous situation in two dimensions [6,12]). Indeed, the natural variable with algebraic correlations is a coarse-grained "electric" field E; however, this variable exhibits no long-range order in *either* phase. Instead, it is the fluctuations of E that distinguish the two phases. It is also instructive to examine the transition from the Coulomb side with the dual angles θ. It allows the mapping of the dimer problem onto a model of interacting vortex loops with a long-range $1/r$ potential. While these loops are dilute in the Coulomb phase, they have to "proliferate" to reproduce a low-temperature crystal phase with frozen dimer positions (thus highly fluctuating dual variables θ). Intuitively, the restoration of the $O(2)$ symmetry would be through an inverted 3D XY transition, which is however incompatible with the critical exponents found numerically (see below). The crucial difference with a simple $O(2)$ spin model can be traced back to the background electric charges ± 1 which couple to the vortex loops and presumably affect their proliferation. We note the similar analysis of Ref. [8], where an unconventional non-LGW transition is predicted in a closely related model.

We now come to the universality class of the transition. The correlation length exponent ν can be extracted from the scaling with L of stiffness LdK^{-1}/dT or Binder cumulant dB/dT derivatives at the critical temperature T_c, which can be calculated thermodynamically in the MC process. Taking into account only the largest $L \geq 48$ (see insets of Figs. 2 and 3), we obtain compatible estimates $\nu^{\rm K} = 0.50(4)$ and $\nu^{\rm col} = 0.51(3)$ (error bars take into account stability of fits toward inclusion of smaller samples and uncertainty on T_c). The specific heat critical exponent α can be extracted from its scaling at the critical point: $C_v(T_c)/N = c_0 + AL^{\alpha/\nu}$, where A is a constant and c_0 the regular part at the transition (c_0 is non-negligible as can be seen for the $L = 16$ sample in Fig. 1). A fit for the largest L (see inset in Fig. 1) gives $\alpha/\nu = 1.11(15)$, leading to $\alpha = 0.56(7)$. Hyperscaling $\alpha = 2 - \nu d$ is thus satisfied within error bars. The last independent exponent can be obtained from the scaling of the columnar order parameter at criti-

cality $m(T_c) \sim L^{-\beta/\nu}$ or from the associated susceptibility $\chi = \langle m^2 \rangle - \langle m \rangle^2 \sim L^{\gamma/\nu}$. Using standard relations between critical exponents, we obtain for the correlation function exponent $\eta = -0.02(5)$. This set of exponents excludes some simple 3D universality classes [such as $O(2)$, $O(3)$ with or without cubic anisotropy], but are compatible with the universality class of an $O(n)$ *tricritical point* at its upper critical dimension $d = 3$, for which $\nu = \alpha = 1/2$ and $\eta = 0$ (up to logarithmic corrections). We also note that the value at T_c of the cumulant of the 3D order parameter m is compatible within error bars (see Fig. 3) with the value 0.56 982... of a tricritical $O(3)$ theory (for $d \geq 3$) [16]. With dimers, we do not have direct access to the XY order parameter $\vec{n}(r)$ for the dual angles θ. We can, however, investigate the fluctuations of the electric flux. ϕ_z is the integer-valued Noether charge associated to the $O(2)$ symmetry ("total angular momentum" if z is interpreted as the time direction): $\phi_z = \kappa \int dxdy(n_1 \partial_z n_2 - n_2 \partial_z n_1)$, where κ appears in the "kinetic" term $\frac{\kappa}{2}(\partial_z \vec{n})^2$ of the dual $O(2)$ action. Above T_c, the typical flux scales as $\sqrt{L}$ and the ratios $\langle \phi_z^4 \rangle / \langle \phi_z^2 \rangle^2$ and $\langle \vec{\phi}^4 \rangle / \langle \vec{\phi}^2 \rangle^2$ are, respectively, equal to 3 and 5/3, in agreement with the Gaussian and $O(3)$-symmetric nature of fluctuations in the Coulomb phase. We believe that the distribution of ϕ is universal at T_c and we measured $\langle \phi^2 \rangle = 0.28(2)$ and $\langle \phi^4 \rangle = 0.25(4)$. The smallness of these quantities at the critical point means that the discrete nature of $\vec{\phi} = (\phi_x, \phi_y, \phi_z)$ cannot be neglected there.

While it may be seen as the only way to reconcile the numerical results with a LGW analysis, the tricritical universality class is rather unexpected here as it would imply a "hidden" fine-tuning of parameters of the effective action. It is also quite possible that the exponents found are close, but not equal, to tricritical exponents, thereby defining a new "non-LGW" [3,8] universality class. The absence of monomers is in fact very similar to the absence of "hedgehogs" in the models studied by Motrunich and Vishwanath [11], which also display a transition from a broken-symmetry phase to a Coulomb liquid. However, our critical exponents do not match those of Ref. [11]. This discrepancy might be due to one or several factors: (i) lattice cubic anisotropies (not present in Ref. [11] but potentially relevant) exist in our model which admits 6 ground states related by cubic symmetry; (ii) the simulations of Ref. [11] may not be in the scaling regime; (iii) the proximity of a tricritical point (for instance at finite monomer doping), could affect finite-size estimations of the exponents and hide the true critical behavior. Finally, even though we simulate systems with N up to 96^3, a first-order transition with a large correlation length can never be excluded from finite-size simulations.

In conclusion, our study has established the crystallization in the cubic dimer model as an example of an unconventional phase transition in a classical model in three dimensions. The conventional LGW approach to phase transitions is currently under attack from many sides [3,8,11,17], but shows considerable resilience in microscopic models [4]. From this perspective, our results are promising since they cannot be described by a strict application of the LGW scheme [1] of an expansion in terms of the low-T order parameter. Further analytical calculations and numerical tests are needed to extend this study, notably to investigate the possible proximity to a tricritical universality class. This will hopefully allow a deeper understanding of the limits of a central concept in statistical physics.

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[1] See, e.g., L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, New York, 1980), 3rd ed.
[2] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[3] T. Senthil *et al.*, Science **303**, 1490 (2004); Phys. Rev. B **70**, 144407 (2004).
[4] A. W. Sandvik *et al.*, Phys. Rev. Lett. **89**, 247201 (2002); A. Kuklov, N. Prokof'ev, and B. Svistunov, *ibid.* **93**, 230402 (2004); L. Spanu, F. Becca, and S. Sorella, Phys. Rev. B **73**, 134429 (2006); J. Sirker *et al.*, *ibid.* **73**, 184420 (2006); A. B. Kuklov *et al.*, cond-mat/0602466.
[5] S. Isakov *et al.*, cond-mat/0602430.
[6] F. Alet *et al.*, Phys. Rev. Lett. **94**, 235702 (2005).
[7] D. Huse *et al.*, Phys. Rev. Lett. **91**, 167004 (2003).
[8] D. L. Bergman, G. A. Fiete, and L. Balents, Phys. Rev. B **73**, 134402 (2006).
[9] O. I. Motrunich and T. Senthil, Phys. Rev. B **71**, 125102 (2005).
[10] P. E. Lammert, D. S. Rokhsar, and J. Toner, Phys. Rev. Lett. **70**, 1650 (1993).
[11] O. I. Motrunich and A. Vishwanath, Phys. Rev. B **70**, 075104 (2004).
[12] A. W. Sandvik and R. Moessner, Phys. Rev. B **73**, 144504 (2006).
[13] T. Banks, R. Myerson, and J. Kogut, Nucl. Phys. **B129**, 493 (1977).
[14] M. S. S. Challa, D. P. Landau, and K. Binder, Phys. Rev. B **34**, 1841 (1986).
[15] K. Binder, Z. Phys. B **43**, 119 (1981).
[16] E. Brézin and J. Zinn-Justin, Nucl. Phys. **B257**, 867 (1985).
[17] L. Balents *et al.*, Phys. Rev. B **71**, 144508 (2005); T. Senthil and M. P. A. Fisher, cond-mat/0510459.
[18] F. Alet *et al.*, J. Phys. Soc. Jpn. Suppl. **74**, 30 (2005); M. Troyer, B. Ammon, and E. Heeb, Lect. Notes Comput. Sci. **1505**, 191 (1998); see http://alps.comp-phys.org.