SU(2)-invariant continuum theory for an unconventional phase transition in a three-dimensional classical dimer model

Stephen Powell and J. T. Chalker

Theoretical Physics, Oxford University, 1 Keble Road, Oxford, OX1 3NP, United Kingdom

We derive a continuum theory for the phase transition in a classical dimer model on the cubic lattice, observed in recent Monte Carlo simulations. Our derivation relies on the mapping from a three-dimensional classical problem to a two-dimensional quantum problem, by which the dimer model is related to a model of hard-core bosons on the kagomé lattice. The dimer-ordering transition becomes a superfluid–Mott insulator quantum phase transition at fractional filling, described by an SU(2)-invariant continuum theory.

PACS numbers: 64.60.Bd, 64.70.Tg, 75.10.Hk

The standard model of symmetry-breaking phase transitions, both classical and quantum, is the Landau-Ginzburg-Wilson (LGW) theory [1], where the critical properties are described by a continuum theory written in terms of the order parameter of the transition. It has recently been argued, however, that in certain two-dimensional quantum systems, continuous phase transitions are possible between symmetry-breaking states with apparently unrelated order parameters, in conflict with the LGW paradigm [2, 3].

Another class of non-LGW transitions occurs in classical systems with constraints that prevent a fully disordered state [4]. As the temperature is raised, these systems instead enter a ‘Coulomb phase’, where correlation functions have power-law forms and strong directional dependence. A naïve application of the LGW theory fails to capture these correlations and so cannot describe a transition between an ordered phase and a Coulomb phase [5].

Recent numerical work [4, 6] indicates that such a transition exists in a classical dimer model on the cubic lattice. This model describes the statistics of close-packed ‘dimers’, objects that occupy two neighbouring sites of the lattice, with every site of the cubic lattice covered by precisely one dimer. There are many configurations that obey this constraint, and if all are given equal weight, the system displays a Coulomb phase [6]. If instead they are given Boltzmann weights that favour parallel dimers, the system orders at low temperatures; the ordered phase is a six-fold degenerate crystal, breaking the lattice symmetry.

In this Letter, we outline two steps that lead to a continuum description of this classical dimer transition. Our first step uses the standard mapping between classical statistical mechanics in 3D and quantum mechanics in 2D, and so provides a bridge between the two classes of proposed non-LGW transitions. In the second step, we show that long-wavelength properties at the resulting 2D quantum transition are described by the SU(2)-symmetric noncompact $CP^1$ (NCC$P^1$) model. This conclusion is consistent with earlier suggestions, on the basis of results for several three-dimensional (3D) quantum models at finite temperature [6, 7], that the classical dimer transition should be described by a gauge theory coupled to multiple matter fields.

Our approach is to identify the [111] direction as imaginary time and map to a model of hard-core bosons on the kagomé lattice. A related mapping has previously been applied to another classical transition that is believed to lie outside the LGW paradigm, the Kasteleyn transition of spin ice in a [100] magnetic field [8]. As in that case, the Coulomb phase of the classical problem maps onto a superfluid phase for the quantum bosons, and the long-range power-law form for the correlation functions is reproduced by the fluctuations of the Goldstone (phase) mode. The dimer crystal becomes a bosonic Mott insulator, with a charge-density-wave order that breaks the symmetry of the kagomé lattice. There is a six-fold degeneracy in the ordering pattern, corresponding to the degeneracy of the crystalline phase.

In contrast to the case of spin ice [8], the quantum phase transition that results is still not amenable to a straightforward application of the LGW theory, and is instead an example of the class of non-LGW quantum transitions described above. The transition is between a bosonic superfluid and a Mott insulator at fractional filling, and is of the type considered by Balents et al. [2]. They showed that, using a dual representation in terms of vortices, the continuum behaviour can be described by a gauge theory whose form is strongly constrained by the symmetries of the original boson problem. In this dual model, the condensed phase of bosons becomes the non-condensed phase of the vortices, where the fluctuations of the photon mode of the gauge theory reproduce the superfluid correlations. The condensation of the vortex fields leads, by the Anderson-Higgs mechanism, to a gap for the photon and short-ranged correlation functions.

In our case, the continuum theory is an SU(2)-invariant gauge theory of a two-component complex vector $\varphi$ minimally coupled to a noncompact $U(1)$ gauge field $A$,

$$\mathcal{L}_0 = \left| (\nabla - iA)\varphi \right|^2 + s|\varphi|^2 + u(|\varphi|^2)^2 + \kappa |\nabla \times A|^2. \quad (1)$$
This can be rewritten in the usual form for $\text{NCCP}^1$ by replacing the terms $s$ and $u$ by a hard constraint $|\varphi| = 1$. Although the method picks out one direction as imaginary time, space-time isotropy is restored in the final form of the theory, a 3D classical model denoted by the three-dimensional derivative operator $\nabla$.

High-precision Monte Carlo data suggest that the dimer model has either a single continuous transition as the temperature is varied, or a very weak first-order transition, with a large but finite correlation length. In both cases, we expect there to be a well-defined continuum regime with correlation length much longer than the lattice spacing, described by Eq. (1). It remains controversial whether this continuum theory itself exhibits a continuous transition [13, 14, 15, 16].

An outstanding puzzle noted in Refs. [4] and [6], which we are unable to resolve, is that the critical exponent values extracted from simulations of the NC[P] model [1, 2] differ from those obtained in direct simulations of the dimer model [4].

The six ground states have been suggested [4, 6] that the critical exponent values extracted from simulations of the dimer model [4] differ from those obtained in direct simulations of the NC[P] model [1, 2] and related quantum spin models [17, 18]. It has been suggested [4, 6] that the discrepancy may be due to the proximity of a tricritical point in the phase diagram of a generalized dimer model; further numerical work is required to clarify this point as well as the nature of the transition.

The configurations of the classical model are close-packed arrangements of hard-core dimers, described by the variables $d_\mu(r) \in \{0, 1\}$, giving the occupation number of the link between the cubic-lattice sites $r$ and $r + \delta_\mu$, where $\delta_\mu$ is a unit vector ($\mu \in \{x, y, z\}$). The close-packing constraint can be expressed as $\sum_\mu [d_\mu(r) + d_\mu(r - \delta_\mu)] = 1$, for all $r$. The energy of a configuration is $E = -n_0$, where $n_0$ is the number of plaquettes (of any orientation) with parallel dimers, though our continuum theory applies equally to other potentials that also favour columnar crystalline order.

At zero temperature, $T = 0$, the dimers maximize $n_0$ by selecting one of the six degenerate columnar ordering patterns, distinguished by the staggered order parameter,

$$m_\mu(r) = \frac{1}{2} (-1)^{r_\nu} [d_\mu(r) - d_\mu(r - \delta_\mu)].$$

The six ground states have $\binom{\pm \delta_x, \pm \delta_y, \pm \delta_z}$, for all $r$. For $T = \infty$, $\langle m \rangle = 0$, and the dimer–dimer correlation function has the 3D dipole form [9]

$$\langle d_\mu(r)d_\nu(0) \rangle \sim \eta_k \frac{3r_\mu r_\nu - |r|^2 \delta_\mu \delta_\nu}{|r|^5},$$

where $\eta_k = (-1)^{r_\nu}$ is $\pm 1$ on the two sublattices.

Monte Carlo simulations show a transition, apparently continuous, from an ordered phase to a Coulomb phase as $T$ is increased, at a critical temperature of $T_c \simeq 1.675$. For $T < T_c$, the lattice symmetry is broken, and $\langle m \rangle$ takes on a nonzero value (oriented along one of the cubic unit vectors $\pm \delta_\mu$). For $T > T_c$, the order parameter vanishes and the correlation functions have a dipolar form.

We now outline a derivation of the continuum theory for this transition, based on a mapping to quantum bosons in 2D. Our first step is to define the imaginary time $\tau = \sum_\mu \tau_\mu$, given by the projection of the 3D position onto the [111] direction. We then map the configurations of a given [111] plane of the classical model to the basis states in a quantum Hilbert space, by simply identifying the presence (or absence) of a dimer with the presence (absence) of a boson. As illustrated in Figure 1, the midpoints of the cubic bonds satisfying $\tau \mod 3 = \frac{1}{2}$ form a set of kagomé planes stacked in the [111] direction, and we use this set as the space-time lattice for the quantum problem.

For this mapping to make sense, we require conservation of particle number. The close-packing constraint implies that

$$\sum_{\mu} \sum_{\mathbf{r} \in \tau} d_\mu(r) = \sum_{\mathbf{r} \in \tau - 1} \left[ 1 - \sum_{\mu} d_\mu(r) \right],$$

where $|\varphi| = 1$. The close-packing constraint can be expressed as $\sum_{\mu} [d_\mu(r) + d_\mu(r - \delta_\mu)] = 1$.
where \( r \in \tau \) indicates a sum over all cubic sites in imaginary-time slice \( \tau \). This implies that if the kagomé plane at \( \tau = n \) has \( n \) bosons and a total of \( N \) sites, then the plane at \( \tau = \frac{N}{3} + 3 \) will have \( n - n \) bosons. We must therefore choose an imaginary-time step \( \delta \tau \) that is even in order to give particle conservation; the smallest choice is \( \delta \tau = 6 \) and so we take only the bonds whose midpoints are at \( \tau \mod 6 = \frac{3}{2} \) to define the quantum problem.

The six distinct ground states of the dimers map to six ordered states of the kagomé bosons, and the example with \( m = -\delta \) is shown in Figure 1. In each ordered state, half of the sites on a given sublattice are occupied, so the density (bosons per site) is \( f = \frac{1}{6} \). The low-temperature phase of the classical model maps to the ordered phase of the bosons, while in the high-temperature phase the bosons condense and there is no spatial order, corresponding to the Coulomb phase with \( \langle m \rangle = 0 \).

The basis states for the quantum Hilbert space are given by the occupation-number states of hard-core bosons on the kagomé lattice. The hard-core nature of the dimers further implies that there is hard-core nearest-neighbour repulsion, and each triangle of the kagomé lattice (of either orientation) can be occupied by at most one boson. The partition function for the classical problem is therefore given by the quantum zero-temperature limit is therefore given by the quantum zero-temperature limit, \( \beta \rightarrow \infty \).

It is in principle possible to find \( T \), and hence \( H \), exactly for a finite lattice, by enumerating all possible configurations of the dimer problem. For even quite small lattices, however, this is a computationally difficult problem, and we have made no attempt to find \( T \) explicitly. Instead, the continuum theory for the transition can be found by using general principles such as symmetry to place constraints on \( H \).

The Hamiltonian will take the form of a generic lattice-boson model, with all hopping terms and interactions that are consistent with symmetry, as in the related mapping for spin ice [3]. The parameters in the Hamiltonian are functions of those in the classical model, and so in our case the hopping and interaction strengths will depend on the classical temperature \( T \). Since the high-temperature phase corresponds to a boson condensate, we expect the ratio of the hopping strength to the interactions to increase with \( T \).

For the mapping to bosons to be useful in the thermodynamic limit, we require that the Hamiltonian should be local, at least in its action on low-energy states. We have no general proof that this is the case, but we argue that it is so in the region of interest, near the transition. In this case, the low energy states of the bosons can be written in terms of states with a finite density of domain walls separating regions with different density-wave orderings.

These one-dimensional domain walls are, in 3D, the intersections of a given (111) plane with two-dimensional domain walls between dimer orderings. Consider a domain wall that moves by a large amount in a single time step, so that one of the two neighbouring domains grows by an area \( \delta A \). In the three-dimensional picture, this domain wall has a section of area \( \delta A \) that runs parallel to the (111) plane. Such a configuration costs entropy and configuration energy that grows with \( \delta A \), and hence has an exponentially suppressed contribution to the transfer matrix.

We defer a full analysis of the symmetry properties of the Hamiltonian \( H \) to a forthcoming paper, and discuss here only a symmetry of particular importance: rotation by \( \frac{\pi}{3} \) about a [111] axis passing through the centre of a kagomé hexagon, and hence through a cubic lattice site with \( \tau \mod 3 = 0 \) (such as the one at the centre of Figure 1). This maps the kagomé lattice onto itself, but is not a symmetry of the cubic lattice, since it exchanges the positions of the cubic sites on the intermediate planes. (For instance, it exchanges cubic sites with \( \tau = 1 \) and \( \tau = 2 \).) We therefore define the operation \( R \) consisting of this rotation followed by a reflection in the (111) plane \( \tau = \frac{3}{2} \), which is a symmetry of the cubic lattice. In terms of the bosons, \( R \) is a rotation followed by a time-reversal operation \( \tau \rightarrow 3 - \tau \), and it commutes with \( H \).

Before addressing the transition, we note that taking full account of the symmetries allows an alternative derivation [3], starting from the quantum model, of the dipolar form of the Coulomb-phase correlation functions. This phase corresponds to the superfluid, where long-range correlation functions are dominated by fluctuations of the Goldstone phase mode \( \phi \), described by the coarse-grained action \( L_\phi \sim |\partial \phi|^2 \). Correlation functions can be found by using the symmetries to express the boson number operators and dimer occupations in terms of the continuum field \( \phi \), giving for instance \( d_\mu \sim \eta_\mu \partial_\mu \phi \).

The continuum theory describing the transition between a superfluid and a Mott insulator at fractional fillings can be expressed in terms of dual vortex fields. We will sketch the derivation of this theory; readers are referred to the papers of Balents et al. [4] for an overview of the approach. In essence, it consists of a transformation from a current-loop representation of the boson problem [4], where the basic degrees of freedom are the currents \( J_\mu(r) \) defined on the links of the space-time lattice, to a gauge field \( A_\mu(r) \) defined on the links of the dual lattice, according to \( J = \nabla \times A \).

Note that the bosons belong on the sites of the kagomé lattice, and so the space-time lattice is not the original
cubic lattice of the dimer problem, but instead consists of stacked kagomé planes. The dual of kagomé is the dice lattice [11,12], and so the gauge field $A_\mu(r)$ is defined on the links of a lattice of stacked dice planes.

The dual theory has a gauge invariance resulting from the redundancy of the definition of $A_\mu$, and can be written in terms of the gauge field $A_\mu(r)$ and matter fields $\psi(r)$ defined on the sites of the dual lattice. In terms of the original bosons, these matter fields represent vortex links of a lattice of stacked dice planes.

The allowed interaction terms can be found by expressing all gauge-invariant bilinears of the fields $\varphi_0$ and $\varphi_1$ in terms of the boson density operators $L^{\mu}$, or equivalently, in terms of the dimer order parameters $m_\mu$. Using the symmetries of the cubic lattice, we find

$$m_\mu \sim \varphi^\dagger \sigma^\mu \varphi,$$

where $\sigma^\mu$ are the Pauli matrices.

Defining the SU(2) Casimir invariant $\Omega = |\varphi_0|^2 + |\varphi_1|^2$, all gauge-invariant combinations of the fields $\varphi_0$ and $\varphi_1$ can be written in terms of $\Omega$ and $m_{x,y,z}$, and it is straightforward to show that $\Omega^2 \sim |\mathbf{m}|^2$. While the action can contain any term involving only $\Omega$, terms involving functions of $m_\mu$ that break SU(2) are strongly restricted by symmetry. The first such term allowed by Eq. (5), of sixth order in $\varphi$, is $m_{x}m_{y}m_{z}$, and is excluded by requiring symmetry under $\mathbf{m} \rightarrow -\mathbf{m}$. The lowest-order combination satisfying all the symmetries is of eighth order, and is given by $\mathcal{L}_1 = v \sum_\mu m_\mu^4$. In order to describe the transition to the particular ordered states with which we are concerned, we require $v < 0$.

The SU(2)-invariant part of the action, given in Eq. (1), takes the standard form for a complex vector minimally coupled to a noncompact $U(1)$ gauge field. We have omitted terms containing higher derivatives or higher powers of the field $\varphi$. The cubic symmetry of the original dimer problem means $\mathcal{L}_0$ must be space–time symmetric, and we have made this explicit in Eq. (1).

It is not firmly established whether this action has any nontrivial fixed points under the RG. As noted in Ref. [3], a conjecture of this sort is difficult to test analytically [19], and the evidence from numerical studies is inconclusive. It is clear from simulations, however, that the transition is, at most, weakly first order, with a very large correlation length, and so a continuum description is appropriate. The fact that $\mathcal{L}_1$ is of eighth order in the field $\varphi$ makes it highly likely that this term is irrelevant in the continuum, and that the effective theory has an emergent $SU(2) \cong O(3)$ symmetry.

Using this assumption, and the expression for the crystalline order parameter given in Eq. (6), we are able to explain two qualitative observations made by Misguich et al. [6] based on their numerical results near the transition. Firstly, the data strongly suggest that the order-parameter distribution is spherical, as expected for an $O(3)$-symmetric theory. Secondly, the dimer–dimer correlations are dominated by a ‘spin-like’ contribution [6]. This follows from the fact that $m_\mu$ (and hence the dimer variables $d_\mu$) couples directly (without derivatives) to a bilinear in the critical field $\varphi$, and forms a three-dimensional representation of SU(2). We therefore find $\langle m_\mu m_\nu \rangle \sim \delta_{\mu \nu} |r|^{-d + 2 - \eta_m}$ [6]. The absence of a weak-coupling fixed point again prevents us from making quantitative predictions about the anomalous dimension $\eta_m$. As noted by Misguich et al. [6], these properties, while explained straightforwardly by the NCCP theory, are incompatible with other, more obvious, candidate continuum theories, such as the O(3) model.

In conclusion, we have derived an NCCP theory to describe the observed phase transition in a classical dimer model on the cubic lattice [4], by means of a mapping to a quantum transition in two dimensions. Simple qualitative predictions based on this mapping are in agreement with numerical results for the dimer system [4,6]. The discrepancies between the observed properties of the NCCP and dimer models, as well as the uncertainty regarding the nature of the transitions, illustrate the need for further numerical studies of both models.

We thank P. Fendley and L. Balents for helpful comments. This work was supported in part by EPSRC Grant No. EP/D050952/1.

[1] L. D. Landau et al., *Statistical Physics* (Butterworth-Heinemann, New York, 1999).
[2] T. Senthil et al., Science 303, 1490 (2004); Phys. Rev. B 70, 144407 (2004).
[3] L. Balents et al., Phys. Rev. B 71, 144508 (2005); Prog. Theor. Phys. Suppl. 160, 314 (2005).
[4] F. Alet et al., Phys. Rev. Lett. 97, 030403 (2006).
[5] D. L. Bergman et al., Phys. Rev. B 73, 134402 (2006).
[6] G. Misguich et al., [arXiv:0803.2196v1].
[7] O. I. Motrunich and T. Senthil, Phys. Rev. B 71, 125102 (2005).
[8] S. Powell and J. T. Chalker, [arXiv:0803.4204v1].
[9] D. A. Huse et al., Phys. Rev. Lett. 91, 167004 (2003).
[10] M. Wallin et al., Phys. Rev. B 49, 12115 (1994).
[11] K. Sengupta et al., Phys. Rev. B 73, 245103 (2006).
[12] L. Jiang and J. Ye, J. Phys.: Condens. Matter 18, 6907 (2006).
[13] O. I. Motrunich and A. Vishwanath, Phys. Rev. B 70, 075104 (2004).
[14] F.-J. Jiang et al., [arXiv:0710.3926v1].
[15] O. I. Motrunich and A. Vishwanath, [arXiv:0805.1494v1].
[16] A. Kuklov et al., [arXiv:0805.2578v1].
[17] A. W. Sandvik, Phys. Rev. Lett. 98, 227202 (2007).
[18] R. G. Melko and R. K. Kaul, Phys. Rev. Lett. 100, 017203 (2008).
[19] For instance, an expansion in $\epsilon = 4-d$, where $d$ is the spatial dimension, has no stable weak-coupling fixed points.