Topological multicritical point in the Toric Code and 3D gauge Higgs Models

I.S. Tupitsyn, A. Kitaev, N.V. Prokof’ev, and P.C.E. Stamp

1 Pacific Institute of Theoretical Physics, University of British Columbia, 6224 Agricultural Road, Vancouver, BC V6T 1Z1, Canada
2 California Institute of Technology, Pasadena, California 91125, USA
3 Department of Physics, University of Massachusetts, Amherst, Massachusetts 01003, USA

(Dated: April 20, 2008)

We report a new type of multicritical point that arises from competition between the Higgs and confinement transitions in a $\mathbb{Z}_2$ gauge system. The phase diagram of the 3d gauge Higgs model has been obtained by Monte-Carlo simulation on large (up to $60^3$) lattices. We find the transition lines continue as 2nd-order until merging into a 1st-order line. These findings pose the question of an effective field theory for a multicritical point involving noncommuting order parameters. A similar phase diagram is predicted for the 2-dimensional quantum toric code model with two external fields, $h_x$ and $h_z$; this problem can be mapped onto an anisotropic 3d gauge Higgs model.

PACS numbers:

Introduction. Topological quantum phases and anyons are well known in connection with the fractional quantum Hall effect, but they are also expected to exist in frustrated magnets. It has long been proposed that a certain class of resonating-valence-bond (RVB) [1] phases carries $\mathbb{Z}_2$-charges and vortices and has a four-fold degenerate ground state on a torus [2]. A qualitative understanding of this phase can be obtained from a so-called toric code model (TCM) [3]. The dimer model on the Kagome lattice is mapped onto the TCM exactly [4] while some other models [5, 6] belong to the same universality class.

The TCM is defined in terms of spin-1/2 degrees of freedom located on the bonds of an arbitrary 2d lattice. The Hamiltonian is as follows:

$$H_{TC} = -J_x \sum_s A_s - J_z \sum_p B_p,$$

where $A_s = \prod_{j \in s} \sigma^x_j$ and $B_p = \prod_{j \in p} \sigma^y_j$ are products of spin operators ($\sigma^x$ are the Pauli matrices) on the bonds incident to a lattice site $s$ and on a boundary of a plaquette $p$, respectively. The ground state corresponds to eigenvalues $A_s = 1$, $B_p = 1$ for all $s$ and $p$. On a surface of genus $g$, it is $4^g$-fold degenerate. Elementary excitations are characterized by eigenvalues $A_s = -1$ (a $\mathbb{Z}_2$ charge on site $s$) and $B_p = -1$ (a $\mathbb{Z}_2$ vortex on plaquette $p$); all excitations are gapped. Each type of quasiparticle is bosonic, but due to nontrivial mutual braiding, they must be jointly regarded as Abelian anyons.

The Hamiltonian [1] has special properties related to its exact solvability: the two-point correlator vanishes and the quasiparticles have flat dispersion. These features do not survive a small generic perturbation, while the topological character of the ground state and the anyonic quasiparticle statistics are robust. Yet a sufficiently strong field can polarize the spins, driving a transition to the topologically trivial phase. Trebst et al [2] studied a perturbation of the form $-h \sum \sigma^z_j$ and solved the problem by reducing it to the 2d transverse-field Ising model, which is mapped to an anisotropic 3d classical Ising model. In this paper we consider a more general Hamiltonian:

$$H_Q = H_{TC} - h_x \sum_b \sigma^x_b - h_z \sum_b \sigma^y_b,$$

where $b$ runs over the bonds of a square lattice and $H_{TC}$ is given by Eq. (1). Note that the fields $h_x$ and $h_z$ induce different types of phase transition. The term with $h_z$ creates virtual pairs of $\mathbb{Z}_2$ charges, which condense when the field strength exceeds a certain threshold. This phenomenon may be described as a Higgs transition, or as vortex confinement. By duality, the field $h_x$ causes the condensation of vortices and charge confinement. The competition of the two terms should result in an interesting phase diagram, which is the subject of this paper.

We approach the problem by reducing the quantum Hamiltonian to a classical anisotropic $\mathbb{Z}_2$ gauge Higgs Hamiltonian on a three-dimensional cubic lattice; see Eq. (2) below. We expect the phase diagram to be qualitatively similar to that for the isotropic case, i.e., model $M_{3,2}$ as defined by Wegner [5]. Monte-Carlo simulations have been performed for the latter model because it is more amenable to numerics. Some properties of the phase diagram in the isotropic case were predicted by Fradkin and Shenker [6]. In particular, the topological phase is bounded by second-order lines corresponding to charge condensation (for $h_x \ll h_z \sim J_x, J_z$) and vortex condensation (for $h_z \ll h_x \sim J_x, J_z$), but the two condensate phases are continuously connected. For the quantum Hamiltonian [2], a connecting path is realized by increasing $h_z$ so as to polarize the spins in the $z$ direction, rotating the field in the $xz$-plane, and decreasing it again. However, the two phase transitions are clearly different, therefore the corresponding lines cannot join smoothly.

A previous numerical study involving $10^3$ sites by Jongeward, Stack, and Jayaprakash [11] showed the two
The classical Hamiltonian:

\[ H = -J_x \sum_s \mu_s^x - J_z \sum_p B_p - h_x \sum_b \sigma_b^x - h_z \sum_{uv} \sigma_{uv}^z. \]  

Note that in the first term we have replaced \( A_s \) by \( \mu_s \) using the gauge-invariance condition, \( \mu_s A_s \equiv 1 \).

We now map this 2-d quantum Hamiltonian onto a (2+1)-d classical one. The overall scheme is standard [11], but some care should be taken to preserve the gauge invariance. We let \( \Delta \tau = \beta/n \), and approximate the quantum partition function \( Z = \text{Tr}[\exp(-\beta H)]/\text{Tr}[\exp(-\Delta \tau H_x)\exp(-\Delta \tau H_z)] \), where \( \text{Tr}[\exp(-\Delta \tau H)] \) is the projector onto the gauge-invariant subspace, and \( H_x, H_z \) are the terms in the quantum Hamiltonian that depend on \( \sigma_b^z, \mu_s^x \) and \( \sigma_{uv}^z, \mu_s^z \), respectively. This expression can be written as a classical partition function on a cubic lattice. The classical variables \( \sigma_b^t, \mu_s^t, \mu_s^z \) correspond to \( \sigma_b^z, \mu_s^x, \mu_s^z \) respectively. But when we change from 2d to 3d, new vertical bonds (along the time direction) appear. The classical spins on the vertical bonds between two time slices correspond to a choice of term in the expansion of \( \mathcal{P} = \prod_{t \in \mathbb{Z}} \{1 + \mu_s^z A_s\} \). Thus we arrive at this classical Hamiltonian:

\[ H_C = -\sum_{uv} \lambda_{|uv|^b}^b \mu_u \sigma_{uv}^z \mu_v - \sum_p \lambda_{|p|^b}^b \prod_{j \in p} S_j. \]  

where \( \lambda_{|uv|^b}^b = -\frac{1}{2} \ln \tanh \tilde{J}_x \) is vertical bonds; \( \lambda_{|p|^b}^b = -\frac{1}{2} \ln \tanh \tilde{h}_x \) is horizontal bonds; \( \lambda_{|uv|^b}^b = -\frac{1}{2} \ln \tanh \tilde{h}_x \) is vertical plaquettes; \( \lambda_{|p|^b}^b = \frac{1}{2} \ln \tanh \tilde{h}_x \) is horizontal plaquettes, where \( \tilde{J}_x = J_x \Delta \tau, \tilde{J}_z = J_z \Delta \tau, \tilde{h}_x = h_x \Delta \tau, \tilde{h}_z = h_z \Delta \tau. \) This model is an anisotropic generalization of the \( Z_2 \) gauge Higgs model [9].

As a final step, we eliminate the redundancy by fixing \( \mu_s \). This only changes the classical partition function by a constant factor since Hamiltonian (4) can be written in terms of the gauge-invariant variables \( S_{uv} = \mu_u \sigma_{uv} \mu_v \):

\[ \tilde{H}_C = -\sum_{b} \lambda_{|b|^b}^b S_b - \sum_{p} \lambda_{|p|^b}^b \prod_{j \in p} S_j. \]  

More detailed calculations show that the quantum and classical partition functions are related by

\[ Z = \left( \frac{1}{2} \sinh(2\tilde{J}_x) \right)^{k/2} \left( \frac{1}{2} \sinh(2\tilde{h}_x) \right)^{m/2} Z_C, \]  

where \( k \) and \( m \) are the number of vertical bonds and plaquettes, respectively.

Of course, Eq. (8) holds only in the limit \( \Delta \tau \to 0 \). However, we take the liberty of parametrizing the general classical Hamiltonian (4) by \( \tilde{J}_x, \tilde{J}_z, \tilde{h}_x, \tilde{h}_z \), even though the corresponding quantum problem may not be defined. In the isotropic case, two parameters will suffice:

\[ \tilde{H}_C = -\lambda_{|b|^b}^b S_b - \lambda_{|p|^b}^b \prod_{j \in p} S_j, \]  

where \( \lambda_{|b|^b}^b = \tilde{h}_z, \lambda_{|p|^b}^b = -\frac{1}{2} \ln \tanh \tilde{h}_x \). This model is equivalent to the 3D classical Ising model (Eq. 9) is also known as the 3D Ising gauge theory [8]. Using high-accuracy results of Ref. [12] for the critical point and the duality relation \( \lambda_{|p|^b}^b = -1/2 \ln \tanh(J/T) \), where \( J \) is the Ising exchange coupling, we obtain \( \lambda_{|p|^b}^b = 0.7614125 \).

At arbitrary values of \( \lambda_{|b|^b}^b \) and \( \lambda_{|p|^b}^b \) the model is self-dual [13], i.e. it maps to itself under the coupling constant transformation \( \lambda_{|b|^b}^b \to -1/2 \ln \tanh(\lambda_{|p|^b}^b) \). This means that the phase diagram has a symmetry, or self-duality, line defined by \( \lambda_{|b|^b}^b = -1/2 \ln \tanh(\lambda_{|p|^b}^b) \). Under the duality mapping (\( \lambda_{|b|^b}^b = 0, \lambda_{|p|^b}^b = 0.7614125 \)) \( \lambda_{|b|^b}^b = 0.221653, \lambda_{|p|^b}^b = \infty \), which gives us two Ising-type critical points on the phase diagram.
To calculate the rest of the phase diagram we performed Monte Carlo simulations using standard single-spin flip updates, supplemented by rare (once per $N^2$ updates) flips of all spins belonging to bonds cut by planes oriented along any one of the crystal axes, or along any of the diagonals to these axes. There are $9N^2$ possible planes satisfying this condition, and we select any of them at random. The plaquette energy (second term in (5)) is conserved by this update. To determine the 2nd-order critical lines, we employed a standard finite-size scaling analysis of the specific heat $C_v$, for linear system sizes $N = 24, 36, 48, 60$ (i.e., for $3N^3$ spins). First-order critical points were identified and located using energy distributions. These distributions are bi-modal (have two maxima) for the first-order transitions and single-modal otherwise. We thermalized our samples for up to $10^6$ MC sweeps (one sweep having $3N^3$ elementary updates). The data were accumulated for $\sim 4 \times 10^8$ MC sweeps.

The resulting phase diagram is presented in Fig.1. The first-order transition coinciding with the self-duality line was observed for $0.2575(5) > \lambda_{\text{bond}} > 0.22635(5)$. Outside of this interval we saw no bi-modal structure in the energy distribution for system sizes up to $N = 60$. The inset of Fig.2 shows the evolution of the energy distribution function along the self-dual line. Even when the bi-modal structure is observed it is extremely weak, developing only for large $N$, and the distribution can be sampled in the minimum without flat-histogram or similar reweighting techniques.

As noted above, these results conflict with previous MC simulations in Ref. [10], who suggest the 1st-order line splits into two 1st-order lines. The inset (a) of Fig.4 shows a closeup of the controversial region. Though we were able to resolve critical points with an accuracy of at least three digits, we observed no splitting of the self-dual 1st-order line into two 1st-order transitions. We also find no evidence for tri-critical points on the Ising-type lines as long as we can resolve two separate transitions. There remains a tiny parameter range between the apparent disappearance of the bi-modal distribution on the self-dual line (this disappearance probably due to our limited system size) and two resolved 2nd-order transitions.

**FIG. 1:** (color online). The phase diagram of the Hamiltonian (9). Circles correspond to the second-order transitions (open and filled symbols are related by the duality transformation). Filled squares describe the first-order self-dual transitions. Bold and dashed lines are used to guide an eye and correspond to the 1st- and 2nd-order transitions, respectively. The phases are: (I) - topological phase; (II) - topologically disordered phase; (III) - magnetically ordered phase. In inset (a) we show the region where all phases meet each other. In inset (b) we show three alternative ways of connecting the lines.

**FIG. 2:** (color online). The distance between two maxima in bi-modal energy distributions along the self-duality line for $N = 60$ as a function of $\lambda_{\text{bond}}$. The inset shows examples of the energy distributions at various values of $\lambda_{\text{bond}}$.

To probe the behavior in this tiny parameter range we need a different approach. We therefore scanned energy distributions at 30 points ($N = 48$) along the line perpendicular to the self-duality line right in the questionable region (short solid line in the inset (a)). If the 1st-order line were to split above the scan, the third maximum would have to emerge in the energy distribution right between the two maxima we observe on the self-dual line - implying that the energy maxima on the self-dual line could not merge smoothly, and right below the split, three maxima would have to be seen in the energy distribution. However all distributions along the scan were found to have only one peak. It is also clear from the main part of Fig.2 that on the self-duality line, the energy maxima approach each other and merge continuously as $\lambda_{\text{bond}}$ increases. The curves presented in Fig.2 follow a power law near the vanishing point, with corresponding critical exponent $\sim 0.55$. We thus conclude that the split 1st-order scenario does not work. Instead there are three possibilities. Either all three lines merge at one point (case (1) in the inset (b), Fig.1); or the 1st-order line ends before or after the point where two 2nd-order lines touch the self-dual
line (cases (2) and (3) in the inset (b), Fig. 1). Unfortunately our data cannot distinguish between the alternatives because the 2nd-order lines seem to touch at extremely small (possibly zero) angle. Formally, option (2) fits the data best. Theoretically, the last two scenarios are less demanding since they fit the existing theory of phase transitions (our data suggest that the 2nd-order transitions cannot merge into a single smooth curve and form a kink at the self-dual line). We are not aware of any effective theory leading to the first scenario.

Phases. Using the two correspondence equations

\[
\tilde{h}_z = -\frac{1}{2} \ln \tanh(\tilde{J}_z) = \lambda_{\text{bond}}; \quad (10a)
\]
\[
\tilde{J}_z = -\frac{1}{2} \ln \tanh(\tilde{h}_x) = \lambda_{\text{pl}}, \quad (10b)
\]

we can reformulate the phase diagram Fig. 1 in terms of the renormalized parameters \( \tilde{J}_z, \tilde{h}_z, \tilde{h}_x \) of the TCM. The resulting phase diagram in terms of the external fields is presented in Fig. 3. Let us go through the phases in this Figure.

The phase (I) corresponds to the topological phase of the model (the “free charge” phase of the 3d gauge Higgs model) remains stable in a rather wide range of fields and breaks down via two Ising type transitions whose critical lines meet with the 1st-order one corresponding to a liquid-gas type transition. The 1st-order line either meets with two 2nd-order lines in one multicritical point, or terminates before or after the point where two 2nd-order lines touch the self-duality line. The construction of an effective field theory for this multicritical region is an interesting open problem.

We thank E. Fradkin, B. Svistunov, S. Trebst, M. Troyer, I. Affleck, and K. Shtengel for discussions. We are also indebted to M. Berciu and J. Heyl whose research clusters were used to perform our MC simulations.

\[\text{References}\]

[1] P.W. Anderson, Science 235, 1196, (1987).
[2] N. Read, B. Chakraborty, Phys. Rev. B 40, 7133 (1989).
[3] A.Yu. Kitaev, Ann. Phys. (N.Y.) 303, 2 (2003).
[4] G. Misguich, D. Serban, V. Pasquier, Phys. Rev. Lett. 89, 137202 (2002); cond-mat/0204428.
[5] N. Read, S. Sachdev, Phys. Rev. Lett. 66, 1773 (1991).
[6] R. Moessner, S. L. Sondhi, Phys. Rev. Lett. 86, 1881 (2001); cond-mat/0007378.
[7] S. Trebst, P. Werner, M. Troyer, K. Shtengel, and C. Nayak, PRL 98, 070602 (2007).
[8] F.J. Wegner, J. of Math. Phys. 12, 2259 (1971).
[9] E. Fradkin and S. Shenker, Phys. Rev. D 19, 3682 (1979).
[10] G.A. Jongeward, J.D. Stack and C. Jayaprakash, Phys. Rev. D 21, 3360 (1980).
[11] M. Suzuki, Progress on Theor. Phys. 56, 1454 (1976).
[12] R. Gupta and P. Tamayo, The critical exponents for the 3d Ising model, US-Japan Bilateral Seminar - Maui, August 28-31, 1996.
[13] R. Balian, J.M. Drouffe, and C. Itzykson, Phys. Rev. D 11, 2098 (1975).