Motivated by cold atom experiments on Chern insulators, we study the honeycomb lattice Haldane-Hubbard Mott insulator of spin-1/2 fermions using exact diagonalization and density matrix renormalization group methods. We show that this model exhibits various chiral magnetic orders including a wide regime of triple-Q tetrahedral order. Incorporating third-neighbor hopping frustrates and ultimately melts this tetrahedral spin crystal. From analyzing the low energy spectrum, many-body Chern numbers, entanglement spectra, and modular matrices, we identify the molten state as a chiral spin liquid (CSL) with gapped semion excitations. We formulate and study the Chern-Simons-Higgs field theory of the exotic CSL-to-tetrahedral spin crystallization transition.
For $U \gg |t_{1,2}|$, degenerate perturbation theory in the Mott insulator [54] with one fermion per site leads to the spin model

$$H_{\text{spin}} = \frac{4t^2}{U} \sum_{\langle ij \rangle} S_i \cdot S_j + \frac{4t^2}{U} \sum_{\langle \langle ij \rangle \rangle} S_i \cdot S_j + \frac{24t^2}{U^2} \sum_{\text{small} \sim \Delta} \hat{\chi}_\Delta \sin \Phi_\Delta + \frac{24t^3}{U^2} \sum_{\text{big} \sim \Delta} \hat{\chi}_\Delta \sin \Phi_\Delta,$$

where $\hat{\chi}_\Delta \equiv S_i \cdot (S_j \times S_k)$ is the scalar spin chirality operator. The sites $\{ijk\}$ in $\hat{\chi}_\Delta$ are labelled going anticlockwise around the small or big triangles of the honeycomb lattice. As shown in Fig. 1(a), the fluxes in $H_{\text{spin}}$ are $\Phi_\Delta = -\phi$ on small (green) triangles, and $\Phi_\Delta = -3\phi + (3\phi)$ on large triangles which do (do not) enclose a lattice site. Classical magnetic ground states of this model, valid for $S = \infty$, have been studied in [48]; here, we report to a numerical study for $S = 1/2$, retaining strong quantum fluctuations.

**ED phase diagram.** For $\phi = 0$, $H_{\text{spin}}$ reduces to the $J_1-J_2$ honeycomb lattice Heisenberg model, with $J_{1,2} = 4t^2_{1,2}/U$. Previous work indicates that $J_2 \gtrsim 0.2J_1$ kills Néel order, leading to incommensurate spirals [55] for $S = \infty$, and competing valence bond crystals for $S = 1/2$ [56–58]. Here, we study the unexplored regime $\phi \neq 0$, using Lanczos ED on clusters up to $N = 32$ spins, varying $t_{2,3}$ and $\phi$ for fixed $U/t_1 = 10$ which puts us in the Mott insulator [48]. We focus on flux values $\pi/4 \leq \phi \leq \pi/2$, which reveals incommensurate phases with large scalar spin chirality; restricting ourselves to this window of flux avoids incommensurate spiral orders [48, 55] expected at small $\phi$, which have strong finite-size effects in ED. Below, we work in units where $t_1 = 1$.

As shown in Fig.1(b), we find that the phase diagram contains four magnetically ordered phases — Néel, tetrahedral and triad-III orders — which are also observed in the classical phase diagram [48]. (i) The Néel order on the honeycomb lattice is translationally invariant, with ferromagnetic order on each sublattice and a single structure factor peak at the $\Gamma$ point of the hexagonal Brillouin zone. (ii) The tetrahedral order has an 8-site magnetic unit cell, with spins pointing toward the four corners of a tetrahedron and structure factor peaks at the three $M$ points. It is a so-called “regular magnetic order”, respecting all lattice symmetries modulo global spin rotations. (iii)/(iv) Triad-I/II both have 6-site magnetic unit cells, with three spins on each sublattice forming a cone and structure factor peaks at the $K$ and $K'$ points. They can be thought of as umbrella states on each triangular sublattice, with their common axis being parallel in the triad-I case and anti-parallel in the triad-II. This yields a net ferromagnetic moment in triad-I and a net staggered moment in triad-II.

We identify these magnetic orders within ED, on clusters with up to $N = 32$ spins, through a careful analysis of the low energy spectrum, extracting quantum numbers of the quasi-degenerate joint states, i.e., the ’Anderson tower’, in each total spin sector, whose energies collapse onto the ground state as $1/N$ leading to spontaneous symmetry breaking in the thermodynamic limit [59, 60] (see Supplemental Material [61]). The phase boundaries in Fig.1(b) are determined [61] by dips in the ground state fidelity $\langle \Psi_0(g)|\Psi_0(g+\delta g) \rangle$ which signal quantum phase transitions [62], where $g$ is a tuning parameter (here, $t_2$ or $\phi$). We substantiate this by studying changes in the finite-size singlet ($E_s$) and triplet ($E_t$) gaps, $\langle \hat{\chi}_\Delta \rangle$, and reorganization of the low energy spectrum. Our results are in contrast to slave-rotor mean field theory of the Haldane Mott insulator [45, 46], in which the ground state is a CSL which simply inherits the band topology of the underlying QAHI.

**Melting tetrahedral order.** The tetrahedral state is a “regular magnetic state” [63] which respects all lattice symmetries in its $SU(2)$-invariant correlations. Given its large scalar spin chirality, it is tempting to speculate that quantum disordering of this state might lead to a CSL. We thus modify the Haldane model in order to frustrate the tetrahedral order. We notice that the tetrahedral state has spins on opposite vertices of the honeycomb hexagon aligned ferromagnetically. Thus incorporating third-neighbor hopping $t_3$ will lead to an additional exchange interactions in $H_{\text{spin}}$, i.e., the Heisenberg exchange $J_3 = 4t_3^2/U > 0$ which will inevitably frustrate tetrahedral order, as well as additional chiral interactions. Below, we present extensive results retaining only $J_3 > 0$ since keeping all chiral terms induced by $t_3$ significantly increases the computational complexity; we have explicitly checked that these additional terms induce very small quantitative differences in the ED spectra, and only slightly shift the phase boundaries in the phase diagram (see Supplemental Material [61]).

One key signature of a CSL is a nonzero spin gap and two-fold ground state degeneracy on the torus. We thus look for regimes where the lowest excited state is a spin-singlet whose energy gap becomes smaller with system size, while the triplet gap remains nonzero. Fig. 2(a) shows the ED phase diagram as we vary $(t_2, t_3)$, where we find a candidate CSL regime. Here, we have fixed $\phi = \pi/3$, at which the coefficient of $\hat{\chi}_\Delta$ on the large-\(\Delta\) vanishes, enormously simplifying the numerics.

Fig. 2(c) shows a representative ED spectrum on an $N = 32$-site magnetic unit cell, with spins pointing toward the four corners of a tetrahedron and structure factor peaks at the three $M$ points. It is a so-called “regular magnetic order”, respecting all lattice symmetries modulo global spin rotations.
and thus do not cross. However, only the total Chern number $t_3 \neq 0$. Background shows ground state chirality $\langle \chi_\Delta \rangle$ on small-$\Delta$. Using ED and DMRG (at indicated points), we find a window of CSL with topological order. (b) Topological robustness of the CSL ground states upon threading flux through one hole of the torus. Energy spectrum as a function of boundary phase $\theta_0$ is shown for $N = 24$ sites, $t_2 = 0.6$, and $t_3 = -0.6$. (c) Energy spectrum for $N = 32$ cluster, with states labelled by total spin $S_{tot}$ and Brillouin zone momenta shown in the inset. We find approximate two-fold ground state degeneracy with total Chern number $C_1 + C_2 = 1$.

torus at $(t_2, t_3) = (0.6, -0.6)$. We find an approximate two-fold ground state degeneracy, both states being spin singlets with crystal momentum $k = (0, 0)$ as expected for a honeycomb lattice CSL, and a spin gap $E_t \approx 0.3$. Threading flux through one hole of the torus (see Fig. 2(b)), we find the two-fold ground state manifold does not with mix with higher excited states, demonstrating that the ground state degeneracy is of topological origin. We have computed the many-body Chern numbers $C = \mp \frac{1}{2} \int d\theta_1 d\theta_2 \text{Im} \langle \partial_{\theta_1} \Psi_1 | \partial_{\theta_2} \Psi_i \rangle$ using twisted boundary conditions on the two ground states $|\Psi_{i=1,2}\rangle$, since two ground states have the same momentum and thus not cross. However, only the total Chern number of this degenerate manifold is meaningful in the thermodynamic limit; we find $C_1 + C_2 = 1$. These results provide strong evidence that $t_3$ melts tetrahedral order, leading to a $\nu = 1/2$ bosonic Laughlin liquid. Our ED results delineate a regime at $\phi = \pi/3$, see Fig. 2(a), which we identify as a CSL candidate.

DMRG results. To further confirm the existence of CSL, we investigate the model $H_{\text{spin}}$ with additional terms generated by non-zero $t_3$, using DMRG [24], on a cylinder of infinite length with circumference up to $L = 8$ unit cells. The characterization of a topologically ordered phase is achieved by: (i) identifying the conformal field theory (CFT) that describes gapless edge excitations via the "entanglement spectrum" [64], and (ii) computing topological $S$ and $T$ matrices that contain information about bulk anyon excitations [22, 51, 65–68]. Simulations were performed for $\phi = \pi/3$, and four different values of $(t_2, t_3)$ marked by red dots on the phase diagram in Fig. 2(a), keeping only the additional $J_3$ exchange term. We present detailed results below for one point $(t_2, t_3) = (0.6, -0.6); we obtain similar results at the other three points. We also performed simulations on smaller width cylinders (upto $L = 6$) keeping $J_3$ and all additional chiral terms from having $t_3 \neq 0$ in $H_{\text{HFI}}$, obtaining similar results.

Randomly initialized DMRG finds two ground states, $|\Psi_{i=1,2}\rangle$, with well-defined anyon flux threading inside the cylinder [66]. Fig. 3 shows the entanglement spectrum $E_i$ of the reduced density matrix for half an infinite cylinder computed for both ground states. Studying these spectra, we can extract universal information about possible gapless boundary excitations, as if the system had an actual, physical edge [64, 69–72]. The spectra $E_i$ are seen to be consistent with corresponding sectors of the chiral $SU(2)_1$ Wess-Zumino-Witten CFT [73]. $E_1$ is associated with the identity primary operator and its Kac-Moody descendants. The computed degeneracy pattern in every tower (labeled by $S_z$) is seen to follow the expected partition numbers (1–1–2–3–5–7–...) [74]. $E_2$ corresponds to the chiral boson vertex operator and its descendants.

The ground states $|\Psi_{i=1,2}^{\text{cyl}}\rangle$ on an infinite cylinder $\infty \times L$ may be used to mimic grounds states on a $L \times L$ torus $|\Psi_{i=1,2}^{\text{tor}}\rangle$ by means of cutting and reconnecting matrix-product states of $|\Psi_{i=1,2}^{\text{cyl}}\rangle$ [66, 67]. Every such ground state $|\Psi_{i=1,2}^{\text{tor}}\rangle$ has a well-defined anyon flux threading inside the torus. The topological $S$ and $T$ matrices of the emergent anyons can be extracted.
from the overlaps $\langle \Psi_{\text{tot}}^\dagger | R_{\pi/3} | \Psi_{\text{tot}} \rangle$, where $R_{\pi/3}$ denotes clockwise $\pi/3$ rotation of a $L \times L$ torus. For $L = 6$, we find
\begin{equation}
S = \frac{1}{\sqrt{2}} \begin{pmatrix} 0.99 & 0.97 \\ 0.96 & -0.97 & e^{i\pi \cdot 0.01} \end{pmatrix}, \tag{3}
\end{equation}
\begin{equation}
T = e^{i \frac{\pi}{2} \cdot 0.96} \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}, \tag{4}
\end{equation}
in excellent agreement with the exact $S$ and $T$ matrices of a chiral semion anyon model, $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ and $e^{i \frac{\pi}{2}}\begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}$. The combined DMRG results thus provide an unambiguous identification of the phase as a CSL.

**Spin crystallization transition.** Our ED results show that the chirality and ground state fidelity vary smoothly going from the tetrahedral state into the CSL. This suggests that the two phases might be separated by an exotic critical point since the tetrahedral state is topologically trivial but breaks $SU(2)$ spin symmetry while the CSL has topological order and no broken symmetries. A powerful route to accessing such exotic transitions is via fractionalizing the spins [76]. We formulate our theory in terms of spin-1/2 boseonic spinons minimally coupled to an Abelian level $k = 2$ Chern-Simons (CS) gauge field. In the CSL, integrating out gapped spinons results in a CS topological field theory. The lowest energy excitations are gapped spinons, which carry unit gauge charge and bind $\pi$-flux, converting them into semions. On the tetrahedral side, spinon condensation produces magnetic order, destroying topological order via the Higgs mechanism.

To construct the field theory for the matter sector, we imagine boseonic spinons with spins polarized along the local Zeeman axes of the underlying tetrahedral order. Adiabatic spinon transport around closed loops on the honeycomb lattice then produces nontrivial Berry phases; we find $\pi$-flux around hexagonal loops and $\pi/2$-flux around triangular plaquettes. Even if long wavelength quantum fluctuations disorder the tetrahedral state, so these Zeeman fields average to zero, we expect the local spin chirality and hence the local fluxes to persist. Diagonalizing this spinon Hofstadter Hamiltonian on the honeycomb lattice, we find 4 equivalent dispersion minima located for our gauge choice, at $\mathbf{Q}_0 \equiv \Gamma$ and $\mathbf{Q}_i \equiv M_i$ $(i = 1, 2, 3$; the three $M$ points of the BZ). We thus study the action $S = \int d^2x d\tau (L_{CS,\phi} + L_{\text{int}})$, where
\begin{equation}
L_{CS,\phi} = \frac{1}{2\pi} e^{i\mu \lambda} a_\mu \partial_\tau a_\lambda + |(\partial_\mu - ia_\mu)\phi_{i}^{\dagger}|^2 + |r|\phi_{i}^{\dagger}|^2 \tag{5}
\end{equation}
describes boseonic spinons minimally coupled to the CS gauge field, while $L_{\text{int}} = L_{\text{int}}^{(1)} + L_{\text{int}}^{(2)}$ captures spinon interactions,
\begin{equation}
L_{\text{int}}^{(1)} = u_1 \sum_i (\rho_i)^2 + u_2 \sum_{i \neq j} \rho_i \rho_j + u_3 \sum_{i \neq j} \mathbf{S}_i \cdot \mathbf{S}_j \tag{6}
\end{equation}
\begin{equation}
+ u_4 \sum_{i \neq j} \phi_{i}^{\dagger} \phi_{j}^{\dagger} \phi_{i} \phi_{j} + u_5 \sum_{i \neq j} \phi_{i}^{\dagger} \phi_{j}^{\dagger} \phi_{i} \phi_{j}
\end{equation}
\begin{equation}
L_{\text{int}}^{(2)} = w_1 \sum_i (\rho_i)^3 + w_2 \sum_{i \neq j \neq k} e^{i j k} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) + \ldots \tag{7}
\end{equation}
Latin indices label the 4 modes at $\mathbf{Q}_i$ $(i = 0, 1, 2, 3$), the notation $[ij \ell k]$ implies all 4 modes are different, and there is an implicit sum on Greek indices which label spin or space-time. We defined $\rho_i \equiv \phi_{i}^{\dagger} \phi_{i}$ and $\mathbf{S}_i \equiv \phi_{i}^{\dagger} \sigma_{\alpha \beta} \phi_{i \beta}$. $L_{\text{int}}^{(1)}$ and $L_{\text{int}}^{(2)}$ respectively list all quartic interactions and important sixth order terms, consistent with momentum conservation, global $SU(2)$ symmetry, and local gauge invariance. $u_{1,2}$ are forward-scattering interactions, $u_{3,4}$ are backscattering terms, and $u_5$ is an Umklapp process. $w_2$ encodes broken time-reversal symmetry. At mean field level, with dominant $u_1$, $w_1 > 0$, we find $r > 0$ leads to the CSL, while tuning $r < 0$ leads to a confining Higgs phase with $\langle \phi_{i=0} \rangle \neq 0$. For $u_2 < 0$, we get simultaneous condensation at all $\mathbf{Q}_i$. The tetrahedral state emerges via a continuous transition for subdominant terms $u_4, u_5 < u_3, w_2$ (see Supplemental Material [61]). Our construction of the field theory for the CSL-tetrahedral transition relies on a nontrivial flux pattern for the spinons, hinting at ‘crystal symmetry fractionalization’ [77] in the CSL.

**Summary.** Using ED and DMRG, we have shown that the Haldane-Hubbard Mott insulator supports unusual chiral magnetic orders, while third-neighbor hopping induces a CSL with topological order. We have argued that this CSL descends from a ‘parent’ tetrahedral state and constructed a CS-Higgs theory for this exotic spin-crystalization transition. Recent work has shown that the kagome lattice admits only a single $SU(2)$ invariant symmetry enriched CSL [78, 79]. However, the honeycomb lattice may admit multiple CSLs with distinct crystal symmetry fractionalization patterns. Future research directions include nailing down the precise nature of this CSL [78–82], and relating this CSL to Gutzwiller projected wavefunctions [50, 51]. Another outstanding issue is fluctuation effects on the CS-Higgs transition proposed here, and in related U(1) symmetric bosonic quantum Hall to charge density-wave insulator transitions [83].

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ment of the Chern-Simons Higgs theory.

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Supplemental Material

Exact diagonalization spectra for magnetically ordered states with $t_3 = 0$

Exact diagonalization (ED) on system sizes of up to $N = 32$ spins is used to construct the phase diagram of the Haldane-Hubbard Mott insulator, with fixed $U = 10$ and varying $t_2$ and flux $\phi$. The magnetic orders present can be identified by analysing the quantum numbers of the low-lying states in each total spin sector of the ED energy spectrum, the so-called ‘quasi-degenerate joint states’ (QDJS), or ‘Anderson tower’. These states collapse onto the ground state as $1/N$ leading to a spontaneous symmetry broken ground state in the thermodynamic limit.

As stated in the main text, we find that the phase diagram contains four magnetically ordered phases - Néel, tetrahedral and triad-I/II orders. In Fig. S4 we present example spectra for these four phases for a $N = 24$ site cluster which has the full point group symmetry of the lattice $C_{6v}$. In this case the QDJS can be characterised by their momenta and irreducible representation (IR) of $C_{6v}$. Properties of the phases include:

- The Néel order is collinear and translationally invariant, with QDJS with momentum at the $\Gamma$ point and energy scaling linearly with $S_{Tot}(S_{Tot} + 1)$ as expected for quantum rotor excitations.
- The tetrahedral order is non-coplanar with QDJS with momentum at the $\Gamma$ and $M$ points and large chirality on small triangles.
- The triad-I order is non-coplanar and has a net ferromagnetic moment (with the ground state lying in a sector with $S_{Tot} \neq 0$), with QDJS at the $\Gamma$ point and the $K, K'$ points as expected.
- The triad-II order is similar in many respects to the triad-I but with a net anti-ferromagnetic moment and oppositely signed chirality on big triangles.

**FIG. S4.** Example ED energy spectra for the four magnetically ordered phases described in the main text for a $N = 24$ spin cluster.

**Ground state fidelity exact diagonalization results**

The phase boundaries were determined by analysing dips in the ground state fidelity, $F(g) = \langle \Psi_0(g)|\Psi_0(g+\delta g)\rangle$ with $g$ a tuning parameter, as well as changes in the low energy spectrum, the finite-size singlet ($E_s$) and triplet ($E_t$) gaps and the scalar spin chirality $\langle \hat{\chi}_s \rangle$ on big and small triangles. In Fig. S5 we show the ground state fidelity as a function of $t_2$ for $N = 18, 24$ and 32 site torus geometries at $\phi = \pi/2, t_3 = 0$. The sharp dips mark the transition from the Néel to the tetrahedral state.
Comparison between ED results for $t_3 \neq 0$ for the full model versus simplified model with only $J_3 > 0$

With $t_3 = 0$, we have found that there is robust magnetically ordered states in the Mott insulating phase of the Haldane-Hubbard model. With $t_3 \neq 0$, we showed that a CSL phase emerges. In Fig. S6 we show the phase diagram, at $\phi = \pi/3$, for (a) the case presented in the main text in which only the additional third-neighbor Heisenberg term $J_3 = 4t_3^2/U$ is considered, and (b) the case in which all of the additional terms are considered, i.e., the Heisenberg term as well as the additional chiral terms, $J_x = 24t_1 t_2 t_3 / U^2$. In Fig. S7 we show an example of the energy spectrum for both cases at $(t_2, t_3) = (0.5, -0.3)$. We see that keeping all of the terms results in only very small shifts in the phase boundaries, showing that it is really the Heisenberg exchange $J_3$ that is the driving force behind melting the tetrahedral order and getting the CSL phase.

To reduce the computational complexity of the ED/DMRG computations on the largest system sizes, we have retained only this Heisenberg term $J_3$ in the key results presented in the main text. However we have also done DMRG computations (on infinite cylinders with widths up to $L_y = 6$) at the four points marked in Fig. S6(b) retaining all the extra chiral interactions, and confirmed that the CSL phase is robust.
Field Theory of the Spin Crystallization Transition

In the main text we constructed a field theory of spin-1/2 bosonic spinons minimally coupled to an Abelian level \( k = 2 \) Chern-Simons (CS) gauge field to describe a continuous CSL-tetrahedral transition. The action is

\[
S = \int d^2x d\tau (\mathcal{L}_{CS,\phi} + \mathcal{L}_{\text{int}}),
\]

with

\[
\mathcal{L}_{CS,\phi} = \frac{1}{2\pi} \epsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda + |(\partial_\mu - i a_\mu) \phi_{i\alpha}|^2 + r |\phi_{i\alpha}|^2
\]

\[
\mathcal{L}_{\text{int}} = u_1 (\sum_i \rho_i)^2 + u_2 \sum_{i \neq j} \rho_i \rho_j + u_3 \sum_{i \neq j} S_i \cdot S_j + u_4 \sum_{[ijk\ell]} \phi_{i\alpha}^* \phi_{j\beta} \phi_{k\alpha} \phi_{\ell\beta} + u_5 \sum_{i \neq j} \phi_{i\alpha}^* \phi_{j\beta} \phi_{i\alpha}^* \phi_{j\beta}
\]

where Latin indices label the 4 modes at \( Q_i \) (\( i = 0, 1, 2, 3 \)), \([ijk\ell]\) implies all 4 modes are different, there is an implicit sum on Greek indices which label spin or space-time, and we have defined \( \rho_i \equiv \phi_{i\alpha}^* \phi_{i\alpha} \) and \( S_i \equiv \phi_{i\alpha}^* \sigma_{i\beta} \phi_{i\beta} \).

At mean field level, we drop all gradient terms. With dominant \( u_1, w_1 > 0 \) and with \( u_2 < 0 \), we find \( r > 0 \) leads to the CSL with \( \langle \phi_{i\alpha} \rangle = 0 \), while tuning \( r < 0 \) leads to a transition into a confining Higgs phase with \( \langle \phi_{i\alpha} \rangle \neq 0 \). The tetrahedral state emerges for subdominant terms \( u_4, u_5 < u_3, w_2 \). Fig. S8 illustrates a concrete example of such a transition, with the square of the tetrahedral order parameter, plotted as a function of \( r \) at \( u_1 = w_1 = 1, u_2 = -0.7, u_3 = w_2 = 0.1 \) and \( u_4 = u_5 = 0.01 \). It exhibits clear linear scaling as expected for the square of a mean-field order parameter.

FIG. S7. Example ED energy spectra for the blue points marked in Fig. S6 for a \( N = 32 \) spin cluster with (a) only the additional Heisenberg exchange \( J_3 \) and (b) all additional terms, Heisenberg \( J_3 \) and chiral \( J_c \), generated by adding third-neighbor hopping with amplitude \( t_3 \). The two lowest lying states in both cases carry total Chern number \( C = 1 \).

FIG. S8. Mean field computation of the squared order parameter \( \Psi_{\text{Tet}}^2 \) for the tetrahedral state within the Chern-Simons-Higgs field theory, for parameter values in the action mentioned in the text, showing a continuous mean field transition at \( r = 0 \).