Percolation transition and colossal magneto resistive effects in a complex network

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Recent experiments have shown the intrinsic topology complexity in self-organized manganites. The coexistence of short- and long-range forces and the diversity of many competing phases have challenged present electronic models based on regular lattices. The challenge is approached here by invoking the concept of small-world network, whose topology interpolates between regular lattices and random graphs. Magnetic phase transition and percolation transition in these complex networks are studied via Monte Carlo simulations and finite-size scaling analyses. The observed ramified percolative fractals, signified field-induced percolation transition, and enhanced colossal magneto resistive effects agree with experiments well. © 2006 American Institute of Physics.

Recently, a wide variety of experimental results and theoretical investigations has demonstrated that many transition metal oxides (TMOs) have dominant states that are spatially inhomogeneous, due to the simultaneous occurrence of several physical interactions, namely, spin, charge, lattice, and orbital, in these systems. Colossal magnetoresistance (CMR) in manganites is found to be closely related to this phenomenon. Computational studies have already shown the tendency of phase separation, localization, and percolation transition in manganites. However, the puzzling percolative magnetotransport and complex real-space phase morphology have so far resisted a complete physical understanding. In fact, these TMOs are not merely complicated systems. They also tend to spontaneously self-organize, with their structures varying widely in size and scales. In contrast to simple crystalline solids, these spontaneously patterned structures can be assembled in various geometries, virtually unrestricted by a crystal symmetry. Therefore, these manganite materials may be appropriately described by mathematical objects known as graphs (or networks). Possible inadequacy of previous Monte Carlo simulations is based on regular lattices with on-site disorder, which are insufficient to describe the topological complexity and the coexistence of short- and long-range interactions. The appropriate description for many complex real-world systems should be as a network, a general connection of nodes and vertices which need not have the structure of a regular lattice. The small-world network model combines both long-range and short-range aspects, and interpolates between regular lattice and random graph. In this letter, by using Monte Carlo simulations and finite-size scaling analyses, we have performed a systematic investigation of magnetic phase transition and percolation transition in these complex networks. The observed ramified percolative fractals, signified field-induced percolation transition, and enhanced colossal magneto resistive effects agree with experimental findings in phase-separated manganites. In the mean time, the puzzle of mean-field type of paramagnetic-ferromagnetic (P-M) phase transition in the double-exchange manganites is well explained.

The Ising-like Hamiltonian invoked here should model the ferromagnetic interactions between Mn$^{3+}$ and Mn$^{4+}$, and their complex distribution in a real manganite, though the other details of manganites are not explicitly included. The Hamiltonian is written as $H=-\sum_{\langle i,j \rangle} J_{ij} S_i S_j - J_{\langle i,k \rangle} S_i S_k - H \sum S_i$, where $\langle i,j \rangle$ denotes a pair of nearest neighbor (NN) and $\langle i,k \rangle$ means a pair of non-NN once a long-range correlation is established between site $i$ and site $k$. These randomly selected long-range correlations are possible, since neither the variable-range hopping nor quenched disorder happens statistically. We consider the following random adding procedure. Starting from a two-dimensional (2D) regular lattice $(N \times N)$, where each spin interacts with its four NNS, each spin is visited and linked additionally to a randomly chosen spin with the probability $P$, provided that these two are not NNS and there is no such an extra link already, as illustrated in Fig. 1 (upper panel). This method differs somewhat from the original one proposed in Ref. 8, but the underlying topology is the same and is easy to be carried out in 2D cases. Here, a certain amount of non-NNS are correlated by long-range links, but the former local properties preserve. Little is known about the percolation transition in 2D small-world systems we consider here, not to mention their application to hard TMOs. Metropolis Monte Carlo simulations and finite-
size scaling calculations are performed for the above small-world model to obtain the physical properties of magnetic phase transition and percolation transition.\(^7\) In particular, percolation theory is invoked to determine the real-space morphology accurately, including the dimension of fractals, the spanning clusters, and the infinity clusters.\(^1^0\)

Firstly, the temperature dependence of magnetization and \(P\) dependence of Curie temperature \(T_C\) are displayed in Figs. 1(a) and 1(b) (lower panel), respectively. Here \(T_C\) is determined by finite-size scaling of Binder’s fourth-order cumulant \((U_N)\), which is plotted as a function of temperature for various \(N\), yielding a unique crossing point. For the cases with small \(P\), lattices with much larger size \((N>100)\) are used. The non-linear \(P\) dependence of \(T_C\) revealed here, especially the rapid increase upon the initial introduction of small-world links, is beyond any simplified mean-field approach. According to finite-size scaling theory,\(^8\) the free energy of an \(N \times N\) system is given by the universal scaling \(F(i,H;N)=N^{-\beta(Y)(iN^{1/\nu}),bH(N^{2/\nu})}\), where \(i=1-T/T_C(\infty)\). \(T_C(\infty)\) is the infinite-lattice transition temperature, and \(H\) is the external ordering field. \(a\) and \(b\) are meric factors making the scaling function universal. \(d\) is the spatial dimension of the system, and \(\nu\) and \(\Delta\) are static critical exponents. The finite-size scaling of the free energy leads to similar relations for the spontaneous magnetization \(M\), the susceptibility \(\chi\), and the specific heat \(C_V\) as \(m=N^{-\beta(Y)I(M)(iN^{1/\nu}), \chi =N^{\beta(\nu)}\chi(iN^{1/\nu}), \text{and} \ C_V=N^{\beta(Y)\gamma(C)(iN^{1/\nu})}\), respectively. \(\alpha\), \(\beta\), and \(\gamma\) are critical exponents which should satisfy the scaling and hyperscaling relations \(\Delta=\beta\delta+\beta+\gamma\), and \(2-\alpha=\nu\beta+\gamma\). For a given size \(N\) and temperature \(T\) (in units of \(1/k_B\)), various thermodynamic quantities such as Binder’s fourth-order cumulant, the specific heat, and the susceptibility can be measured: \(U_N=1-[(m^4)]/[3(m^2)^2], \ C_V=[(H^2)-\langle H \rangle^2]/T^2 N, \text{and} \ (\cdot \cdot \cdot)\) and \([\cdot \cdot \cdot]\) represent the thermal average (10^\(\text{th}\)) and the average over different configurations (10^\(\text{th}\)), respectively. Close to \(T_C\), the critical exponent \(\nu\), describing the divergence of the correlation length near \(T_C\) as \(\xi \sim |T-T_C|^{-\nu}\), is related to the temperature dependence of the fourth-order cumulant as \(U_N(T)=U^*+U_1(1-(T/T_C))^{1/\nu}\), with \(U^*\) and \(U_1\) independent of \(T\) and \(N\). Thus, we have \(\Delta U_N/\Delta T \sim -N^{1/\nu}\), from which the value of \(\nu\) can be estimated. We have found that all the critical exponents fall into the class of mean-field critical behavior (the detailed calculation not shown here): e.g., when \(P=0.01, \nu=0.97\pm0.03, \beta/\nu=0.42\pm0.02, \alpha/\nu=0.05\pm0.01,\) and \(\gamma/\nu=1.21\pm0.04; \text{when} \ P=0.7, \nu=0.93\pm0.070, \beta/\nu=0.480\pm0.005, \alpha/\nu=0.034\pm0.008,\) and \(\gamma/\nu=1.023\pm0.003). The obtained mean-field type of phase transition in small-world network is in excellent agreement with experimental findings\(^1^1\) and supplements the calculations based on double-exchange, which leads to Heisenberg type of phase transition.\(^1^2\) In fact, we have also studied double-exchange Hamiltonian [Eq. (1) in Ref. 12] in small-world networks, with the same mean-field type of \(P-M\) transition obtained.

Besides the macroscopic magnetic properties, microstructure of phase separation and percolation transition near \(T_C\) are studied. The evolution of real-space phase morphology (spin configuration) below \(T_C\) as a function of temperature and \(P\) is displayed in Fig. 2 (upper panel). Here, phenomenologically, the spin up (green) and spin down (yellow) can be regarded as two competing phases. With the increase of small-world links, a crossover from larger droplet phase to finer mist one is found.\(^1^3\) Such variations in microstructure agree with the neutron experiments, i.e., the phases exist in the form with somewhat a reduced dimension (e.g., liquid-like droplets in \(\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3\) and “red cabbage” 2D sheets or one-dimensional filament in \(\text{Pr}_{0.65}\text{Ca}_{0.35}\text{MnO}_3\)).\(^1^4\) The percolating fractals at \(T_C\) are identified with red color in the...

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**FIG. 1.** (Color online) Upper panel: Illustration of complex networks with small-world links. Lower panel: (a) Temperature dependence of magnetization and (b) \(P\) dependence of \(T_C\).

**FIG. 2.** (Color online) Upper panel: Real-space phase morphology in \(100^2\) networks with spin up (green) and spin down (yellow) representing two competing phases. From left to right, \(T/T_C=0.85, 0.90, 0.97,\) and 1.0, respectively, and from top to bottom, \(P=0, 0.001, 0.01, 0.1, 0.3,\) and 0.7, respectively. The largest cluster of spin up at \(T_C\) is plotted in red on the right. Lower panel: The evolution of the largest cluster in \(100^2\) networks at 1.1\(T_C\) as a function of external magnetic field and \(P\). From left to right, \(P=0, 0.001, 0.01, 0.1, 0.3,\) and 0.7, and from top to bottom, \(H/J=0, 0.01,\) and 0.02, respectively. The electrodes in each case are applied from top to bottom. The absence of infinite spanning cluster is clear when \(P \neq 0\) and \(H/J = 0\).
right column and their fractal dimension \( D_f \) is shown in Fig. 3(a). Due to the double-exchange mechanism or as the definition in Ref. 3, the transport path is open only between two parallel spins. The reduced \( D_f \) indicates that the electrical transport paths are much closer to a one-dimensional filament. Our previous numerical simulations have revealed that CMR in ferromagnetic state depends strongly on the microstructure of transport paths. When the current is localized in a single channel, CMR reaches the maximum [inset of Fig. 3(a)]. The ramified percolating clusters in small-world networks indicate a filamentlike transport path and consequently an enhanced CMR effect. This finding is also consistent with a recent experiment of enhanced CMR in \((\text{La}_0.7\text{Pr}_{0.3})_3\text{Ca}_{0.7}\text{MnO}_3\), where the current is found to take complex paths.\(^{16}\) To explore the colossal effects further, another kind of CMR, that is related to the enlargement of metallic component near/above \( T_C \), is studied. Here field-induced percolation transition is thought to be the fundamental mechanism. In Fig. 2 (lower panel), the evolution of the largest spin-up cluster is displayed as a function of external magnetic field and \( P \). One can see immediately that the largest percolating cluster disappears so long as small-world links are introduced and consequently a more obvious field-induced percolation transition. Percolation threshold \( f_{cP} \) and critical exponent \( (\beta_P) \) of this field-induced percolation transition are calculated in Figs. 3(b) and 3(c) for small-world systems \( (P \geq 0.001) \), respectively. The small ratio of \( \beta_P \) indicates a sharp percolation transition in small-world networks. Extended to manganites, this will lead to a sharp \( I-M \) transition, accompanied with a significant CMR effect.

To summarize, we have developed a complex network model for the self-organization in manganites. The consistent picture of giant cluster coexistence, magnetic phase transition, percolation transition, and colossal magnetoresistive effects provides a further understanding of self-organization in manganites and demonstrates that the topological complexity in manganites is beyond the description in a regular lattice. In particular, the puzzle of the coexistence of percolative CMR effects and mean-field type of \( P-M \) transition in the double-exchange manganites is well understood.

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**References**


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**Fig. 3.** (Color online) (a) \( P \)-dependence of \( D_f \) of spin-up clusters at \( T_C \). Detailed calculation method refers to Ref. 10. Inset shows low-field CMR as a function of effective number of transport paths \( N_{eff} \) (Ref. 15). (b) \( P \)-dependence of \( f_{cP} \). Inset shows the finite-size scaling of \( f_{cP} \) (the strength of spanning cluster). (c) \( P \)-dependence of \( \beta_P \). Inset shows the finite-size scaling of \( f_{cP} \) (the strength of infinity cluster), which satisfies the scaling \( f_{cP} \sim (f - f_{c})^{\beta_P} \) near \( f_{c} \).