Dynamical and transport properties of a simple single-band spin-fermion lattice model for (III,Mn)V diluted magnetic semiconductors (DMS) is here discussed using Monte Carlo simulations. This effort is a continuation of previous work (G. Alvarez et al., Phys. Rev. Lett. 89, 277202 (2002)) where the static properties of the model were studied. The present results support the view that the relevant regime of $J/t$ (standard notation) is that of intermediate coupling, where carriers are only partially trapped near Mn spins, and locally ordered regions (clusters) are present above the Curie temperature $T_C$. This conclusion is based on the calculation of the resistivity vs. temperature, that shows a soft metal to insulator transition near $T_C$, as well on the analysis of the density-of-states and optical conductivity. In addition, in the clustered regime a large magnetoresistance is observed in simulations. Formal analogies between DMS and manganites are also discussed.

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I. INTRODUCTION

Diluted magnetic semiconductors (DMS) are attracting much attention lately due to their potential for device applications in the growing field of spintronics. In particular, a large number of DMS studies have focused on III-V compounds where Mn doping in InAs and GaAs has been achieved using molecular beam epitaxy (MBE) techniques. The main result of recent experimental efforts is the discovery of ferromagnetism at a Curie temperature $T_C\sim\text{110 K}$ in Ga$_{1-x}$Mn$_x$As, with Mn concentrations $x$ up to 10%. It is widely believed that this ferromagnetism is “carried induced”, with holes donated by Mn ions mediating a ferromagnetic interaction between the randomly localized Mn$^{2+}$ spins. In practice, anti-site defects reduce the number of holes $n$ from its ideal value $n=x$, leading to a ratio $p=(n/x)$ substantially smaller than 1.

Until recently, theoretical descriptions of DMS materials could be roughly classified in two categories. On one hand, the multi-band nature of the problem is emphasized as a crucial aspect to quantitatively understand these materials. In this context the lattice does not play a key role and a continuum formulation is sufficient. The influence of disorder is considered on average. On the other hand, formulations based on the possible strong localization of carriers at the Mn-spin sites have also been proposed. In this context a single impurity-band description is considered sufficient for these materials. Still within the single-band framework, but with carrier hopping not restricted to the Mn locations, recent approaches to the problem have used dynamical mean-field or reduced-basis approximations. An effective Hamiltonian for Ga$_{1-x}$Mn$_x$As was derived in the dilute limit and studied in Ref. [14]. All these calculations are important in our collective effort to understand DMS materials.

However, it is desirable to obtain a more general view of the problem of ferromagnetism induced by a diluted set of spins and holes. To reach this goal it would be better to use techniques that do not rely on mean-field approximations and, in addition, select a model that has both the continuum and impurity-band formulations as limiting cases. Such an approach would provide information on potential procedures to further enhance $T_C$ and clarify the role of the many parameters in the problem. In addition, these general considerations will be useful beyond the specific details of Ga$_{1-x}$Mn$_x$As, allowing us to reach conclusions for other DMS. An effort in this direction was recently initiated by Mayr and two of the authors. A detailed Monte Carlo study of a simple model for DMS already allowed us to argue that $T_C$ could be further enhanced --perhaps even to room temperature-- by further increasing $x$ and $p$ from current values in DMS samples. These predictions seem in agreement with recent experimental developments since very recently Ga$_{1-x}$Mn$_x$As samples with $T_C$ as high as 150 K were prepared, a result believed to be caused by an enhanced free-hole density. Also samples with $T_C\sim\text{127 K}$ and $x>0.08$ were reported in Ref. [17] and, very recently, a $T_C$ of 140K was achieved on high quality GaMnAs films grown with Arsenic dimers. There seems to be plenty of room to further increase the critical temperatures according to these theoretical calculations.

The model used in Ref. [15] was a single-band lattice Hamiltonian, also studied by other groups, which does not have the multi-band characteristics and spin-orbit couplings of the real problem. However, it contains spin and holes in interaction and it is expected to capture the main qualitative aspects of carrier-induced ferromagnetism in DMS materials. The choice of a single-band model allows us to focus on the essential aspects of the problem, leaving aside the numerical complexity of the multi-band Hamiltonian, which unfortunately cannot be studied with reliable numerical techniques at present without introducing further approximations. Note that a quite similar philosophy has been followed in the related area of manganites for many years. In fact, it is well-known that the orbital order present in those compounds can only be studied with a two-band model. However, single-band approaches are sufficient to investigate the competition between ferromagnetic and anti-ferromagnetic states, an effect...
recently argued to be at the heart of the colossal magnetoresistance phenomenon. As a consequence, a qualitatively reliable study of the single-band DMS model—with itinerant holes and localized classical spins—is expected to be important for progress in the DMS context as well.

In our previous publication, the phase diagram of the single-band model for DMS was already sketched. This phase diagram is reproduced in Fig. 1. The only parameter in the Hamiltonian is the ratio \( J/t \), where \( J \) is the local antiferromagnetic coupling between the spins of carriers and localized Mn\(^{2+}\) ions, and \( t \) is the carrier-hopping amplitude (for details, see the full form of the Hamiltonian in the next section). Due to its large value 5/2, the Mn spin is assumed to be classical for numerical simplicity. At small \( J/t \), individual carriers are only weakly bounded to the Mn spins. Even for small realistic values of \( x \), the carrier wave functions strongly overlap and a large-bandwidth itinerant band dominates the physics. In this regime, \( T_C \) grows with \( J/t \).

This portion of the phase diagram is referred to as ‘weak coupling’ in Fig. 1 and in our opinion it qualitatively corresponds to the continuum-limit approach pursued in Refs. 15. In the other extreme of large \( J/t \), the previous effort\(^{15} \) found a \( T_C \) that is much suppressed, converging to zero as \( J/t \) increases (at least at small values of \( x \)). The reason for this behavior is the strong localization of carriers at Mn spin locations, to take advantage of the strong \( J \) coupling. The localization suppresses the mobility and the carrier-induced mechanism is no longer operative. However, when several Mn spins are close to one another small regions can be magnetized efficiently. As a consequence, a picture emerges where small islands of ferromagnetism are produced at a fairly large temperature scale \( T^* \) (>\( T_C \)) that grows with \( J \), but a global ferromagnetic state is only achieved upon further reducing the temperature such that the overlaps of wave functions induce a percolation-like process that aligns the individual preformed clusters. The proper procedure to distinguish between these two regimes is through an analysis of short- and long-distance spin correlations. In our opinion, the effort of Refs. 9,10 belongs to this class, and it corresponds to the ‘strong coupling’ region of Fig. 1. Between the weak and strong coupling domains, an intermediate region provides a natural interpolation between those two extreme cases. The Curie temperature is optimal (i.e., the largest) in this intermediate zone, at fixed values of \( p \) and \( x \). In this regime, there is sufficient interaction between the clusters to become globally ferromagnetic, and at the same time the \( J \) is sufficiently strong to induce a robust \( T_C \). If chemical control over \( J/t \) were possible, this intermediate region would be the most promising to increase the Curie temperature (again, at fixed \( x \) and \( p \)).

However, it may even occur that the DMS materials are already in the intermediate optimal range of \( J/t \) couplings. An indirect way to test this hypothesis relies on calculations of dynamical and transport properties, which are presented in this paper, and its comparison with experiments. In particular, the experimentally measured d.c. resistivity \( \rho_{dc} \) of DMS compounds has a nontrivial shape with a (poor) metallic (d\( \rho_{dc}/dT \) >0) behavior below \( T_C \), which turns to insulating (d\( \rho_{dc}/dT \) <0) at higher temperatures. This nontrivial profile resembles results reported in the area of manganites, which also have a metal-insulator transition as a function of temperature\(^{22} \), although in those materials the changes in resistivity with temperature are far more dramatic than in DMS. The formal similarities DMS-manganites have already been remarked in previous literature\(^{23} \) and suggest a common origin of the \( \rho_{dc} \) vs. temperature curves. In Mn-oxides it is believed that above the Curie temperature, preformed ferromagnetic clusters with random orientations contribute to the insulating behavior of those materials\(^{20,21} \). For DMS, a similar rationalization can be envisioned if the state of relevance above \( T_C \) has preformed magnetic clusters. From the previous discussion\(^{15} \) it is known that the intermediate \( J/t \) region can have clusters without collapsing \( T_C \) to a very small value. At the Curie temperature, the alignment of these preformed moments leads to a metallic state. An explicit calculation of the resistivity—using techniques borrowed from the mesoscopic physics context—is provided in this paper, and the results support the conjecture that clustered states can explain the transport properties of DMS. These unveiled analogies with manganites are not just accidental. Clearly, approaches to DMS that rely on mobile carriers and localized spins in interaction have close similarities with the standard single-band double-exchange model where only one \( e_g \)-orbital is considered. The key difference is the presence of strong dilution in DMS as compared with manganites.

It is interesting to remark that in agreement with the ‘clustered’ state described here, recently Timm and von Oppen have shown that correlated defects in DMS are needed to describe experimental data. Their simulations with Coulombic effects incorporated lead to cluster formation, with sizes well beyond those obtained from a random distribution of Mn sites as considered here. In this respect, the results of Ref. 23 provide an even more dramatic clustered state than ours. If the Mn spins were not distributed randomly in our simulations but in a correlated manner, the state above \( T_C \) would be even more insulating than reported below and the physics would resemble much closer that observed in manganites. Note also that
Kaminski and Das Sarma have also independently arrived to a polaronic state that qualitatively resembles the clustered state discussed here. It is also interesting that in recent ion-implanted (Ga,Mn)P:C experiments that reported a high Curie temperature, the presence of ferromagnetic clusters were observed and they were attributed to disorder and the proximity to a metal-insulator transition. Even directly in (Ga,Mn)As, the inverse magnetic susceptibility deviates from the Curie law at temperatures above $T_C$ (Fig. 2(b) of Ref. 2), which may be an indication of an anomalous behavior. In manganites, these same anomalies in the susceptibility are indeed taken as evidence of the formation of clusters.

The paper is organized as follows: In Section II the details of the method of simulation, definitions, and conventions are presented. Section III describes the results for the density-of-states (DOS) of this model, the appearance of an “impurity band” at large $J/t$, and the relation of the DOS with the optimal $T_C$. The temperature and carrier dependence of the optical conductivity and Drude weight are presented in Section IV with results compared with experiments. In Section V the resistance of a small cluster is calculated and also the optical conductivity and Drude weight are presented in Section VI. Large effects are observed. Section VII describes the characteristics of the clustered-state regime above $T_C$. Finally, in Section VIII the ‘transport’ phase diagram is presented, and it is discussed in what region it appears to be the most relevant to qualitatively reproduce results for Ga$_{1-x}$Mn$_x$As MBE-grown films.

II. METHOD AND DEFINITIONS

A. Hamiltonian Formalism

There are two degrees of freedom in the DMS problem described here: (i) the local magnetic moments corresponding to the 5 electrons in the $d$ shell of each Mn impurity, with a total spin $S/2$, and (ii) the itinerant carriers produced by the Mn impurities. Since these Mn impurities substitute Ga atoms in the zinc-blende structure of GaAs, there is, in principle, one hole per Mn. However, it has been found that the system is heavily compensated and, as a consequence, the actual concentration of carriers is lower. In the present study, both the density of Mn atoms, $x$, and the density of carriers, $n$, are treated as independent input parameters. Moreover, the ratio $p = n/x$ is defined, which is a measure of the compensation of the system, e.g. for $p = 0$ the system is totally compensated and for $p = 1$ there is no compensation.

The Hamiltonian of the system in the one-band approximation can be written as:

$$\hat{H} = -t \sum_{<ij>,\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + J \sum_I \mathbf{S}_I \cdot \hat{\mathbf{S}}_I,$$

(1)

where $\hat{c}_{i\sigma}$ creates a carrier at site $i$ with spin $\sigma$. The carrier-spin operator interacting antiferromagnetically with the localized Mn-spin $\hat{S}_I$ is $\hat{s}_I = \hat{c}^\dagger_{i\uparrow} \hat{c}_{i\downarrow} \hat{\mathbf{S}}_I$. Through nearest-neighbor hopping, the carriers can hop to any site of the square or cubic lattice. The interaction term is restricted to a randomly selected but fixed set of sites, denoted by $I$. Note that in addition to the use of a single band, there are other approximation in the model described here: (i) The Hubbard $U/t$ is not included. This is justified based on the low-carrier concentration of the problem, since in this case the probability of double occupancy is small. In addition, Mn-oxide investigations have shown that an intermediate or large $J$ coupling acts similarly as $U/t$, also suppressing double occupancy. (ii) A nearest-neighbors anti-ferromagnetic coupling between the Mn spins is not included. Again, this is justified as long as $x$ is small. (iii) Finally, also potential disorder is neglected (together with the spin, the Mn sites should in principle act as charge trapping centers). This approximation is not problematic when the Fermi energy is larger than the width of the disorder potential (i.e. large $p$ and $x$). However, in the $(p, x)$ range analyzed in this paper it becomes more questionable to neglect this effect. Its influence will be studied in a future publication.

In the present study the carriers are considered to be electrons and the kinetic term describes a conduction band. However, in Ga$_{1-x}$Mn$_x$As the carriers are holes and the valence band has to be considered instead. Although the latter is more complicated, the simplified treatment followed here should yield similar results for both cases.

The local spins are assumed to be classical which allows the parametrization of each local spin in terms of spherical coordinates: $(\theta_i, \phi_i)$. The exact-diagonalization method for the fermionic sector is described in this section, following Ref. 20. The partition function can be written as:

$$Z = \prod_i \left( \int_0^\pi d\theta_i \sin \theta_i \int_0^{2\pi} d\phi \left( Z_p(\theta_i, \phi_i) \right) \right).$$

(2)

where $Z_p(\theta_i, \phi_i) = \text{Tr}(e^{-\beta \hat{K}})$ is the partition function of the fermionic sector, $\hat{K} = \hat{H} - \mu \hat{N}$, $\hat{N}$ is the number operator, and $\mu$ is the chemical potential.

In the following, an hypercubic lattice of dimension $D$, length $L$, and number of sites $N = L^D$ will be considered. Since $\hat{K}$ is a Hermitian operator, it can be represented in terms of a hermitian matrix which can be diagonalized by an unitary matrix $U$ such that

$$U^\dagger KU = \begin{pmatrix} \epsilon_1 & 0 & \cdots & 0 \\ 0 & \epsilon_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \epsilon_{2N} \end{pmatrix}.$$  

(3)

The basis in which the matrix $K$ is diagonal is given by the eigenvectors $u_1^{|0\rangle}, u_2^{|0\rangle}, \ldots, u_N^{|0\rangle}$, where the fermionic operators used in this basis are obtained from the original operators through $u_m = \sum_{j\sigma} U^\dagger_{m,j\sigma} c_{j\sigma}$, with $m$ running from 1 to $2N$.

Defining $u_m^{|n\rangle} = |n_m\rangle$ and denoting by $n_m$ the eigenvalues
of \( \hat{n}_m \), the trace can be written
\[
\text{Tr}_y(e^{-\beta \hat{K}}) = \sum_{n_1, \ldots, n_{2N}} \langle n_1 \ldots n_{2N} | e^{-\beta \hat{K}} | n_1 \ldots n_{2N} \rangle
\]
\[
= \sum_{n_1, \ldots, n_{2N}} \langle n_1 \ldots n_{2N} | e^{-\beta \sum_{\lambda=1}^{2N} \epsilon_{\lambda} n_{\lambda}} | n_1 \ldots n_{2N} \rangle, \tag{4}
\]

since in the \( \{ u_m, |0 \rangle \} \) basis, the operator \( \hat{K} \) is \( \sum_{\lambda} \epsilon_{\lambda} \hat{n}_{\lambda} \), and the number operator can be replaced by its eigenvalues. Thus, Eq. (4) can be rewritten as
\[
Z = \prod_{i}(\int_{0}^{\pi} d\theta_i \sin \theta_i \int_{0}^{2\pi} d\phi_i) \frac{2N}{\lambda=1} (1 + e^{-\beta \epsilon_{\lambda}}), \tag{5}
\]
which is the formula used in the simulations.

### B. Monte Carlo Method

The integral over the angular variables in Eq. (5) can be performed using a classical Monte Carlo simulation. The eigenvalues must be obtained for each classical spin configuration using library subroutines. Finding the eigenvalues is the most time consuming part of the numerical simulation. The integrand is clearly positive. Thus, “sign problems” in which the integrand of the multiple integral under consideration can be non-positive, are fortunately not present in our study.

Although the formalism is in the grand-canonical ensemble, the chemical potential was adjusted to give the desired carrier density, \( n \). To do so, the equation \( n(\mu) - n = 0 \) was solved for \( \mu \) at every Monte Carlo step by using the Newton-Raphson method. This technique proved very efficient in adjusting with precision the desired electronic density and, as a consequence, our analysis can be considered as in the canonical ensemble as well, with a fixed number of carriers.

Usually, 2,000-5,000 Monte Carlo iterations were used to let the system thermalize, and then 5,000-10,000 additional steps were carried out to calculate observables, measuring every five of these steps to reduce autocorrelations.

Since for fixed parameters there are many possibilities for the random location of Mn impurities, results are averaged over several of these disorder configurations. Approximately 10-20 disorder configurations were generally used for small lattices (4\(^3\) and 10\(\times\)10) and 4-8 for larger lattices (6\(^3\) and 12\(\times\)12). The inevitable uncertainties arising from the use of a small number of disorder configuration does not seem to affect in any dramatic way our conclusions below. This is deduced from the analysis of results for individual disorder samples. The qualitative trends emphasized in the present paper are present in all of these configurations.

### C. Observables

Quantities that depend on the Mn degrees of freedom (\( \theta_i \) and \( \phi_i \) in the previous formalism) are calculated simply by averaging over the Monte Carlo configurations. Note that any observable that does not have the continuous symmetry of the Hamiltonian will vanish over very long runs. Thus, it is standard in this context to calculate the absolute value of the magnetization, \( |M| = \sqrt{\sum_{ij} \hat{S}_i \cdot \hat{S}_j} \), as opposed to the magnetization vector. Another useful quantity is the spin-spin correlation, defined by:
\[
C(x) = \frac{1}{N(x)} \sum_y \hat{S}_{y+x} \cdot \hat{S}_y \tag{6}
\]
where \( N(x) \) is the number of non-zero terms in the sum. The correlation at a distance \( d \) is averaged over all lattice points that are separated by that distance, but since the system is dilute, the quantity must be normalized to the number of pairs of spins separated by \( d \), to compare the results for different distances.

The observables that directly depend on the electronic degrees of freedom can be expressed in terms of the eigenvalues and eigenvectors of the Hamiltonian matrix \( \hat{K} \). The DOS, \( N(\omega) \), is simply given by \( \sum_\lambda \delta(\omega - \epsilon_\lambda) \). However, the majority and minority DOS, \( N_\uparrow(\omega) \) and \( N_\downarrow(\omega) \), were also calculated in this study. \( N_\uparrow(\omega) \) indicates the component that aligns with the local spin, i.e., \( N_\uparrow(\omega) \) is the Fourier transform of \( \sum_i < \hat{c}_\uparrow^\dagger(t) \hat{c}_\uparrow(0) > \), where \( \hat{c}_\uparrow = \cos(\theta_i/2) c_\uparrow + \sin(\theta_i/2) e^{-i\phi_i} c_\downarrow \). Then:
\[
N_\uparrow(\omega) = \sum_\lambda \delta(\omega - \epsilon_\lambda) \left\{ \sum_i U_{\uparrow,\lambda}^\dagger U_{\lambda,i} \cos^2(\theta_i/2) + U_{\uparrow,\lambda}^\dagger U_{\lambda,i} \sin^2(\theta_i/2) + (U_{\uparrow,\lambda}^\dagger U_{\lambda,i} \exp(-i\phi_i) + U_{\downarrow,\lambda}^\dagger U_{\lambda,i} \exp(i\phi_i)) \times \cos(\theta_i/2) \sin(\theta_i/2) \right\}, \tag{7}
\]
where for sites \( i \) without an impurity \( \theta_i = \phi_i = 0 \) is assumed. A similar expression is valid for \( N_\downarrow(\omega) \). The optical conductivity was calculated as:
\[
\sigma(\omega) = \frac{\pi (1 - e^{-\beta \omega})}{\omega N} \int_{-\infty}^{+\infty} dt \frac{e^{i\omega t}}{2\pi} \langle \hat{j}_x(t) \cdot \hat{j}_x(0) \rangle, \tag{8}
\]
where the current operator is:
\[
\hat{j}_x = i \hbar e \sum_{j\sigma} (\hat{c}_{j+\hat{x},\sigma}^\dagger \hat{c}_{j,\sigma} - H.c.), \tag{9}
\]
with \( \hat{x} \) the unit vector along the \( x \)-direction. For \( \omega \neq 0 \), \( \sigma(\omega) \) can be written as:
\[
\sigma(\omega) = \sum_{\lambda \neq \lambda'} \frac{\pi t^2 e^2 (1 - e^{-\beta \omega})}{\omega N} \times \left| \sum_{j\sigma} (U_{\uparrow,\lambda}^\dagger U_{\lambda,\sigma} - U_{\downarrow,\lambda}^\dagger U_{\lambda,\sigma}) \right|^2 \frac{(1 + e^{\beta(\rho_\lambda - \rho_{\lambda'})})(1 + e^{-\beta(\rho_\lambda - \rho_{\lambda'})})}{(1 + e^{\beta(\rho_\lambda - \rho_{\lambda'})})^2} \times \delta(\omega + \rho_\lambda - \rho_{\lambda'}). \tag{10}
\]
Both \( N(\omega) \) and \( \sigma(\omega) \) were broadened using a Lorentzian function as a substitute to the \( \delta \)-functions that appear in
not completely separated from the unperturbed band. For this reason, both the unperturbed band and the impurity band have to be considered in quantitative calculations. To illustrate this, Eq. (11) was calculated in order to gather additional information. The optical conductivity in the Fermi regime is considered at strong coupling, then two spin-split bands ("impurity bands") will appear for this model, each with weight proportional to \(x\), at each side of the unperturbed band which would have weight \(x\), but the chemical potential \(\mu\) lies within it.

Eqs. (4) and (11). The width of the Lorentzian used was \(\epsilon = 0.05\) in units of the hopping, \(t\).

The optical conductivity in \(d\) dimensions obeys the sum rule:

\[
\frac{D}{2} = \frac{\pi e^2}{2N\hbar} \langle -\hat{T} \rangle - \int_0^\infty \sigma(\omega) d\omega, \tag{12}
\]

where \(D\) is the Drude weight and \(\hat{T}\) is the kinetic energy:

\[
-\hat{T} = t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.). \tag{13}
\]

Although the Drude weight gives a measure of the d.c. conductivity properties of the cluster, the "mesoscopic" conductivity was also calculated in order to gather additional information. The details are explained in Section III.

**III. DENSITY OF STATES**

In this section, the density-of-states calculated at several couplings is shown and discussed. A few basic facts about the DOS of the model, Eq. (11), are presented first. If carrier localization effects are not taken into account and a ferromagnetic state is considered at strong \(J/t\) coupling, then two spin-split bands ("impurity bands") will appear for this model, each with weight proportional to \(x\), at each side of the unperturbed band which would have weight \(2(1-x)\) (Fig. 2). For partially compensated samples, \(p < x\), the chemical potential will be located somewhere in the first spin-split band, and, as a consequence, only this band would be relevant in the model Eq. (11).

In practice, Monte Carlo simulations show that, in the regime of interest where \(T_C\) is optimal, the impurity band is not completely separated from the unperturbed band. For this reason, both the unperturbed band and the impurity band have to be considered in quantitative calculations. To illustrate this, Figure 3 shows \(N(\omega)\) vs. \(\omega\) for different \(J/t\)’s in two dimensions. With growing \(J/t\), the "impurity band" begins to form for \(J/t \geq 3.0\), and at \(J/t = 6.0\) it is already fairly separated from the main band. However, note that for this extreme regime of \(J/t\), \(T_C\) is far lower than for \(J/t = 3.0\), as discussed before in Ref. 15. In fact, the optimal \(J/t\) for the \((x, p)\) parameters used here was found to be in the range 2.0-4.0. This implies that the model shows the highest \(T_C\) when the "impurity band" is about to form, but it is not yet separated from the main band. This introduces an important difference between our approach to DMS materials, and the theoretical calculations presented in Ref. 9. Figure 3(a)-(c) indicates that a similar behavior is found in three dimensions. In this case, once again, the optimal \(T_C\) occurs for intermediate \(J/t\), as seen in Fig. 3(d) where the phase diagram obtained from a \(6^3\) lattice with \(x=0.25\) and \(p=0.3\) is shown.

The physical reason for this behavior is that at very large \(J/t\), the states of the impurity band are highly localized where the Mn spins are. Local ferromagnetism can be easily formed, but global ferromagnetism is suppressed by the concomitant weak coupling between magnetized clusters.

Both, Figures 3 and 4 represent results obtained at particular values of parameters \(x=0.25\), \(p=0.3\), and \(T/t = 0.01\). However, results for several other sets \{(\(x, p, T\)}\} were gathered as well (not shown). The \(x\) dependence of the DOS is simple: increasing \(x\) produces a proportional increase in the number of states of the impurity band, and a corresponding decrease of the main band weight (see Fig. 4). In terms of \(p\), increasing the effective carrier concentration by a small amount was found to simply shift the chemical potential to the right. Concerning the temperature dependence of the DOS, at low temperature the states contributing to the impurity band are polarized, i.e. the system is ferromagnetic, as shown by the different weights of the majority and minority bands (Figs. 4 and 5). As the temperature increases, spin disorder grows due to thermal fluctuations, and when \(T \sim T^*\), i.e. in the paramagnetic regime, the bands become symmetric.

It appears that the only change that a small increase in the carrier concentration produces is an increase in the chemical potential. However, experimentally the appearance of a pseudo-gap at the Fermi energy has been reported. Although the finite size effects in the present theoretical calculation do not allow for a detailed study of \(N(\omega)\) at or very near the Fermi energy with high enough precision, in certain cases a pseudo-gap was indeed observed in the present study at the chemical potential, particularly when the system is in the clustered regime. While this result certainly needs confirmation, it is tempting to draw analogies with the more detailed calculations carried out in the context of manganites, where the presence of a pseudo-gap both in theoretical models and in experiments is well established. Pseudo-gaps are also present in under-doped high temperature superconductors. Given the analogies between DMS materials and transition-metal oxides unveiled in previous investigations, it would not be surprising that DMS presents a pseudo-gap in the clustered regime as well. More work is needed to confirm these speculations.

Results presented in this section for the DOS qualitatively agree with those found in Ref. 12 using the dynamical mean-
field technique (DMFT) in the coupling regime studied there. However, the DMFT approach is a mean-field approximation local in space and, as a consequence, the state emphasized in this paper— with randomly distributed clusters— cannot be studied accurately with such a technique.

Experimental evidence of the formation of the impurity band for Ga$_{1-x}$Mn$_x$As has been provided by Okabayashi et al. in Refs. 31-32 (see also Ref. 33). It is interesting to remark that half the total width of the impurity band obtained in our simulations is about 2$t$ (see, e.g., Figs. 3 and 4, and using $t=0.3eV$ this is equal to 0.6eV, in good agreement with the width 0.5eV estimated from the photoemission experimental measurements mentioned before.

The local DOS is studied next. The purpose of this analysis is to further understand the inhomogeneous state that forms as a consequence of Mn-spin dilution and concomitant carrier localization. The local DOS is shown in Fig. 5 on an 8×8 lattice at $x=0.25$, $p=0.4$, $J/t=2.5$, and $T/t=0.05$. In this particular case only, an arrangement of classical spins was introduced ‘by hand’ such that the clusters are clearly formed. In this way, sites can easily be classified in three groups, as discussed below. Despite using a particularly chosen spin configuration, the resulting DOS is similar to those obtained previously (Fig 5) using a truly random distribution of spins.

Lattice sites are classified as follows: the first group is defined to contain lattice sites that have a classical spin and belong to a spin cluster. The second class is composed of sites that have an isolated classical spin, i.e., nearby sites do not have other classical spins. Finally, lattice sites without classical spins in the same site or its vicinity belong to the third class. $N_I(\omega)$, $N_{II}(\omega)$, and $N_{III}(\omega)$ denote the local DOS at sites corresponding to each of the three classes, respectively. It can be observed that $N_I(\omega)$ contributes to states inside the impurity band (note the sharp peak near -1), but also contributes to the main band since the $J/t$ used is intermediate. $N_{II}(\omega)$ contributes a sharp peak near zero, and also has weight in the main band. This can be explained as follows: the electron is weakly localized at an isolated site yielding a state at $\omega_I \approx -J$ or, since $\mu \approx -J$ for $p \approx 0.4$, $\omega_{II} = \mu \approx 0$ (see Fig 5). This interesting result shows that many of the states near zero in Figs 3 and 4 may be localized, and they do not contribute to the conductivity. Finally, in $N_{III}(\omega)$ the empty sites contribute weight only in nearly unperturbed states, i.e., states that belong to the main band. In conclusion, the local carrier density is very inhomogeneous and this fact has an important effect on the form of the site-integrated DOS. Our results show that

THREE DIMENSIONS

![Figure 3: $N_I(\omega)$ and $N_{II}(\omega)$ vs. $\omega-\mu$ for a 10×10 periodic system with 26 spins ($x \sim 0.25$) and 10 electrons ($p \sim 0.4$) at $T/t = 0.01$. Results are shown for (a) $J/t = 2.0$, (b) $J/t = 3.0$, (c) $J/t = 4.0$, and (d) $J/t = 6.0$. $\omega-\mu$ is in units of the hopping, $t$. The results are averages over eight configurations of disorder (but there is no qualitative difference in the results from different configurations).](image)

![Figure 4: $N_I(\omega)$ and $N_{II}(\omega)$ vs. $\omega-\mu$ for a 6×6 periodic system with 54 spins ($x \sim 0.25$) and 16 electrons ($p \sim 0.4$) at $T/t = 0.01$. Results are shown for (a) $J/t = 2.0$, (b) $J/t = 4.0$, (c) $J/t = 6.0$. $\omega-\mu$ is in units of the hopping, $t$. The results are averages over eight configurations of disorder (but there is no qualitative difference in the results from different configurations).](image)
The frequency of this peak, transitions from the impurity band to the unperturbed band. Intermediate frequencies is due to inter-band transitions, i.e. coupling exists, when applied to DMS materials. As well, which is shown in Fig. 6(a) for a two-dimensional lattice. This optical conductivity has two main features: (i) a zero-frequency or Drude peak and (ii) a finite-frequency broad peak which is believed to correspond to transitions from the impurity band to the main band, as argued below. From Fig. 6(a), it is observed that inter-band transitions are not much relevant at weak coupling \( J/t = 1.0 \), but they appear with more weight at intermediate couplings \( J/t = 2.0 - 3.0 \), where \( T_C \) is optimal. It is worth remarking that at \( J/t \) strong enough, e.g. \( J/t = 6.0 \), when the impurity band is well-formed, the finite-frequency peak is weaker in strength than for the optimal \( J/t \) due to localization. In fact, if \( J/t \) were so large that the “impurity band” is completely separated from the unperturbed band, then carrier localization would be so strong that inter-band transitions would not be possible. The Drude peak is plotted separately in Fig. 6(b) as a function of \( J/t \) at low temperatures. As expected, when \( J/t \) increases and localization sets in, the conductivity of the cluster decreases. Similar results for the optical conductivity and Drude weight are found in three dimensions (see Fig. 7).

The rise in absorption that appears for \( J/t \geq 2.5 \) at intermediate frequencies is due to inter-band transitions, i.e. transitions from the impurity band to the unperturbed band. The frequency of this peak, \( \omega_{\text{inter}} \), depends upon \( J/t \) as well as carrier concentration \( p \), but for \( J/t \geq 2.5 \) (which is an intermediate value) and \( p = 0.4 \) (a realistic value), it was observed that \( 0.5t \leq \omega_{\text{inter}} \leq 1.0t \). The model parameter \( t \) was previously estimated \(^{15} \) to be \( t \sim 0.3\text{eV} \), yielding \( 0.15\text{eV} \leq \omega_{\text{inter}} \leq 0.3\text{eV} \), in agreement with experiments (see below).

The temperature dependence of \( \sigma(\omega) \) is shown in Fig. 8 and it is as follows: for \( T \leq T_C \), the Drude weight, \( D \), decreases in intensity as temperature increases and the same behavior is observed for the finite-frequency peak. When \( T \geq T_C \), \( D \) increases slightly at first and then remains constant as the temperature is increased further. This slight raise in \( D \) is subtle and could be linked to the decrease in resistiv-
ity observed for $T > T_C$ for intermediate $J/t$ as explained in the next section, since the system is clustered just above $T_C$. Since both the optical conductivity and Drude weight decrease with temperature, to satisfy the sum rule the kinetic energy must also decrease as temperature increases. This is indeed observed (not shown) and is to be expected since localization of the wave function is stronger above $T_C$.

FIG. 8: Temperature dependence of the optical conductivity of model Eq. (1). Shown is $\sigma(\omega)$ vs. $\omega$ for a 10×10 periodic system with 26 spins ($x \sim 0.25$), $J/t = 2.5$, $p = 0.3$, and for different temperatures, as indicated. *Inset*: Drude weight, $D$, vs. temperature $T$.

A broad peak at around 0.2eV is experimentally observed in the optical conductivity of Ga$_{1-x}$Mn$_x$As, as shown in Fig. 9 which is reproduced from Ref. 3. This feature has been explained before in two different ways: (i) as produced by transitions from the impurity band to the GaAs valence band, or (ii) as caused by inter-valence band transitions. Due to the frequency range and temperature behavior observed, our study supports the first possibility, i.e., that the finite-frequency peak observed for Ga$_{1-x}$Mn$_x$As at around 0.2 eV is due to transitions from the impurity band to the main band. Recent observations also appear to support this view.

The Drude weight increases in intensity with increasing carrier density, as can be seen from Fig. 10. In fact, the ratio $p$ of carriers to Mn concentration, which is a measure of the compensation of the samples, could explain, within the framework of this model, the different behavior observed at low frequencies for GaMnAs and InMnAs. In the former case, no tail of the Drude peak is found. However, for InMnAs, a clear Drude tailing is observed with increasing intensity as the temperature increases. At large enough doping, our calculations based on model Eq. (1) predict a Drude-like peak for $\sigma(\omega)$ which could correspond to the regime valid for InMnAs, while for low doping this study predicts a very small Drude peak, which is the case for GaMnAs. Unfortunately, the precise carrier concentrations for both materials are not known experimentally with precision.

FIG. 9: Absorption coefficient $\alpha(\omega)$ spectra for a metallic sample prepared by low temperature annealing. The temperatures from down to top are 300, 250, 200, 150, 120, 100, 80, 60, 40, 20, 10 and 4.2 K. (from Katsumoto et al.)

FIG. 10: $p$-dependence of the optical conductivity. Shown is $\sigma(\omega)$, including the Drude weight, vs. $\omega$ for a 10×10 lattice, $x = 0.25$, $J/t = 2.5$, $T/t = 0.01$, and different values of $p$. In the direction of the arrow, $p$ takes the values 0.08, 0.12, 0.20, 0.30, 0.38, and 0.5. *Inset*: Drude weight, $D$, vs. fraction of carriers, $p$.

V. CONDUCTANCE AND METAL-INSULATOR TRANSITION

The conductance, $G$, is calculated using the Kubo formula adapted to geometries usually employed in the context of
The actual expression is

$$G = 2\frac{e^2}{h} \text{Tr} \left[ (i\hbar \hat{v}_x) \text{Im} \tilde{\hat{G}}(E) (i\hbar \hat{v}_x) \text{Im} \tilde{\hat{G}}(E) \right], \quad (14)$$

where $\hat{v}_x$ is the velocity operator in the $x$ direction and $\text{Im} \tilde{\hat{G}}(E)$ is obtained from the advanced and retarded Green functions using $2\text{Im} \tilde{\hat{G}}(E) = \hat{G}^R(E) - \hat{G}^A(E)$, where $E$ is the Fermi energy. The cluster is considered to be connected by ideal contacts to two semi-infinite ideal leads, as represented in Fig. 11. Current is induced by an infinitesimal voltage drop. This formalism avoids some of the problems associated with finite systems, such as the fact that the conductivity is given by a sum of Dirac $\delta$ functions, since the matrix eigenvalues are discrete. A zero-frequency delta peak with finite weight corresponds to an ideal metal – having zero resistance – unless an arbitrary width is given to that delta peak. In addition, in numerical studies sometimes it occurs that the weights of the zero-frequency delta peak are negative due to size effects.

For these reasons, calculations of d.c. resistivity using finite close systems are rare in the literature. All these problems are avoided with the formulation described here.

The entire equilibrated cluster as obtained from the MC simulation is introduced in the geometry of Fig. 11. The ideal leads enter the formalism through self-energies at the left/right boundaries, as described in Ref. 35. In some cases a variant of the method explained in Ref. 35 was used in this paper to calculate the conductance (this modification was suggested to us by J. Vergés). Instead of connecting the cluster to an ideal lead with equal hoppings, a replica of the cluster was used at the sides. This method, although slightly slower, takes into account all of the Monte Carlo data for the cluster, including the periodic boundary conditions. In addition, averages over the random Mn spin distributions are carried out. The physical units of the conductance $G$ in the numerical simulations are $e^2/h$ as can be inferred from Eq. (14). In Fig. 12 the inverse of the conductance, which is a measure of the resistivity, is plotted for a three-dimensional lattice at weak, intermediate, and strong coupling, at fixed $x=0.25$ and $p=0.3$. For the weak coupling regime ($J/t=1.0$) the system is weakly metallic at all temperatures. In the other limit of strong couplings, $1/G$ decreases with increasing temperature, indicating a clear insulating phase, as a result of the system being in a clustered state at the temperatures explored with carriers localized near the Mn spins. At the important intermediate couplings emphasized in our effort, the system behaves like a dirty metal for $T < T_C$, while for $T_C < T < T^*$, $1/G$ slightly decreases with increasing temperature, indicating that a soft metal to insulator transition takes place near $T_C$. For $T > T^*$, where the system is paramagnetic, $1/G$ is almost constant. Note that for strong enough $J/t$, $T_C \to 0$ and therefore no metallic phase is present.

FIG. 11: Geometry used for the calculation of the conductance. The interacting region (cluster) is connected by ideal contacts to semi-infinite ideal leads.

FIG. 12: Dependence of the theoretically calculated resistivity, $\rho$, with temperature in three dimensions. Shown is $\rho = L/G$ vs. $T$ on $4^3$ lattices, 16 spins ($x = 0.25$), and 5 carriers ($p = 0.3$) for the $J/t$'s indicated. An average over 20 disorder configurations has been performed in each case. Units are shown in two scales, $a \hbar/(2e^2)$ on the left and $m$Ωcm on the right, with $L = 4$ and assuming $a = 5.6$ Å. The estimated critical temperatures are also shown (the arrows indicate the current accuracy of the estimations).

Similar qualitative behavior is found for the two-dimensional case (Figs. 13 and 14). Furthermore, in Fig. 13, the spin-spin correlations have been plotted to show the distribution of $T_C$ and $T^*$ and their relation to the resistivity.

It is interesting to compare our results with experiments. For Ga$_{1-x}$Mn$_x$As, data similar to those found in our investigations have been reported. A typical result for resistivity versus $T$ can be found in Ref. 3. The qualitative behavior of the resistivity in these samples agrees well with the theoretical results presented in Fig. 12, if intermediate couplings are considered. On the other hand, stronger or weaker couplings are not useful to reproduce the data, since the result is either insulating or metallic at all temperatures, respectively (defining metallic and insulator regimes by the slope of the resistivity vs. temperature curves).

Furthermore, even the experimental numerical values of the resistivity are in agreement with the results presented here (even though model Eq. 11 does not include a realistic treatment of the GaAs host bands). This can be shown as follows. The conductivity of a three-dimensional sample is related to the conductance by $\sigma = G/L$, where $L$ is the side length of the lattice. Hence the resistivity is $\rho = L/G$. The units of $G$ are, as explained before, $\hbar/(2e^2)$, and in our case $L = 4a$, where $a$ is the lattice spacing. Assuming $a = 5.6$ Å, then the values shown in Fig. 12 are obtained. Note that...
in Fig. 12, the minimum resistivity for $J/t=2.5$ is 3.3 mΩcm, whereas the minimum possible value for that carrier doping and cluster size used is 1.5 mΩcm, which corresponds to the case $J/t=0$. In spite of the label ‘metallic’ for these results, the absolute values of the resistivity are high. Similarly, in the metallic phase of the sample shown in the experimental results of Ref. 4, the minimum resistivity is only $\sim 3-6$ mΩcm. Both in theory and experiments, the metallic phase appears to be ‘dirty’, which is likely due to the reduced number of carriers, and localizing effect of the disorder.

For $J/t$ intermediate or strong, localization of the wave function is observed at intermediate temperatures. This implies that carriers tunnel between impurity sites without visiting the main band, leading to insulating behavior. Below $T_C$ conduction is favored by the ferromagnetic order and, as a consequence, as temperature decreases conductance increases. To further understand why the conductance (resistance) has a minimum (maximum) around $T_C$ it is helpful to consider the three states: FM, clustered, and paramagnetic (PM) as depicted for a special spin configuration in Fig. 15 on an $8 \times 8$ lattice. This configuration is not truly random but it was chosen ‘by hand’ for simplicity so that the spin clusters can easily be recognized. In the case of a random configuration of spins a similar reasoning can be drawn. For the FM state of Fig. 15 conduction is possible and indeed the measured conductance is $G \approx 2.8(2e^2/h)$. For the two possible clustered states represented in Figs. 15b) and (c), the conduction is reduced due to the different alignment of spins in different clusters. This is verified by calculating the conductance which is $G \approx 0.0$ in those cases. For a paramagnetic spin arrangement with spin pointing in random directions (not shown), the conductance is small but finite, $G \approx 0.5(2e^2/h)$.

It follows that the clustered state has the minimum conductance, and this explains the observed behavior of the resistivity with a maximum near $T_C$, i.e., when the system is clustered.

The inverse of the Drude weight, $D^{-1}$, also shows a peak around $T_C$ as seen in Fig. 16 where the same Mn-spin configuration as in Fig. 14 was used. This provides further evidence for the metal-insulator transition near $T_C$ described here.

It is also interesting to remark that the optimal value of $J/t$ changes with $x$ (e.g., for small $x$, $J/t$ optimal is also small). Since $J/t_{optimal}$ approximately separates the metal from the insulator, working at a fixed $J/t$ (as in real materials) and varying $x$, then an insulator at high temperatures is found at small $x$, turning into a metal at larger $x$. This is in excellent agreement with the experimental results of Ref. 4, using a careful annealing procedure (while results of previous investigations with as grown samples had found an insulator-metal-insulator transition with increasing $x$). The issue discussed in this paragraph is visually illustrated in Fig. 17 for the benefit of the reader.

VI. MAGNETORESISTANCE

The magnetoresistance percentage ratio was calculated using the definition $MR = 100 \times (\rho(0) - \rho(B))/\rho(B)$. Figure 15 shows the magnetization, $|M|$, and the resistivity as a function of the applied field $B$ on a $12 \times 12$ lattice, $x=0.15$, $p=0.4$, $J/t=1.0$, and low temperature. Note that in two di-
mensions at \( x = 0.25 \) and \( p = 0.3 \), the intermediate coupling corresponds to \( J/t = 2.5 \), but at \( x = 0.15 \), now \( J/t = 1.0 \) corresponds to optimal coupling since as \( x \) decreases the optimal \( J/t \) also decreases. For these parameters, \( T_C \) was estimated to be \( 0.02t \) and \( T^* \approx 0.06t \). The value in Teslas of the magnetic field was calculated assuming \( g = 2.0 \) and \( S = 5/2 \) for the localized spins. The units of the resistivity are \( \hbar/(2e^2) \) for the two-dimensional lattice.

In our simulations it was observed that \(|M|\) increases with increasing magnetic field. At zero magnetic field \(|M|\) is 60% of its maximum value, while at 12 T it has reached \( \sim 80\% \). This is in agreement with the experimental results in Fig. 3 of Ref. 8 where the magnetization is 50% of its maximum value at zero field, but it reaches 70% of that maximum value at 4 T. In our simulations it was also observed that \( 1/G \) decreases with increasing magnetic field, showing at all fields a negative magnetoresistance. Near \( T_C \) the resistivity decreases by 20%-30% increasing the field from zero to 12 T, while the decrease in resistivity at higher temperatures is much smaller. The present computational results agree very well with the experimentally measured dependence of the resistivity and magnetization on magnetic fields. For example, in Fig. 2(b) of Ref. 3 the decrease in resistivity is 25% near \( T_C \approx 60 \) K when increasing the field from zero to 15 T. A much smaller decrease in resistivity is observed at higher temperatures \( (T > 120 \) K). It is also indicated in that experimental reference that the magnetoresistance is between 30% and 40% at 12 Tesla.

It is interesting to remark that substantial magnetoresistance effects have been reported in thin films consisting of nanoscale Mn\(_{11}\)Ge\(_3\) ferromagnetic clusters embedded in a dilute ferromagnetic semiconductor matrix. The characteristics of these materials are analogous to our clustered state, that also show a robust MR effect due to magnetization rotation of spontaneously formed clusters.

VII. MORE ABOUT CLUSTER FORMATION

It was discussed before in this paper and in previous publications that a clustered state is formed above \( T_C \) for inter-
mediate and large $J/t$ couplings. This state is a candidate to describe DMS materials since it explains both the resistivity maximum around $T_C$, as well as the decrease in resistivity with increasing applied magnetic field. In addition, it provides an optimal $T_C$. This clustered state is formed only for intermediate or larger $J/t$ and when the compensation is strong, $p < 0.4$. Since for large $J/t$ the carriers are localized, the problem becomes one of percolation theory, which has already been treated using different approaches and approximations. Here, only a very simple way of visualizing this state will be presented. First, consider a two-dimensional lattice with 5% Mn spins represented as black dots, as shown in Fig. 19. The carrier wave function, $\psi(r)$, is considered to be localized around a Mn spin and it is assumed to be a step function for simplicity, i.e. $\psi(r)$ is non-zero only if $r < r_1$ where $r_1$ is the localization radius introduced by hand. Sites where the wave function is not zero are the black areas of Fig. 19(b). In this case, sites can be classified into connected regions, and that feature is indicated in Fig. 19(c) using different shades. Each region is correlated and will correspond to a FM cluster. In this case all spins belong to some large cluster. As the concentration $x$ grows, the clusters will tend to merge. As $x$ decreases, these clusters will become more and more isolated.

Recent experimental work on (Ga,Cr)As have revealed unusual magnetic properties which were associated with the random magnetism of the alloy. The authors of Ref. 38 explained their results using a distributed magnetic polaron model, that resembles the clustered-state ideas discussed here and in Refs. 15, 23, 24.

FIG. 19: Percolation picture for the formation of the clustered-state regime. (a) Two-dimensional lattice representing randomly-located classical spins as black dots with $x=0.05$. (b) Black areas represent non-zero carrier wave function, assuming a step-function profile for the wave functions with radius equal to 2 sites, as explained in the text. (c) Same as (b) but now showing connected regions (which could in practice correspond to the FM clusters discussed in the text) indicated with different shades of gray.

VIII. CONCLUSIONS

In this paper, dynamical and transport properties of a single-band model for diluted magnetic semiconductors have been presented. The calculations were carried out on a lattice and using Monte Carlo techniques. The optical conductivity, density of states, and resistance vs. temperature agree with experimental data for Ga$_{1-x}$Mn$_x$As if the model is in a regime of intermediate $J/t$ coupling. In this region, the carriers are neither totally localized at the Mn sites nor free, as in previous theories. The state of relevance has some characteristics of a clustered state, in the sense that upon cooling from high temperatures first small regions are locally magnetized at a temperature scale $T^*$ – causing a mild insulating behavior – while at an even lower temperature $T_C$ the alignment of the individual cluster moments occurs – causing metallic behavior. This is in agreement with previous investigations. 10,15,23,24

One of the main conclusions of the paper is summarized in Fig 24 where the ‘transport’ phase diagram is sketched. The low-temperature ferromagnetic phase is metallic (although often with poor metallicity). The clustered state between $T^*$ and $T_C$ has insulating properties, and the same occurs in a good portion of the phase diagram above these two characteristic temperatures. Note that here the terms metallic and insulating simply refer to the slope of the resistivity vs. temperature curves. The values of the resistivities in the two regimes are not very different, similarly as observed experimentally.

This and related efforts lead to a possible picture of DMS materials where the inhomogeneities play an important role.
FIG. 20: Sketch of the phase diagram indicating the conducting and insulating regions, as obtained in the present investigations. The dashed area in the paramagnetic phase indicates the crossover region from a mild metallic weak coupling regime to a mild insulating strong coupling regime.

In this respect, these materials share characteristics with many other compounds such as manganites and cuprates, where current trends point toward the key importance of nanocluster formation to understand the colossal magnetoresistance and underdoped regions, respectively. “Clustered” states appear to form a new paradigm that is useful to understand the properties of many interesting materials.

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