The rapidly developing field of ferromagnetism in diluted magnetic semiconductors, where a semiconductor host is magnetically doped by transition metal impurities to produce a ferromagnetic semiconductor (e.g. $Ga_{1-x}Mn_xAs$ with $x \approx 1 - 10\%$), is discussed with the emphasis on elucidating the physical mechanisms underlying the magnetic properties. Recent key developments are summarized with critical discussions of the roles of disorder, localization, band structure, defects, and the choice of materials in producing good magnetic quality and high Curie temperature. The correlation between magnetic and transport properties is argued to be a crucial ingredient in developing a full understanding of the properties of ferromagnetic semiconductors.

I. INTRODUCTION

The study of semiconductors (i.e. intrinsically insulating materials with band gaps in the $\sim 1$ eV range) which are also ferromagnetic has a long, but perhaps somewhat intermittent, history. Back in the 1960s and early 1970s there was a great deal of interest in Eu-based chalcogenide materials which exhibited ferromagnetism with Curie temperature around 50K or less. These were strongly insulating systems with rather poor semiconducting transport properties. In the 1980s there were major efforts in magnetically doped II–VI ternary and quaternary semiconductor alloys, e.g. CdMnSe, CdMnTe, PbSnMnTe etc., but most of these materials exhibited spin glass or related disordered magnetic behavior and any ferromagnetism invariably had very low ($\leq 5K$) transition temperature. The idea of a diluted magnetic semiconductor, where a small ($< 10\%$) concentration of magnetically active atoms (most often Mn although Co and Cr have also been used occasionally) is distributed at the cation sites of the host semiconductor, is appealing because such a system may have both semiconducting and ferromagnetic properties. Making such materials has, however, been problematic because the magnetic transition metal (i.e. Mn) is not thermodynamically stable in the semiconductor host (e.g. GaAs), and tends to segregate.

The need for actively controlling and manipulating the carrier spin degree of freedom (in addition to the charge degree of freedom) in semiconductors leading to novel multifunctional magneto-opto-electronic capabilities has created the emerging interdisciplinary field of spintronics (or spin electronics). A key component of spintronics is the development of new ferromagnetic semiconductors. Following the successful development of $Ga_{1-x}Mn_xAs$ and $In_{1-x}Mn_xAs$ as ferromagnetic semiconductors (with $x \approx 1 - 10\%$), using careful low-temperature molecular beam epitaxy (MBE) technique, intensive worldwide activity has led to claims of ferromagnetism (some at room temperatures and above) in several magnetically doped semiconductors, e.g. $GaMnP$, $GaMnN$, $GeMn$, $GaMnSb$. It is at present unclear whether all these reports of ferromagnetism (particularly at room temperatures or above) are indeed intrinsic magnetic behavior or are arising from clustering and segregation effects associated with various Mn-complexes (which have low solubility) and related materials problems. The observed ferromagnetism of $GaMnAs$ is, however, well-established and is universally believed to be an intrinsic diluted magnetic semiconductor (DMS) phenomenon.

The Mn dopants in $GaMnAs$ serve the dual roles of magnetic impurities providing the local magnetic moments and of acceptors producing, in principle, one hole per Mn atom. The number density $n_v$ of the charge carriers (holes in $GaMnAs$), however, turns out to be by almost an order of magnitude lower than the number density $n_i$ of the Mn ions, making the system to be a highly compensated doped semiconductor. This high level of compensation is believed to be a crucial ingredient in the underlying DMS ferromagnetic mechanism. In particular, the precise role played by the relative values of the local moment density $n_i$ and the hole density $n_v$ in giving rise to DMS ferromagnetism is currently being debated in the literature to the extent that there is no agreement even on whether the heavy compensation ($n_c \ll n_i$) in the system helps or hinders ferromagnetism. An important question in this context is to obtain the functional dependence of the ferromagnetic transition temperature (“Curie temperature”) $T_c$ on magnetic moment and hole densities $n_i$ and $n_c$. In $Ga_{1-x}Mn_xAs$ the early experimental results indicated a nonmonotonic behavior of $T_c(x)$ with $T_c$ first increasing with the Mn concentration $x$, reaching a maximum of about 110K for $x \approx 5\%$, and then decreasing with further increase of Mn concentration above this optimum value. A strong correlation between the magnetic transition temperature and transport properties of $GaMnAs$ was also reported in these findings with the system exhibiting relatively stronger metallic behavior close to this optimum Mn doping level ($\lesssim 5\%$). Recent experimental studies of $Ga_{1-x}Mn_xAs$ under carefully controlled annealing conditions seem to suggest that the metastable nature (and high defect content) of low temperature MBE grown $GaMnAs$ may be playing an important role in determining magnetic properties – in particular, careful annealing.
could, under suitable conditions, lead to an enhancement of $T_c$ with increasing Mn content leading to an eventual saturation of the transition temperature in the $x = 5-8\%$ range without the nonmonotonic $T_c(x)$ behavior observed earlier. These annealing studies\textsuperscript{12,13} confirm the close connection between carrier transport properties and ferromagnetism in DMS materials showing that typically $T_c$ values are the highest in GaMnAs samples with nominally highest conductivities (and presumably the highest hole densities). It has therefore been suggested that, in agreement with the mean-field theory (MFT) for DMS ferromagnetism originally derived in Refs.\textsuperscript{14,15} in a different context and recently rediscovered in Refs.\textsuperscript{16,17}. $T_c$ in GaMnAs grows monotonically as $T_c \propto n_e^{1/3}$ when the carrier density increases for a fixed Mn concentration. This simple Weiss MFT\textsuperscript{14,15,16,17,18} then implies a convenient technique for enhancing the ferromagnetic transition temperature in GaMnAs, namely, to increase the hole density as much as possible. The general validity of this Weiss MFT-based assertion remains questionable, and it has been argued\textsuperscript{19,20} that this prediction holds only in perturbative regime of small $J$ and small $n_e$.

The GaMnAs annealing studies bring up important and interesting questions regarding the nature and role of metastable defects in the system that are presumably being healed during annealing leading to $T_c$ enhancement. Two different kinds of GaMnAs lattice (atomistic) defects have been discussed in this context. First, there are As antisite (As$_{Ga}$) defects, As atoms sitting at Ga sites, that are invariably present in the low temperature MBE growth required for DMS GaMnAs. These As antisite defects act as double donors with each As defect capturing two holes in GaMnAs. The second type of defects that has been much discussed recently, is the Mn interstitial defect, where the “defective” Mn atom sits at an interstitial site in the GaAs lattice instead of occupying a substitutional cation site replacing a Ga atom. The Mn interstitials are thought to be particularly deleterious in affecting the magnetic properties of GaMnAs because they have two adverse effects: first, they act as donors (similar to As antisite defects) capturing holes; second, the Mn interstitials typically have strong local direct antiferromagnetic coupling to any neighboring substitutional Mn atoms, thereby suppressing the net effective Mn magnetic moment available for DMS ferromagnetism. The quantitative abundance of As antisites and Mn interstitials in GaMnAs is difficult to estimate because there is really no direct experimental technique to observe these defects. It is, however, widely believed that the low-temperature MBE technique, crucial for the homogeneous single-phase growth of GaMnAs, invariably generates both of these defects with their relative importance varying from sample to sample depending on the uncontrollable details of growth and processing. In addition to the atomistic As antisite and interstitial defects in GaMnAs, there are invariably many other unintentional (as well as unknown and uncontrolled) defects and impurities (both charged and neutral) in GaMnAs because low temperature MBE, in general, produces materials of rather poor quality. This poor quality of GaMnAs is reflected in the transport properties as even the best GaMnAs samples seem to have very low carrier mobilities. The measured hole mobilities in the so-called “metallic” GaMnAs systems are only about 1 – 50 cm$^2$/V·s corresponding to a typical carrier mean free path of 0.1 – 1 nm. Such small values of mean free paths would indicate a strong tendency toward carrier localization in GaMnAs, and indeed there are reports of reentrant metal-insulator transitions in GaMnAs as a function of the Mn content $x$. Specifically, it has been reported\textsuperscript{11} that Ga$_{1-x}$Mn$_x$As is an insulator for small ($x < 3\%$) and large ($x > 7\%$) values of $x$ whereas it is metallic (albeit with very small mean free paths) in the intermediate range of $x$ ($\sim 5\%$) where the ferromagnetic transition temperature is maximized. Other experimental studies (often using careful sample annealing procedures) do not find such reentrant metal-insulator transition behavior\textsuperscript{12,13}.

It is important to emphasize that the existence of DMS ferromagnetism seems to be independent of the system being metallic or insulating. For GaMnAs, both metallic and insulating samples are ferromagnetic with the transition temperature typically being higher for metallic systems although this may not necessarily be a generic behavior. Many other systems exhibiting DMS ferromagnetism, e.g., InMnAs, GeMn, GaMnSb, GaMnN, are however strongly insulating, and as such, metallicity (i.e. itinerant nature of the carriers), is not a necessary precondition for the existence of ferromagnetism in DMS systems. Additionally, in Ga$_{1-x}$Mn$_x$As samples exhibiting reentrant metal-insulator transitions the ferromagnetic behavior appears to be completely continuous as a function of $x$ with the only observable effect being a variation in $T_c$, which is expected since different GaMnAs samples, even with nominally the same value of $x$, show wide variations in $T_c$ values. The real DMS carriers mediating the ferromagnetic interaction between the local moments are generically likely to be far from free holes in the valence band of the host semiconductor material. They are, in all likelihood, extended or bound carriers in the impurity (or the defect) band which forms in the presence of the Mn dopants. There is a great deal of direct experimental support for the relevance of this impurity band picture for DMS ferromagnetism, and first principles band structure calculations also confirm the impurity band nature of the carriers active in DMS ferromagnetism. Both the impurity band nature of the carrier system and the presence of strong charge and spin disorder in the system (due to the random Mn dopants as well as other defects, disorder, and impurities invariably present in the DMS material) make carrier localization a relevant issue in DMS ferromagnetism. We believe that understanding the correlation between transport and magnetic properties is a key ingredient in DMS physics.

In the next section of this review we critically discuss some of the proposed theoretical models (and their va-
lidity or applicability) for DMS ferromagnetism emphasizing the connection between magnetization (as well as the Curie temperature) and transport properties. We conclude in section III with a brief discussion of (many) open questions and some possible future directions in the subject.

This article is is more of a theoretical perspective; it is not meant to be an exhaustive review of the vast literature on ferromagnetic semiconductors. We only discuss some of the key developments in the subject in order to highlight the physical mechanisms and the important system parameters controlling ferromagnetism in diluted magnetic semiconductors.

II. THEORIES

The fact that the DMS are ferromagnetically independent of their weakly metallic or strongly insulating nature implies a robust character for the underlying mechanism leading to the long range magnetic order in these systems. Clearly the ferromagnetic mechanism should not depend crucially on the carrier system being “free” valence band holes since the strongly insulating DMS systems do not have any free holes. The currently accepted picture for DMS ferromagnetism is that it is the local anti-ferromagnetic coupling between the carriers (i.e., holes in GaMnAs) and the Mn magnetic moments that leads to long range ferromagnetic ordering of Mn local moments. The carrier system also becomes spin-polarized in the process with the carrier magnetic moment directed against the Mn magnetic ordering by virtue of the anti-ferromagnetic hole-Mn coupling, but the total magnetic moment of the spin polarized carriers is extremely small since \( n_c \ll n_i \) and \(|S| > |s|\) where \( S \) and \( s \) are respectively the Mn and the hole spin. The relevant DMS effective magnetic Hamiltonian can be written as

\[
H_M = \int d^3r J(r) S(r) \cdot s(r),
\]

where \( S(r) \) and \( s(r) \) are respectively the Mn and hole spin densities. The coupling \( J(r) \) between Mn local moments and hole spins can, in principle, be ferromagnetic \( (J < 0) \) or antiferromagnetic \( (J > 0) \), but the effective interaction between the Mn local moments mediated by the holes (through \( H_M \)) is always ferromagnetic. The magnitude of \( J \) must come from a first principles band structure calculation or from experiments.

Since the Mn moments are localized at specific lattice sites, it is sensible to write Eq. (1) in the more conventional form

\[
H_M = J \sum_i \int d^3r \delta(r - R_i) S_i \cdot s(r),
\]

where the sum over \( i \) goes over the Mn sites in the GaAs lattice, and we have assumed the exchange coupling \( J \) to be a constant. The \( J S_i \cdot s \) local exchange coupling defined in Eq. (2) is sometimes referred to as the Zener model (or the \( s - d \) coupling although in the context GaMnAs, where the carriers are holes, the coupling is more like an \( p - d \) exchange coupling between Mn \( d \) levels and the \( p \) valence band).

The magnetic Hamiltonian defined in Eqs. (1) and (2) is, of course, one of the most well-known interaction Hamiltonians in all of condensed matter physics. Depending on the relative magnitudes of hole and Mn moment densities \( n_h \) and \( n_i \), and the coupling strength \( J \), \( H_M \) describes the Kondo model or the Kondo lattice model or \( s - f \) (or \( s - d \)) Zener model or the double exchange model or the RKKY model or (in the presence of strong disorder) the (RKKY) spin glass model. Most of the earlier studies of this exchange Hamiltonian have concentrated on the low impurity-density limit, \( n_i \ll n_c \), where the local moments are a perturbation on the carrier Fermi surface. The DMS systems provide an interesting novel regime for studying \( H_M \), namely the regime of low carrier density \( n_i \gg n_c \). There has not been much earlier work focused on the low carrier-density limit of the Kondo lattice Hamiltonian or the RKKY spin glass Hamiltonian, which is the appropriate parameter regime for GaMnAs. We emphasize that Kondo physics plays no essential role in DMS systems, but because of the strong inherent disorder in these systems spin glass physics may very well be playing a role at lower values of \( n_i/n_c \).

The simplest way to understand DMS ferromagnetism on a qualitative level is to neglect all disorder effects, and assume that the system can be thought of as a collection of local moments of density \( n_i \) interacting with itinerant holes of density \( n_c \). In the weak coupling regime \( (J < t, E_F \text{ where } t \text{ and } E_F \text{ are the band width and the Fermi energy of the carrier system}) \) it is then possible to “eliminate” the carrier degrees of freedom by mapping the problem into the corresponding RKKY problem of Mn local moments interacting indirectly via the holes through \( H_M \). This carrier-polarization-mediated RKKY exchange interaction is essentially a second order perturbation theoretic calculation in \( J \), leading to the following interaction Hamiltonian between the Mn spins (assuming, for the sake of simplicity, a single parabolic hole band)

\[
H_i = \sum_{i \neq j} J_{ij} S_i \cdot S_j,
\]

with

\[
J_{ij} \propto |J|^2 \left[ \frac{\sin(2k_F R) - (2k_F R) \cos(2k_F R)}{(2k_F R)^3} \right],
\]

where \( k_F \propto n_c^{1/3} \propto E_F^{1/2} \) is the Fermi wave vector for the holes and \( R = |R_{ij}| = |R_i - R_j| \) is the distance between the Mn impurities at \( i \) and \( j \) lattice sites. This oscillatory RKKY indirect exchange magnetic coupling between local moments placed in an electron gas arises from the spin polarization induced in the electron system by the local moment, and is a perturbative effect of the local moments.
on the carrier system (valid in the limit of small $J$). In
the DMS systems an approximate average distance be-
tween the Mn local moments is $\bar{R} \sim n_i^{1/3}$, making typical
values of $k_F R \sim (n_c/n_i)^{1/3}$. For ferromagnetism to occur
(remembering that the real GaMnAs system is intrinsi-
cally strongly substitutionally disordered) one must avoid
the strong frustration effects associated with random sign
changes in the magnetic interaction of Eq. \(\mathcal{K}\) arising
from the oscillatory terms in Eq. \(\mathcal{L}\), which can only be
guaranteed when $k_F R \ll 1$. This then necessitates the condi-
tion $n_c/n_i \ll 1$, making strong compensation, i.e.,
$n_c \ll n_i$, a necessary condition for ferromagnetism in the
system.

We note that a Weiss MFT calculation can easily be
carried out for the coupled Mn-hole magnetic problem
defined by the Zener-RKKY model of Eqs. \(\mathcal{A}\)–\(\mathcal{I}\). For a
simple single-band degenerate hole model, the result for
$T_{c,\text{MF}}$ in the Weiss MFT was obtained a very long time
ago, \(\text{\cite{1,3,5}}\).

$$T_{c,\text{MF}} = \frac{S(S+1)}{3} s^2 J^2 D(E_F)n_i, \quad \text{(5)}$$

where $S$ is the local spin moment and $s$ is the carrier
spin. The carrier density of states $D(E_F)$ in Eq. \(\mathcal{J}\),
in the degenerate one band free carrier system, is given
by $D(E_F) \propto E_F^{3/2} \propto n_c^{1/3}$. Thus $T_{c,\text{MF}}$ increases mono-
tonically with the exchange coupling, the local moment
density, and the carrier density as

$$T_{c,\text{MF}} \propto J^2 n_c^{1/3} n_i, \quad \text{(6)}$$

where $n_c$ and $n_i$ are treated as independent density pa-
rameters. Based on this simple Weiss MFT (and its
various extensions incorporating spin wave corrections
and/or explicit spin-orbit coupling effects in the GaAs va-
locence band), quantitative predictions have been made
about the dependence of the ferromagnetic transition tem-
perature in various DMS systems on the system pa-
rameters (carrier and local moment densities, effective
exchange coupling strength, etc.). In addition, we have
recently shown \(\text{\cite{21}}\) that the MFT for the model defined by
Eqs. \(\mathcal{I}\) and \(\mathcal{J}\) can be extended to the nondegenerate
carrier system more appropriate for the localized holes
in the strongly insulating DMS materials. In contrast to
the degenerate results of Eq. \(\mathcal{K}\), which is appropriate for
the metallic (“extended”) carrier system (e.g. free
valence band holes), the nondegenerate MFT provides a
transition temperature dependence given by

$$T_{c,\text{MF}} \propto |J|(n_c n_i)^{1/2}. \quad \text{(7)}$$

Thus, the dependence of $T_{c,\text{MF}}$ on the system parameters
changes drastically in the localized nondegenerate limit.
More details can be found in Ref. \(\text{\cite{22}}\).

The simple Weiss mean-field theory (Eqs. \(\mathcal{A}\) and \(\mathcal{B}\))
model based on the degenerate valence band holes in-
teracting with the Mn local moments (and its obvious
extensions) has been used extensively in the literature.

The question, therefore, arises about its validity, or more
generally, about its quantitative reliability. It is argued
that the molecular MFT should apply well in DMS sys-
tems because of the large length scales (e.g. $k_F^{-1}$) involved
in the problem. We believe that there are good reasons
to question the validity of the Weiss MFT as applied to
DMS ferromagnetism. First, strong disorder in the sys-
tem invariably brings in some effects of frustration which
should become more significant at larger values of car-
rier density, making the simple MFT defined by Eqs. \(\mathcal{B}\)
and \(\mathcal{C}\) increasingly incorrect at higher carrier densities
(even for the metallic system). In fact, $T_c$ should vanish
in the disordered system as $n_c \to n_i$. Second, MFT in
this problem being equivalent to a second order pertur-
baion theory in the exchange coupling $J$ (i.e. Eqs. \(\mathcal{B}\)
and \(\mathcal{C}\)), the validity of Weiss mean-field theory becomes
highly questionable for large values of $J$ where carriers
may bind to individual local moment sites to lower their
energy forming an impurity band. There is significant
experimental evidence for impurity band formation in DMS
materials, which is not included in the MFT. Therefore
mean-field predictions will fail at larger values of $J$ where
DMS magnetic properties should be dominated by im-
purity band physics not caught by Eqs. \(\mathcal{B}\) and \(\mathcal{C}\). We
have recently developed a dynamical mean-field theory
(DMFT) picture \(\text{\cite{23,24}}\) of DMS ferromagnetism where im-
purity band physics is explicitly included. Third, in the
limit of $n_i \gg n_c$, where DMS ferromagnetism prevails,
disorder effects are extremely strong (as is obvious from
the insulating nature of most DMS materials and from
the extremely low mobilities of the so-called “metallic”
DMS materials which may very well also be insulating
at $T = 0$), and therefore the degenerate “metallic” Weiss
MFT approach based on the carriers being the free ex-
tended valence band holes of the host semiconductor may
be fundamentally flawed. A more appropriate picture in
this disordered localized regime may be the percolation
picture of DMS ferromagnetism recently developed by
us \(\text{\cite{25}}\) where each hole is bound in a cluster of magnetic
impurities forming a bound magnetic polaron. With de-
creasing temperature, these bound magnetic polarons co-
alesce eventually leading to a magnetic percolation tran-
sition at $T_c$ where a magnetic percolation cluster spans
the whole system. This polaron percolation picture of
DMS ferromagnetism is strongly supported \(\text{\cite{25}}\) by direct
numerical simulations and by experimental studies show-
ing strongly concave magnetization curves in many DMS
systems which follow naturally from our theory \(\text{\cite{25,26}}\).

Below we provide some details on the dynamical mean-
field and polaron percolation theories of DMS ferromag-
netism.

### A. Dynamical mean-field theory

In this section we briefly describe the “dynamical
mean-field theory” (DMFT). Due to size limitations, we
are not able to give detailed description of this formalism
all of the relevant physics may be determined from the paramagnetic state (with components parallel ($Z$) with components parallel ($Z$) and$0$ with components$00$), and then all of the relevant physics may be determined from the local (momentum-integrated) Green function defined by

$$
G_{\text{loc}}(i\omega_n) = a_0^3 \int \frac{d^3p}{(2\pi)^3} \frac{1}{i\omega_n + \mu - \epsilon(p) - \Sigma_{\sigma}(i\omega_n)}, \quad (8)
$$

where we have normalized the momentum integral to the volume of the unit cell $a_0^3$, and $\mu$ is the chemical potential. $G_{\text{loc}}$ is in general a matrix in spin and band indices and depends on whether one is considering a magnetic or non-magnetic site. Since $G_{\text{loc}}$ is a local function, it is the solution of a local problem specified by a mean-field function $g_0$, which is related to the partition function $Z_{\text{loc}} = \int dS \exp(-S_{\text{loc}})$ with action

$$
S_{\text{loc}} = \sum_{\alpha\beta} g_{0\alpha\beta}^0 (\tau - \tau') c_\alpha^\dagger(\tau)c_\beta(\tau'),
$$

on a magnetic site and

$$
S_{\text{loc}} = \sum_{\alpha\beta} g_{0\alpha\beta}^b (\tau - \tau') c_\alpha(\tau)c_\beta(\tau'),
$$

on a non-magnetic site. Here $c_\alpha(\tau)$ ($c_\alpha^\dagger(\tau)$) is the destruction (creation) operator of a fermion in the spin state $\alpha$ and at time $\tau$. $g_0(\tau - \tau')$ plays the role of the Weiss mean field (bare Green function for the local effective action $S_{\text{loc}}$) and is a function of time. The magnetic-site mean-field function $g_{0\alpha\beta}^0$ can be written as $g_{0\alpha\beta}^0 = a_0 + a_1 \mathbf{m} \cdot \sigma_{\alpha\beta}$ with $\mathbf{m}$ the magnetization direction and $a_1$ vanishing in the paramagnetic state ($T > T_c$). Since the spin axis is chosen parallel to $\mathbf{m}$, $g_{0\alpha\beta}^0$ becomes a diagonal matrix with components parallel ($g_{0\alpha \alpha}^0 = a_0 + a_1$) and antiparallel ($g_{0\alpha \beta}^0 = a_0 - a_1$) to $\mathbf{m}$. It is specified by the condition that the local Green function computed from $Z_{\text{loc}}$, namely $\delta \ln Z_{\text{loc}} / \delta g_{0\alpha\beta}^0 = (g_{0\alpha\beta}^0 - \Sigma)^{-1}$ is identical to the local Green function computed by performing the momentum integral using the same self energy.

Within this approximation we calculate the normalized magnetization of the local moments with the semicircle density of states, $D(\omega) = \sqrt{4t^2 - \omega^2}/2t$, where $t$ is a bandwidth of the system. The normalized magnetization $M(T)$ is given by $M(T) = \int (dS) \cdot \hat{S} \exp(-S_{\text{loc}}) / Z_{\text{loc}}$. As the temperature is increased, the spins disorder and eventually the magnetic transition temperature is reached. Above this temperature, $g_0$ is spin-independent. By linearizing the equation in the magnetic part of $g_0$ with respect to $a_1$ we may obtain the ferromagnetic transition temperature $T_c$. The details on the calculation of $T_c$ are given in Refs. 19,20. In Fig. 1 we show the calculated $T_c$ as a function of carrier density for $x = 0.05$ and various couplings $J$, and the corresponding density of states are given in the inset. When $J < t$ the impurity band formation does not occur (see the inset for $J = 0.5t$, $1.0t$).

In Fig. 1 we show the calculated $T_c$ as a function of carrier density for $x = 0.05$ and various couplings $J$, and the corresponding density of states are given in the inset. When $J < t$ the impurity band formation does not occur (see the inset for $J = 0.5t$, $1.0t$).

In Fig. 2 we show the normalized magnetization of the local moments as a function of temperature for different values of $J = 1.0, 1.5, 2.0t$ and $x = 0.05$, and for various hole densities, $n_c/n_l$. For the small coupling constant $J = t$ the impurity band is not formed, but for $J = 1.5, 2.0t$ we have a spin-polarized impurity band. For relatively high density ($n_c/n_l = 0.4$) the calculated magnetization looks similar to the Weiss mean-field results. But for low density ($n_c/n_l = 0.04$) we have a linear $M(T)$ in the intermediate temperature range. Near the critical temperature $T_c$ the critical behavior of the magnetization for all density is given by $M(T) \propto (T_c - T)^{1/2}$.

For different exchange couplings we have similar results (i.e., linear behavior at low densities and intermediate temperature ranges).

FIG. 1: Calculated ferromagnetic transition temperature $T_c$ as a function of carrier carrier density $n_c/x$ for $x = 0.05$ and various exchange couplings $J$. Inset shows the majority spin density of states at $T = T_c$ and for $x = 0.05$ and $J = 0.5t$, $1.0t$.ина.
In particular, it should be possible to obtain the $M(T)$ behavior for the localized carrier case also from DMFT by incorporating impurity band localization in the DMFT formalism. Our current theory does not include localization, and the impurity band (or valence band) carriers in our DMFT calculations are all delocalized metallic carriers. First principles band theory calculations indicate that the actual exchange coupling in Ga$_{1-x}$Mn$_x$As may be quite important for understanding DMS magnetism, but now the carriers are pinned down with the localization radius $\rho_l$. The magnetic impurities, and the total magnetization of the sample is not trivial and has been found in our earlier work:

$$T_c \sim sSJ \left( \frac{a_0}{a_B} \right)^3 \left( \frac{n_i}{n_c} \right)^{\frac{1}{2}} \sqrt{\frac{n_i}{n_c}} \exp \left( -\frac{0.86}{\left( a_B^3 n_c \right)^{\frac{1}{2}}} \right).$$

The limit of applicability of Eq. (12) is determined by the condition $a_B^3 n_c < 1$. The dependence of $T_c$ on $a_B^3 n_c$ is shown in Fig. 3.

Since $n_e < n_i$, one polaron includes many magnetic impurities, and the total magnetization of the sample is that of impurities:

$$\frac{M(T)}{M_0} = \nu \left( 0.86 + \left( a_B^3 n_c \right)^{\frac{1}{2}} \ln \frac{T_c}{T} \right).$$

Here $0.64 = 0.86^3$ is the critical value of the parameter $r^3 n$ at which the infinite cluster appears, and $T_c$ is the Curie temperature of the ferromagnetic system under consideration, derived in Ref. 22.

B. Perculation theory

Our percolation theory for DMS$^{22}$ applies strictly in the regime of strongly localized holes where the dynamical mean-field theory for delocalized carriers described above has little validity. These two theories, mean-field theory and percolation theory, are therefore complementary.

The percolation theory assumes the same model of carrier-mediated ferromagnetism, but now the carriers are pinned down with the localization radius $\rho_l$. The disorder, averaged out in the mean-field theory, plays a key role in the carrier localization. The magnetic impurities are assumed to be completely randomly distributed in the host semiconductor lattice in contrast to the mean-field case where the carrier states are free and the disorder is neglected.

As we have demonstrated in Ref. 22, the problem of ferromagnetic transition in a system of bound magnetic polarons can be mapped onto the problem of overlapping spheres well-known in the percolation theory.\(^{22}\) The latter problem studies spheres of the same radius $r$ randomly placed in space (three-dimensional in our case) with some concentration $n$. Overlapping spheres make “clusters;” as the sphere radius $r$ becomes larger, more and more spheres join into clusters, the clusters coalesce, and finally, at some critical value of the sphere radius, an infinite cluster spanning the whole sample appears. This problem has only one dimensionless parameter, $r^3 n$, and therefore can be easily studied by means of Monte-Carlo simulations.

Each sphere of the overlapping spheres problem corresponds to a bound magnetic polaron, which is a complex formed by one localized hole and many magnetic impurities with their spins polarized by the exchange interaction with the hole spin. The concentration $n$ of spheres coincides with the concentration $n_c$ of localized holes. The expression for the effective polaron radius in terms of the physical parameters of the system under consideration is not trivial and has been found in our earlier work:

$$r^3 n = \left[ 0.86 + \left( a_B^3 n_c \right)^{\frac{1}{2}} \ln \frac{T_c}{T} \right]^3. \quad (11)$$

FIG. 2: The normalized DMFT impurity magnetization as a function of temperature for (a) $J = 1.5t$, (b) $J = 1.0t$, and (c) $J = 2.0t$, for $x = 0.05$ and for $n_e/n_i = 0.4, 0.2, 0.1, 0.04$ (from the top). The dashed line in (a) represents the magnetization calculated for the simple Weiss mean field theory for the local moment spin $S = 5/2$. 

The limit of applicability of Eq. (12) is determined by the condition $a_B^3 n_c < 1$. The dependence of $T_c$ on $a_B^3 n_c$ is shown in Fig. 3.

Since $n_e < n_i$, one polaron includes many magnetic impurities, and the total magnetization of the sample is that of impurities:

$$\frac{M(T)}{M_0} = \nu \left( 0.86 + \left( a_B^3 n_c \right)^{\frac{1}{2}} \ln \frac{T_c}{T} \right), \quad (13)$$
where the universal function $V(y)$ is the infinite cluster’s volume in the model of overlapping spheres; it depends only on the product $y$ of the spheres’ diameter and the cubic root of their concentration. One can see that the shape of the magnetization curve is determined by only one dimensionless parameter $a_B^3 n_c$, while the expression (12) for $T_e$ is more complicated and depends on all parameters of the model. Fig. 4 shows the temperature dependence of the magnetization at two values of $a_B^3 n_c$; the curve is more concave at smaller values of this parameter. The concave shape of the curve is consistent with the experimental magnetization data in $\text{Ge}_{1-x}\text{Mn}_x$ and low-$T_e$ III-V samples where our polaron percolation picture applies better due to stronger carrier localization associated with lower values of $a_B^3 n_c$. Our magnetization results also agree with the numerical results of Ref. 23. Very recently, a direct numerical Hartree-Fock calculation has convincingly verified the magnetic polaron percolation picture for the localized regime.

FIG. 4: The solid lines show the relative magnetization of the magnetic impurities [Eq. (13)] for $a_B^3 n_c = 10^{-3}$ (curve 1) and $10^{-2}$ (curve 2). The dashed lines show the relative magnetization of localized holes, whose contribution to the total sample magnetization is small.

field theory, while being a powerful qualitative tool, is obviously too simplistic to be taken seriously for quantitative analyses of DMS properties. In real DMS systems spatial fluctuations (i.e., disorder associated with random positions of the magnetic dopants) and thermal fluctuations of magnetic moments as well as impurity band and discrete lattice effects (all neglected in the Weiss mean field theory) are likely to be of real importance even if the magnetic coupling can be assumed to be a simple local exchange coupling between local impurity moments and carrier spins. In addition, the mean field theory averages out the oscillatory exchange coupling between the impurity moments, which must be important at higher carrier densities, particularly in the presence of strong spatial disorder. For example, the mean field theory incorrectly predicts the ground state to be ferromagnetic for all values of $n_c$ and $n_l$, whereas in reality of course the system is a spin glass for larger values of $n_c$. The mean field theory is qualitatively valid only for very small values of the carrier-local-moment exchange coupling $J$ where impurity band effects are weak, and applies only in the limit of $n_c \ll n_l$ where disorder and oscillatory aspects of exchange can be neglected. In addition, the standard mean field theory is valid only for degenerate metallic systems although a nondegenerate localized version of the mean field theory has recently been developed.

FIG. 3: Curie temperature $T_e$ as a function of the dimensionless parameter $a_B^3 n_c$. At $a_B^3 n_c \lesssim 1$, $T_e$ is given by Eq. (12). At $a_B^3 n_c \gtrsim 1$, Eq. (12) (being beyond limits of its applicability) predicts decline of $T_e$ (dotted line); in reality, $T_e$ grows monotonically with $a_B^3 n_c$ (solid line), though its exact behavior is unknown.

III. CONCLUSION

When carriers are present with a carrier density $n_c$ in a semiconductor containing a certain magnetic impurity density $n_l$ of local magnetic moments, a Weiss mean field theory, developed years ago within the Zener-RKKY effective magnetic Hamiltonian describing the local exchange coupling between local moments and carrier spin, would always predict ferromagnetism with a mean field transition temperature $T_e^{\text{MF}}$ varying linearly in $n_l$ and $n_c^{1/3}$. This Weiss mean field theory, appropriately modified by the complicated spin-orbit coupled multiband valence band structure of GaAs, has been extensively used in making quantitative predictions about the magnetic properties of GaMnAs. This Weiss mean

There have been recent theoretical developments going beyond the simple Weiss mean field theory where impurity band effects (both for metallic and insulating DMS systems) are explicitly included in the dynamical mean field and magnetic polaron percolation theories. The DMFT theory predicts, in contradiction with the Weiss mean field theory, that the ferromagnetic transition temperature $T_e$ is not monotonic in the carrier density (and the coupling strength $J$), and may vanish for larger values of $n_c$. While the definitive quantitative theory for DMS ferromagnetism, taking into account complete band structure complications of the system
along with disorder, fluctuation, and nonperturbative strong-coupling (i.e. $J$ not necessarily small) effects in a consistent manner is still lacking, it is increasingly clear that disorder and impurity band aspects of the real DMS systems are extremely important in understanding DMS magnetic properties, and theories\textsuperscript{19,20,21,22} that include these effects should be of qualitative and quantitative significance in explaining DMS magnetic properties.

The observed correlation between transport and magnetic properties in DMS systems, e.g. the more metallic systems typically having more convex magnetization curves as a function of temperature whereas more insulating systems having extreme non-mean-field like concave magnetization versus temperature curves (with considerable missing magnetic moments), is perhaps a strong indicator of the underlying mechanism of DMS ferromagnetism.\textsuperscript{21} This correlation indicates a carrier-mediated magnetic interaction origin of DMS ferromagnetism. In particular, two very recent theoretical publications\textsuperscript{21,26} have discussed in considerable details this correlation between metallicity and DMS ferromagnetism. In Ref. \textsuperscript{21} it has been argued that the appropriate picture for DMS ferromagnetism in strongly disordered insulating materials is the bound magnetic polaron percolation picture whereas at higher densities (and/or lower disorder), where the system is metallic, the dynamical mean-field picture (which becomes equivalent to the Weiss mean field picture at low values of exchange coupling insufficient to cause the impurity band formation) is more appropriate. In Ref. \textsuperscript{21} a detailed numerical simulation of the disordered DMS model has been carried out qualitatively validating this picture. The question therefore arises regarding the nature of the DMS ground state: Is it localized and insulating or extended and metallic or is there a transition between the two as a function of carrier density? If there is a true metal-insulator transition, then the percolation picture holds in the insulating phase and the dynamical mean field picture holds in the metallic phase. Although there have been experimental claims of metal-insulator transitions in GaMnAs systems as a function of Mn content, the current experimental situation is sufficiently murky that is possible that all GaMnAs systems are in fact insulating at $T = 0$ for all values of the Mn content. It would therefore be desirable to develop a dynamical mean field theory (or even just the Weiss mean field theory) of DMS ferromagnetism explicitly incorporating disorder effects so that the magnetic properties can be studied continuously through the metal-insulator transition (or crossover, as the case may be).

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