Proposed outline of the long PRB article critically examining continuum and discrete mean field treatments of magnetic behavior in Diluted Magnetic Semiconductors

Donald J. Priour, Jr. and S. Das Sarma

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Abstract

We critically discuss the shortcomings of the continuum Weiss-Dietl Virtual Crystal Approximation (VCA), a model which leads to a frequently cited (but manifestly incorrect) formula for the dependence of T_c on the impurity concentration x_i and the density of (hole) carriers, n_c. We quickly summarize *lattice mean field theory*, which takes into account the discrete fcc crystal structure of $Ga_{1-x}Mn_xAs$.

We consider mean field theories in light of Monte Carlo T_c results, reiterating that the DMS parameter space corresponds to a strongly disordered regime (in a sense opposite to the realm where MFT applies) where the ferromagnetic thermal phase transition occur via the percolation of magnetic clusters with strong parallels to the theoretical description by Kaminski and Das Sarma in terms of the percolation of magnetic polarons. Nonetheless, we obtain the critical exponents at the 1% level, showing that despite the strong disorder there is very little deviation from the simple cubic Heisenberg model.

We discuss the T^* phenomena mentioned by Dagotto et al, and we examine special types of disorder (e.g. impurity superlattice).

Finally, we obtain the $T = 0$ phase diagrams for the RKKY model for DMS, the *nn* FM and *nnn* AF model examined by Binder et al, and bond disordered models such as the Edwards-Anderson model, arguing that the $T = 0$ transitions in each case constitute zero temperature magnetic percolation critical transitions. We also speculate briefly about the nature of non-ferromagnetic phase. [Note: the abstract needn't be this long; I just wanted to sketch the paper's suggested content for the purpose of the outline.]

1 Chapter I: Introduction

This is a brief introductory section summarizing, and striving to unify the themes discussed in the long paper. However, the introduction also reviews previous theoretical efforts, particularly simple mean field theories such as the Curie Weiss continuum MFT.

2 Chapter II: a critical examination of DMS Mean Field Theories

2.1 The Virtual Crystal Approximation (VCA)

The VCA, a continuum mean field theory, neglects the crystal lattice and consequently does not correctly predict even the qualitative behavior of T_c (e.g. the non-monotonicity in n_c for fixed x_i).

2.2 Lattice Mean Field Theory

By considering a mean field theory which takes into account the discrete structure of the fcc lattice, one can capture qualitative aspects of T_c trends and the shape (concave or convex) of the $m(T)$ curve.

2.3 Critique of simple Mean Field Theories, such as the VCA

2.3.1 MFT difficulties arising purely from strong disorder

Site Disorder Difficulties arise with MFT in the strong disorder limit when the interaction scale l is small in comparison with the average separation between impurities, $l_s \equiv n_i^{-1/3}$. In fact, this regime is better understood in terms of random sphere percolation theory, in a sense opposite to the

$l_s \ll l$ "mean field" limit. We offer Monte Carlo evidence to support our assertion that much of the DMS parameter regime (with a finite interaction range $l \sim a$ and dilute impurity concentrations x_i on the order of or less than 10%), corresponds to the strongly disordered regime mentioned above where simple mean field theoretical treatments are manifestly not tenable.

Bond Disorder In addition to the strongly disordered site models mentioned above, where the typical separation between impurities greatly exceeds the decay length l of the coupling $J(r)$, we also consider situations in which there is comparatively little site disorder (e.g. in a regular cubic lattice), but very strong bond disorder. For sufficiently broad distributions of bond strengths, we use an approach very similar to that applied for models with strong site disorder where the thermal ferromagnetic phase transition was viewed in terms of random sphere percolation, and we obtain an analytic formula for T_c (modulo an unknown overall constant) valid in the limit of very broad bond strength distributions.

In our study of models with strong bond disorder, consideration is given mainly to systems with purely FM couplings between moments (though the absolute magnitude of the coupling will vary greatly). Again, we provide Monte Carlo evidence as a direct numerical verification of the theoretical T_c formula, and to assess the regime of validity of the Handrich result [K. Handrich, Phys. Status Solidi B **32**, K55 (1969)] which should be valid only when the width of bond strengths is small in comparison with the mean bond strength.

2.3.2 Further problems with VCA-type MFT where AF couplings are appreciable

Another weakness of simple mean field theories becomes evident when antiferromagnetic couplings (e.g. from RKKY oscillations) become strong enough to partially or completely disrupt ferromagnetic ordering. Since theories such as Curie-Weiss continuum MFT always assume a ferromagnetic ground state, major problems certainly occur when n_c/n_i is large enough to eliminate ferromagnetism as the favored (i.e. lowest energy) low temperature state. Graphs of juxtaposed VCA and Monte Carlo T_c results are discussed to highlight the increasingly serious problems with MFT as larger n_c/n_i values are examined. Ultimately, the MC Curie temperatures fall to zero while the VCA results continue to rise, even deep in the "spin glass" regime with $n_c/n_i \sim 1$ (where a non-zero ferromagnetic T_c would be nonsensical). It is noted that discrete MFT fares somewhat better than its continuum counterpart for the larger values of n_c/n_i.

3 Chapter III: Simple (random) disorder versus special types of disorder

We examine the effect on T_c of situations more complicated than simple random doping. The impact of introducing correlations among impurities or arranging Mn dopants in regular superlattices can be a difficult question to properly assess with the aid of Mean Field Theories, so emphasis will be given to the results of Monte Carlo calculations. However, some lattice MFT results will be discussed as well.

3.1 Relaxing the discretization condition

A very simple way to modify the manner in which Mn dopants are distributed is to remove the requirement that magnetic ions reside only on fcc crystal lattice sites in favor of a continuous distribution in which impurities are randomly assigned to arbitrary positions.

3.1.1 Negligible AF couplings ($n_c/n_i \ll 1$)

Detailed Monte Carlo data show very close agreement (generally to within 1% or better) between Curie temperatures obtained for discretely and continuously distributed impurities. This close agreement exists for essentially the entire x_i and l regime appropriate to DMS, with the proviso that AF couplings (and hence n_c/n_i) are kept small. Analytic arguments are provided to account for the surprisingly close agreement of the continuum and discrete T_c's, as well as other thermodynamic quantities (such as $m(T)$) calculated for $T \leq T_c$. In passing, it is emphasized that the close match of variables calculated for the discrete and continuous systems does *not* imply that one can accept VCA T_c formulae.

3.1.2 Appreciable AF couplings for larger n_c/n_i

We compare thermodynamic variables (particularly T_c) for discrete and continuous impurity distributions for situations where antiferromagnetic couplings are significant. The goal is to examine T_c for the two types of distributions while steadily increasing n_c/n_i to see where (or if) the agreement breaks down.

3.2 Impurity Superlattices

In both Monte Carlo and MFT calculations, we examine situations in which magnetic impurities are organized in regular arrays. One thing we didn't do previously was to compare superlattice and random disorder Curie Temperatures for systems with the AF local superexchange interaction switched on. An appreciable local AF coupling might impact T_c's of random disorder configurations more than regular impurity superlattice, though not necessarily enough to yield higher Curie temperatures for the superlattice case.

4 Chapter IV: The $T = 0$ phase diagrams of models with competing interactions and magnetic percolation

We consider several models which allow for significant competing AF couplings in conjunction with strong disorder, and we obtain the low temperature phase diagram in each case. A feature common to each model is a phase boundary marked by zero temperature magnetic percolation critical behavior as a NF phase gives way to a FM phase via the percolation of magnetic clusters.

- Damped and undamped RKKY models, already described in our recent PRL are considered. We will also discuss Monte Carlo T_c results and obtain some critical exponents (β/ν and the Binder cumulant at T_c) for a DMS RKKY model with moderate damping. The expectation is that the latter quantities will be very close to those of the simple cubic Heisenberg model, suggesting that our model belongs to a universality class very close to that of the (non-disordered) simple cubic Heisenberg model.

- The *nn* FM and *nnn* AF model examined by Binder *et al* in 1995. (In addition to obtaining the low temperature phase diagram, we also obtain the critical exponent ratio β/ν and the Binder cumulant evaluated at T_c). It is quite possible that our results will be very close to the corresponding values calculated for the simple cubic Heisenberg model, in contrast to the larger ($\sim 10\%$) deviations found by Binder *et al.*

- The Edwards-Anderson model, a bond disordered system showing magnetic percolation. Again, we obtain β/ν and the Binder cumulant at the 1% level to examine the impact specifically of increasingly prevalent AF couplings (but no site disorder) on the universality class. Based on preliminary results, shifts in the exponents are expected to be very slight.

4.1 Speculation as to the nature of the non-ferromagnetic (NF) phase

4.1.1 Short-ranged coupling between impurities

Intuition would suggest that in the very dilute limit, where $l \ll l_s$, the NF phase should behave more like a usual paramagnet and have relatively little glassy character. For one thing, as the highly dilute limit is approached, determining the ground state becomes increasingly straightforward task, and can be accomplished for very dilute systems via a technique akin to a "real space" renormalization group calculation.

In this procedure for finding the lowest energy state, one first forms small spin clusters by aligning individual impurity spins with those of their nearest neighbors, as dictated by the coupling between them. These small groups of spins (usually spin pairs which are either collinear or singlets, depending on the sign of the coupling among them) are then regarded as a new set of individual spins, and the effective coupling between the new "spins" is calculated. The RG-like procedure is iterated until it terminates with all of the spins in the system are assigned to a single large cluster.

4.1.2 Longer-ranged $J(r)$, $l \geq l_s$

In the opposite regime, where the range of $J(r)$ is at least comparable to l_s, complicated glassy behavior is a much stronger possibility in the NF phase. There may also be substantial glassiness if one considers a local AF superexchange interaction for systems with higher impurity densities (i.e. $x_i \sim 0.1$). There will no doubt be some overlap in this part of the paper with our Rapid Communication with Euyheon Hwang.

4.2 Monte Carlo studies of "glassy" behavior in the Ferromagnetic phase

In the DMS context, we consider the possibility of some glassy behavior even fairly deep in the ferromagnetic phase. We concentrate on n_c/n_i values which are moderate though definitely not enough to disrupt the ferromagnetic order of the ground state. Starting with a high temperature (purely random) spin configuration, we operate within Heat-Bath Monte Carlo and abruptly cool the system to $T = 0$ [this is identical to the spin relaxation procedure used by Walker and Walstedt [PRB **22**, 3816 (1980)] in the spin glass $n_c/n_i \sim 1$ regime). The potential computational intricacies of this task will be mitigated by the fact that instead of the more demanding annealing procedure one would use to seek the lowest energy state, we are only waiting for the system to relax fully to a local energy minimum; hence, we should be able to access reasonably large systems.

Based on preliminary findings we anticipate that close enough to the FM/NF phase boundary (though on the FM side), a kind of spin glassiness will appear as the system size L is made larger, preventing the relaxation to a state with ferromagnetic ordering for very large L. To operate in a quantitative manner, we will calculate the normalized correlation length ξ/L; depending on whether for large L the quantity ξ/L is an increasing or decreasing function in the system size, one can determine whether glassy behavior is preventing relaxation to a state with long range FM order in the thermodynamic limit. We will seek the boundary in the FM region separating systems which can relax from the high temperature configuration to states with FM order and those which cannot.

5 Chapter V: Conclusions

Salient points and major results are reiterated.