Magnetic Susceptibility of Insulating *n*-Doped Semiconductors

Recently, a number of calculations[1-5] have attempted to describe quantitatively the temperature (T) dependence of the donor magnetic susceptibility $\chi_D(T)$ in insulating, n-doped semiconductors,[2,4] and to explain the apparent absence of a magnetic ordering transition due to the (antiferromagnetic) exchange coupling between donor spins down to very low T (~10 mK). These include numerical cluster calculations[2,4] and a numerical renormalization group (RG) scheme,[5] as well as two simple models[1,3,4] which profess to calculate χ_D to within acceptable experimental accuracy (~ 5% – 10%) by correcting shortcomings of the pair approximation (PA)—a much less laborious method. While all the above models fit experimental data[2,4] with use of hydrogenic exchange there is some flexibility in parameters (donor density, Bohr radius, and for Faraday rotation,[2] a scale factor). Thus it is of interest to compare results of various calculations for the same parameters.

This is illustrated in Fig. 1, which plots the inverse of $\chi_D(T)/\chi_C(T)$ [$\chi_C(T) \propto T^{-1}$ is the free spin (Curie) susceptibility] for a prototype of a doped semiconductor: a random distribution of spin $\frac{1}{2}$ at a density n and antiferromagnetic Heisenberg exchange $J(r) = J_0 \exp(-\alpha r)$ with $n\alpha^{-3} = 0.001$. The PA (dotted line) convolutes the nearest-neighbor probability density[1] $p(r)$ with the χ of a pair of donors to obtain the ensemble averaged $\chi_p(T)$. The solid line is obtained by using Rosso's prescription[1]: convolute an analytically calculated[1] distribution of spin pairs with separation r, $\tilde{p}(r)$, obtained by pairing spins in a hierarchy of decreasing coupling strength, with the χ of the pair. The dashed line is for a modified pair approximation (MPA),[3,4] which uses $\chi_p(T)$ to identify the number of isolated spins at any T, and define a T-dependent clustering volume $v(T)$. $\chi_{MPA}(T)$ is then obtained as an analytic function of $\chi_p(T)$ and $\chi_C(T)$ from an approximate ensemble average in $v(T)$. The open and closed circles are results of the RG calculation for two "samples."

As can be seen, the MPA and RG results are in good agreement with each other, and the former has been shown[3] to agree within $\approx 5\% - 10\%$ with numerical cluster calculations for the same parameters in a similar concentration range. Rosso's method, on the other hand, yields a much larger χ. This can be traced back to his expression $\tilde{p}(r) = 4\pi n r^2 [1 - \int_0^r \tilde{p}(r')dr']^2$, in

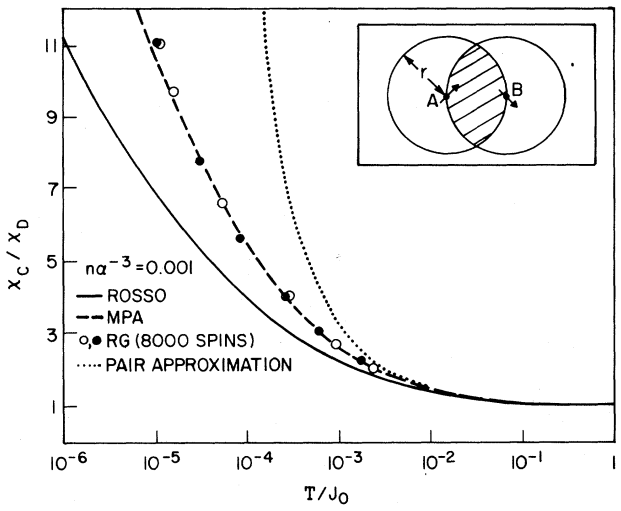

FIG. 1. Inverse donor susceptibility (relative to Curie value) as a function of temperature; inset: prospective spin pair A-B.

which the factor in square brackets squared, representing the probability that two spins at a distance r (A and B in Fig. 1, inset) are not already paired, is written as a product of the individual probabilities. The problem is that the distribution of neighboring spins of A and B are not independent, since their relevant spheres overlap; thus multiplying the probabilities is only approximate. This can be shown to overestimate χ_D: about 60% of the discrepancy in Fig. 1 is removed with the correct $\tilde{p}(r)$ (which, however, has to be calculated by numerical simulation), the rest being inherent to the unrenormalized pairing scheme.[5] Thus the MPA[3,4] appears to be a more convenient and accurate method of calculating χ_D than the scheme proposed by Rosso.[1] Further, it is easily generalized for indirect-gap semiconductors[4] with a nonmonotonic $J(r)$.

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