

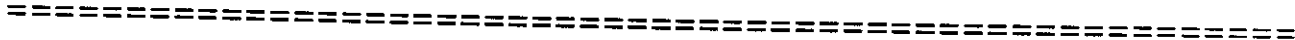


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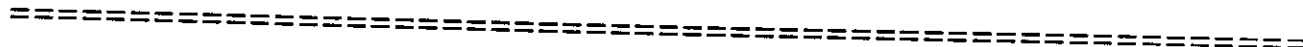
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**SPRING COLLEGE IN CONDENSED MATTER
 ON QUANTUM PHASES
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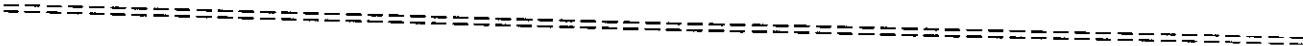


**Background material for lectures 1 - 2 -3 on
 METAL-INSULATOR TRANSITION IN
 DISORDERED MATERIALS (THEORY)**

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These are preliminary lecture notes, intended only for distribution to participants.



Absence of Spin Diffusion in Most Random Lattices

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We examine the metallic phase of the positionally disordered Anderson-Hubbard model as a prototype of a strongly correlated, disordered metal. We find that the low-temperature thermodynamics is dominated by spin excitations in rare regions, leading to non-Fermi-liquid behavior as $T \rightarrow 0$, characterized by a diverging susceptibility, a specific heat rising faster than T , and a vanishing spin diffusion coefficient. We argue that the results should, in principle, apply throughout the metallic phase of random alloys which undergo a transition, as a function of concentration, to an insulating phase with local moments.

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Recent experiments on weakly metallic samples of uncompensated doped semiconductors (Si:P, Ge:Sb, Si:B) using magnetic [1] and thermodynamic [2] probes have provided strong evidence that highly disordered correlated metals contain localized moments [3-5]. These dominate the magnetic susceptibility and specific heat at low temperatures (< 1 K). Experiments on compensated materials (Si:P;B) show even stronger effects [6].

The idea of local moments existing in disordered systems on the metallic side of the metal-insulator (MI) transition is not new [4]. A recent study [5] of the positionally disordered Hubbard model in three dimensions found local moment instabilities on $\sim 10\%$ of the sites at densities $\sim 25\%$ above the critical density n_c of the MI transition. The issue is whether such moments persist down to low temperatures, so that they are an integral part of the low-energy description, or are quenched (due to coupling to other electrons) at a high-energy scale resulting in (finite) renormalization of Fermi-liquid parameters, but no dramatic consequences.

In this Letter we examine this question in some detail, focusing on the consequences of *quenched randomness*. Our principal result is that at *any* composition in such dirty metallic systems, rare statistical density fluctuations give rise to local moments which are so weakly coupled to the itinerant electron fluid that they cannot be effectively quenched via either the Kondo mechanism or RKKY interactions. These residual moments give rise, in the $T \rightarrow 0$ limit, to a divergent magnetic susceptibility $\chi(T)$ and specific-heat coefficient $\gamma(T) \equiv C_v(T)/T$, and a vanishing spin diffusion coefficient. These effects will occur at any composition provided the system undergoes a MI transition as a function of composition to an insulating phase with local moments. Far away from the transition the effects will be very small and only appear at exponentially low temperature, but as the transition is approached the effects should become much larger. This implies that a *minimal* phenomenological description of such a metallic disordered system at low temperatures is not in terms of a single-component Fermi fluid, but must consist of

two entities—including both the local moments and the itinerant electron fluid. This is in contrast to uniform systems (such as heavy fermions [7]) which form local moments at intermediate temperatures but (barring other instabilities such as superconductivity) exhibit Fermi-liquid behavior as $T \rightarrow 0$, characterized by a *finite* χ and γ , albeit with very large [7] renormalization $\sim 10^3$. These differences [5], due to the quenched disorder, are analogous to Griffiths singularities [8] in the disordered phase of classical random magnets, which can dominate the dynamical properties [9], and for quantum systems, the static properties as well [10]. Alternative explanations [11-13] of the experimental observations have been based on renormalization-group treatments of interacting electrons in a disordered medium, but these have focused on long-wavelength rather than localized effects.

For concreteness, we first consider a specific model—the Anderson-Hubbard model with sites positioned randomly in a d -dimensional continuum. Such a model is a rather good caricature of doped semiconductor [14] systems; further, as we shall argue later, most of our arguments can be generalized to systems with other kinds of quenched random disorder. The Hamiltonian is

$$H = \sum_{i\sigma} (\epsilon_i - \mu) n_{i\sigma} + \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where the sites i are distributed *randomly* in d dimensions with density n and some spread in the on-site energies ϵ_i . The hopping integral $t_{ij} \sim t_0 \exp(-r_{ij}/a)$, where $t_0 \sim U$, the on-site Coulomb repulsion, μ is the chemical potential, and σ the spin index. This model is believed to have a transition from an insulating state to a metallic state for $d > 2$ as the site density n is increased. In $d = 3$, the critical density n_c is expected to be near the Mott criterion [15,16] value ($n_c^{1/3} a \approx \frac{1}{4}$) especially close to half filling, which we primarily consider.

Well above n_c , most of the sites will be coupled to an infinite cluster by hopping elements $t_{ij} \sim U$. Nevertheless, there exist large density fluctuations because of the random distribution of sites. Thus, for example, the density

of isolated sites which have their nearest neighbor at a distance greater than r is given by $n_l(r) \sim n \exp(-c_d \times nr^d)$, with c_d a dimensionality-dependent constant. For sufficiently large r , such strongly isolated sites are occupied by single electrons and because of their weak coupling to the surroundings form local moments [3,5], analogous to d or f levels in the Anderson model [3], whereas the other, well-coupled sites are like conduction electron levels. The exchange coupling J_i of a moment at strongly isolated site i (with a nearest neighbor k at distance r_i) with the rest of the system is of order $J_i \sim t_{ik}^2/u \sim \exp(-2r_i/a)$, which falls off relatively rapidly with r_i . u is an energy involving U and $\epsilon_i - \mu$, which does not depend on r_i for such isolated sites. Such a local moment (Fig. 1), in the absence of J_i , would give a divergent Curie susceptibility $\chi_c(T) \sim \mu^2/T$. However, the coupling to other sites can quench the local moment.

Since quenched moments do not contribute significantly to the susceptibility, the low-energy magnetic behavior is controlled by the density of moments $\rho_u(\epsilon)$ which are *not* quenched at an energy scale above ϵ . Since these moments will only have a Curie susceptibility at temperature T if $\epsilon < T$, the resulting susceptibility is approximately $\chi(T) \sim (\mu^2/T)\rho_u(T)$. The entropy from the unquenched sites gives rise to a contribution to the specific heat $C_v(T) \equiv T\gamma(T) \approx T d\rho_u(T)/dT$. One mechanism for quenching local moments is through coupling to the sites which has formed a "Fermi fluid," i.e., via the Kondo effect [17]. This quenching is effective below the Kondo temperature given by [18] $T_K \approx E_0(J_i\rho_F)^{1/2} \times e^{-1/J_i\rho_F}$, where E_0 is of the order of the bandwidth and ρ_F is the density of states at the Fermi level. Note that because of the strong (exponential) dependence of J_i , which in turn depends exponentially on r_i , the Kondo temperature for relatively isolated sites is *extremely* low, as can be explicitly seen by substituting for J_i in T_K . If the Kondo effect were the only mechanism for quenching moments, then $\rho_u(T)$ would be simply $n_l(r_T)$ where the size of the isolation hole r_T around sites not quenched to temperature T is given by $T_K(r_T) = T$. This would give

$$\chi(T) \sim (n\mu^2/T) \exp\{-f_d \ln^d[\ln(T_0/T)]\}, \quad (2)$$

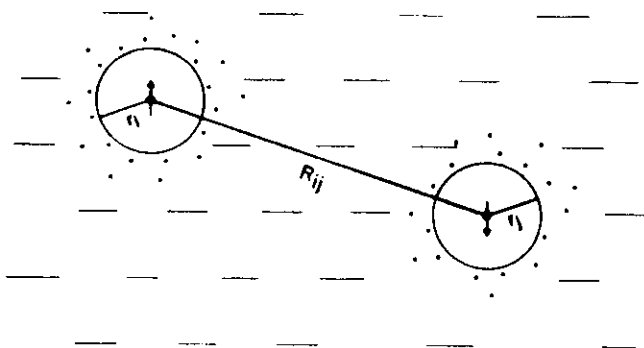


FIG. 1. Two isolated sites i and j with local moments separated by a distance R_{ij} in the midst of a Fermi liquid.

where $T_0 \sim t$, and $f_d = c_d n(a/2)^d$. This $\chi(T)$ diverges at low T in all dimensions, as does $\gamma(T)$ [19].

This arises because, even though the density $n_l(r)$ has a rapid falloff with r , the few sites in the tail of the distribution are too weakly coupled to be quenched effectively via the Kondo effect. Consequently, in the absence of any other quenching mechanism, they would give a divergent susceptibility, and dominate the thermodynamics at low enough temperatures, and the system would not be a Fermi liquid in the conventional sense as $T \rightarrow 0$.

In real systems, we must also consider quenching of the local moments due to interactions with other local moments. In the metallic phases of interest, this occurs via the conduction electron mediated RKKY interaction. Between two spins with separation R_{ij} coupled to the conduction electrons via exchanges J_i and J_j (see Fig. 1), the effective RKKY exchange is $K_{ij} \sim J_i J_j \rho_F g_d(k_F R_i, k_F R_j) / |R_{ij}|^d$, with g_d an oscillatory function of its arguments, typically varying on a scale of unity, and exhibiting randomness in a dirty metal arising from the behavior of the conduction electron wave functions near the Fermi surface [20]. The RKKY interactions between local moments at large separation ($R_{ij} \gg k_F^{-1}$) are thus randomly ferromagnetic or antiferromagnetic. For spin- $\frac{1}{2}$ local moments, however, the latter have a much stronger effect due to the factor of 3 difference in exchange energy between a singlet and triplet. Since we are interested in a *lower* bound on the susceptibility, we first assume that the RKKY interactions are purely antiferromagnetic with $g_d = 1$, and then return to the more realistic case.

Bhatt and Lee [21] have shown that *exponentially* decaying antiferromagnetic interactions J_{ij} between randomly placed spin- $\frac{1}{2}$ impurities (e.g., insulating Si:P) give rise to a "random singlet" phase with the spins paired into singlets (or occasionally grouped in larger clusters) with a distribution of separations. In the simplest approximation, the most strongly coupled pair of spins are paired, then the strongest coupled pair of the *remaining* spins are paired and the process continued until all the spins are exhausted. The susceptibility is due to spins which are eventually paired with an energy smaller than ϵ , $\rho_u(\epsilon)$, as discussed above. If all the exchanges J_i were equal, this would lead to $\rho_u(\epsilon) \sim \epsilon/J^2 \rho_F$, yielding a *finite* susceptibility as in uniform systems.

With the broad spectrum of J 's which occurs in our case, the behavior is somewhat more subtle. Most of the spins with largest J , i.e., J_0 , will pair with those with comparable J . Some, however, will find a rarer spin with a smaller J , J_1 , with which they can bind more strongly than the unpaired J_0 spins. Because of the rarity of the J_1 spins, this will only happen occasionally. (Indeed, the resulting pairing strengths K_{01} when it does occur will usually be comparable to the typical coupling strength K_{11} between J_1 spins.) Thus the J_1 spins will again pair primarily with spins of their own ilk. A good approximation to the number of unpaired spins at temperature T is

thus given by the density $n_l(r_T)$ of those with isolation holes of size r_T such that the RKKY interaction $K_T = J(r_T)^2 \rho_F R_T^{-3}$ between them and similarly isolated spins is of order T . The typical separation between such spins is $R_T \sim [n_l(r_T)]^{-1/d}$. By substituting for $\rho_u(T) \sim n_l(r_T)$ we then obtain a low-temperature susceptibility:

$$\chi(T) \sim [J^2(r_T) \rho_F]^{-1} \sim \exp[C_d \ln^{1/d}(T_0/T)]. \quad (3)$$

This diverges as $T \rightarrow 0$ albeit more slowly than any power of T , as does $\gamma(T)$ (up to extra $\ln T$ factors).

Several factors might affect the susceptibility. First, excitation of an already paired singlet of intervening spins can give rise to an effective indirect interaction \tilde{K} between spins, larger than the direct interaction. In the insulating case with exponential decay of K_{ij} , this is an important effect [21], especially in low dimensions. In our case, on the other hand, because of the power-law dependence of K_{ij} on R_{ij} , this can only be an important effect if the unpaired spins of interest are located near the opposite ends of the preformed singlet. This can be shown to occur only rarely and thus it does not significantly affect the results.

A potentially more important effect is due to the ferromagnetic nature of some of the interactions (and effective interactions). If the system remains in a random singlet phase, then these should only enhance the susceptibility via the formation at temperature T of clusters with larger magnetic moments. It is possible, however, that the competition between the ferromagnetic and antiferromagnetic interactions drives the system towards a spin-glass phase with broken spin rotational symmetry at $T=0$. Interactions decaying as $1/R^d$ are believed to be marginal for classical Heisenberg spin glasses, i.e., a positive temperature spin-glass transition ($T_c > 0$) might occur in their presence if it did not do so in their absence [22]. If $T_c > 0$, $\chi(T)$ should exhibit a cusp and then saturate to a finite value at $T=0$. If, however, $T_c = 0$, $\chi(T)$ is likely to be more strongly divergent than Eq. (3), probably a Curie form due to excitations of size of order the T -dependent spin-glass coherence volume [22].

A random singlet phase appears most likely in three dimensions for a spin- $\frac{1}{2}$ system due to the dominance of antiferromagnetic interactions. If so, the susceptibility of Eq. (3) is probably a lower bound, although it may asymptotically be the correct form. But, in any case, the zero-temperature metallic phase will *not* be a "normal" dirty metal with Pauli susceptibility, linear specific heat, and no broken symmetries; it will have a divergent susceptibility, a broken spin symmetry, or both.

In a random singlet phase with no spin-nonconserving interaction, the spin transport will be anomalous. Spins will tend to get "trapped" by the localized moments at low temperature so the spin diffusion coefficient $D_s(T) \rightarrow 0$ as $T \rightarrow 0$. If the spin is carried between the local moments by the same Fermi liquid quasiparticles which carry the charge then the Wiedmann-Franz law gives

$$D_s(T) = [\chi_0/\chi(T)]\sigma/K_0, \quad (4)$$

where χ_0 and K_0 are the susceptibility and compressibility of a noninteracting Fermi gas and σ is the conductivity of the actual system [11,12]. In a metallic phase with a finite conductivity at $T=0$, this yields $D_s(T) \sim \chi^{-1}(T)$. Note that at any *fixed* temperature the susceptibility and other properties will be essentially homogeneous on sufficiently long length scales ($\gg [\rho_u(T)]^{-1/d}$), thus Eq. (4) should obtain. Further understanding of the transport processes is needed to validate or invalidate this result, in particular the effects of the RKKY coupling between the local moments.

We now consider the generality of our results. In one-dimensional systems, the results do not apply directly for a variety of reasons, including the absence of Fermi-liquid behavior even in a spinless system. Nevertheless, other arguments again suggest a divergent susceptibility [23]. In higher dimensions, however, our results should, at least in principle, be quite general. All that is needed is the possibility of forming an isolated spin in a region of radius r which is sufficiently isolated from the rest of the system that its exchange with the conduction electrons, $J \sim e^{-br}$. This may be on single sites as we have considered, or on clusters of sites. If this *can* occur, in a random alloy, then it will *always do so* with probability no smaller than e^{-Cr^d} since any possible event in a region of size r will occur with at least this probability. Thus we expect that in the presence of electron-electron interactions in *any random alloy* which has a metal-insulator transition to an insulating phase with local moments as a function of concentration, isolated moments, and the associated destruction of the dirty Fermi liquid will occur for *any concentration*. This should obtain provided the Fermi level in the alloy lies *below* the electron affinity level of the pure insulating component and between the odd (lower) and even (higher) electron states of *any* cluster embedded in the insulating matrix. Exceptions would be systems in which it is impossible to isolate an *odd* number of electrons, or those which are metallic at all compositions. The best systems for observing the effects discussed here are clearly those near to a metal-insulator transition; deep in the metallic phase they will occur only at inaccessibly low T .

So far, we have assumed only Heisenberg spin interactions. In the presence of spin-orbit interactions, crystal fields, etc., the spin diffusion would of course no longer exist even in a conventional dirty Fermi liquid. Nevertheless, the thermodynamic properties of the random singlet phase should still persist at least for weak symmetry-breaking perturbations. With predominantly antiferromagnetic RKKY exchange, clusters of even numbers of spins will typically have nondegenerate ground states with a gap. Odd-numbered clusters will, because of time-reversal invariance, have degenerate Kramers doublet ground states. This strongly suggests that the basic

mechanism which causes the random singlet phase (i.e., weakly coupled spins interacting directly and via excitation of intervening pairs with a gap) will persist. In the most general case the pairs will not have any good quantum number except time reversal but the weakly coupled pairs will nevertheless still give rise to divergent susceptibilities and specific-heat coefficients of the same form as the isotropic case studied here.

Our results cast doubts over perturbative field theoretic approaches to the MI transition from the metallic side [11,12] which leave out the effects of rare regions. Such difficulties may be related to the direct breakdown of the spin transport in perturbation theory investigated recently [13]. This field-theoretic treatment to two-loop order finds a transition as disorder is increased from a metallic phase with both charge and spin diffusion to a metallic phase with charge diffusion but no spin diffusion, *before* the onset of charge localization (MI transition) at still higher disorder. Our results suggest that quite generally the zero-temperature spin diffusion coefficient at long wavelengths is zero in the metallic phase—presumably their transition is destroyed by nonperturbative effects.

For a random site model with an energy scale $\sim 1-10$ eV and $n \sim 1.5n_c$, we estimate that these effects should be observable at millikelvin temperatures. However, the estimates are exponentially sensitive to input parameters, and therefore difficult to make reliable. It would nevertheless be of interest to look at the magnetic and thermodynamic behavior of other atomically disordered metal-insulator composites (where the metal atom has unpaired spins and little tendency to form atomic pairs with zero spin) near the MI transition, to see how universal these features are. Other candidate systems include disordered heavy fermions (with low or zero superconducting temperatures) where the Fermi liquid in the crystalline material is already fragile, and low-dimensional systems (e.g., δ -doped semiconductors) where some of these ideas can be tested more quantitatively.

In conclusion, we have shown that for the positionally disordered Anderson-Hubbard model, the low-temperature thermodynamics (in the absence of instabilities like superconductivity) is *not* that of a Fermi liquid, even deep in the metallic phase, but rather a random singlet metal with a divergent susceptibility and specific-heat coefficient, and concomitant absence of spin diffusion in the long-wavelength limit. This behavior, due to rare fluctuations, should be ubiquitous and may be observable in other quenched disordered systems [24].

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ESR Studies of Compensated Si:P,B near the Metal-Insulator Transition

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We have studied the ESR properties of three compensated *n*-type Si:P,B samples near the metal-insulator transition covering the low-temperature regime from 30 mK to 10 K. We find that both the susceptibility and the ESR linewidth increase dramatically as the temperature is lowered, and in the metallic Si:P,B samples the susceptibility increase is more than in similar uncompensated Si:P samples. We compare results for the insulating phase with numerical calculations, then discuss the metallic region in light of various theoretical models for the low-temperature thermodynamic behavior.

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In a simple picture of the metal-insulator (MI) transition the low-temperature excitations in the insulating phase involve localized electrons, while in the metallic phase they involve itinerant electrons. Within this picture one expects that the magnetic properties of these two phases are drastically different—the Fermi-liquid-like metallic phase is expected to have a small, nearly temperature-independent susceptibility, while the insulating phase should have weakly interacting local magnetic moments with a large Curie-type susceptibility. However, numerous ESR [1–4], NMR [5–8], and thermodynamic measurements [9–15] have shown that this simple picture is inadequate, at least in the extensively studied case of phosphorus-doped silicon (Si:P). The magnetic properties of Si:P are found to be surprisingly similar in the metallic and insulating phases near the MI transition and show characteristics of local magnetic moments. This observation suggests that local magnetic moments persist into the disordered metallic phase and dominate the low-temperature thermodynamic properties [1,9,12–15] as well as the spin dynamics [7,8]. Milovanovic, Sachdev, and Bhatt [16] have numerically solved a disordered Hubbard model with randomly placed centers within a self-consistent-field approximation and found local moment instabilities at a few percent of the sites in the metallic phase, in rough agreement with the experimental result in Si:P. A Fermi-liquid theory incorporating the local moments has been formulated by Sachdev [17]. Bhatt and Fisher [18] have very recently given arguments that these local moments persist down to the lowest temperatures, notwithstanding the Kondo effect or the local-moment-local-moment interaction. However, these theoretical approaches do not address all aspects of the effects of local moments in the disordered metal, e.g., how they affect the critical conductivity behavior at the MI transition.

Attempts to clarify the above issues by comparing compensated and uncompensated semiconductors near the MI

transition have raised more questions. Recent NMR measurements in boron-compensated Si:P [19] are in qualitative agreement with similar earlier measurements in uncompensated Si:P [7] and are interpreted in terms of interactions of ²⁹Si nuclei with local moments. However, the critical conductivities of Si:P [20] and Si:P,B [21,22] behave quite differently and one finds a steeper conductivity onset for the uncompensated case. Fitting the conductivity near n_c by the critical form $\sigma \propto (n - n_c)^\mu$, the critical exponent is $\mu = 0.5$ and 0.9 for Si:P and Si:P,B, respectively.

In this Letter we report low-temperature ESR measurements for three Si:P,B samples in the vicinity of the MI transition and compare both their spin susceptibility and ESR linewidth with previously determined values for uncompensated samples [4]. The three samples had electron concentrations of $(2.6, 4.9, \text{ and } 8.0) \times 10^{18} \text{ cm}^{-3}$ and compensation values, defined as the ratio of acceptor to donor doping densities, of 0.6, 0.5, and 0.5, respectively. The electron density n was determined from the room-temperature Hall coefficient and the compensation from the value of n and the donor doping density N_D measured by neutron activation. This procedure is described in detail elsewhere [21,22]. The samples were in the form of a stack of ten thin slabs, $12 \times 9 \times 0.4 \text{ mm}$ each, cut thinly to minimize eddy-current losses. The doping profile of each slab was measured at room temperature with a resistivity technique and found to span $\pm 7\%$. This is somewhat more than the $\pm 2\%$ density variation of the uncompensated Si:P samples used in the earlier control experiment [4]. However, the density variation is not expected to significantly affect the susceptibility, which is found to vary gradually as n goes through n_c . The ESR techniques in this experiment and in the earlier Si:P study [4] were identical. Again the ²⁹Si NMR signal was used for calibrating the ESR spectrometer in absolute susceptibility units. We estimate an absolute accuracy of $\pm 20\%$ for our susceptibility values.

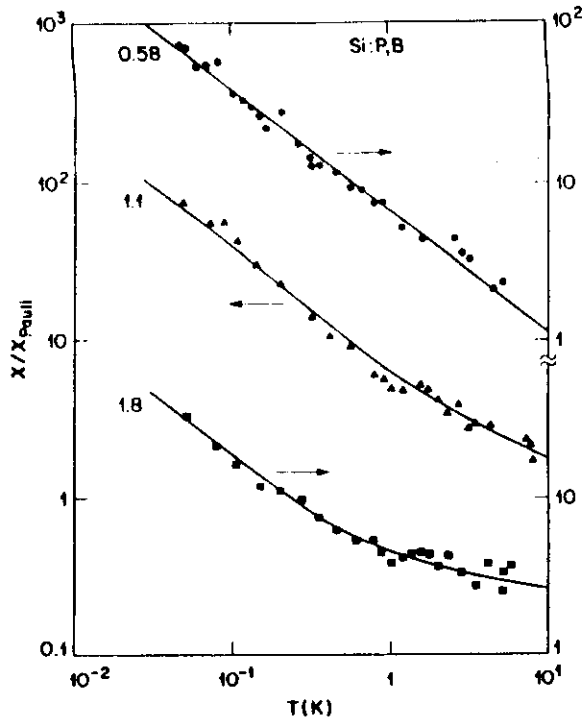


FIG. 1. Temperature dependence of normalized susceptibility χ/χ_{Pauli} of three Si:P,B samples with different normalized electron densities, $n/n_c = 0.58, 1.1,$ and 1.8 . Solid lines through data are a guide to the eye.

In Fig. 1 we show the enhancement of the susceptibility χ (relative to $\chi_{\text{Pauli}} = 3n\mu_B^2/2k_B T_F$) as a function of temperature for all three compensated samples. These data are qualitatively similar to the uncompensated Si:P data [4], i.e., the susceptibility increases towards lower temperatures approximately as a power law $\chi \propto T^{-\alpha}$. As shown in Fig. 2, this temperature dependence is observed over our entire temperature range for insulating samples. In this figure we have compared the normalized susceptibilities $\chi/\chi_{\text{Curie}} \propto T^{1-\alpha}$ ($\chi_{\text{Curie}} = n\mu_B^2/3k_B T$) of compensated and uncompensated Si:P and find, using least-squares fits, that the exponent $\alpha = 0.75 \pm 0.05$ for Si:P,B is somewhat larger than the value of 0.62 ± 0.03 for Si:P. The dashed lines in Fig. 2 represent a quantitative theoretical calculation of the susceptibility using no adjustable parameters as explained below.

The susceptibility of uncompensated Si:P for $n < n_c$ was explained by Bhatt and Lee (BL) using a quantum spin- $\frac{1}{2}$ random Heisenberg antiferromagnetic Hamiltonian [23]. We have performed a similar computer calculation of the susceptibility of a model appropriate for a compensated doped semiconductor deep in the insulating phase. The model consists of distributing donor and acceptor sites at random in a 3D continuum. The negatively charged acceptors provide a fixed random Coulomb potential while the electrons are allowed to occupy the donor sites with the lowest-self-consistent energies, neglecting quantum-mechanical (hopping, exchange)

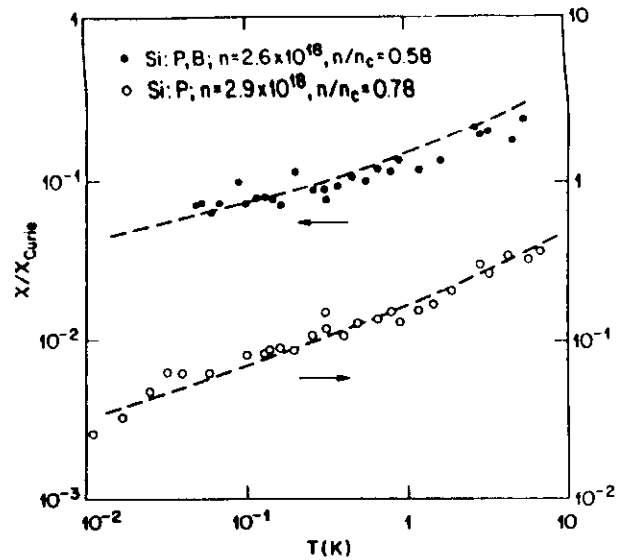


FIG. 2. Comparison of measured normalized susceptibilities χ/χ_{Curie} (circles) of insulating Si:P and Si:P,B samples with theoretical calculation (dashed lines) described in the text.

terms. The ground state is tested for stability against one- and two-electron hops. The susceptibility is then calculated in the manner of BL using the antiferromagnetic spin- $\frac{1}{2}$ Heisenberg exchange Hamiltonian:

$$H = \sum_{i,j} J(r_{ij}) \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where the sum over i and j includes the electron occupied donor sites. For the exchange constant we use the asymptotic hydrogenic result [24] $J(r) = J_0(r/a)^{5/2} \exp(-2r/a)$, where $a = 16 \text{ \AA}$ ($n_c^{1/3} a = 0.25$ for Si:P) and $J_0 = 140$ K. The high-temperature curvature of the theoretical lines in Fig. 2 is due to the asymptotic formula chosen for $J(r)$. This formula underestimates J at small r and these are the values relevant at high temperatures. A theoretical estimate of the exponent α , obtained from the low-temperature behavior of the dashed lines in Fig. 2, is found to be slightly larger in the compensated case. This is due to the rearrangement of the electron occupied donor sites, which results for the compensated case in a distribution differing from the Poisson distribution at short distances. In summary, the theory with no adjustable parameters is in remarkable agreement with the experimental results for the insulating phase.

The difference between Si:P and Si:P,B is more dramatic on the metallic side of the MI transition—the susceptibility enhancement is unexpectedly large in Si:P,B at the lowest temperatures even for the very metallic sample $n/n_c = 1.8$. As shown in Fig. 3, comparing Si:F and Si:P,B samples with similar values of $n/n_c \approx 1.1$, the compensated system shows a factor of 3 to 5 larger local moment fraction than the uncompensated one for $T < 0.1$ K. This is in contrast to the theoretical results of Milovanovic, Sachdev, and Bhatt [16] who find for the disordered Hubbard model that the fraction of local moment-

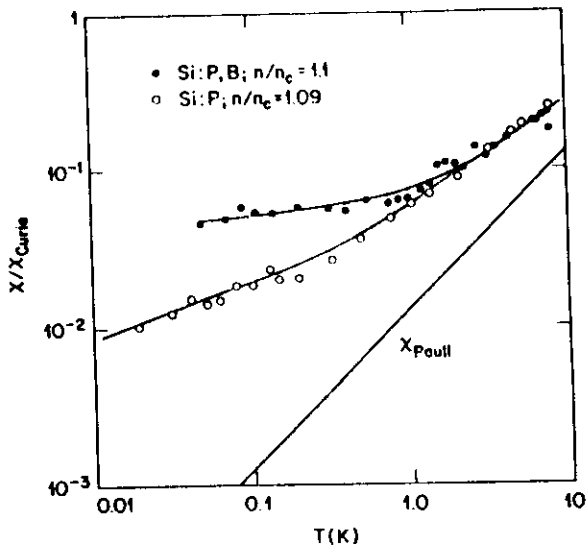


FIG. 3. Comparison of normalized susceptibilities χ/χ_{Curie} of uncompensated and compensated Si:P in the metallic regime.

decreases at carrier concentrations away from half filling of the band. One possible cause of this discrepancy is the presence of random fields in the experimental system arising from the negatively charged acceptors and positively charged donors. These are not included in the disordered Hubbard model calculation. Another possibility is the emergence of ferromagnetic exchange interactions due to the departure from half filling.

Assuming that the increased χ is due to an increase in the number of local moments rather than to ferromagnetic interactions and further that the strength of spin-flip scattering of itinerant electrons increases with the number of local moments we would expect the spin-flip rate τ_s^{-1} to be higher in compensated samples. This increased spin-flip rate could account for the critical-exponent difference between uncompensated Si:P and compensated Si:P,B, provided τ_s^{-1} is just below or equal to $k_B T/h$ in Si:P within the T range from 3 to 100 mK. With this particular value of τ_s^{-1} , the higher spin-flip rate of Si:P,B (which should be checked by the magnetoresistance measurements) could put it (but not Si:P) into the spin-flip universality class [25,26]. However, within the same scaling approach for the spin-flip universality class, χ is not expected to diverge as T tends to zero, in contrast to the experimental evidence in Si:P,B. Thus, the one-component (i.e., the long-wavelength mode) scaling theory requires a coincidence of parameters to explain the critical-conductivity differences between Si:P and Si:P,B, and even then needs local moments to explain the susceptibility of Si:P,B.

The ESR line is broadened by the hyperfine interaction between the electrons and the P nuclei (hyperfine interaction with the nuclei of negatively charged B^- acceptors is very small due to the Coulomb repulsion) but motionally narrowed by the rapid electron spin motion. In the

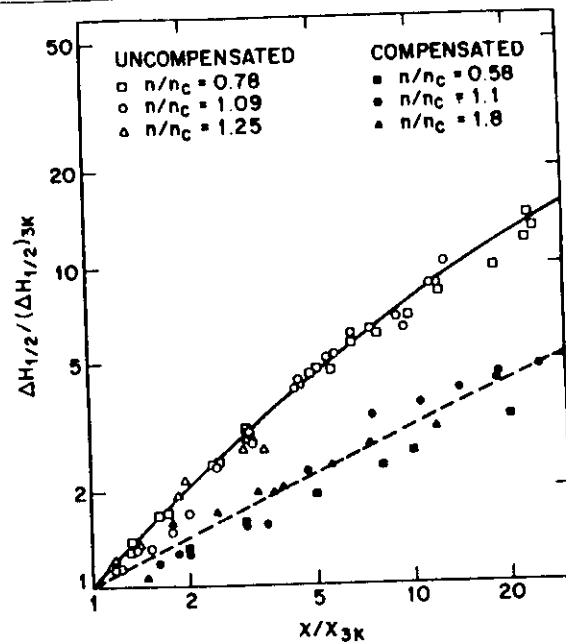


FIG. 4. Log-log plot of ESR linewidth vs susceptibility for uncompensated and compensated Si:P. Both quantities have been normalized by their values at a temperature $T = 3$ K.

Fermi-liquid picture the spin motion is diffusive and can be tied to the Fermi-liquid properties of the sample [27]. In the localized moment picture the low-temperature linewidth is dominated by the fast spin-lattice relaxation of the local moments which then relax the itinerant electrons through the exchange processes [28]. The localized moments form clusters and spin motion via exchange processes determines their motional line narrowing [29]. In previous measurements of the uncompensated samples [4] the linewidth was observed to increase towards lower temperatures with the increase apparently proportional to the susceptibility increase. This simple proportionality is also predicted in the lowest-order disordered Fermi-liquid model [4,27] and it was argued that this observation supports the validity of the scaling theory description.

We find a broader ESR line in the compensated samples than in the uncompensated samples with similar values of n/n_c . The extra linewidth of Si:P,B samples might be expected, given the electron repulsion away from the B^- ions. This leads to an increase of both the electron wave function and the hyperfine interaction at P^+ sites. In Fig. 4 we have plotted the normalized linewidth as a function of normalized susceptibility for both the compensated and uncompensated Si:P. The normalization was done with the $T = 3$ K values of the linewidth $(\Delta H_{1/2})_{3K} = 0.9, 1.1, \text{ and } 1.6$ G (0.45, 0.45, and 0.60 G) and the susceptibility $\chi_{3K}/\chi_{Pauli} = 3.0, 3.2, \text{ and } 3.4$ (4.5, 2.9, and 2.5) in the compensated (uncompensated) low-, medium-, and high-density samples, respectively. We find several interesting features in the data of Fig. 4. First, for the compensated samples the linewidth is not

proportional to the susceptibility. Second, the similar results for the insulating and metallic samples suggest that the same mechanism, presumably the local moment relaxation, is causing the line broadening in both phases.

A zeroth-order estimate of the linewidth within the localized spin model, assuming that the linewidth comes from the spin-lattice relaxation of the local moments, can be obtained as follows. The half-width $\Delta H_{1/2} \approx 1/T_1 \approx \frac{1}{2} \gamma_c H_{\text{hf}}^2 \tau_c$, where the hyperfine field $H_{\text{hf}} = 21 \text{ G}$ [30] and τ_c is the correlation time for the hyperfine interaction when a spin excitation diffuses within a given cluster. The correlation time τ_c is expected to scale inversely with the characteristic exchange interaction J , which has a wide distribution in our disordered system. If we make the drastic assumption that the distribution of J values (including further neighbor interactions) can be described by a single parameter α , we can obtain τ_c by averaging J^{-1} over the distribution $P(J) = J^{-\alpha}$ from the hyperfine energy $\hbar \gamma_c H_{\text{hf}}$ to the thermal energy $k_B T$. This will give a linewidth of

$$\Delta H_{1/2} \propto H_{\text{hf}} (\hbar \gamma_c H_{\text{hf}} / k_B T)^{1-\alpha}. \quad (2)$$

In qualitative agreement with Fig. 4, Eq. (2) predicts a linewidth which for $\alpha > 0.5$ has a weaker temperature dependence than the temperature dependence of the susceptibility, $\chi \propto T^{-\alpha}$. An exact proportionality between the linewidth and susceptibility is accidentally achieved when $\alpha = \frac{1}{2}$. Computer calculations such as those done for the uncompensated system [29] are necessary to check the merits of this rather simplified argument.

In conclusion, our ESR studies of boron-compensated Si:P near the MI transition support the two-fluid model of localized spins and itinerant electrons in the metallic phase. The interaction between the two "fluids" leads to the spin-flip scattering of the itinerant electrons. The strength of this spin-flip scattering may affect the critical conductivity exponent. In the insulating phase the susceptibility is found to be in quantitative agreement with the computer simulations of a generalization of the Poisson distributed random antiferromagnet to take into account the effect of compensation.

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Effective-Field Theory of Local-Moment Formation in Disordered Metals

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We present a simple new effective-field theory for the metallic state of a disordered interacting Fermi liquid, taking into account its instability towards the formation of local-moment states. We find a generalization of the compensation theorem of the single-impurity Anderson model, namely, that strongly localized magnetic instabilities occur even when the mean-field single-quasiparticle states are extended. The theory clarifies the understanding of recent thermodynamic and spin-resonance measurements in phosphorus-doped silicon.

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Many theoretical analyses^{1,2} have recently addressed the subject of the metal-insulator transition (MIT) in a disordered interacting-electron gas. Using a renormalized weak-disorder perturbation theory, but including the effect of interactions exactly within lowest order in disorder, these investigations have led to an understanding of many transport properties in the disordered metallic phase. However, these theories remain unsatisfactory in explaining the low-temperature thermodynamics as well as the region near the MIT.³⁻⁷ Here we present a new mean-field theory of the *disordered metallic state*. Our theory is directly motivated by experiments on doped semiconductors and should serve as an improved starting point for a complete theory of the MIT.

We take a point of view that is complementary to recent approaches;² we treat the noninteracting disordered Hamiltonian *exactly* in a numerical calculation, but account for the interactions in a Hartree-Fock-type approximation.⁸ Such an approach is crucial in accounting for the instability of an interacting-electron gas towards the formation of localized magnetic states.⁹ This instability is not directly apparent in a disorder perturbation theory even though it can occur for *weak* disorder. Additional motivation comes from the understanding of the insulator through magnetic and optical measurements in doped semiconductors¹⁰ where a correct treatment of disorder effects was crucial.

We discuss our approach in the framework of a disordered Anderson-Hubbard model,

$$H = - \sum_{i \neq j, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} (\epsilon_i - \mu) c_{i\sigma}^\dagger c_{i\sigma},$$

where i, j extend over all the sites in the system (not necessarily on a lattice), $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and σ is the spin index. The off-diagonal disorder in the hopping matrix elements t_{ij} will produce local environments favoring the formation of local moments; we present below a theoretical criterion for this to occur. The on-site energies ϵ_i are weakly random variables [$(\langle \epsilon_i - \langle \epsilon_i \rangle \rangle^2) < \max(t_{ij})$]. We find that an appreciable number of local moments can occur in weak disorder under conditions in which the

mean-field single-quasiparticle states near the Fermi level are extended. The localization length of the local moments appears to be finite even in the metallic state; this strong localization may be viewed as a *generalization of the compensation theorem⁹ for the single-impurity Anderson model*.

We begin by reviewing a well understood special case of H ; the *single-impurity⁹ Hamiltonian* H_S . We obtain H_S by placing sites i, j on a cubic lattice with hopping matrix elements $t_{ij} = t$ for all nearest-neighbor bonds except for the six bonds connected to the impurity site 0, for which $t_{0i} = t_{i0} = w$. We choose a density of one electron per site ($\epsilon_i = 0, \mu = U/2$). For $w = 0$, a single electron at the origin has energy $-U/2$, while a second electron will cost energy $U/2$; for small w , therefore, the model is related by a canonical transformation to the *symmetric Anderson model*. Using the extensive numerical and analytic renormalization-group analyses¹¹ on this model, the temperature dependence of the local spin susceptibility of the site 0, χ_0 , can be obtained (Fig. 1). At high temperatures, $T \gg U$, interactions are irrelevant and $\chi_0 = (g\mu_B)^2/8kT$. For $T < U$ two types of behavior occur. (i) For small w , χ_0 is enhanced to $(g\mu_B)^2/4kT$ at intermediate temperatures due to the formation of a local moment at the origin, but is eventually quenched by the Kondo effect at $T \ll T_K$ (the Kondo temperature). (ii) For larger w one obtains a Fermi liquid¹² and the susceptibility is directly quenched via the onset of the Pauli spin susceptibility. The boundary between these two types of behavior sketched in Fig. 1 is obtained as described below.

Some features of the local-moment formation deserve mention. (i) The Hartree-Fock calculation is adequate to determine the boundary between the local-moment and Fermi-liquid regimes.¹¹ The Kondo effect, which needs renormalization-group methods, only becomes important at $T \leq T_K$. (ii) In the Fermi-liquid regime, we may perform a nonmagnetic Hartree-Fock factorization of H_S to obtain $(H_S)_{\text{HF}} = \sum_{i,j} t_{ij} c_{i\sigma}^\dagger c_{j\sigma}$. $(H_S)_{\text{HF}}$ is a single-impurity Hamiltonian which can be exactly diagonalized

We first discuss the case of a density of 1 electron per site (this corresponds to uncompensated SiP). The calculations were carried out at temperatures of $T=0.1t_0$ and $T=0.01t_0$ for a number of sample sizes and densities. We found that, at a fixed density of electrons, the number of local moments was quite accurately proportional to the total number of electrons for system sizes greater than twenty sites. This is as would be expected if the system size is much greater than the localization length of the local moments. The ratio of the number of local-moment instabilities to that of electrons was found to increase monotonically with decreasing density from

$$P_{ab} = \frac{\sum_i |m_a(i)|^2 |m_b(i)|^2}{\sum_i |m_a(i)|^4 + \sum_i |m_b(i)|^4}$$

Only the larger of a pair of eigenvalues k_a and k_b with $P_{ab} > P_m$ was accepted as representing a local moment. We chose values of P_m between 0.1 and 0.5. Variations of P_m in this range produced relative changes in the number of local moments which varied from $< 1\%$ at high temperatures and high densities up to $\sim 25\%$ at the lowest temperatures and densities.

We first discuss the case of a density of 1 electron per site (this corresponds to uncompensated SiP). The calculations were carried out at temperatures of $T=0.1t_0$ and $T=0.01t_0$ for a number of sample sizes and densities. We found that, at a fixed density of electrons, the number of local moments was quite accurately proportional to the total number of electrons for system sizes greater than twenty sites. This is as would be expected if the system size is much greater than the localization length of the local moments. The ratio of the number of local-moment instabilities to that of electrons was found to increase monotonically with decreasing density from

All of the above discussion has concentrated on an electron filling factor of 1 electron per site. As in the single-impurity Anderson model, this is the most favorable condition for the formation of local moments. To explore the consequences of changing the number of

We also studied the properties of the single-particle wave functions, $\psi_a(i)$, and the eigenvectors, $m_a(i)$, of these two sets of eigenvectors, our experience shows that every eigenvector $m_a(i)$ which is localized around the site r_i (say) is associated with an eigenvector $\psi_a(i)$ which is peaked at r_i and has an eigenenergy close to the Fermi level. Exactly the same correspondence is present in the single-impurity Hamiltonian H_S . We evaluated the inverse participation ratios $P_{H_a} = \sum_i |\psi_a(i)|^4$ and $P_{X_a} = \sum_i |m_a(i)|^4$. We plot in Fig. 2 the average of $P_{H_a}, P_H = (P_{H_a})$ over many samples and for states within $0.1t_0$ of the Fermi energy for a fixed density of electrons $\rho a^3 = 0.02$. On a log-log plot, P_H decreases monotonically as a function of the number of sites in the system with a slope ≈ 0.73 , which is reasonable since the correlation length is comparable to system size, and is evidence that all the states within $0.1t_0$ of the Fermi level are extended. For the same samples, the behavior of $P_{X_a} = (P_{X_a})$ is quite different. It remains independent of the system size at a value of around 0.5 (for $T=0.01t_0$) showing quite convincingly that all of the local-moment states are localized on length scales of order the spacing between the sites (at higher temperatures P_X increases towards its $T = \infty$ limit of $P_X = 1$).

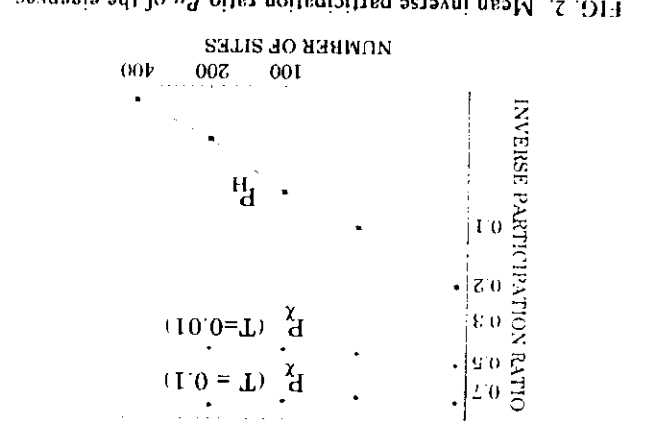


FIG. 2. Mean inverse participation ratio P_H of the eigenvectors $\psi_a(i)$ of H , and P_X of the eigenvectors $m_a(i)$ of X , at a density $\rho a^3 = 0.02$, and the filling factor $\nu = \frac{1}{2}$ for different system sizes. We used an upper cutoff $P_m = 0.5$ for the cross inverse participation ratio P_{ab} . The values of P_X are shown at two temperatures $T=0.01$ and $T=0.1$. They are independent of system size suggesting that the eigenvectors $m_a(i)$ are localized. Values of P_H show no appreciable T dependence and decrease with system size suggesting that the $\psi_a(i)$ are extended.

MAGNETIC PROPERTIES OF DISORDERED SYSTEMS NEAR A METAL-INSULATOR TRANSITION

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Abstract. - Using doped semiconductors as a paradigm, the low-temperature magnetic and thermodynamic behaviour of a disordered system undergoing a metal-insulator transition is described, and compared with various theoretical approaches from the metallic and insulating phases. Issues addressed include universal behaviour in the insulating phase, local moments in the metallic phase, and effects of compensation.

1. Introduction

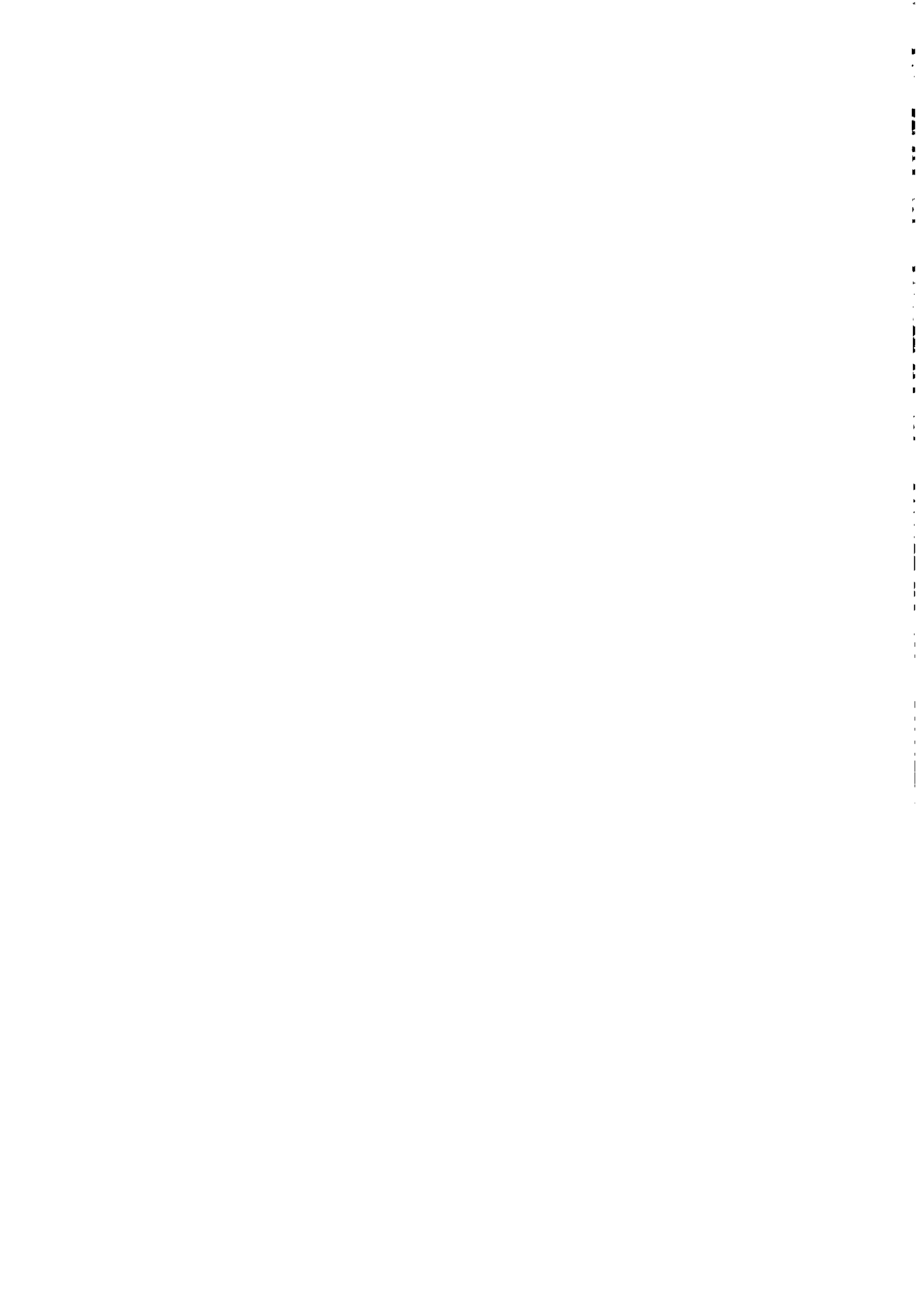
Progress in the understanding of the properties of disordered systems undergoing a metal insulator (MI) transition during the past decade [1] has hinged on the scaling theory of localization. Following the seminal papers for non-interacting electrons in a disordered medium [2, 3], the role of electron interactions has been incorporated into the scaling description [4-7]. These studies suggest that the critical behaviour at the MI transition in disordered systems depends on spin-dependent effects (e.g. spin-flip or spin-orbit scattering, magnetic field) which appear as cut-offs in the scaling equations. This leads to various universality classes for the critical exponents of the transport coefficients (conductivity, Hall coefficient, etc.). Thus the magnetic properties of disordered systems near the MI transition could yield valuable clues towards unraveling the transport behaviour.

Experiments have been performed on a variety of systems such as (i) doped semiconductors, (e.g. uncompensated Si:P (Silicon doped with phosphorus) and compensated Si:P; B); (ii) metal-semiconductor mixtures (e.g., Au-Ge, Nb-Si) and (iii) magnetic semiconductors.

Except for uncompensated silicon [8], the exponent μ characterizing the $T = 0$, the conductivity onset $\sigma \sim |x - x_c|^\mu$ is $\mu \approx 1$. (Here x is the concentration, pressure, uniaxial stress, or magnetic field, and x_c is the value at the MI transition). In contrast, uncompensated doped silicon shows a much sharper onset, with $\mu \approx 0.5 - 0.6$. Recent work [9-15] has focussed towards the resolution of this controversy, through magnetic and thermodynamic measurements at low temperatures, as well as magnetoresistance data in doped silicon. Similar measurements on the other systems would be invaluable in furthering our understanding of the MI transition and the applicability of scaling ideas for thermodynamic quantities

We limit ourselves to doped semiconductors, comparing various theoretical scenarios with experiments on Si:P and Si:B. Doped semiconductors are in some sense the most basic disordered system, because the impurity electron is in a shallow hydrogenic 1s state, with a Bohr radius a_B ($\sim 20 \text{ \AA}$ in Si) that is much larger than lattice spacing because of the large dielectric constant of the host semiconductor. Consequently, it is well modelled as an ensemble of hydrogen atoms, *randomly distributed in three-dimensional space* (i.e. the discreteness of the underlying lattice is unimportant at the densities of interest $n \sim n_c \approx (1/4a_B)^3$). Additional complications due to mass anisotropy, many conduction band minima etc., necessary for quantitative calculations, are of little concern for the qualitative physics, and so will not be discussed here.

At low n , each donor impurity electron is bound to the impurity, in a 1s state; the system behaves magnetically as an ensemble of spins with $s = 1/2$, with very weak exchange interactions, leading essentially to a Curie susceptibility $\chi \sim 1/T$. At high densities, on the other hand, the electrons delocalize, and if we were to take the analogy with lattice systems, we would expect a T -independent Pauli spin-susceptibility. Thus the low T magnetic behaviour considerably with n . It is this change, as well as the associated effect on the low temperature thermodynamics, and its relation with the MI transition and the electronic transport properties that we wish to discuss in the following sections. Section 2 is devoted to the insulating phase, where we believe we have an approximate theory and a good physical understanding of the magnetic behaviour. Section 3 discusses recent developments in our understanding of the behaviour in the vicinity of the MI transition, implications for the disordered metal, and the effect of compensation. Finally, in section 4, we summarize our conclusions.



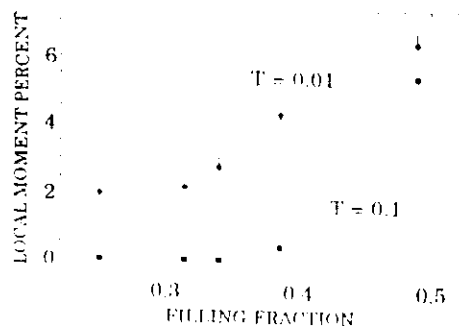


FIG. 3. The ratio of the number of local moments to the total number of electrons, f_{lm} , as a function of filling factor for a constant density of electrons $\rho a^3=0.02$ at two different temperatures (measured in units of t_0).

electrons per site we repeated all of the calculations with decreasing values of the chemical potential μ down to a filling fraction of 0.25. We show in Fig. 3 results for f_{lm} , the ratio of the number of local-moment instabilities to the total number of electrons, as a function of filling factor for a constant density of electrons $\rho a^3=0.02$. The value of f_{lm} in an effective-field calculation increases with falling temperature; at $T=0.01t_0$, f_{lm} is expected to be close to its asymptotic zero-temperature value. We see from Fig. 3 that f_{lm} is a maximum at half-filling; however, the falloff with decreasing filling fraction is rather gradual.

While our calculations have been done on a model Hamiltonian, we have chosen the model to capture the essential aspects of disorder and electron correlation. It is thus gratifying that our estimate for the number of local-moment instabilities of $\sim 10\%$ of the sites at densities within 50% of the critical density ρ_c is in good agreement with experimental estimates of 10%–25% from NMR³ and thermodynamic⁵ measurements. A larger U/t_0 suggested by Ref. 15 would in fact improve agreement. We regard this agreement to be a vindication of the basic physical picture of the phenomenological two-fluid (the itinerant electrons and the localized moments) model of metallic doped semiconductors.^{3,5,17}

To conclude, we have shown in this paper that a system of interacting electrons in weak disorder displays a strong instability towards the formation of localized moments on length scales much shorter than the localization length of the electrons' Hartree-Fock wave functions. This phenomenon has been argued to be related to the *compensation theorem* of the single-impurity Anderson model where competing ferromagnetic (due to the spatial extent of the impurity wave function) and antiferromagnetic interactions (due to superexchange) cancel each other, leading to a very localized spin polarization. Any complete theory of the MIT has therefore to account for the presence of the electron local moments and the effect of interactions between the local moments and the itinerant electrons. Two steps in this direction have been taken: (a) the determination of the Fermi-liquid

properties of a two-fluid model of itinerant electrons and local moments¹⁸ and (b) the study of the very low-temperature properties of a disordered system with local moments.⁶ An important question which remains open is the precise role of the local-moment instabilities in the critical behavior of charge transport near the MIT.

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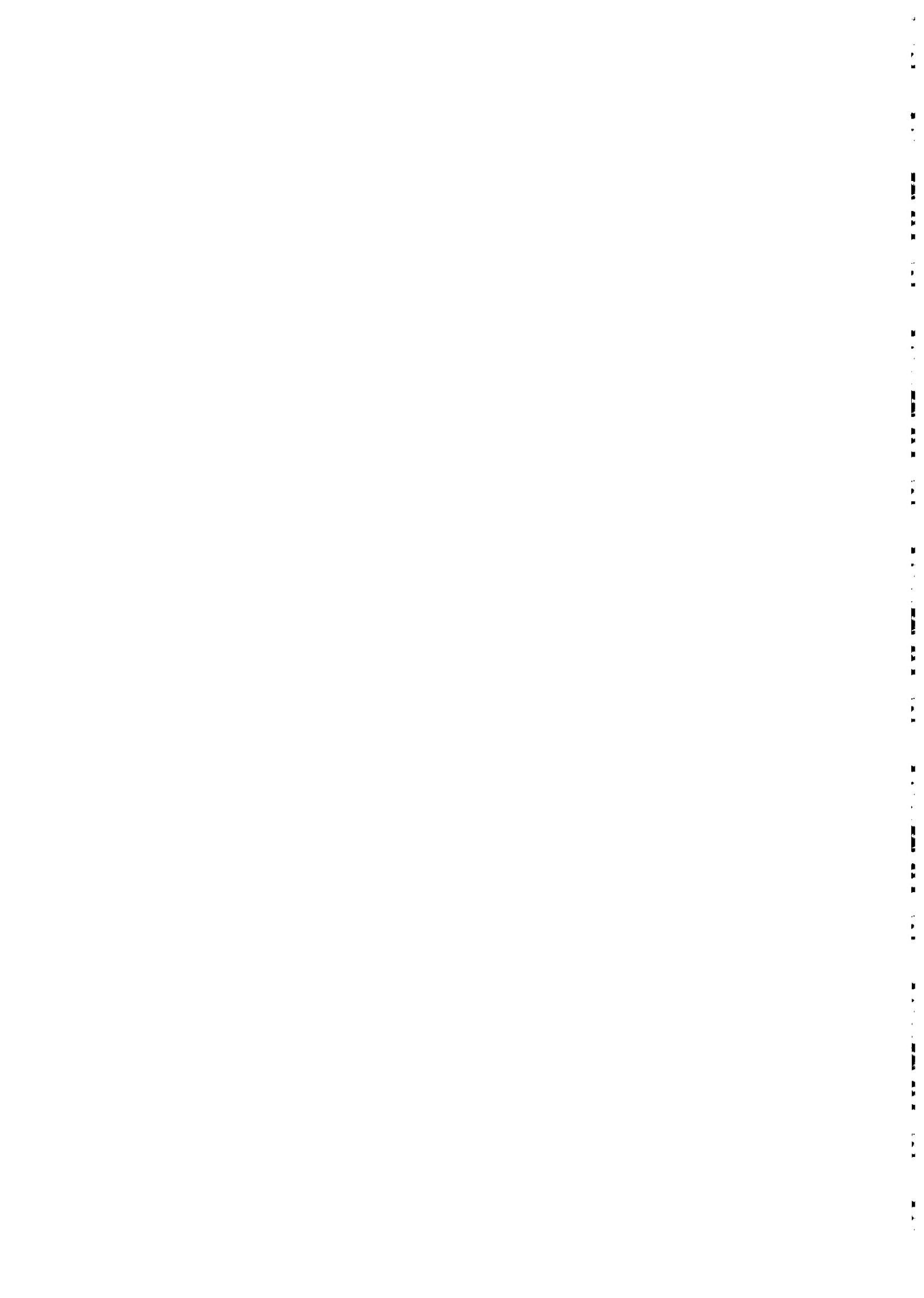
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2. The insulating phase

The magnetic character of the insulating phase is by and large understood by now for the "fruit-fly" of disordered systems, the random ensemble of hydrogenic atoms, which is realized in n-doped uncompensated semiconductors. We will only summarize the results here and the reader is referred to a previous review [16] for details. At low densities, deep in the insulating phase, where charge fluctuations are unimportant (at low energy scales) the low energy behaviour can be described in terms of the Heisenberg Hamiltonian:

$$H = \sum_{ij} J(\mathbf{r}_{ij}) \mathbf{S}_i \cdot \mathbf{S}_j \quad (1)$$

$J(r)$, the direct antiferromagnetic exchange interaction between pairs of hydrogen atoms varies roughly as $J(r) \sim J_0 \exp(-2r/a_B)$. Though the microscopic $J(r)$ can be calculated only in the low density limit, we will argue that a similar exchange Hamiltonian with $J(r)$ varying exponentially with distance describes the low-energy behaviour throughout the insulating phase, and experiment suggests that it may also persist somewhat into the metallic phase.

Despite the superficial similarity of equation (1) to a lattice Heisenberg Hamiltonian, the magnetic character of the random antiferromagnet is quite different from that of a lattice of hydrogen atoms (e.g., simple cubic or bcc). For the lattice, the dominant nearest neighbour interactions would lead to simple Neel ordering at a temperature $T_N \sim J(r_0)$ where r_0 is the nearest neighbour distance, implying an ordered ground state for arbitrarily small density, n ($\sim r_0^{-3}$). The random antiferromagnet, on the other hand, is best described as a "valence-bond" insulator, i.e. pairs of sites coupled strongly to each other form an inert singlet ground state (valence-bond) because of the large energy gain due to quantum fluctuations in this spin-1/2 system. That this happens to strongly coupled pairs is not so surprising, because of the wide distribution of initial (bare) couplings covering many orders of magnitude in this highly disordered system; in fact, the necessity of a hierarchical scheme has been pointed out by a number of workers [17]. What is more significant is that this wide distribution and hierarchical scheme works down to extremely low energy scales, as shown by the numerical renormalization group calculations [18] of Bhatt and Lee (BL). As a result, the low temperature magnetic and thermodynamic properties are well described by an ensemble of coupled pairs of spins with a *renormalized* distribution $P_R(J)$ of pair couplings J , analogous to that used in the context of the quasi-1d organic systems [19] which are the one dimensional counterpart of this system. Both experiment and the numerical calculation suggest that the susceptibility at low temperatures $T < 10$ K for densities $0.2n_c < n < n_c$ behaves *approximately* as

$\chi(T) \sim T^{-\alpha}$ where $\alpha \approx 0.6$. In the numerical calculation, α is weakly dependent on T (logarithmically); however, the experiments are consistent with a constant α over almost three decades in T . (The same situation is true in the quasi-1d systems). Further, the experimental $\chi(T)$ at low T is almost independent of n as well, strongly suggesting that some sort of fixed point behaviour has been reached in the entire range of densities.

Within the hierarchical pair approach, the singular behaviour of $\chi(T)$ is viewed as a consequence of an infrared singularity which develops in the *renormalized* pair distribution $P_R(J) \sim J^{-\alpha}$. Because of this singularity the low- T thermodynamics in the insulating phase is dominated by spin excitations, even when charge (electron-hole) excitations are added, as, for example, in the Hubbard model with randomly positioned sites. Indeed, as long as one is in the insulating state, an effective spin Hamiltonian with exchanges varying exponentially with distance at long distances is likely to emerge as the low energy description, though $J(r)$ is not the bare hydrogenic exchange.

In the non-interacting valence bond picture, all thermodynamic properties can be calculated explicitly as integrals over the distribution $P_R(J)$, and compared with experiment. The resulting fit in terms of a single parameter α (which is motivated by the numerical studies), and *no further adjustable parameters* to the susceptibility [20], specific heat [10], as well as the scaling behaviour of the non-linear magnetization [21] is very good. Further, by including the interactions between the spin pairs and hyperfine interactions [22], a satisfactory agreement can be obtained for the dramatic temperature dependence of the ESR line width and position [23] as well, suggesting that this gives a good starting point for the spin dynamics as well.

This valence-bond insulator is the disordered counterpart of the RVB picture put forth for the high- T_c superconductors by Anderson *et al* [24]; however, it has no "resonance" in the valence bonds. Further, our result is crucially dependent on the existence of a high degree of disorder, so that the hierarchy is well-defined, and it appears not to depend crucially on dimension, at least for $d = 1-3$ [18]. Finally, it should be emphasized that while this gives a good description, it is a zeroth order model, from which perturbative expansions *may* be necessary, depending upon the question asked; as for example, in the case of spin diffusion [22].

3. Beyond the critical density

The traditional picture of the metallic phase beyond n_c has been in terms of a Fermi liquid, much like systems with translational symmetry (fluids and crystalline solids), especially because at large density, interaction effects are less important than the one electron kinetic energy. This would suggest that in the ab-

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sence of magnetic transitions in the insulating phase, the thermodynamic properties across the MI transition would be well described by the Brinkman-Rice [25] result for the MI transition in the half-filled Hubbard model. Namely, the divergent susceptibility would be quenched in the metallic phase at low temperatures at a value $\chi(0) \sim m^*/m$, with an effective mass, diverging as $m^* \sim (n - n_c)^{-1}$, leading to a divergent χ at n_c at $T = 0$. The same divergence is found for the specific heat $\gamma \equiv C/T$, and the ratio (χ/γ) is four times the free electron value. Unfortunately, such a scenario is not borne out by the experimental results on Si:P (Fig. 1), which shows $\chi(T)$ vs. T on a double logarithmic plot for concentrations on both sides.

It is quite conceivable that properties at low-temperatures where Fermi liquid theory is supposed to apply are drastically modified in the presence of disorder, and calculations based on perturbative scaling approaches [5-7] suggest that this is indeed so, particularly in the absence of spin scattering and magnetic fields. The RG equations, involve a dimensionless conductance t , an action parameter γ_2 , and a quasiparticle density of states renormalization z , which vary on the length scale l as:

$$\frac{dt}{dl} = -\frac{\epsilon}{2}t + t^2 \left[4 - 3 \left(\frac{1 - \gamma_2}{\gamma_2} \right) \ln(1 + \gamma_2) \right] \quad (2a)$$

$$\frac{d\gamma_2}{dl} = \frac{t}{2} (\gamma_2 + 1)^2 \quad (2b)$$

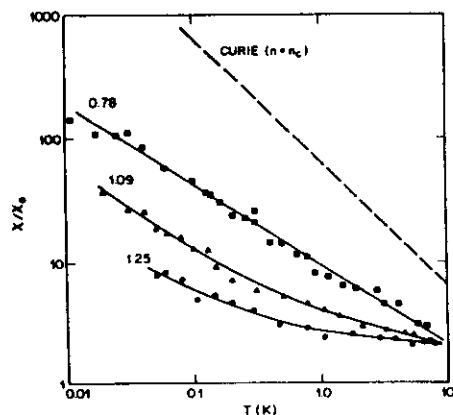


Fig. 1. - Spin susceptibility of Si:P normalized to the Pauli value as a function of temperature for three values of the reduced density n/n_c indicated on a double logarithmic plot. Dashed line is the Curie susceptibility corresponding to the MI transition density n_c .

$$\frac{dz}{dl} = \frac{t}{2} z (3\gamma_2 - 1). \quad (2c)$$

Here $t = \Lambda^{d-2} / 4\pi^2 N_1 D$, where Λ is the cut off in momentum space, N_1 the bare density of states at the Fermi level, and D the charge diffusion constant. Equations (2) are to lowest order in $\epsilon \equiv d - 2$, the

dimensionality above two dimensions, and are appropriate for the non-degenerate band case, though similar equations with slightly different coefficients can be written down for the degenerate (multi-valley) case. Identifying the physical conductivity σ , specific heat γ and magnetic susceptibility χ as:

$$\sigma \sim \Lambda^{d-2} / t \quad (3a)$$

$$\gamma = N_1 z \quad (3b)$$

$$\chi = N_1 z (1 + \gamma_2), \quad (3c)$$

one may show that these equations imply a strong T -dependent enhancement of both χ and γ , $\chi \sim T^{-4\epsilon/(d+3\epsilon)}$ and $\gamma \sim T^{-3\epsilon/(d+3\epsilon)}$ as T is reduced. However, at low T the parameters flow to strong coupling, where equations (2) are no longer applicable.

This dependence of $\chi \sim T^{-2/3}$ and $C = \gamma T \sim T^{1/2}$ (for $\epsilon = 1$) are qualitatively in agreement with experimental results (Figs. 1 and 2). However, from equa-

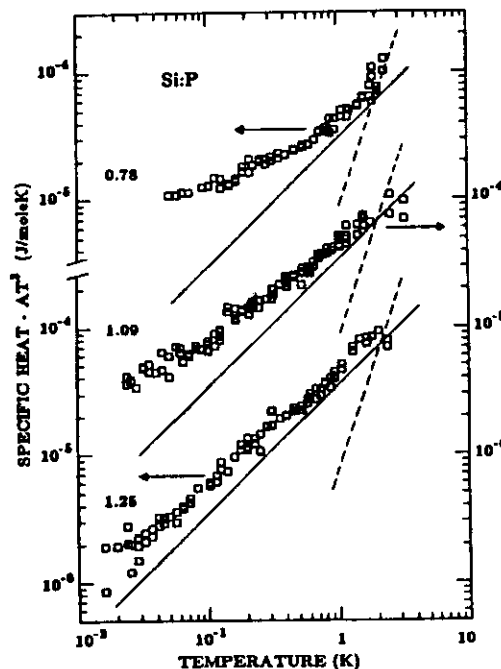


Fig. 2. - Electronic specific heat of the same three samples versus temperature. Also shown is the "free electron" (solid line) and phonon (dashed line) specific heat. Below 1 K, the specific heat for the insulator (top curve) is consistent with $C \sim T^{1-\alpha}$ with $\alpha \approx 0.6$.

tions (2) and (3), we can also write down equations for the variation in susceptibility χ/χ_0 , specific heat γ/γ_0 , and conductivity σ/σ_0 (where symbols with the subscripts 0 refer to the bare, high temperature values), in terms of each other, which are independent of cutoff to lowest order in ϵ and can be integrated up to (down to) any desired length scale (tempera-

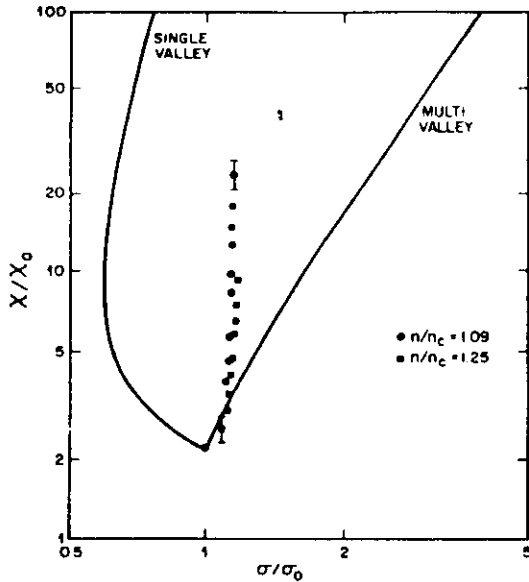


Fig. 3. - Plot of susceptibility as a function of conductivity for metallic samples along with results of the scaling theory for single and multi valley case.

ture). Such *implicit* plots, which have no adjustable parameters, except for the starting point at high temperature, are shown in figures 3 and 4a. The various symbols represent experimental data [10] from the two metallic Si:P samples as the temperature is varied, while the two solid curves labelled SV and MV stand for the non-degenerate (single valley) case, and the multi-valley case appropriate for silicon. Despite fitting the results at high temperature, the experimen-

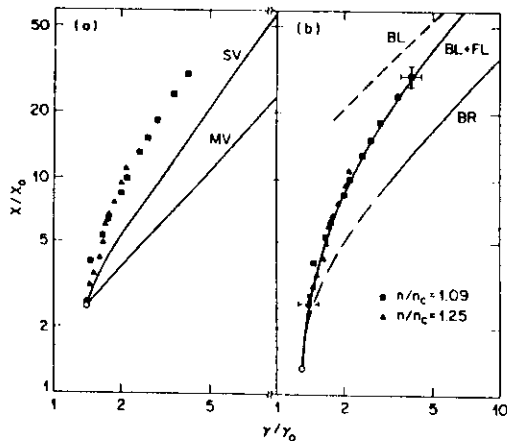


Fig. 4. - Plot of the susceptibility versus specific heat γ for metallic samples. In (a) the experimental data are compared with the single and multi valley scaling theory, while (b) compares it with the Brinkman-Rice and the two-fluid (BL + FL) model. Dashed line is the asymptotic low temperature result where BL pairs dominate.

tal data do not fit the theory well, and the fits do not improve much by changing the starting point for the RG equation. We mention in passing that with spin scattering or finite magnetic field, the divergences in χ and γ at low T are quenched in the RG equations, so these would not fit the data even qualitatively.

The large enhancement of χ relative to γ suggests a magnetic instability of the Fermi liquid, namely the formation of local moment (or long-lived quasi localized spin fluctuations). This is found in studies of the disordered Hubbard model [26], which suggests a continuity with the thermodynamics of the insulating phase, where it was dominated by localized spins interacting with each other. Following this line of thought, we may write a generalization of the results of the insulating phase to include a Fermi-liquid contribution to γ and χ in a two fluid model:

$$\gamma / \gamma_0 = m^* / m + (T / T_0)^{-\alpha} \quad (4a)$$

$$\chi / \chi_0 = m^* / m + \beta (T / T_0)^{-\alpha} \quad (4b)$$

We assume an $\alpha \simeq 0.62$, taken from the susceptibility and specific heat data for the $n / n_c = 0.78$ sample (Figs. 1 and 2), independent of n , $\beta = 10.5$ from the spin pair model for $\alpha = 0.62$, and a mass enhancement $m^* / m = 1.3$ from earlier measurements [29]. Then equations (4) contain only one adjustable parameter T_0 (which measures the fraction of localized spins), which may be eliminated by considering the plot of χ / χ_0 vs. γ / γ_0 (as for the scaling theory) where (T / T_0) is an implicit parameter. The resulting curve is shown in figure 4b as (BL + FL), and clearly fits the data rather well approaching the BL result at low T . The Brinkman-Rice result (BR), where the control parameter is the vicinity to the transition, is shown as well.

Finally, in figure 5, we show the Wilson ratio $(\chi / \chi_0) / (\gamma / \gamma_0)$ as a function of temperature T for the three Si:P samples near n_c . The insulating sample approaches a constant value ≈ 9.3 close to the BL re-

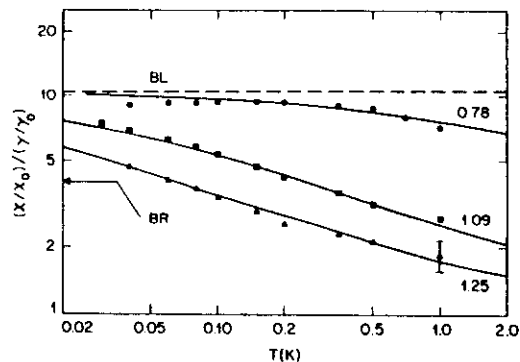


Fig. 5. - Wilson ratio as a function of temperature for the three samples and fits using the two-fluid model. Note the constant value for the insulating sample below $T \sim 0.2$ K, close to the Bhatt-Lee model value (dashed line).

sult of 10.5, and much above the BR value of 4. By adjusting T_0 for each sample the solid curves are obtained from equations (4), implying that the ratio of spins for the three samples in ascending density, is 20:5:2. (Assuming nearly 100 % localized in the insulating sample gives 25 % and 10 % localized spins in the two metallic samples).

The existence of local moments in the metallic phase as $n \rightarrow n_c^+$ can also be directly inferred from the phosphorus NMR measurements [14] which see a dramatic loss of signal from nuclei coupled to the itinerant electron gas as n_c is approached. Silicon NMR measurements [13, 15] are also consistent with the two-fluid picture [27, 15]. Bulk magnetization measurements [11] at higher temperatures and susceptibility measurements [28] have also provided evidence in favor of local moments in the metallic phase.

The idea of local moments just above n_c is quite old – it was proposed well before the scaling theory on the basis of susceptibility and specific heat measurements by a number of workers [29]. What is new is that by going to lower temperatures and measuring both χ and C on a series of samples, it has been possible to not only test different theoretical models, but also provide an idea of the interactions between the local moments in the poor metal.

A number of questions are raised by the proposition of local moments in a metal – e.g. why do they not get quenched by a Kondo effect, and what is their effect on transport properties? It has recently been shown [30] that for randomly (Poisson) distributed sites, that the Kondo effect is not capable of quenching the susceptibility even deep in the metallic phase, because of the presence of rare regions consisting of an odd number of sites with low density ($\ll n_c$). The RKKY interaction between these rare regions is more effective, but still does not appear to prevent a divergence in $\chi(T)$ as $T \rightarrow 0$, suggesting a breakdown of a pure Fermi liquid description. Such effects would clearly be enhanced in the vicinity of n_c ; the positionally disordered Hubbard model has ~ 10 % local moments near n_c [26].

The above considerations also give some justification for why a description of *thermodynamics* in terms of a two-fluid model is appropriate – the exchange between these moments is much more efficient than that between the moments and the “itinerant part” of the electron gas. Nevertheless, the two non-interacting fluids (Eq. (4)) is clearly a zeroth order description.

The local moments provide a T -dependent spin-flip scattering for transport within a Fermi liquid picture [31]. Analysis of the magnetoresistance data [12] shows that in uncompensated Si:P, the spin-flip rate remains close to $k_B T$ down to millikelvin temperatures, while in compensated Si:P; B and Ge:Sb the rate is actually higher. Recent susceptibility measurements on compensated Si:P; B by ESR show an *enhanced* susceptibility over uncompensated Si:P. This is entirely consis-

istent if the spin-flip scattering is due to local moments – the higher rate corresponds to their larger number, evidenced by the higher χ . (In the one-fluid scaling theory, on the other hand, large spin-flip scattering rate implies no divergence in $\chi(T)$, contrary to the stronger divergence seen in experiment.) The differences in spin-flip scattering may be responsible for the differences in the conductivity exponent, though incorporating the local moments within a scaling theory for transport is not yet complete.

Finally, the ESR line width at small fields was found to be proportional to the susceptibility in uncompensated Si : P; this is easier understood in the disordered Fermi-liquid [9, 32], than in the BL model [22]. However, this proportionality *does not* occur in the compensated samples. In fact the slower divergence in linewidth compared to the uncompensated case correlates very well with the faster divergence of $\chi(T)$ with a BL picture, and is under investigation.

4. Concluding remarks

Through an extensive effort involving a series of measurements and theoretical modelling of both transport and thermodynamic properties in doped semiconductors, a consistent picture of the MI transition in disordered systems seems to be emerging. The data favour the appearance of local moments in the disordered metal, and a pure Fermi liquid picture of the disordered metal may break down in a more serious way than perturbative scaling approaches to the MI transition (from the metallic side) would suggest. The effect of the local moments for the thermodynamics is to form a second component in a two-fluid description which is the counterpart of the localized valence bonds (spin pairs) in the insulating phase. For the transport, they provide spin flip scattering, and their greater abundance in compensated silicon provides a plausible explanation of the different effective exponents for the conductivity onset seen in uncompensated and compensated systems. Thermodynamic and magnetic experiments on amorphous metal-semiconductor mixtures would be invaluable in furthering our understanding of the MI transition, and the issue of the pervasiveness of local moment formation in disordered metals.

Acknowledgments

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Magnetic Properties of Doped Semiconductors

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Abstract

Doped semiconductors, being a physical realization of an ensemble of one-electron (hydrogenic) atoms distributed randomly in space, are in a sense the simplest disordered system. Our current understanding of their magnetic properties is reviewed, for densities on both sides of a critical density n_c at which the system undergoes a transition (at zero temperature) from an insulating phase ($n < n_c$) to a metallic phase ($n > n_c$). It is argued that the insulating phase is well modeled in terms of a disordered Heisenberg anti-ferromagnet, and quantitative agreement with experiment can be obtained. In contrast, the metallic phase just beyond n_c is not as well understood, and a number of possible candidate models are described. Finally, the issue of the effect of magnetic properties on the metal-insulator transition is addressed.

1. Introduction

Recent progress on the subject of electron localization in disordered systems, following the advent of the scaling theory of localization in 1979 [1, 2], has concentrated on transport properties [3]. This is natural, since the phenomenon of localization has direct bearing on transport coefficients. However, as has become clear in the last couple of years, the nature of metal-insulator (MI) transition in real, three-dimensional, disordered systems may depend on a variety of factors. Especially relevant are effects involving the electron spin (spin scattering, magnetic field), which lead to different universality classes [3, 4]. For each class, a different exponent μ characterises the onset of the conductivity in the metallic phase at $T = 0$:

$$\sigma \sim (n - n_c)^\mu. \quad (1)$$

In eq. (1), n is the microscopic variable (e.g., concentration of impurity in semiconductor systems, which is what we shall mean in the rest of this paper, or fraction of metallic component in metal-semiconductor mixtures, though it may as well be any quantity which couples to microscopic variables of the system, e.g., uniaxial stress or magnetic field). n_c is the critical density at the MI transition. Experimentally, there appear to be at least two families of systems [5] with different exponents $\mu \approx \frac{1}{2}$ and $\mu \approx 1$. In light of the predicted sensitivity to spin coupling fields, a more careful look into magnetic properties (a subject which has a venerable history for doped semiconductors [6]), at low temperatures would clearly be very informative. This issue forms the subject of the present article.

Semiconductors doped with shallow impurities which undergo a transition from insulating to metallic behavior as a function of dopant concentration, are natural candidates for such a study. [Examples include elemental Si or Ge with group III (B, N) or group V (P, As, Sb) impurities or compounds like GaAs doped with Si, CdS doped with In, etc.] This is because the microscopic Hamiltonian is much better known, than, for example, the metal-semiconductor alloy

systems, and the behavior is well-characterized both in the extreme insulating and extreme metallic limits. In addition, the system (as illustrated in this article for the case of donors in Si) is amenable to both static (susceptibility and non-linear magnetization) and dynamic (ESR, NMR) probes of the magnetic behavior.

This paper is organized as follows. In Section 2, after a brief introduction to the doped semiconductor system, we give a general overview of the "expected" magnetic behavior as a function of dopant concentration, based on highly simplified models. In Section 3 we discuss the magnetic behavior in the insulating phase ($n < n_c$) in some detail, and describe what evidence exists to suggest that our understanding of the magnetic properties is in reasonable shape. Section 4 deals with the metallic phase just beyond n_c , whose magnetic behavior is, relatively speaking, poorly understood, though there are a number of plausible scenarios which could explain the qualitative behavior. Towards the end, we discuss which experiments could help distinguish between the different models, and also the difficulties associated with interpretation. Finally, Section V summarizes the conclusions.

It should be pointed out that while this is a review of magnetic properties, it is written with an emphasis on issues involved in the interplay between magnetic properties and the MI transition. Further, we focus on phosphorus doped silicon (Si:P), on which the most detailed work has been done in recent years. Consequently, a number of interesting experimental and theoretical papers (particularly 1980 and before) which form the history of this subject, are not mentioned, and others discussed inadequately; the interested reader is referred to the review articles by Holcomb [6, 7] in this regard.

2. Simplified overview of doped semiconductors and their magnetic properties

Shallow impurities in semiconductors (e.g., P in Si) are, in some sense, the simplest disordered system. All but one electron (or hole, for p -type impurities) of the substitutional impurity go into chemical bonding, and the final electron (or hole) at low impurity concentration is very weakly bound to the impurity nucleus. (A similar situation is also true for interstitial impurities, e.g., Li in Si.) The wavefunction (for the case of the electron, like in Si:P, which we concentrate on from now on), is given by the Bloch wave at the conduction band minimum of the host semiconductor with an envelope which satisfies a hydrogenic Schrödinger equation [8]. The effective mass is the conduction band mass, and the coulomb potential due to the singly charged nucleus is screened by the host dielectric constant. As a consequence, the Rydberg for such a hydrogen atom is $Ry^* \sim 30$ meV for impurities in Si (~ 10 meV in Ge), and the Bohr radius $a^* \sim 20$ Å in Si

($\sim 50 \text{ \AA}$ in Ge). Complications due to multiple conduction band minima (as in Si or Ge) and short range "central-cell" potentials (due to core mismatch between impurity and the host atom), do not affect the physics of the magnetic properties but are necessary when quantitative fits are required. In particular, they reduce a^* to 17 \AA in Si:P, and further reduce the exchange interactions by an order of magnitude [9]. However, we shall not dwell on this issue here.

With such large Bohr radii and small energy scales of the impurity electrons, the host acts simply as an inert medium, characterized by only its zero frequency dielectric constant and conduction band effective mass. Further, at the concentrations of interest [$n \sim n_c \approx (4a^*)^{-3}$], typical impurity distances ($50\text{--}200 \text{ \AA}$) are much larger than the Si-Si distance ($\approx 2.5 \text{ \AA}$), and impurity interactions are small ($< 100 \text{ K}$, often much less) compared to the growth temperature. Consequently, the system is well represented [10] by a random (Poisson) distribution of hydrogen atoms in *continuum* 3D space, neglecting chemical clustering effects as well as discreteness of the P positions (on the Si lattice). This will turn out to be crucial for our understanding of the magnetic properties.

In Si:P at very low concentrations n , with each electron bound to its P nucleus in a hydrogenic $1s$ state with zero orbital angular momentum, the magnetic susceptibility at a temperature T due to the impurity is the Curie susceptibility of free spins with $S = \frac{1}{2}$:

$$\chi_c = \frac{ng^2 \mu_B^2 S(S+1)}{3k_B T} = \frac{n\mu_B^2}{k_B T} \quad (2)$$

where $g \approx 2$ is the gyromagnetic ratio, μ_B the Bohr magneton and k_B Boltzmann's constant.

On the other hand, at high concentrations $n \gg n_c$, when the electrons are delocalized and the potential of the P nuclei is well screened, the spin-susceptibility is the Pauli susceptibility of n electrons distributed in the v -fold degenerate Si conduction band with longitudinal and transverse effective mass m_l and m_t :

$$\chi_p = \mu^2 N(E_F) = \frac{3m_l^2}{2E_F} \quad (3)$$

where

$$E_F = \pi^2 (3\pi^2 n v)^{2/3} 2m^* \quad (4)$$

is the Fermi energy,

$$m^* = (m_l m_t)^{1/2} \quad (5)$$

is the average effective mass, and $N(E_F) = dn/dE_F$ is the density of states at the Fermi level.

There is, in addition, an orbital diamagnetic [11] contribution to the total susceptibility. For isotropic conduction band minima, as in the case of free electrons, the diamagnetic term is $1/3$ of the paramagnetic contribution so the total susceptibility $\chi_i = \frac{2}{3}\chi_p$. In Si and Ge, however, with large mass anisotropy, the diamagnetic term in fact overwhelms the paramagnetic term, and the total donor susceptibility χ_i turns out to be negative. Early experiments by Quirt and Marko [12] and Sasaki and Kinoshita [11] demonstrated the validity of eqs. (2) & (3) in the low and high density limits. We will, for the most part, concentrate on the spin susceptibility which dominates at low temperatures in the insulating phase, and can be extracted even in the metallic phase using electron spin resonance techniques.

One obvious question which arises is, how does the $T \rightarrow 0$

divergent Curie susceptibility for the donor spins go over into the Pauli value which is finite at $T = 0$? It is well known from the work of Herring [13] that in the dilute limit, the interactions between donor spins is a sum of pairwise Heisenberg exchange interactions described by the (quantum mechanical) Heisenberg Hamiltonian:

$$H = \sum_{\langle ij \rangle} J(r_{ij}) S_i \cdot S_j \quad (6)$$

where the exchange interaction $J(r_{ij})$ can be shown to be antiferromagnetic [13] for all separations r_{ij} of the pair of spins S_i and S_j . We use $J > 0$ for antiferromagnetic interactions in contrast to normal convention, in order to avoid minus signs in various equations. For hydrogenic wavefunctions, Herring and Flicker [14] have calculated the asymptotic form of the exchange at large distances (given in Rydbergs):

$$J(r) = 1.636 \left(\frac{r}{a^*} \right)^{5/2} e^{-2r/a^*} \quad (7)$$

which agrees well with numerical computations [15] for a pair of hydrogen atoms at distances $r \geq 5a^*$.

For antiferromagnetically interacting spins, standard mean field theory (or lowest order high temperature expansion) for the susceptibility in the paramagnetic (high temperature) phase gives the expression:

$$\chi^{-1} = \frac{k_B}{n\mu_B^2} (T + \theta) \quad (8)$$

where θ is an average exchange field at the donor site, also known as the Curie-Weiss temperature. We consider first, for simplicity, and also because we can make concrete estimates, the hypothetical case of donor spins on a lattice (say simple cubic or body centered cubic). Then the Curie-Weiss θ is given approximately by:

$$k_B \theta = \frac{Z}{4} J(R) \quad (9)$$

where Z is the nearest neighbor coordination number. ($Z = 6$ for sc and $Z = 8$ for bcc), and R is the nearest neighbor distance ($R \equiv n^{-1/3}$ for sc and $R = \sqrt{3}(4n)^{-1/3}$ for bcc). In eq. (9) we have neglected exchange couplings with further neighbors, which turns out to be a good approximation at low concentrations. For sc, the effect of next neighbor coupling exceeds 10% of the nearest neighbor coupling only for n close to n_c ; the corresponding density for bcc is around $n_c/4$. Equation (8) suggests that the divergence of the Curie susceptibility is quenched below $T \sim \theta$, and using eqs. (7) and (9) to estimate θ near n_c we get $k_B \theta \approx 0.025 \text{ Ryd}$ for sc and $\approx 0.02 \text{ Ryd}$ for bcc. In the mean field approximation the average zero temperature susceptibility ($\frac{2}{3}\chi_{\perp} + \frac{1}{3}\chi_{\parallel}$) is given by [16]:

$$\chi(0) = \frac{n\mu_B^2}{3k_B \theta} \quad (10)$$

which is of the same order of magnitude as the Pauli susceptibility of the metal [eq. (3)] evaluated at n_c . The exact estimates from the mean field approach are not quantitative, e.g., the actual nearest neighbor spin- $\frac{1}{2}$ Heisenberg antiferromagnet has an antiferromagnetic transition at a Neel temperature $T_N \approx 0.95J$ for sc and $T_N \approx 1.2J$ for bcc [17] as opposed to eq. (9), and there are spin wave corrections to the zero tem-

perature susceptibility [18]. However, this does not alter the basic result that the divergence of the Curie susceptibility is quenched as soon as the concentration is finite, and that no strong anomaly in the low temperature susceptibility is expected around n_c for the lattice case (of course, there must be an eventual transition from antiferromagnetic to paramagnetic ground state, probably somewhere in the metallic regime). Even for structures such as the fcc lattice, where a simple antiferromagnetic state is not favored due to frustration effects [19], a more complicated ordering is expected to take place. The ordering temperature may be suppressed somewhat, but is usually within an order of magnitude. Consequently, the same general remarks should apply.

Since the mean field analysis qualitatively applies to the lattice case, one may be tempted to apply it to the random distribution of spins. In the random case, one would not expect the ordered state to be a simple antiferromagnet, but instead one in which spins are frozen in random directions, i.e., a spin-glass phase [20] because of frustration effects arising from plaquettes with an odd number of spins.

A first guess might be to generalize the Curie-Weiss temperature appearing in eq. (8), from eq. (9) to

$$k_B \theta = \frac{1}{4} \int_0^{\infty} 4\pi n r^2 J(r) dr, \quad (11)$$

which would suggest, using eq. (10), that the susceptibility is quenched at a value which is independent of n ! If we use eq. (7) for $J(r)$, this value turns out to be $\chi_0 \approx 3.6 n_c \mu_B^2$, of the same order of magnitude as the Pauli susceptibility at n_c . If this hadn't raised one's suspicions, the surprisingly large value of the Curie-Weiss θ [$\approx 0.09(n/n_c)$ in Rydbergs with the same $J(r)$] compared to the lattice case for small n (a factor of 50–100 larger at $n \approx 0.2n_c$) certainly would.

The reason for this strange result is not far to seek. While the analog of eq. (11) is reasonable for weak disorder, in a highly random system like the Poisson distributed donor spins interacting via a short range (exponential) exchange interaction, which varies over many orders of magnitude depending on the spin in question, it is improper to average the Curie-Weiss temperature. In fact the experimental data for the susceptibility at low temperature ($20 \text{ mK} < T < 4 \text{ K}$) show a continual curvature on a χ^{-1} vs. T plot, implying that eq. (8) is not valid anywhere in this temperature range. One must instead average the susceptibility itself, which can only be done by resorting to an approximation (as discussed in the next section). Furthermore, the ordering temperature, if any, would not be related to an ensemble averaged exchange field θ at a site, but to an energy scale such that spins connected by bonds of larger magnitude form some sort of a percolating cluster. To what extent these ideas are borne out we shall see in the next section.

3. Magnetic behavior in the insulating phase

To calculate the thermodynamic properties (e.g., magnetic susceptibility, specific heat, etc.) of an ensemble of a quenched random distribution of (quantum) spin- $\frac{1}{2}$ interacting according to the Heisenberg Hamiltonian [eq. (6)], one would have to perform an average over the free energy (quenched average), for which no known techniques exist except in special cases. Even to do the problem numerically for a finite size system is prohibitive because for an ensemble

of N spins, there are 2^N states. With no symmetries of the Hamiltonian except for total spin S^2 and S_z for an arbitrary set of couplings, the size of the Hamiltonian matrix grows exponentially with N . Consequently, one has to resort to various approximation techniques.

The simplest approximation, which was suggested over twenty-five years ago [21], is the so called nearest neighbor pair approximation. In this approximation one considers each spin as being only influenced by its nearest neighbor. The distribution of nearest neighbor distances for randomly distributed spins is Poisson, and given in three dimensions by:

$$P(r) = 4\pi n r^2 e^{-4\pi n r^3}. \quad (12)$$

From eq. (12), the mean nearest neighbor distance $\langle r \rangle \approx 0.54 n^{-1/3}$, but the rms deviation is comparable, which coupled with the exponential dependence of $J(r)$ on r , leads to a very broad distribution in the magnitude of J , i.e., $P(J) \equiv P(r) dr/dJ$ covers many orders of magnitude, as shown in Fig. 1 for Si:P at a concentration $n \approx 8 \times 10^{17} \text{ cm}^{-3}$.

The susceptibility (or specific heat) in this approximation is exactly calculable, for it is given by an ensemble average of the result for a pair of spin- $\frac{1}{2}$, for which the energy spectrum is trivial to calculate. The eigenstates consist of a non-degenerate singlet $S = 0$ ground state (for antiferromagnetic interactions), and a three-fold degenerate ($S = 1$, triplet) excited state in zero magnetic field, at an energy J above the ground state. The triplet is split linearly by the Zeeman coupling to the magnetic field $h_0[\Delta E = g\mu_B h S_z, S_z = 0, \pm 1]$. Remembering that the density of pairs is $\frac{1}{2}n$, the ensemble averaged susceptibility is given by:

$$\chi_p(T) = \frac{4n\mu_B^2}{k_B T} \int_0^{\infty} \frac{P(r) dr}{3 + e^{J(r)/k_B T}}. \quad (13)$$

Equation (13) reduces, as it should, to the Curie result when $k_B T \gg J(r)$ for all r , whereas $\chi_p(T \rightarrow 0) \rightarrow 0$ as all pairs drop into their singlet ground state and freeze out. Equation (13), in conjunction with Fig. 1 which shows the distribution of nearest neighbor exchange, explains why the Curie-Weiss behavior is not seen in doped semiconductors in

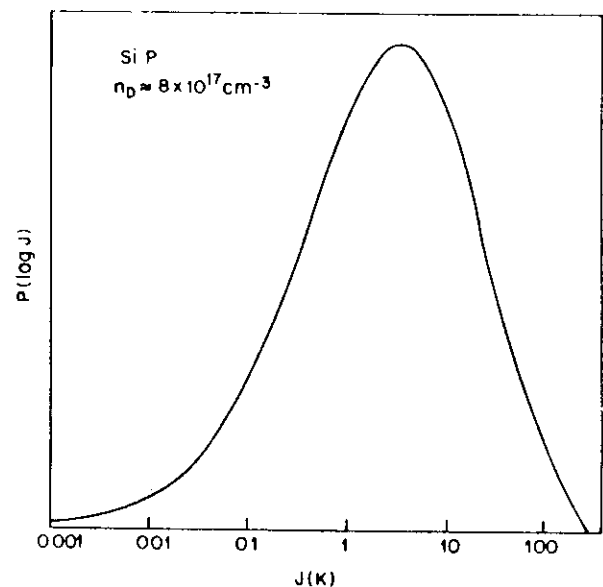


Fig. 1. Distribution of the logarithm of the nearest neighbor exchange in Si:P at $n \approx 8 \times 10^{17} \text{ cm}^{-3} \approx 0.2n_c$.

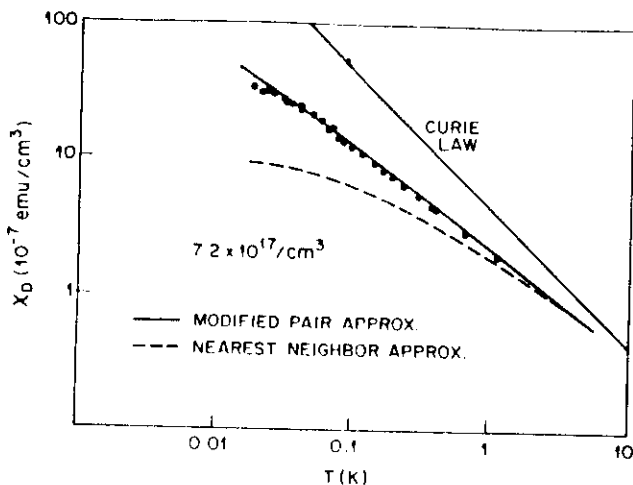


Fig. 2. Experimental susceptibility and the result of the nearest neighbor as well as the modified pair approximation for Si:P at $n \approx 7 \times 10^{17} \text{ cm}^{-3}$. (From Ref. 9).

any temperature range. The broad distribution of the *magnitude* of the exchange goes up to values of order the Rydberg. Thus, at temperatures where the donor electrons (or acceptor holes) are in their ground state (i.e. $T \ll \text{Rydberg}$), one is always in the midst of the distribution $P(J)$, and the high- T Curie Weiss result is inapplicable.

Of course, in a pair approximation, one does not expect to get an ordered low temperature state, though eq. (13) does give a maximum susceptibility at a temperature which can be calculated by putting in eqs. (7) and (12). Unfortunately, this is of little use because, as several workers have recognized [9, 12, 22], the susceptibility obtained using eqs. (12) and (13) does not agree at all with experimental results [9] once either drops by about 20% below the Curie result. In other words, though eq. (13) describes correctly the departure from Curie law as the temperature is lowered, its validity is over too limited a range to be of much use. This is demonstrated in Fig. 2, which plots the experimental susceptibility as well as the nearest neighbor pair result for Si:P for a typical concentration $n \approx 0.2n_c$.

The reason why the nearest neighbor approximation does not work is that it does not take into account further neighbor correlations. Namely, the nearest neighbor B of a given spin A may have a third spin C closer to it than A. In the singlet ($S = 0$) ground state of the pair BC the spin B is equally up or down, with a zero net exchange field on A. Thus the coupling between A and B is proportional to the extent that the pair BC is in the excited state and is strongly reduced compared to when B is free.

Although naively one might have expected the nearest neighbor approximation to underestimate the effect of neighbors by neglecting all but the nearest neighbor, the above argument shows how in fact it overestimates the effect of neighbors. Thus, the susceptibility given by eq. (13) tends to be a gross underestimate, once further neighbor correlations become important.

Various alternatives to the pair approximation have been suggested, including grouping spins in three [12], numerical diagonalization of clusters of spins [9, 23, 24] as well as a couple of remedies to the pair approximation [22, 25]. The grouping into three is rather ad-hoc, and can be shown to overestimate the susceptibility at low temperatures. The numerical cluster scheme would be expected to be correct at high temperatures when the clusters (defined by interactions

$J > T$) are small (cluster size $\leq 8-10$). The other two alternatives basically tried to remedy the problem with the pair approximation described earlier. In one, the pair approximation (which essentially gives the probability of a spin being isolated) was used to define a temperature dependent clustering volume. An approximate ensemble average was then performed using the notion that spins within this volume were paired and that the susceptibility was due to left-over unpaired spins. An analytic result was obtained in this "modified" pair approximation [9]:

$$\chi_{\text{MPA}}(T) = \frac{\chi_c(T)[1 - (\chi_p(T)/\chi_c(T))^2]}{2 \ln [\chi_c(T)/\chi_p(T)]} \quad (14)$$

where $\chi_c(T)$ is the Curie susceptibility [eq. (2)] and $\chi_p(T)$ the susceptibility in the nearest neighbor approximation [eq. (13)]. Results calculated on the basis of eq. (14) were in good agreement with both experiment (Fig. 2) and numerical cluster calculations [9, 22].

While the procedure above may seem ad-hoc, its success points to the fact that most of the physics is in proper pairing of spins in a hierarchical fashion. There is in fact a tangential allusion to this in the early work of Sonder and Schweinler [21], but the actual implementation had to wait over twenty years. Rosso [25] suggested that the main error in eq. (13) was that the distribution of pairs could not be given eq. (12), but instead by the distribution of pairs obtained hierarchically in order of increasing distance (decreasing interaction). Unfortunately, this turns out, unlike Rosso had originally claimed, to be a highly non-trivial calculation, and the approximate form used by Rosso turns out to be in error by $\sim 30\%$ once the susceptibility dropped below about half the Curie value [26, 27]. Nevertheless, this sort of idea forms the basis for the renormalization scheme [28] to be discussed below, and we shall discuss the differences to Rosso's calculation as we go along.

The renormalization scheme implemented by Bhatt and Lee [28] is based on the observations that (i) the distribution of the *logarithm* of couplings (Fig. 1) is very wide, and (ii) for a spin- $\frac{1}{2}$ antiferromagnet, quantum fluctuations lead to a significant reduction in the ground state energy. (i) suggests a scaling scheme which is built on perturbation theory in the ratio of small couplings and large couplings. (ii), when applied to pairs, implies a three-fold increase (from $J/4$ to $3J/4$) in the *magnitude* of the quantum mechanical (singlet, $|\uparrow\downarrow - \downarrow\uparrow\rangle$) ground state energy of the pair, compared to the classical Neel type state ($|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$). This means that a pair of strongly coupled spins (coupling $\sim J$) would rather form a singlet $S = 0$ ground state than try to build up correlations with other spins they are weakly coupled with (couplings $\sim j$), since the gain in energy in the former case ($J/2$) far exceeds that in the latter ($\sim j$). This suggests starting at short length scales (where the effective Hamiltonian is in terms of $S = \frac{1}{2}$, and the de-ordering quantum effects are largest), with the largest coupling and proceeding hierarchically down the distribution of couplings. Perturbation theory can be used to find the effective couplings on a longer length (lower energy) scale, and by iterating the procedure, quantum effects at longer length scales (lower temperature) can be investigated. It is this second part that is missing from Rosso's scheme, where pairs are simply identified, and removed from consideration in the next stage.

Consider, as an example, the cluster of spins

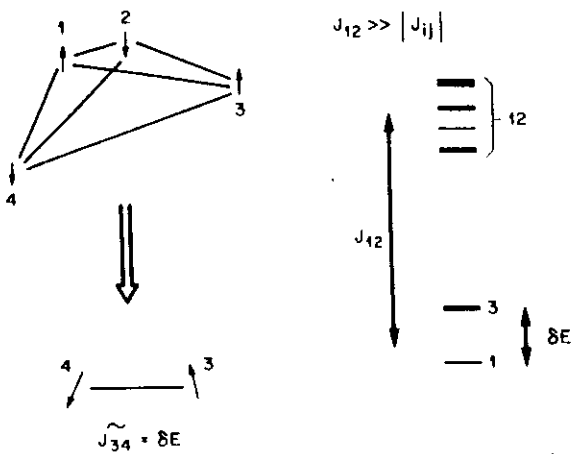


Fig. 3. Renormalization of four-spin cluster to an effective two-spin cluster at low temperatures.

Fig. 3, where spins 1 and 2 are coupled antiferromagnetically and much more strongly than any other pair [$J_{12} \gg |J_{ij}|$ for all $(i, j) \neq (1, 2)$]. Then the energy spectrum ($2^4 = 16$ states) of the cluster divides into a low-lying singlet-triplet manifold and twelve states separated from it by an energy of order J_{12} . At low temperatures $T \ll J_{12}$, when only the lower manifold enters the thermodynamics, the cluster of four spins can be replaced by two spins with an effective coupling \tilde{J}_{34} which equals the singlet-triplet splitting, δE

$$\tilde{J}_{34} = \delta E = J_{34} + \frac{(J_{13} - J_{21})(J_{24} - J_{14})}{2J_{12}} + O\left(\frac{1}{J_{12}^2}\right). \quad (15)$$

Thus, in effect, the pair (1, 2) has disappeared, leaving behind the pair (3, 4), with a renormalized interaction, \tilde{J}_{34} .

For interactions which fall off exponentially with distance, such a renormalization is most important when the pair (1, 2) lies close to the direct line connecting spins 3 and 4 (as in one-dimension, where it is more than the direct coupling J_{34}), and in such cases the correction is predominantly antiferromagnetic, though exceptions are possible. Furthermore, only bonds between spins which are both coupled to at least one of the spins being "decimated" are renormalized to $O(1/J_{12})$. [This is evident from eq. (15), since $\tilde{J}_{34} = J_{34}$ to $O(1/J_{12})$ if either $J_{13} = J_{21} = 0$ or $J_{14} = J_{24} = 0$.] This defines the renormalization procedure - and the strongest coupled spin pair (1, 2) is identified and "decimated" after renormalizing bonds between each pair of spins (3, 4) connected to the pair (1, 2). Then the next strongest pair is identified and removed likewise, which sets up the iterative renormalization procedure. Bhatt and Lee [28] implemented such a scheme numerically by distributing up to 10 000 spins into a three dimensional cube with periodic boundary conditions, interacting according to

$$J(r) = J_0 e^{-r/a^*} \quad (16)$$

with the parameter a^* adjusted to cover the relevant range of $0.001 < na^{*3} < 0.04$. They discarded two spins at a time, until the number of spins remaining was $\approx 1\%$ of the original number.

One of the results of Bhatt and Lee was that the couplings remain widely distributed in magnitude under the scaling procedure. Thus, considering the situation where the largest

coupling constant has been scaled to J , it is a good approximation to take the spin pairs decimated as being effectively frozen in their singlet ground state at a temperature $T = J$, and the remaining spins $n(T)$ as free at that temperature, since their couplings $\ll T (= J)$. In this approximation the susceptibility is given by

$$\chi(T) = \frac{n(T)\mu_B^2}{k_B T} \quad (17a)$$

and the specific heat by

$$C(T) = T \frac{dS}{dT} = k_B T \log 2 \frac{dn(T)}{dT}. \quad (17b)$$

A better approximation would be to use the pair approximation with the renormalized distribution of interactions:

$$P_R(J) = \frac{1}{n} \frac{dn(J)}{dJ} \quad (18)$$

according to which

$$\chi(T) = \frac{4n\mu_B^2}{k_B T} \int \frac{P_R(J) dJ}{3 + e^{J/k_B T}} \quad (19a)$$

and the specific heat is given by:

$$C(T) = \frac{3n}{2T^2 k_B} \int \frac{J^2 e^{J/k_B T} P_R(J) dJ}{(3 + e^{J/k_B T})^2} \quad (19b)$$

Bhatt and Lee [28] checked for convergence by implementing the next order cluster renormalization scheme (details of which are given in their papers) and found good agreement (2-3%) between the two schemes down to the scales studied. The calculated susceptibility versus temperature is shown on a double logarithmic plot in Fig. 4, which clearly bears a striking resemblance to the experimental results of Andres *et al.* [9], as well as subsequent work by Murayama *et al.* [29], Sarachik *et al.* [30] and Paalanen *et al.* [31]. In fact, by using the correct exchange interactions [9] for Si:P with effective Bohr radius $a^* \approx 16 \text{ \AA}$ a quantitative fit to the experimental data can be obtained [32]. Unlike a canonical spin-glass like Cu:Mn or Au:Fe [33], the susceptibility in this quantum spin- $\frac{1}{2}$ antiferromagnet keeps on rising down to millikelvin temperatures [34]. The reason for this difference is the combined effects of extreme disorder (nearest neighbor exchange couplings which vary over many orders of magnitude) and the large energy associated with quantum fluctuations for the spin- $\frac{1}{2}$ case (the canonical spin glasses have $S = 7/2$ or $5/2$). These two effects conspire to destroy any global magnetic ordering in doped semiconductors down to temperatures well below those accessible to experiment. [Actually, below about 10 mK in Si:P or Si:As one has to include hyperfine coupling to the impurity nuclear spin in the Hamiltonian of eq. (6).] That this is a quantum effect is demonstrated [35] by considering the corresponding Ising system, for which the decimation procedure corresponding to Fig. 3 would remove the large coupling J_{12} , but leave ones $O(J_{13}, J_{14}, J_{23}, J_{24})$ behind, unlike the Heisenberg case. Thus there isn't a rapid "dilution" of couplings with decimation, and the long tail to lower couplings in $P_R(J)$ is not generated.

The susceptibility in Bhatt and Lee's calculation (as well as experiments) is reasonably well described by $\chi \sim T^{-x}$ where x is weakly n -dependent and relatively temperature independent in the concentration and temperature range of interest (except for weak, logarithmic dependence on T). This implies [via either eqs. (17a) and (18), or eq. (19a)] that $P_R(J) \sim J^{-x}$.

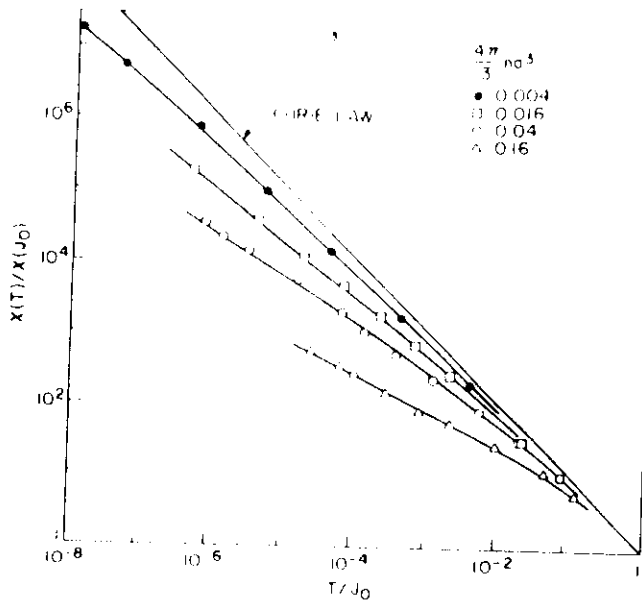


Fig. 4. Susceptibility versus temperature calculated using the renormalization scheme on a double logarithmic plot. (From Ref. 28).

With that distribution of renormalized couplings between spin-pairs, the magnetization may be shown [30] to obey the scaling relation [36]:

$$\frac{g\mu_B M(H, T)}{k_B T \chi(T)} = f_s \left(\frac{g\mu_B H}{k_B T} \right) \quad (20)$$

with

$$f_s(y) = \left[\int_0^y dx \frac{x^{-2} \sinh x}{1 + e^x + 2 \cosh x} \right] / \left[\int_0^y dx \frac{x^{-2}}{3 + e^x} \right] \quad (21)$$

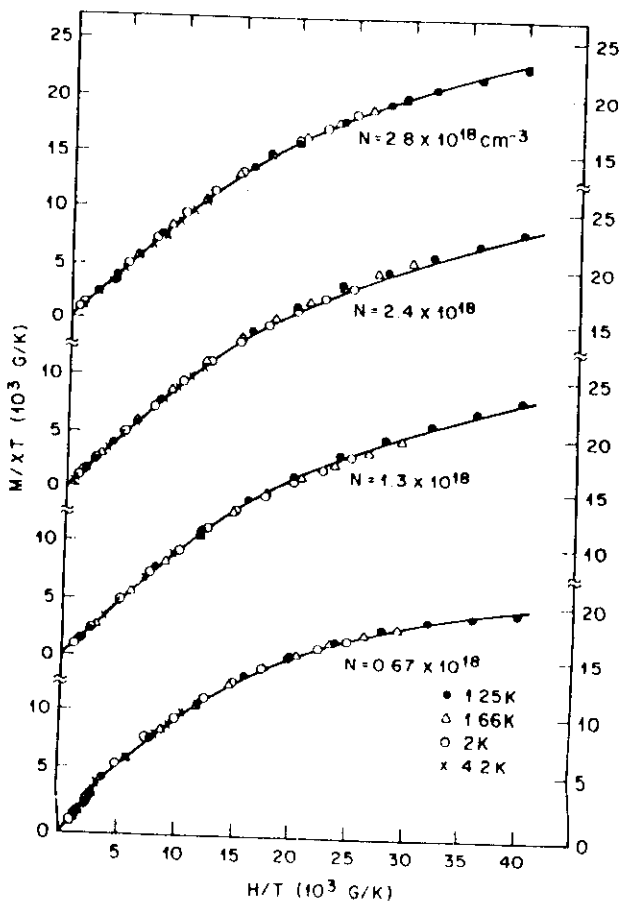


Fig. 5. Scaling plot for the magnetization (eq. 20) in Si:P for different samples. $\alpha \approx 0.79$ for bottom sample, $\alpha \approx 0.65$ for rest. (From Ref. 30)

Such a scaling relation is in fact very well obeyed by the data of Sarachik *et al.* [30] in Si:P, which is reproduced in Fig. 5. The solid lines is the theoretical expression of eq. (21) using no adjustable parameters (α determined from the susceptibility).

The hierarchical nature of couplings and quantum fluctuations have strong effects on electron spin dynamics [29, 37, 38] as well. In particular, Murayama *et al.* [29] found a strong increase in the ESR linewidth in insulating Si:P, as the temperature was reduced. Simultaneously, there was a shift in the resonance position, amounting to an apparent "g-shift" of almost 40%! Very recently, Sachdev and Bhatt [39] have calculated the apparent g-shift and linewidth using the scaling approach of Bhatt and Lee. The essential ingredients, in addition to the exchange Hamiltonian [eq. (6)] and Zeeman term, is the hyperfine coupling to the phosphorus nuclear spins I_i , which is the source of the linewidth. Thus the total Hamiltonian becomes:

$$H = \sum_{i>j} J_{ij} S_i \cdot S_j + A \sum_i I_i \cdot S_i + h \sum_i S_{iz} \quad (22)$$

In this picture, for large fields, the normal "width" of the ESR line for an isolated donor nucleus plus electron (which is $A/2$, since the ESR spectrum consists of two lines separated by A) is "exchange-narrowed" by the rapid diffusion of the electron spin over several donor sites. For a crystalline antiferromagnet with exchange J , the width is given by

$$T_2^{-1} = A^2/J. \quad (23a)$$

However, in this case, since the distribution of the magnitude of near-neighbor exchanges covers many orders of magnitude, the diffusion is very strongly correlated (the spin excitation keeps hopping back and forth along strong bonds). Thus the electron spin effectively gets localized on a cluster of N spins within a dephasing time, leading instead to:

$$T_2^{-1} = \frac{A}{2\sqrt{N}}. \quad (23b)$$

As the temperature is lowered, strongly coupled spins drop out into their singlet states, and the number of sites available to diffuse to reduces. Thus N gets lowered, leading to a broader ESR line as well as an apparent g-shift in the resonance line when the external frequency (magnetic field h) is of order the hyperfine coupling, A . Both quantities depend on the external frequency, and by fitting the width data of Murayama *et al.* at one frequency, Sachdev and Bhatt were able to fit the width as a function of T at another frequency, as well as the frequency dependent g-shift. Their results are shown in Figs. 6(a) and (b).

Thus by now there appears to be a fair body of work which indicates that we have quite a good understanding of the magnetic properties of doped semiconductors in the insulating phase. The localized spin model analysed according to the scaling method of Bhatt and Lee provides a quantitative fit to both static and dynamic magnetic properties. One obvious question that arises is what happens as $n \rightarrow n_c$ and the electron gets delocalized? In fact, the data of Jerome *et al.* [38] in Si:P already show that electrons are no longer localized on single donors at $n \approx 10^{18} \text{ cm}^{-3}$. Why then does the localized model work at concentrations up to 2.7×10^{18} ? The answer hinges on the two points — firstly, though delocalization effects would render the microscopic model invalid, the scaling

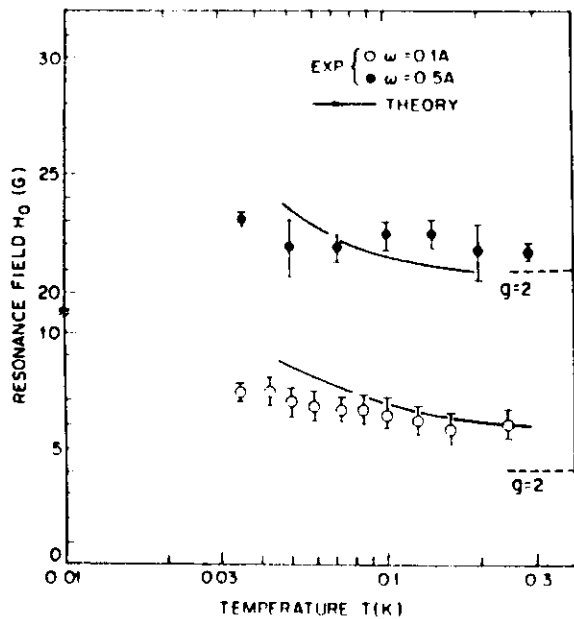
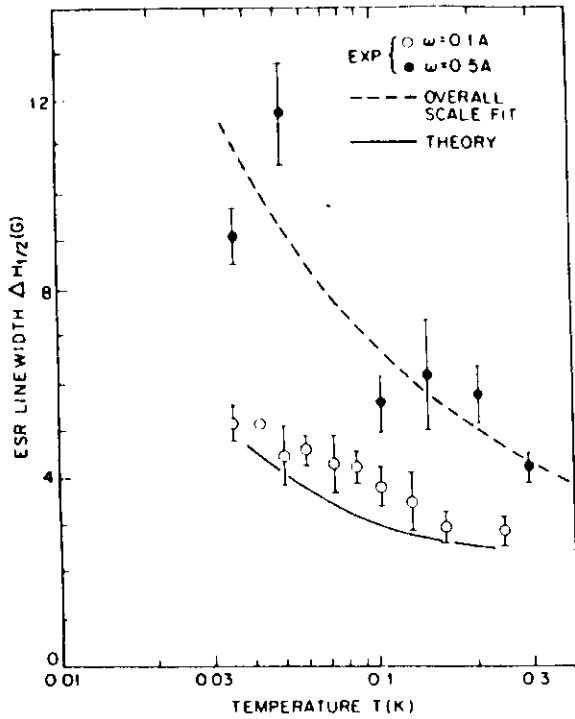


Fig. 6. Linewidth (a) and Resonance Field (b) as a function of temperature for $n \approx 0.5n_c$. Experimental Data from Ref. [29], and theoretical results from Ref. [39]

pliable as a starting point, an effective localized spin description appears likely to emerge at low temperatures, with interactions falling off exponentially at large distances since the states are localized. Secondly, since the spin-Hamiltonian exhibits a singular density of excitations at low energies ($P_R(J) \sim J^{-2}$), it probably swamps effects due to, e.g., electron hole excitations, and dominates the low temperature behavior. In this way one can reconcile the observations of Jerome *et al.* [38] with those of Sarachik *et al.* [30] and Murayama *et al.* [29].

4. The metallic phase

Above the critical density n_c , the system becomes conducting at $T = 0$, and the canonical description of the electronic

properties is in terms of itinerant electrons. Nevertheless, standard free electron theory for metals does not work until $n \geq 2n_c$, and correlation and disorder effects are quite prominent especially in the vicinity of n_c .

There have been many attempts to address the magnetism of a correlated metal, especially in terms of Stoner enhancement and spin fluctuation effects near a magnetic instability. Such a description may be appropriate in the absence of disorder, e.g., the Hubbard model or the lattice of donors. However, in view of the fact that disorder appears to prevent any global magnetic ordering in the insulating phase, we shall restrict ourselves to non-magnetic metallic states as well.

One procedure which circumvents the complications due to magnetic ordering is the Gutzwiller variational method. This method puts in correlations into a free fermion many body ground state wavefunction in which donor sites can be occupied by two electrons, by reducing the amplitude for such double occupancy which is treated as a variational parameter. Such a calculation in the context of the metal-insulator transition in a one-electron per site model was done by Brinkman and Rice [41]. They found that as the on-site electron-electron repulsion U was increased, the system underwent a transition from metal to insulator at $U = U_c$, and that both the low temperature specific heat C and zero temperature susceptibility $\chi(0)$ were enhanced by an effective mass m_{eff}^* which diverged as $(U_c - U)^{-1}$.

$$C(T) \sim \gamma T \quad (24a)$$

and

$$\chi \rightarrow \chi(0) \quad (24b)$$

with

$$\chi(0) \sim \gamma \sim m_{eff}^*/m^* \quad (25)$$

Further, they found that the ratio $\chi(0)/\gamma$ was four times the free electron value:

$$\frac{\chi(0)}{\gamma} = 4 \left(\frac{\chi(0)}{\gamma} \right)_{fc} \quad (26)$$

Such a scenario could fit in well with the insulating susceptibility data which does tend to diverge as $T \rightarrow 0$ for all $n < n_c$. A plausible extrapolation of the data in the metallic phase is shown in Fig. 7; the limiting $T = 0$ values of χ decrease from ∞ as n goes past n_c , and the plateau in χ extends to higher temperatures.

Unfortunately, such a scenario is not borne out by the ESR (spin susceptibility) data of Paalanen *et al.* [31, 42] for Si:P which are shown in Fig. 8. Instead of levelling off, the data in the metallic phase are also T -dependent down to 10 mK, and appear to be diverging as $T \rightarrow 0$! (This neglects

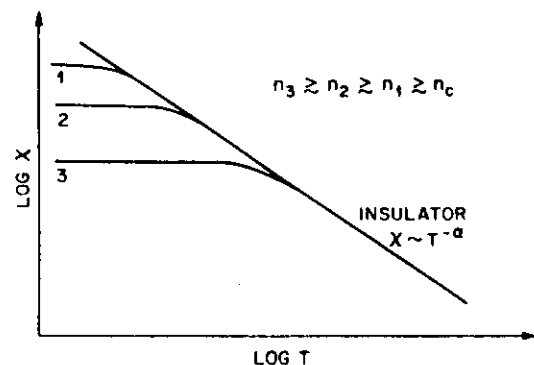


Fig. 7. "Expected" spin susceptibility beyond n_c .

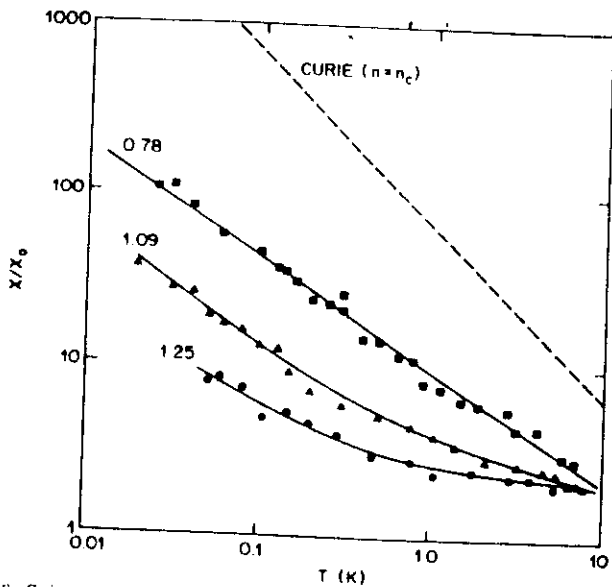


Fig. 8. Spin susceptibility as a function of temperature for samples close to, and on either side of n_c . Data from Paalanen *et al.* (Ref. 31).

spin-flip processes which come in at lower temperatures and should cause $\chi(T)$ to level off). Consequently if one wishes to apply the Brinkman-Rice scheme to Si:P, one will have to generalize it to explain the behavior in this range of temperature, and also to explain why the scale for levelling off is below 10 mK.

Another method of attack has been weak disorder perturbation theory for interacting electrons [3, 4, 42, 43], in which one starts by putting in disorder into a clean metal. Disorder is measured by the parameter $(k_F l)^{-1}$, where k_F is the Fermi wavevector, and l the elastic mean free path for electrons. The results are obtained to leading order in $(k_F l)^{-1}$ but all orders in e-e interactions. Such a perturbative renormalization scheme suggests that spin scattering effects are of paramount importance, and determine the universality class of the metal-insulator transition. Consequently, the critical exponents of various quantities (such as conductivity), as well as the low-temperature behavior of various thermodynamic quantities may depend on the universality class a particular system belongs to. This behavior is summarized in Table I. *It should be borne in mind that these are extrapolations based on perturbative results.* The renormalization group equations are perturbatively accessible in dimensionality close to $d = 2$. Thus, these results amount to an ϵ -expansion where $d = 2 + \epsilon$, to lowest order in ϵ , extrapolated to $\epsilon = 1$. In

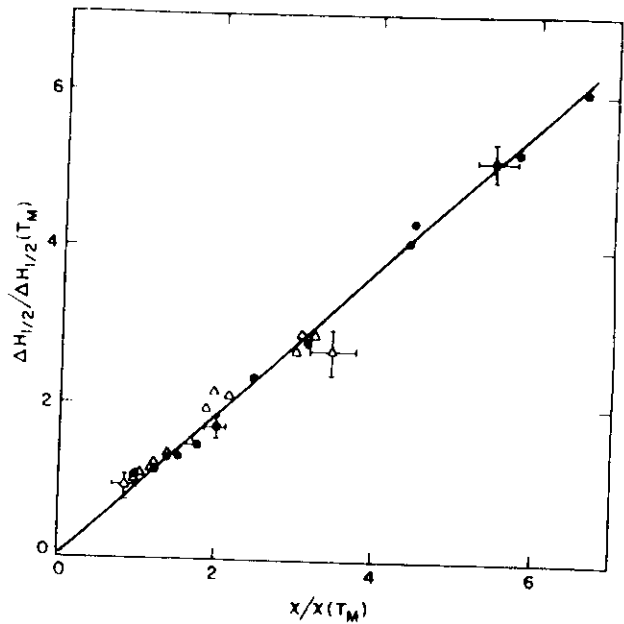


Fig. 9. Plot showing the proportional enhancement of the susceptibility and linewidth near n_c . (From Ref. 42).

addition, the results for pure potential scattering rely on the applicability of the perturbative results to the strong coupling regime.

With this caveat in mind, we can see that the only scenario that bears resemblance to Si:P is the potential (no spin-flip) scattering case for interacting electrons, where $\chi(T) \sim T^{-4.5}$ and $C(T) \sim T^{2.5}$ implying a divergent susceptibility in the metal as $T \rightarrow 0$! (This continues of course only down to a temperature of order $\hbar/(k_B \tau_s)$ where τ_s is a spin-flip/spin-orbit scattering time). Further, the exponents 4/5 and 2/5 are only estimates of the lowest order expansion, so should not be relied on quantitatively.

Sachdev [45] has recently extended these results to ESR linewidth, and finds explicitly to this lowest order, in agreement with results based on Kubo formalism [42], that the ESR linewidth and susceptibility in this regime are enhanced proportionately. This is quantitatively borne out by the data [42], as exhibited in Fig. 9. In Fig. 9 the enhancement of the ESR linewidth relative to its value at a fixed high temperature is plotted versus the corresponding enhancement of the spin-susceptibility for two samples with $n/n_c = 1.09$ and 1.25, and the straight line fit through the data has a slope of 0.9 as compared to the theoretical prediction of 1.

The basic mechanism behind this enhancement is not

Table I. Universality classes for the metal insulator transition in disordered systems

	Scattering		
	Potential	Spin flip	Spin orbit
Non-interacting electrons			
Conductivity exponent	1	1/2	No transition (?)
Singular corrections to specific heat, magnetic susceptibility and density of states	NO	NO	NO
Interacting electrons			
Conductivity exponent	?	1	1
Singular corrections to:			
specific heat	$C \sim T^{2.5}$	$C \sim T^{6.5}$	
magnetic susceptibility	$\chi \sim T^{-4.5}$	NO	NO
density of states	Singular	Pseudogap	Pseudogap

Note: Results are based on lowest order ϵ expansion about $d = 2$. For details see Ref. 45.

dissimilar to the insulating phase — a slowing down of spin diffusion due to electron–electron interactions in the presence of disorder. For further details, the reader is referred to the work of Sachdev [45].

The similarity in the behavior of the low temperature susceptibility across n_c may give rise to the suspicion that spin pair excitations similar to those in the insulating phase, extend beyond n_c (e.g., due to unpaired sites well below the Fermi energy). This has indeed not been ruled out [31], and such pairs have also been invoked by Gan and Lee [46] to explain the anomalous NMR relaxation observed in just metallic samples by Paalanen *et al.* [47].

If spin pairs were really the cause of the susceptibility rise in the metallic phase, one may use eqs. (17a) and (18b) in conjunction with $\chi(T) \sim T^{-\alpha}$ to get the result that [48]:

$$\left(\frac{\chi T}{C}\right) \approx \frac{\pi^2}{3(1-\alpha) \ln 2} \left(\frac{\chi T}{C}\right)_{T_c} \quad (27)$$

A similar numerical factor (smaller by 10–15% for relevant values of α) is obtained from eqs. (19a) and (19b). For $\alpha = 0.65$, the coefficient implies an enhancement of 13 times the free electron value, as compared to the Brinkman–Rice result [eq. (26)] of 4. The Castellani DiCastro result [4], on the other hand is:

$$\left(\frac{\chi T}{C}\right) \sim T^{-1.5} \quad (28)$$

which diverges as $T \rightarrow 0$. This is one method of distinguishing between the various models. It should however, be kept in mind that this will not be an easy task, since there are effects by which the numbers 4 and 13 could be changed somewhat and the $T^{-1.5}$ behavior is very weak. Besides, it is unclear to what extent this last result (eq. 28) should be relied upon, since it is a perturbative result extrapolated to strong coupling.

5. Conclusions

It has become clear in recent years that disordered systems have a rich structure in their magnetic properties. In dealing with extreme disorder, as in the case of Poisson distributed donor spins at low density, disorder coupled with quantum fluctuations completely destroys the chance for magnetic order at low temperature. Thus the magnetic phase diagram of doped-semiconductors (as a function of temperature and density) is quite different from the case where the impurity spins were on a lattice [49], or the non-disordered Hubbard model [50] — in these cases, there is clearly an antiferromagnetic state (at least for non-frustrated structures) over some density and temperature range. The combined effect of disorder and quantum spin fluctuations gives rise to a susceptibility which appears to diverge in the $T \rightarrow 0$ limit in the insulator, though the divergence is weaker than the Curie law $\chi(T) \sim T^{-1}$, and seems to be reasonably fit by a form $\chi(T) \sim T^{-\alpha}$. In Si:P α appears to level off to a value $\approx 2/3$ as $n \rightarrow n_c$, but similar experiments on Si:B [51] where Boron is an acceptor (hence a spin- $\frac{1}{2}$, unlike the spin- $\frac{1}{2}$ phosphorus), suggest smaller values for α near n_c . Incidentally, the $\chi \sim T^{-\alpha}$ behavior has been seen also in quasi-1D organic [36, 52] as well as the narrow gap semiconductor $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$ [53], and it would be worth investigating how well the scaling relation (20) works in this last system, to see the universality of such

behavior in disordered systems. The model of the disordered Heisenberg antiferromagnet [28] works well for both static properties such as susceptibility and magnetization, as well as dynamic properties like ESR linewidth and position.

The new surprise is that this divergent behavior of the susceptibility and slowing down of spin diffusion persists in the metallic phase. Thus the disordered metal is also quite different from the ordered metal, where Fermi liquid theory works, and e–e interactions only “renormalize” various parameters. This is apparent even in perturbation theory in the limit of weak disorder, where in the absence of spin scattering, a slowing down of spin diffusion and proportional enhancement of susceptibility and ESR linewidth is predicted at low temperatures (long length scales). Within this perturbative approach, spin-dependent effects are relevant, and can alter the universality class of the metal-insulator transition. This provides a plausible explanation of a long-standing controversy, named the different conductivity exponents [eq. (1)] seen in uncompensated semiconductors and amorphous alloy systems, but magnetic experiments on the latter are needed to decide the issue.

Finally, it should be emphasized that the Heisenberg antiferromagnet and weak disorder perturbation theories are models based on the extreme insulating and metallic limits. Consequently, it is of extreme importance to generalize either to tackle the region near n_c . One obvious effort would be to generalize the disordered antiferromagnet to the highly disordered Hubbard model to include charge fluctuation effects in addition to spin fluctuations, and extend its applicability to n_c and beyond.

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and transforming them into heat. The nonlinearity of the fluorescence reabsorption is of a somewhat unusual nature: It grows exponentially with exciton density but to a first approximation does not alter the exciton dynamics. We have shown that such a nonlinear reabsorption affects the fluorescence decay as well as the shape of the fluorescence spectrum. One should be careful not to confuse these effects with the possible formation of polyexcitons or other excited species in the crystals at high excitation levels. NFR may be useful for experimental determination of the absorption coefficients of electronically excited species.

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Scaling Studies of Highly Disordered Spin- $\frac{1}{2}$ Antiferromagnetic Systems

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A numerical method is developed to study the scaling of distribution of couplings of highly random antiferromagnetic Ising and quantum Heisenberg spin- $\frac{1}{2}$ systems. The method shows how freezing into inert local singlets prevents ordering down to temperatures well below the median nearest-neighbor coupling or bare exchange percolation threshold in positionally disordered systems with Heisenberg exchange varying exponentially with distance (e.g., doped semiconductors, quasi one-dimensional salts). This is contrasted with the Ising system.

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Considerable effort has gone into the search for magnetic order, possibly of the spin-glass type,¹ in doped semiconductors (e.g., Si:P, CdS:In)^{2,3} at donor concentrations (n) below the insulator-metal transition (n_{MI}). However, no anomaly is seen in the magnetic susceptibility³ or Faraday rotation,² attributable to magnetic ordering caused by the antiferromagnetic (af) exchange coupling between donor electrons down to temperatures well below the median nearest-neighbor exchange or the coupling percolation threshold. Because the radius a of the donor electron (much greater than the host lattice spacing) sets the range of the exchange coupling, J , doped semiconductors constitute a three-dimensional (3D) system of spin $\frac{1}{2}$ distributed randomly in

space in essentially a continuum way, whose magnetic properties are characterized by the Heisenberg Hamiltonian

$$H = \frac{1}{2} \sum_{i \neq j} J(\vec{r}_i - \vec{r}_j) \vec{S}_i \cdot \vec{S}_j, \quad (1)$$

where $J(r)$ falls off exponentially³ with r . (We use $J > 0$ for af exchange.)

The lack of ordering has been attributed in varying degrees to (i) the broad distribution of exchange couplings [typically varying by 10^4 – 10^5 , Fig. 1(a)]; (ii) the short-range nature of $J(r)$; and (iii) the quantum character of spin $\frac{1}{2}$, all of which distinguish this system from conventional spin-glasses.¹ Because of (i), cluster calculations²⁻⁵ have proved to be quite successful in pro-

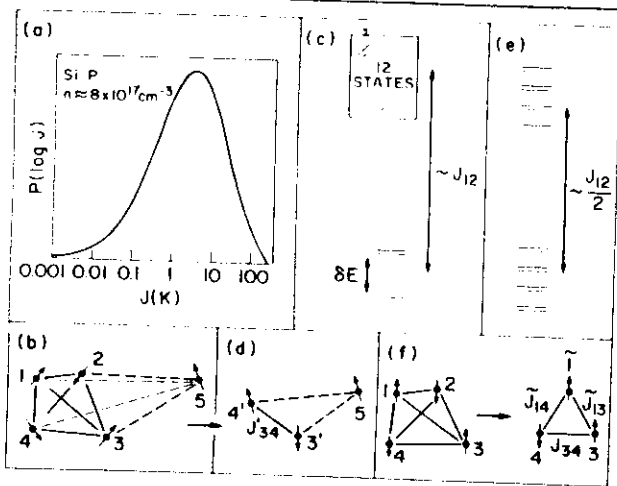


FIG. 1. (a) The distribution of nearest-neighbor couplings in Si:P at a typical concentration. Note the logarithmic scale along the horizontal axis. (b) A four-spin cluster with a neighbor, 5. (c) Eigenstates of the Heisenberg four-spin cluster for $J_{12} \gg |J_{ij}|$ ($i, j \neq 1, 2$). (d) Equivalent Heisenberg pair ($3', 4'$) (with renormalized couplings to neighbor 5 in second scheme). (e) Eigenstates of the Ising four-spin cluster. (f) Equivalent Ising three-spin cluster.

viding agreement with experimental results over a wide temperature range. However, limitations imposed by finite cluster size⁶ prevent these methods from addressing the question of magnetic ordering at lower temperatures (T).

In this Letter, we investigate this possibility by studying the scaling properties of the spatially random Heisenberg (H) spin- $\frac{1}{2}$ system with exponential interactions $J(r) = J_0 \exp(-2r/a)$ at low densities $na^D \ll 1$, prototype of the doped semiconductor system in 3D. Further, by comparing with the corresponding Ising system,

$$H = \frac{1}{2} \sum_{i,j} J(\vec{r}_i - \vec{r}_j) S_i S_j, \quad (S_i = \pm \frac{1}{2}), \quad (2)$$

we are able to determine the extent of the role of (iii). The technique, similar to that used for the 1D random Heisenberg spin- $\frac{1}{2}$ chain with nearest-neighbor exchange,^{7,8} takes advantage of the broad distribution of exchange couplings to iteratively discard high-lying excitation levels of the system (which are irrelevant at low T) and transform it to a scaled version with the same low-lying states. Physical quantities (e.g., magnetic susceptibility) are extracted from the energy-level distributions at appropriate stages.

To understand the philosophy of the calculation, consider a four-spin cluster (1, 2, 3, 4) with H in-

teractions J_{ij} [Fig. 1(b)]. If $J_{12} \gg |J_{ij}|$ for all $(i, j) \neq (1, 2)$, the energy spectrum splits into a low-lying singlet-triplet manifold and twelve excited states separated from it by $\sim J_{12}$ [Fig. 1(c)]. The splitting of the low-lying singlet and triplet is

$$\delta E = J_{34} + (J_{13} - J_{23})(J_{24} - J_{14})/2J_{12} + O(1/J_{12}^2). \quad (3)$$

Thus for $T \ll J_{12}$, the thermodynamics of the four-spin cluster is adequately represented by a spin pair ($3', 4'$) with an effective coupling $J_{34}' = \delta E$ [Fig. 1(d)], the renormalization being due to the polarization of the essentially "frozen" spin pair (1, 2). Thus the simplest scaling procedure involves deleting the strongest spin pairs (1, 2) in the system after renormalizing bonds between all pairs (3, 4) of (neighboring) spins connected to the strongly coupled pair.⁹ This procedure reduces the number of spins by two, and is iterated to scale the system down as desired.

The next approximation in a cluster-perturbative scheme is to replace four-spin clusters by an equivalent spin pair. At each iteration, the four-spin cluster (1, 2, 3, 4) is formed from the strongest af-coupled pair (1, 2) and spins 3 and 4 coupled most strongly to (1, 2). The coupling between the renormalized spins $3'$ and $4'$ [Fig. 1(d)] is obtained as before. We calculate the renormalized couplings J_{35}' and J_{45}' of the new pair ($3', 4'$) to each neighboring spin 5 originally coupled to the four-spin cluster [Fig. 1(c)] by fitting the eigenvalues¹⁰ of the reduced Hamiltonian ($H_r = \frac{1}{2} \sum_{i,j=1}^4 J_{ij} \vec{S}_i \cdot \vec{S}_j$) within the subspace consisting of the low-lying singlet-triplet set of (1, 2, 3, 4) and the doublet on 5, to those of a three-spin cluster ($3', 4', 5$) [Fig. 1(d)]. The system is scaled down by repeated application as before.

A similar scaling procedure when applied to the Ising four-spin cluster removes only eight states [Fig. 1(e)] corresponding to an antiferromagnetic configuration of spins 1 and 2. The remaining states are represented by replacing the spin pair 1-2 with a single spin $\frac{1}{2}$ with magnetic moment $\mu = 0$, labeled $\bar{1}$ in Fig. 1(f), and couplings $\bar{J}_{13} = J_{13} - J_{23}$, $\bar{J}_{14} = J_{14} - J_{24}$. This procedure generates arbitrary magnetic moments and signs of couplings; decimation of a spin pair (ij) into a spin k at an arbitrary stage would yield $\mu_k = \mu_i - \text{sgn}(J_{ij})\mu_j$, and $J_{ki} = J_{ii} - \text{sgn}(J_{ij})J_{ji}$ with a neighboring spin i . As the system is iterated, the distributions of positive and negative J 's approach each other; thus we exhibit results for the distribution of $\ln|J|$.

The scaling schemes outlined above have been

implemented numerically for both systems using a CRAY-1 computer in 1D, 2D, and 3D. Samples of up to 10 000 spins were distributed randomly in a D -dimensional cube and with periodic boundary conditions. All couplings larger than a threshold J_c (initial, as well as generated) were kept. J_c was adjusted to give an average of 15-30 couplings per spin initially. Figure 2(a) shows a typical plot of the width of the distribution of the nearest-neighbor couplings [on a logarithmic scale, as in Fig. 1(a)] normalized to its initial value for the two systems in 3D. (The results using the two schemes for the H system are practically the same, implying convergence of the cluster-perturbation theory.) The slow change for the H system (further-neighbor distributions show even *slower* variation) is in marked contrast to the rapid contraction in the Ising case. This contraction is accompanied by the formation of large clusters with long-range interactions of both sign, strongly suggestive of eventual development into a frustrated Ising spin-glass.¹¹ The lack of such behavior in the Heisenberg system is shown even more dramatically in 2D [Fig. 2(b)] which exhibits invariance of the width of

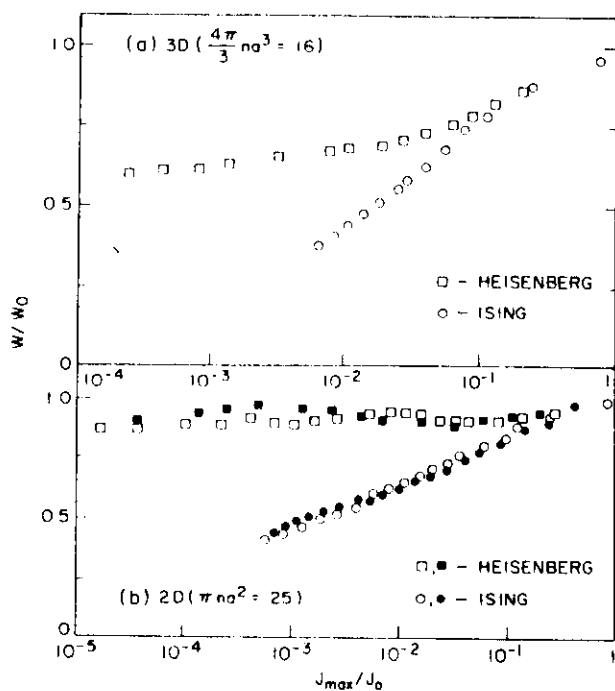


FIG. 2. Width of the distribution of the logarithm of the nearest-neighbor coupling for the spatially random Heisenberg and Ising systems as a function of maximum coupling (temperature), normalized to the bare (initial) value in (a) 3D, (b) 2D.

couplings in the H system (i.e., the system scales into itself as the temperature is lowered).

At each iteration, energy levels discarded are equal to the largest coupling (J_M) in the system. For the highly disordered system under consideration, where couplings and energy levels span several orders of magnitude, it is a good approximation to take, at $T = J_M$, all discarded levels as "frozen," and the remaining spins as free. This yields a magnetic susceptibility

$$\chi(T = J_M) = N(J_M)\chi_c(J_M)/N(J_0), \quad (4)$$

where $\chi_c(J_M) = N(J_0)\mu_B^2/k_B J_M$ is the Curie susceptibility of $N(J_0)$ spins $\frac{1}{2}$ at $T = J_M$ and $N(J_M)$ is the effective number of free spins $\frac{1}{2}$ remaining when the largest coupling equals J_M . Figure 3 shows the normalized magnetic susceptibility $\chi(T)/\chi(J_0)$ obtained from both methods (which agree to well within 2%-3%) for the 3D Heisenberg system, for various donor densities n ($4\pi na^3/3 = 0.004 - 0.16$). The Curie susceptibility is also shown. $\chi(T)$ shows no sign of an anomaly or even saturation at any of the concentrations studied, over many orders of magnitude in T , down to where only 1%-2% of the spins remain. At this stage statistical variation in $\chi(T)$ between different samples is $\sim 5\% - 10\%$. Another limitation is the introduction of ferromagnetic (f) couplings (this occurs when a four-spin cluster has a triplet ground state). Usually the f couplings are found to scale down with the af ones. Towards the end, howev-

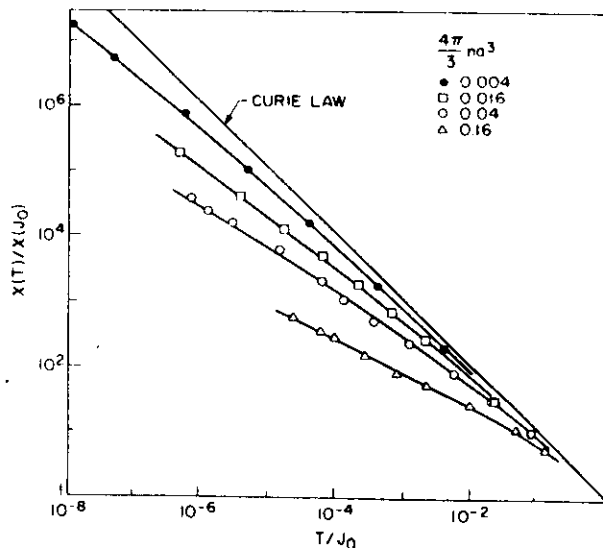


FIG. 3. Magnetic susceptibility of the spatially random 3D Heisenberg spin- $\frac{1}{2}$ system with exponential exchange for various concentrations, n .

er, there are a sizable number of large ($>J_c$) f bonds which must be handled using a larger basis set than our truncation procedure allows for. These "spins 1," however, have been taken into account in computing $\chi(T)$ at the lower temperatures.¹²

In 2D, invariance of the distribution width leads to a straight line on the logarithmic plot¹²: $\chi(T) \sim T^{-\alpha}$ with $\alpha(<1)$ depending on concentration. [In 1D, the distribution gets wider with scaling, leading to a $\chi(T)$ in agreement with previous results.^{7,8}] This behavior is a manifestation of the rapid scaling down of the upper cutoff J_M due to the quantum mechanical nature of inert local singlet ground states which prevent the generation of larger couplings [Eq. (3)] in contrast to, e.g., the Ising system. The concentration range in Fig. 3 covers the insulator-metal transition¹³ in doped semiconductors $4\pi n_{MI} a^3/3 \approx 0.065$ at which stage the electrons get delocalized, and a model in terms of localized moments is no longer valid. Thus the present calculations show that in the insulating regime in doped semiconductors, well below the delocalization transition, there is no magnetic ordering due to the exchange coupling of donor electrons down to temperatures much below those currently accessible to experiment.¹⁴ In our attempt to search for possible ordering in the Heisenberg case [as indicated by a saturation or maximum in $\chi(T)$] we have carried out calculations for power law couplings [$J(R) \sim R^{-m}$], and find maxima in $\chi(T)$ only for $m < 3$.¹⁵ Because of the narrower distribution of couplings, the results are expected to be less quantitative; however, they do indicate the possibility of no magnetic-ordering transition in the random 3D Heisenberg spin- $\frac{1}{2}$ system with short-range interactions.

In conclusion, we find very different scaling behavior for the positionally disordered Ising and Heisenberg spin- $\frac{1}{2}$ systems with short-range interactions. The former forms large clusters and develops long-range interaction as expected; the latter, however, exhibits scale invariant behavior in 2D, and shows no tendency for ordering. In 3D too, the development of frustration is strongly arrested (orders of magnitude in tem-

perature compared to the Ising case), thus showing the importance of the quantum nature of strongly disordered systems in the suppression of magnetic order.

We acknowledge helpful discussions with P. W. Anderson, S. Geschwind, W. L. McMillian, T. M. Rice, and R. E. Walstedt, and the computational help of B. Chambers.

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⁹We note that if $J_{14} = J_{24} = 0$, the renormalization of J_M is $O(1/J_{12}^2)$; consequently, we do not consider such bonds.

¹⁰This procedure yields $(J_{35}' - J_{45}')^2$ and $J_{35}' + J_{45}'$. The ambiguity between J_{35}' and J_{45}' is resolved by looking at the results when the pair (1, 2) is essentially decoupled. In a very small number of cases ($< 0.1\%$) we find small negative values of $(J_{35}' - J_{45}')^2$; in such cases, it is set equal to zero.

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Dielectric function near a polarization catastrophe

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ABSTRACT

The metal-insulator transition in a disordered system is described in terms of a divergence of the dielectric constant of the insulating phase (polarization catastrophe). The results of optical measurements are compared with theory within the framework of a scaling picture of the transition. Also described are recent theoretical and experimental developments regarding the role played by the low-frequency hopping modes that are characteristic of the disordered system, in the description of the transition.

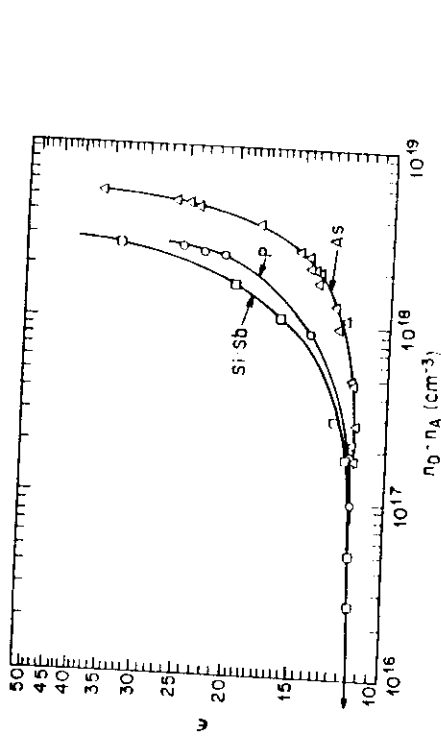
§ 1. INTRODUCTION : THE POLARIZATION CATASTROPHE

Metal-insulator (MI) transitions in disordered systems with monovalent (or open shell) atoms have been studied in a number of systems: doped semiconductors, expanded metals and metal-insulator composites, to name but a few (Mott 1974). In the original picture (Mott 1949) the MI transition, considered to arise from correlation effects, was viewed as discontinuous because of the assumption of a finite static dielectric constant in the insulating phase as the metallic phase was approached, typically by varying the density (composition) to a critical value n_c . For the Anderson transition (Anderson 1958) produced by pure disorder, the situation remained controversial for a long time. In recent years, the rapid growth of the 'localization industry' (Anderson 1983) following the advent of the scaling theory of localization (Abrahams, Anderson, Licciardello and Ramakrishnan 1979, Wegner 1979) has led to a near consensus (see, however, Mott and Kaveh 1981, Kaveh and Mott 1982) that the transition is continuous, and can be described using renormalization group theory in terms of a diverging length, fixed points and critical exponents, much as for a conventional second-order phase transition. A similar attempt has been made for models including both electron-electron interactions and disorder (McMillan 1981, Grest and Lee 1983, C. Castellani, C. DiCastro, G. Forgacs and E. Tabet 1983 (unpublished work), Finkelshtein 1983), but the situation is not as clear. Results for a number of systems†

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‡ Doped semiconductors (Rosenbaum, Andres, Thomas and Bhatt 1980, Paalanen, Rosenbaum, Thomas and Bhatt 1982, Thomas, Ootuka, Katsumoto, Kobayashi and Sasaki 1982, Newman and Holcomb 1983), amorphous alloys (Dodson, McMillan, Mochel and Dynes 1981, Nishida, Yamaguchi, Furubayashi, Morigaki, Ishimoto and Ono 1982, Hertel, Bishop, Spencer, Rowell and Dynes 1983) and magnetic semiconductors (von Molnar, Briggs, Floquet and Remenyi 1983).

Fig. 1



The dielectric constant ϵ of n-doped Si as a function of donor concentration $n_D - n_A$ for P, Sb and As donors (Castner 1980).

have all indicated a continuous critical onset of the $T = 0$ d.c. conductivity in the metallic phase.

Actually, evidence for a possibly continuous transition was to be found in earlier measurements on the insulating side. D'Altroy and Fan (1956) found a strong enhancement of the microwave dielectric constant in doped Ge, and similar effects were found in Na-NH₃ solutions (Mahaffey and Jerde 1968). This was followed by measurements on n-doped Si and Ge by Castner and co-workers (Castner, Lee, Cieloszyk and Salinger 1975, Castner, Lee, Tan, Moberly and Symko 1980). Their results for P, Sb- and As-doped Si are shown in fig. 1, where the strong non-linear increase of the donor polarizability $4\pi\chi_D = \epsilon - \epsilon_h$ (where ϵ_h is the dielectric of the constant host) with dopant concentration n is clearly seen as n becomes a sizeable fraction of n_c . These results were interpreted in terms of a Clausius-Mossotti model of the polarizability of induced dipoles, according to which

$$\chi_D = \frac{n\alpha_D}{1 - (4\pi n\alpha_D/3\epsilon_h)} \quad (1)$$

where α_D is the polarizability per donor and in general depends on n . Castner (1979) attempted to evaluate χ_D self-consistently for a lattice of donors.

The nonlinear enhancement of the dielectric constant with n can also be viewed in terms of the closing of an effective optical gap in the excitation spectrum. In fact, the zero-frequency dielectric constant is given by a Kramers-Kronig relation as an integral over the optical absorption coefficient (see, for example, Capizzi, Thomas, DeRosa, Bhatt and Rice 1980); this is discussed further in § 2. The conventional formula for the dielectric constant

of a semiconductor in terms of the optical gap E_g is (see, for example, Castner 1980):

$$\epsilon = \epsilon_h + \frac{4\pi\hbar^2 n e^2}{m^* E_g^2} \quad (2)$$

Bhatt and Rice (1981) showed that eqn. (2), where E_g is obtained from a lattice calculation, describes the enhancement of ϵ in Si. P quite well up to $n \approx 0.5n_c$. Clearly, however, the lattice is only an approximation for randomly placed donors. Furthermore, for a system without translational invariance, eqn. (2) cannot hold as $n \rightarrow n_c$, since there are no k -selection rules for optical absorption. A generalization to allow for all transitions (as in the theory of the optical gap in amorphous materials (Tauc 1970)) with a constant density of states at the mobility edges yields $\epsilon - \epsilon_h \sim E_g^{-1}$, where E_g is now the mobility gap, which is expected to vanish linearly as $n \rightarrow n_c$. It is interesting to note that both this analysis and that following from a Clausius-Mossotti model yields a dielectric constant diverging as $(n_c - n)^{-1}$, which is not far from what is experimentally observed in Si: P (Capizzi *et al.* 1980, Hess, DeConde, Rosenbaum and Thomas 1982, Paalanen, Rosenbaum, Thomas and Bhatt 1983).

A more general framework within which to consider the divergence of the dielectric constant was established with the advent of the scaling theory of localization (Abrahams *et al.* 1979). The MI transition is signalled by the divergence of a characteristic length ξ , called the localization length, of the form $\xi = \xi_0 |n/n_c - 1|^{-\nu}$. According to the scaling theory, the difference between the insulating and metallic phases is apparent only on length scales longer than ξ ; below ξ their properties are the same. Since the conductivity for a d -dimensional metal ($d > 2$) is e^2/\hbar divided by a length raised to the power $d - 2$, and the only relevant length near n_c is ξ , it follows that for a $3d$ system in the metallic phase the $T = 0$ d.c. conductivity is given by

$$\sigma = C_0 \frac{e^2}{\hbar \xi} \quad (3)$$

where C_0 is a numerical prefactor. The conductivity thus goes continuously to zero as $n \rightarrow n_c$, with a form $\sigma \sim (n - n_c)^\nu$ characterized by the critical exponent ν ; below n_c , of course, $\sigma = 0$. From perturbation theory estimates for a non-interacting system, a value of $\nu \approx 1$ is expected (Abrahams *et al.* 1979, Hikami 1981, Vollhardt and Wölfle 1982); however, non-perturbative effects as well as electron-electron interaction effects could change that (McMillan 1981, Grest and Lee 1983). Arguing similarly that the metallic form of the zero-frequency dielectric constant

$$\epsilon(q) = 1 + \frac{\kappa^2}{q^2} \quad (4)$$

where κ^{-1} is the Thomas-Fermi screening length, should be valid in the insulating phase for wave-vectors $q > \xi^{-1}$ (Rosenbaum *et al.* 1980), below which $\epsilon(q)$ should saturate, one obtains

$$\epsilon(0) \sim \kappa^2 \xi^2 \quad (5)$$

as $n \rightarrow n_c$, so that the divergence of the dielectric constant is given by an exponent twice that of the conductivity in the metallic phase. This argument

has been further amplified to include interaction effects (Imry, Gefen and Bergman 1982, Gefen and Imry 1983; see also Lee 1982) and $\epsilon(0) \sim \xi^{-3}$ is obtained, where η is termed the anomalous dimension. Experiments on Si: P (Rosenbaum *et al.* 1980, Paalonen *et al.* 1983) give $\eta \approx 0$. Although direct measurements of the critical behaviour of the dielectric constant in the insulating phase have not been made on other systems undergoing a localization transition, $\eta \approx 1$ is indicated from other experiments on Nb-Si (Hertel *et al.* 1983).

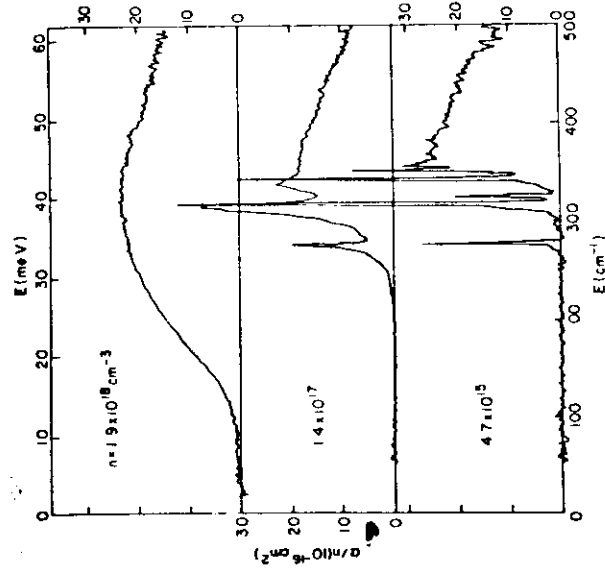
It should be pointed out that a similar polarization catastrophe occurs for systems undergoing a macroscopic percolation transition of metallic regions in an insulating medium (Dubrov, Levinshstein and Shur 1976, Bergman and Imry 1977, Grannan, Garland and Tanner 1981, Stroud and Bergman 1982). However, the mechanism and exponents are quite different, and we limit our discussion to quantum localization. In § 2 are described the evolution of the optical conductivity, as studied most extensively in Si: P, and its relation to the divergence of the dielectric constant. Section 3 is devoted to a discussion of the surprising role played by hopping processes, hitherto neglected in the scaling description of the MI transition, in the divergence of the dielectric constant. Conclusions are drawn in § 4.

§ 2. OPTICAL CONDUCTIVITY AND THE 'ZERO-FREQUENCY' DIELECTRIC CONSTANT

At very low densities ($n < 10^{-3}n_c$) the far-infrared optical conductivity $\sigma(\omega)$ in an uncompensated n-doped semiconductor consists of a set of extremely sharp resonances corresponding to excitation of the donor electrons from the ground state to the optically allowed higher bound states of the isolated donor ($2p, 3p, \dots$) which culminate at the ionization energy E_i . At higher energies the absorption spectrum is continuous, and due to excitation to continuum (conduction band) states. As n is increased the sharp lines broaden, and the continuum moves down in energy, swallowing up the bound-state resonances one at a time. The broadening (Capizzi, Thomas, DeRosa, Bhatt and Rice 1979) is characteristically asymmetric towards lower energies, and has distinct features corresponding to the most likely clusters, donor pairs. Larger clusters come into play once $n \gtrsim 0.07n_c$, but do not give rise to any specific features, and the optical conductivity with its weight moving to lower frequencies is best thought of in terms of a statistical average over an ensemble of cluster sizes (Bhatt and Rice 1979, Thomas, Capizzi, DeRosa, Bhatt and Rice 1981). The evolution of the normalized optical absorption $\alpha(\omega)$ (proportional to $\sigma(\omega)$) as a function of donor density is shown in fig. 2, in which the bottom curve at a density three orders of magnitude below n_c corresponds to the isolated donor limit, and the middle curve to the region where pair spectra can be seen; the top curve, for which $n \sim n_c/2$, represents an almost featureless spectrum produced by random clusters, with a greatly reduced absorption threshold. (Similar spectra are also obtained from expanded metals below n_c , for example, fluid Hg; see Bhatt and Rice (1979).)

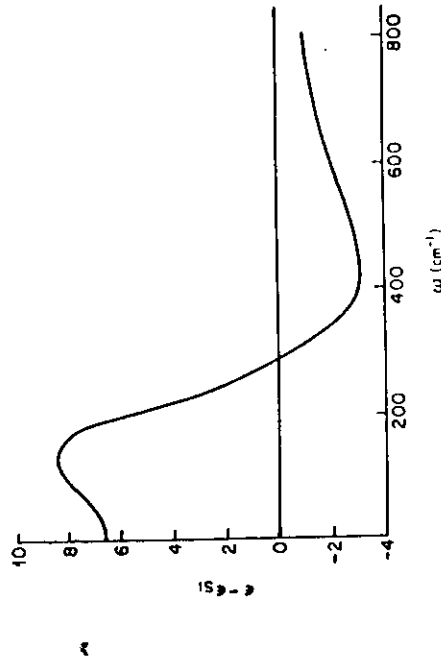
The dielectric function at far-infrared frequencies may be obtained from the standard Kramers-Kronig integral over the optical conductivity arising from

Fig. 2



The variation of the normalized optical absorption α/ϵ_1 of P donors in Si at different concentrations n (Thomas *et al.* 1981).

Fig. 3



The dielectric function $(\epsilon - \epsilon_1)$ of P donors in Si at $n = 1.9 \times 10^{18} \text{ cm}^{-3}$, obtained by Kramers-Kronig analysis of the optical absorption.

the donors :

$$\epsilon(\omega) = \epsilon_b + 4\pi X_D(\omega), \tag{6}$$

where

$$X_D(\omega) = \frac{2}{\pi} \int_0^\infty \frac{\sigma(\omega') d\omega'}{\omega'^2 - \omega^2} \tag{7}$$

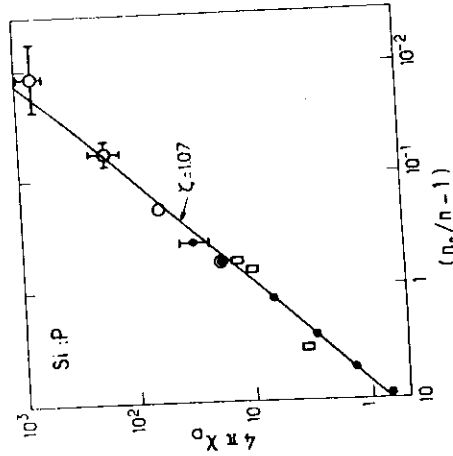
and ϵ_b is the dielectric constant of the host material (e.g. Si), which is frequency-independent in this regime. The donor part, $4\pi X_D(\omega)$, is shown in fig. 3 for the largest density from fig. 2 ($n = 1.9 \times 10^{18} \text{ cm}^{-3}$).

The dielectric constant ϵ is given by the d.c. ($\omega \rightarrow 0$) limit of $\epsilon(\omega)$, and its variation as $n \rightarrow n_c$ from below is found to fit the critical form suggested by scaling theories :

$$4\pi X_D \sim [n_c(n-1)]^{-\zeta} \tag{8}$$

with $\zeta = 1.1 \pm 0.15$. This is depicted in fig. 4 which is compiled from a variety of measurements : low frequency measurements (Castner *et al.* 1975), Kramers-Kronig analysis of the optical conductivity (Capizzi *et al.* 1980) and microwave frequency measurements (Hess *et al.* 1982).

Fig. 4



The optical divergence of the 'zero-frequency' dielectric constant $4\pi X_D$ in Si:P (data from (□) Castner *et al.* (1975), (●) Capizzi *et al.* (1980) and (○) Hess *et al.* (1982)).

The exponent ζ is approximately twice that found for the onset of the d.c. conductivity in the metallic regime, $\nu = 0.5 \pm 0.07$ (Paalanen *et al.* 1982). As stated above, a ratio $\zeta/\nu = 2$ is expected for the non-interacting system, while for the interacting system $\zeta/\nu = 2 - \eta$, where η is the anomalous dimension of ϵ . Thus η is small for Si:P, in contrast amorphous Nb-Si, for which a value of $\eta \approx 1$ has been reported (Hertel *et al.* 1983).

Within the scaling theory of localization, the low-frequency optical conductivity near n_c differs in the insulating and metallic phases, up to a characteristic frequency ω_c which exhibits critical slowing ($\omega_c \rightarrow 0$ as $n \rightarrow n_c$), and is given by the same form above ω_c . (This is the frequency equivalent of the length dependence of σ discussed in the original formulation of Abrahams *et al.* 1979). As shown for the non-interacting system (Shapiro and Abrahams 1981, Shapiro 1982, Imry *et al.* 1982),

$$\sigma(\omega) \sim \begin{cases} \omega^{1/3}, & \omega > \omega_c \approx 1/N_0 \xi^3 \\ \omega^2, & \omega < \omega_c, n < n_c \\ \sigma(0), & \omega < \omega_c, n > n_c. \end{cases} \tag{9}$$

A Kramers-Kronig analysis of eqn. (9) in the insulating phase implies a divergence in $\sigma \sim \xi^2$ coming from frequencies of order ω_c ; little contribution is obtained from frequencies much below ω_c . Even with the logarithmic enhancements of the ω^2 term produced by resonance effects (Mott 1974), not included in this formalism (Vollhardt and Wölfle 1980), the critical divergence remains the same. Thus the existence of another contribution to the divergence of ϵ , discussed in § 3, turns out to be a novel and unexpected feature of this quantum transition, which is distinct from conventional phase transitions.

§ 3. THE HOPPING CONDUCTIVITY

It was found in the early 1960s (Pollak and Geballe 1961) that the low-frequency a.c. conductivity ($\hbar\omega \ll k_B T$) deep in the insulating phase of compensated doped semiconductors was much larger than the d.c. value, and had a frequency dependence of the form $\sigma(\omega) \sim \omega^s$, with $s \approx 0.8$. A theory of the a.c. conductivity for the Anderson insulator (non-interacting electrons), with a constant density of states at the Fermi level, was proposed by Austin and Mott (1969). They considered a localized electron hopping between a pair of sites separated by a distance $r_\omega = (a/2) \ln(\omega_p/\omega)$ (where ω_p is a typical phonon frequency), with a Debye dipolar relaxation involving phonon emission or absorption, and obtained a conductivity

$$\sigma(\omega) = C e^2 N_0^2 a^3 k_B T \omega \ln^4(\omega_p/\omega). \tag{10}$$

Here N_0 is the density of states at the Fermi level, a the extent of the localized electronic wavefunction and C a numerical constant. The sublinear ω dependence of eqn. (10) was in good accord with the experimental data (Pollak and Geballe 1961).

Thus at $T = 0$, the relaxation process gives zero conductivity, apparently resolving the problem of an infinite dielectric constant implied by a Kramers-Kronig integration of a $\sigma(\omega)$ with a sublinear ω dependence (see, however, Bhatt 1984). On the other hand, resonant (zero-phonon) hopping processes lead to a conductivity

$$\sigma(\omega) \sim N_0^2 \omega^2 \ln^4(\omega_c/\omega), \tag{11}$$

as shown by Mott (see, for example, Mott 1974), which would yield a finite contribution to ϵ that could be absorbed into the 'optical' dielectric constant.

It was recognized by Pollak (1970) that electron-electron interactions could lead to strong modifications of the properties of the disordered insulator, giving rise, for example, to the so-called 'Coulomb gap' in the single-particle density of states at the Fermi level. As shown by Efros and Shklovskii (1975), Coulomb interactions—no matter how small—constitute a singular perturbation in the one-electron density of states tied to the Fermi energy E_F . They used the classical Hamiltonian

$$\mathcal{H} = \sum_i \epsilon_i n_i + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_{ij}} n_i n_j \quad (12)$$

with random on-site energies ϵ_i . This is like the Anderson model but without quantum-mechanical hopping terms, including instead the long-range charge fluctuation (Hartree) interactions among the electrons. The one-electron energies for this Hamiltonian are given by

$$E_j = \epsilon_j + \sum_{i \neq j} \frac{e^2}{r_{ij}} n_i \quad (13)$$

Efros and Shklovskii (1975) argued that the ground state of the system described by this Hamiltonian is defined not only by the condition that single-particle energy levels $E_i < E_F$ are full and $E_j > E_F$ are empty, but also by the condition for stability against particle hops, i.e.

$$E_j - E_i - e^2/r_{ij} > 0 \quad (14)$$

for any occupied level E_i and unoccupied level E_j . This implies that for any given difference δE between the single-particle energies of occupied and unoccupied levels, there must be a spatial separation $r > e^2/\delta E$ between them. Because of this, strongly correlated nature of the ground state, there can be at most $n(\delta E) \sim (\delta E)^d$ levels within δE of E_F , and consequently the density of states is $N(E) \lesssim (E - E_F)^2$. Thus there is a singular modification of $N(E)$ at E_F , leading to $N(E_F) = 0$ for arbitrarily weak Coulomb interactions, but $N(E)$ rises to its non-interacting value N_0 within an energy interval $\Delta \sim e^2 N_0^{1/2}$ of E_F . This has been confirmed in numerical simulations (Baranovskii, Efros, Gelmont and Shklovskii 1979, Davies, Lee and Rice 1982). We note that this singular perturbation holds for interactions falling off more slowly than r^{-d} in d dimensions.

Although Coulomb interactions cause $N(E)$ to be suppressed near E_F , they lead to an *enhancement* of the hopping conductivity. In particular, as shown by Pollak (1971) and later by Efros (1981), the equivalent of the low-frequency Austin-Mott formula (eqn. (10)) for an interacting system at low temperatures ($T \ll \Delta$) is

$$\sigma(\omega) = C' e^4 N_0^2 \sigma^d \omega \ln^3(\omega_p/\omega), \quad (15)$$

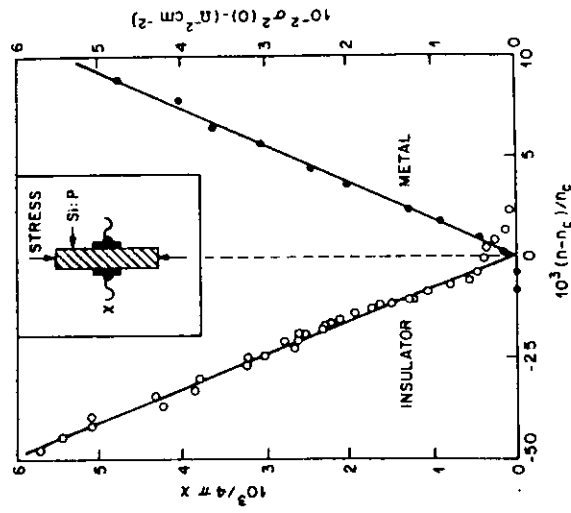
where C' is a numerical constant. As explained most succinctly by Efros (1981), eqn. (15) differs from the result for a non-interacting system (eqn. (10)) because a large number of sites with low bare (non-interacting) energies ϵ_i , which would be filled in the absence of interactions, remain unoccupied in the interacting system because of the Coulomb repulsion of nearby occupied sites. However, low-energy excitation processes involving a *transfer* of electrons from occupied

to unoccupied sites are certainly possible. This effectively enlarges the phase space available for these electron-hole excitations from $k_B T$ around E_F in the non-interacting system to the Coulomb interaction between the pair of sites involved in the hopping process, $e^2/r\omega$. Replacing $k_B T$ in the Austin-Mott formula gives an expression identical to eqn. (15), apart from numerical factors. (Note that eqn. (15) implies a *finite* hopping conductivity with a sublinear frequency dependence in the limit $T \rightarrow 0$.)

Shklovskii and Efros (1981) have also considered the modification of the zero-phonon hopping conductivity arising from resonance processes. They obtained $\sigma(\omega) \sim \omega \ln^3(\omega_c/\omega)$ at $T=0$, rather similar to eqn. (15), but for finite T their formula includes a factor $1 - \exp(-\hbar\omega/k_B T)$, which implies that $\sigma(\omega) \sim \omega^2 \ln^3(\omega_c/\omega)$ at $\hbar\omega \ll k_B T$ and hence yields a non-divergent contribution to $\epsilon(0)$ which can be absorbed into the optical dielectric constant, as for the non-interacting system.

It was realized by Bhatt and Ramakrishnan (1984) that the large density of low-lying hopping modes in a Coulomb insulator belies the expectation that the divergence of the length scale of quantum-mechanical hopping, i.e. ξ , and the consequent swallowing up of the phase space for long-distance classical charge interaction effects, will render any effects of the Efros-Shklovskii (ES) gap unimportant as the MI transition is approached from the insulating side. Thus, they argued, an ES-type analysis of the hopping conductivity is relevant even in the limit $n \rightarrow n_c^-$, where $\xi \rightarrow \infty$, provided a few modifications are made:

Fig. 5



The inverse donor polarizability at 31 kMz and the square of the d.c. conductivity, both extrapolated to $T=0$, in Si:P as a function of $n - n_c$, using the stress-tuning technique illustrated in the inset (Paalanen *et al.* 1983).

Ramakrishnan (1984) obtained an a.c. conductivity in the limit $T \rightarrow 0$ of the form

$$\sigma(\omega) = \frac{C^* \epsilon \omega}{\ln(\omega_p/\omega)} \quad (16)$$

where C^* is a numerical constant and ϵ is the zero-frequency limit of the 'optical' dielectric constant. It is interesting to note that eqn. (16) implies an a.c. conductivity which is independent of the parameters of the system (N_0 , ξ , and so on), except in so far as they enter through ϵ . A Kramers-Kronig analysis of eqn. (16) yields a contribution to the total dielectric function $\epsilon(\omega)$, in addition to the optical part, which is weakly infrared-divergent and has the form

$$\delta\epsilon(\omega) = 8C^* \epsilon [\ln \ln(\omega_p/\omega) + O(1)] \quad (17)$$

in the low-frequency limit. Equation (17) shows that this contribution scales directly with ϵ . In addition, because of its infrared divergent form it remains relevant at the low a.c. frequencies prevailing in typical measurements (of about a kilohertz), which are over ten orders of magnitude removed from typical microscopic frequencies, and remain well below any critically slowing frequency at experimentally accessible values of $n - n_c$. Since $\epsilon(\omega)$ is proportional to ϵ , the low-frequency dielectric function exhibits the same divergence as the optical one. This is found in the measurements by Paalanen *et al.* (1983), in which the MI transition is approached by tuning the critical density n_c with uniaxial stress in Si:P (Paalanen *et al.* 1982, Bhatt 1981, 1982). Their data for the inverse donor polarizability as a function of stress are depicted in fig. 5 (along with the square of the d.c. conductivity in the metallic phase) and imply an exponent $\zeta \approx 1$ for ϵ at the low frequency of the measurement.

Although both the a.c. conductivity and the dielectric function show a strong critical divergence as $n \rightarrow n_c^-$, from eqns. (16) and (17) the ratio $\omega\epsilon(\omega)/\sigma(\omega)$, in which the factor ϵ cancels out, is predicted to remain constant (no critical or cross-over behaviour), except for small logarithmic variations of the frequency factors. This is shown in the inset to fig. 6 for the measurements of Paalanen *et al.* (1983), and demonstrates the proportionality convincingly. Shown in the main part of fig. 6 is the frequency variation of the conductivity and the dielectric function, which is similar to that predicted by hopping theories (including eqns. (16) and (17)).

It should be emphasized that the existence of a hopping conductivity in the limit $T \rightarrow 0$ with a near-linear frequency dependence, and the constancy of the ratio $\omega\epsilon(\omega)/\sigma(\omega)$ with $n - n_c$, are consequences of Coulomb interactions and show the importance of electron-electron interaction effects in the description of the MI transition in real disordered systems.

§ 4. CONCLUSIONS

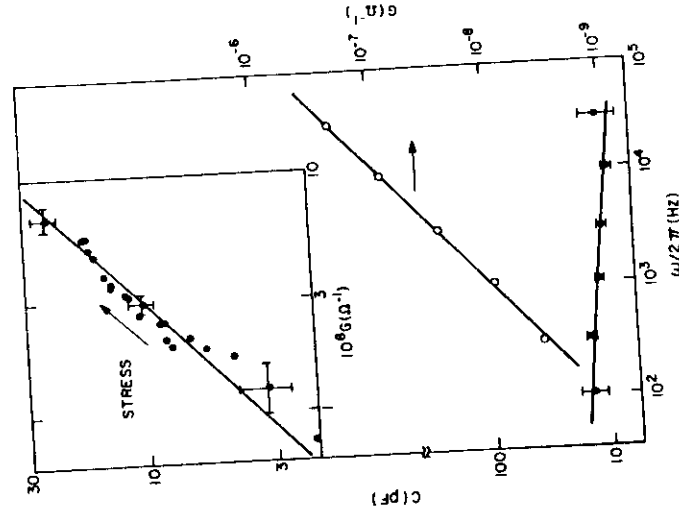
The past few years have witnessed a progressive accumulation of experimental evidence for the divergence of the dielectric polarizability in a three-dimensional disordered insulator as the MI transition is approached. The divergence is of the critical form $\epsilon \sim |n_c - n|^{-\zeta}$, as suggested by a scaling picture of the localization transition with similarities to conventional second-order phase transitions. For the one system in which detailed measurements of the

- (1) the critical divergence of the extent of the localized states, ξ , was incorporated into the analysis;
 - (2) the ES Hamiltonian and hopping conductivity calculated from it were valid only for processes occurring over length scales larger than ξ ; and
 - (3) the electron-electron interaction was screened by the 'optical' dielectric constant ϵ arising from processes occurring over length scales smaller than ξ , which had a critical divergence (as discussed in §§ 1 and 2).
- Further, they found that the length scale defined by the ES gap.

$$r_s \sim e^2/\epsilon\Delta \sim (\epsilon/\epsilon_0 N_0)^{1/2},$$

diverges as $n \rightarrow n_c^-$ with the same exponent as ξ for systems with $\eta = 0$, and the ratio $(r_s/\xi) \approx 1/\epsilon\epsilon_0 N_0^{1/2} \sim 10$, determined by the Mott criterion for n_c (see, for example, Mott 1974). Thus the classical description of the density of states has transition is approached; however, the modification of the density of states has to be taken into account. Using the ES form $N(E) \sim (E - E_F)^2$, Bhatt and

Fig. 6



The variation of the conductance G (○) and donor capacitance C (◻) with frequency, fitted to the forms ω^s and ω^{s-1} with $s = 0.9 \pm 0.1$. The inset shows the crucial proportionality between the real and imaginary parts of the conductance, extrapolated to $T = 0$, at 31 kHz, as $n \rightarrow n_c^-$ by the application of stress. (Paalanen *et al.* 1983.)

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dielectric function are available, namely Si:P, ζ is found to be 1.1 ± 0.15 , approximately twice the exponent for the onset of conductivity in the metallic phase, i.e. $\sigma \sim (n - n_c)^\nu$ with $\nu = 0.5 \pm 0.07$. This ratio agrees with the prediction of the scaling theory for non-interacting electrons. It is interesting that in another well-studied system, amorphous Nb-Si (Hertel *et al.* 1983) while ν is found to be near unity, one infers that $\zeta \approx 1$ (by using tunnelling data and scaling relations), although no direct measurements of ϵ are available.

A novel feature of this quantum ($T = 0$) transition in a disordered system with long-range electron-electron interactions is the existence of a large density of low-frequency excitations. These hopping modes, at frequencies far below the critically slowing frequency, remain relevant to the dielectric polarizability, point and give a non-negligible contribution to the dielectric polarizability, which is weakly infrared-divergent. For $\zeta/\nu = 2$, as in Si:P, the magnitude (prefactor) of this contribution scales directly with the (divergent) 'static' dielectric constant coming from the critical region of the optical conductivity $\sigma(\omega)$ ($\omega \sim \omega_c$). As a result, the impedance angle $\omega\epsilon(\omega)/\sigma(\omega)$ of Si:P at very low frequencies ($\omega \ll \omega_c$) shows essentially no variation as the MI transition is approached, although both the real and imaginary parts of ϵ diverge. However, for systems with a significantly different ζ/ν ratio, a cross-over behaviour for the ratio would be expected. Finally, this complexity in the critical behaviour of the dielectric function points to the doubly appropriate term 'polarization catastrophe', i.e. both as $n \rightarrow n_c^-$ and as $\omega \rightarrow 0$.

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