# Knight Shifts and Spin Dynamics in Disordered Systems

M.J.R. Hoch and S.T. Stoddart

Department of Physics and
Condensed Matter Physics Research Unit,
University of the Witwatersrand, Johannesburg

## 1. Introduction

The metal insulator (MI) transition is a problem that has received much attention in solid state physics. Heavily doped semiconductors have featured prominently in this work with Si:P the archetypal system.

In order to explain the observed low temperature properties, such as the magnetic susceptibility, of MI systems in the vicinity of the critical concentration, $n_c$, of dopant atoms, a phenomenological two–fluid model has been proposed [1]. The present work is concerned with interpreting $^{29}$Si NMR relaxation time measurements and Knight shifts for Si:P and Si:(P,B) in the vicinity of $n_c$. The results are analyzed in terms of available theory in the context of the two–fluid model.

## 2. The Two–Fluid Model and the Bhatt–Lee Theory

For the just metallic or just insulating phases of MI systems, the two–fluid model distinguishes between two types of electron spins. As the transition is traversed, the proportions of the two fluids change. The fluids are comprised of localized moments associated with isolated dopant atoms, or small clusters of dopant atoms, on the one hand, and delocalized moments on the other. In broad terms, the localized moments dominate in determining the magnetic properties in the vicinity of $n_c$, while the delocalized moments determine the electrical properties, such as the conductivity.

For $n < n_c$, the localized moments constitute a disordered antiferromagnetic system. The exchange Hamiltonian may be written in the usual way as

$$H = -\sum_{i<j} J_{ij}\, \underline{S}_i \cdot \underline{S}_j \ ,$$

where $J_{ij}$ is the exchange coupling between spins i and j and $\underline{S}_i$ and $\underline{S}_j$ are the spin operators.

In order to explain the behaviour of the magnetic susceptibility $\chi$ with temperature for $n \leq n_c$, Bhatt and Lee [2] have developed a theory in which the exchange coupling $J_{ij}$ between nearest neighbour pairs of localized moments is used to separate the moments into two groups. In simple terms, spin pairs with $J_{ij} >> kT$ are tightly coupled or *frozen* in the singlet state and effectively do not contribute to $\chi$. The remaining spins do contribute and the susceptibility may be written in terms of the Curie law susceptibility as

$$\chi = \frac{n_e(T)}{n}\, \chi_{Curie} \qquad (1)$$

Numerical procedures were used to determine $n_e(T)$, the effective number of spins at temperature T. Good quantitative agreement was obtained with available experimental susceptibility data. Bhatt and Lee used the following form for the J distribution in their calculations : $P(J) \propto J^{-\alpha}$, with $0.6 < \alpha < 0.8$. This led to $\chi \propto T^{-\alpha}$, as observed.

## 3. $^{29}$Si Spin Relaxation and Localized Electron Spin Dynamics ($n < n_c$)

Previous work [3] has provided strong evidence that localized moments dominate in determining the $^{29}$Si spin lattice relaxation times at low temperatures. These moments constitute an exchange coupled reservoir to which the nuclear spin system is coupled via the dipolar interaction. Hoch and Holcomb [3] have analyzed available $T_1$ results using a model which allows for spin diffusion to the localized moments, which exhibit fluctuations in orientation with a frequency related to the strength of the exchange coupling to neighbouring spins. Frozen spin pairs have been excluded by introducing an effective number of spins in the spirit of the Bhatt–Lee approach to the susceptibility.

Available $T_1$ data, measured at various fields B, at 1.5 K and 13.5 mK were fitted reasonably well by choosing the spectral function for the spin fluctuations to have the form $f(\omega) \propto 1/\omega$ and using calculated values for other quantities, such as the spin diffusion coefficient D.

The best fits were obtained by keeping the diffusion barrier radius, b, constant independent of the field used. Calculations, however, suggest that b should vary as $\ell n$ B.

We now propose that the form of the spectral function can be obtained from the form of the J distribution used by Bhatt and Lee. An outline of the treatment is given below. Converting the J distribution into a $\tau$ distribution and integrating over all correlation times for the unfrozen spins gives

$$J(\omega) = \int_{\hbar/kT}^{\infty} P(\tau)\, J(\omega,\tau)\, d\tau \quad ,$$

with $P(\tau) \propto 1/\tau^{2-\alpha}$. The form of the $J(\omega,\tau)$ may be chosen in various ways corresponding to different possible forms for the correlation function. Our calculations suggest that the form of $J(\omega)$ is not very sensitive to this, and for simplicity, we use an exponential correlation function, leading to a Debye form for $J(\omega,\tau)$. If we put $\alpha = 1$, this leads to $J(\omega) \propto 1/\omega$, as used in the work referred to above. Numerical integration is, in general, necessary for other values of $\alpha$.

For values of $\alpha < 1$, we obtain a spectral function which varies as $1/\omega^{\alpha}$ and therefore more slowly with frequency than the $1/\omega$ form. This permits b to vary when fitting the experimental data. Further details will be published elsewhere.

The approach to the spectral function for an amorphous antiferromagnet, outlined above, is consistent with the ideas of the Bhatt–Lee theory. Susceptibility measurements as a function of n and T and nuclear relaxation measurements as a function of n, B and T can be explained in terms of the properties of the localized fluid component.

## 4. $^{29}$Si Knight Shifts ($n > n_c$)

Knight shifts have previously been measured as a function of dopant concentration n at 4.3 K and 1.5 K [4,5,6] in various magnetic fields. At high concentrations the Knight shifts tend towards the Pauli susceptibility behaviour ($\chi_p \propto n^{1/3}$), as expected for a metal. At lower concentrations the values fall below the Pauli susceptibility predictions.

Using a tight binding approximation based on the approach given by Kaveh and Liebert [7], we have given a semi–quantitative explanation [8] for the observed Knight shift behaviour for both Si:P and Si:(P,B). The delocalized moment fluid determines the Knight shift.

In order to see whether there is any temperature dependence of the Knight shift, we made measurements on two just metallic samples at temperatures down to 50 mK in an Oxford dilution refrigerator. The samples were in the form of a stack of wafers, which were well anchored thermally to the high purity copper tail used in the refrigerator. The field of 1 T was supplied by a high homogeneity superconducting solenoid.

The results are shown in Figure 1.

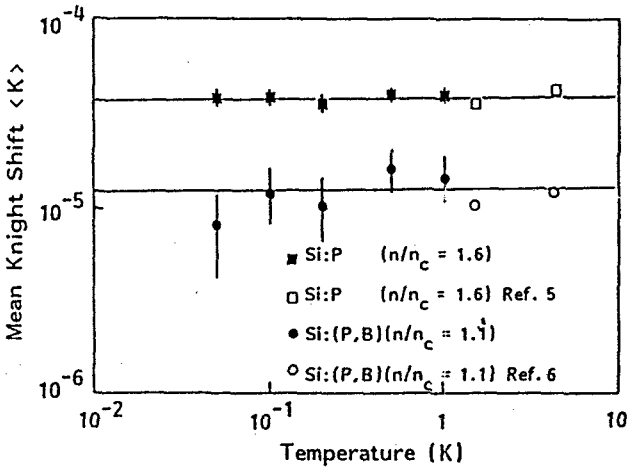


**Figure 1**

**The mean Knight shift for Si:P ($n/n_C$ = 1.6) and Si:(P,B) ($n/n_C$ = 1.1) as a function of temperature down to 50 mK.**

Within experimental uncertainty it can be seen that there is no temperature dependence of the mean Knight shift <K> over the temperature range 4 K – 50 mK for either Si:P or Si:(P,B).

In terms of the two–fluid model this suggests that there are very weak magnetic

interactions between the localized and delocalized spins. The local susceptibility of the delocalized electrons does not change with temperature.

## 5. Conclusion

Measurements of the $^{29}Si$ relaxation rates and Knight shifts as a function of donor concentration, magnetic field and temperature have provided evidence which supports the two–fluid model for the MI transition in Si:P. The $T_1$ measurements provide information on the spin dynamics of the localized moments, while the Knight shifts probe the properties of the delocalized moments.

The relaxation rate results may be interpreted using ideas based on the Bhatt–Lee theory for the magnetic susceptibility. The form of the spectral function for spin fluctuations in the amorphous antiferromagnet system has been deduced using an accepted form for the distribution of exchange couplings.

Knight shifts may be explained using a tight binding model for the delocalized fluid. No temperature dependence of $\langle K \rangle$ has been found over the range 4 K – 50 mK. This may be interpreted to mean that interactions between the two fluids, which occupy spatially distinct regions in the sample, are very weak.

## 6. References

1. H. Alloul and P. Dellouve, Phys. Rev. Lett. **59**, 578 (1987).
   S. Sachdev, R.N. Bhatt and M.A. Paalanen, J. Appl. Phys. **63**, 4285 (1988).
2. R.N. Bhatt and P.A. Lee, Phys. Rev. Lett. **48**, 344 (1982).
3. M.J.R. Hoch and D.F. Holcomb, Phys. Rev. B **38**, 10550 (1988).
4. S. Kobayashi, Y. Fukagawa, S. Ikehata and W. Sasaki, J. Phys. Soc. Jpn. **45**, 1276 (1978).
5. M.J. Hirsch and D.F. Holcomb, Phys. Rev. B **33**, 25201 (1986).
6. M.J.R. Hoch, U. Thomanschefsky and D.F. Holcomb, Physica B **165/166**, 305 (1990).
7. M. Kaveh and A. Liebert, Phil. Mag. Lett. **58**, 247 (1988).
8. S.T. Stoddart and M.J.R. Hoch – to be published in Phys. Rev. B.