Enhanced spin susceptibility in phosphorus-doped silicon

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The influence of the many-valley isotropic effect of the conduction band with a variational N_d dependence on the metal-nonmetal transition of doped semiconductors is investigated further in the calculation of spin susceptibility. A previously developed Gutzwiller method for finite temperature is used. Good agreement with experimental findings is found.

Work to date has concentrated much effort on spin susceptibility χ_s around the metal-nonmetal transition critical point N_c in Si:P.[1] Above N_c, there are up to now the data[2] of Quirt and Marko and the calculation[3] of Chao and Berggren (CB) which show clearly the temperature and donor concentration dependence N_D on χ_s.

In recent works[4] I have shown the influence of the many-valley isotropic effect of the conduction band with a variational N_D dependence of the wave function on the metal-nonmetal transition of doped semiconductors. In this report I show that such a scheme, to some extent, has a remarkable effect on χ_s of Si:P when it is used in the CB approach, which is an extension of the Gutzwiller method for finite temperature. The χ_s obtained is written as

$$\chi_s(T)=\eta_\chi(T)\chi_0(T)\ , \tag{1}$$

where η_χ is an enhancement factor and χ_0 is the Pauli spin susceptibility.[3] CB have used an anisotropic wave function and adjusted the intradonor Coulomb interac-

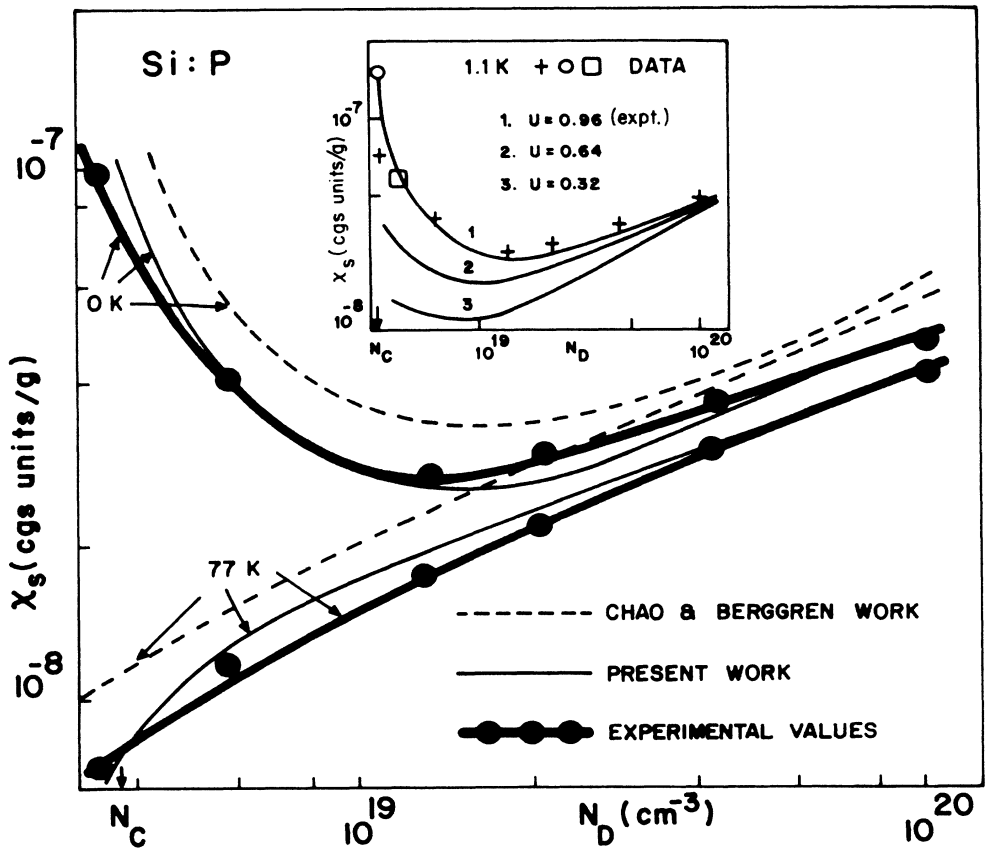

FIG. 1. χ_s as a function of N_D. Inset for $T=1.1$ K; □, Ref. 1; +, Ref. 2; ○, Ref. 12; ——, present work.

tion or correlation energy[5–7] U in order to get the experimental N_c. Here the calculation for χ_s is performed, in the wake of the CB approach, but for the experimental U within the former above scheme.[4,8,9] In Fig. 1 a reasonable fitting with experimental data[2] found for χ_s is shown as a function of N_D. From the metallic side, metal-nonmetal transition takes place when the number of doubly occupied sites is zero. I find $N_c = 3.5 \times 10^{18}$ cm^{-3} while the experiment is 3.7×10^{18} cm^{-3}.[10] I also show, in the inset, the results of χ_s for 1.1 K, as well as its dependence on U.[11] The χ_s shows good agreement when compared to the available experimental data.[2,12] I expect that such results may motivate in the future a more thorough treatment along the concentration region presented.

[1]D. F. Holcomb, in *Localization and Interaction in Disordered Metals and Doped Semiconductors,* edited by D. M. FinLayson (Scottish Universities Summer School in Physics, Edinburgh, 1986), p. 313.

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[3]K. A. Chao and K.-F. Berggren, Phys. Rev. Lett. **34**, 880 (1975).

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[5]J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963); **281**, 401 (1964).

[6]The correlation energy U in the isotropic case of hydrogen donor gives $U \simeq 0.63e^2/\kappa a$, where κ is the dielectric constant and a the donor wave-function radius.

[7]See, e.g., J. C. Slater, *Quantum Theory of Molecules and Solids* (McGraw-Hill, New York, 1968), Vol. I, p. 58.

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[9]The experimental value of U is $U \simeq 0.96E_D$ (E_D being the ionization energy of the system considered). The ratio U/E_D is rather insensitive to mass anisotropic (cf. Ref. 8).

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[11]That is in effect an enhancement of χ_s due to U. The values of U are obtained from Refs. 6 and 9, and a lower value of them is used for the sake of comparison.

[12]S. Ikehata and S. Kobayashi, Solid State Commun. **56**, 607 (1985).