Spin susceptibility and effective mass in shallow doubly doped semiconductor systems

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In light of a recent investigation of the conductivity and metal-insulator transition in the shallow double donor Si:P,As, the spin susceptibility $\chi$, and effective mass $m^*$ of the systems Si:P,As and Si:P,Sb have been calculated. The electronic systems are described by a Gutzwiller scheme to finite temperature. The results for the doubly doped systems predict an enhancement of $m^*$ and $\chi$, similar to that of the single-donor system Si:P in the vicinity of the transition.

The spin susceptibility $\chi$, effective mass $m^*$, and metal-insulator (MI) transition have been widely studied in recent years for single-donor states in doped semiconductors, and yet the nature of the state near the transition remains unclear. Recently Newman and Holcomb (NH) reported measurements of electrical conductivity in the shallow double-donor system Si:P,As and found its critical concentration $N_c$ for the MI transition between the $N_c$ of the shallow single-donor system Si:P and Si:As. In the wake of their measurements we have worked out a single method that provides an $N_c$ for the MI transition, a first step to study further these doubly doped systems, which have a merit of increasing disorder because of the different impurity binding energies present in them.

In a real system the impurities will, of course, be randomly distributed, but we shall ignore this randomness and assume that the impurities are distributed over a regular lattice (sc, fcc, bcc, and diamond) (Refs. 7–11) of the host material (i.e., silicon in our case), and then average these different arrangements of the impurities as well as the different type of hopping integrals $T_{i,j}$, which appear in the calculation. The randomness produces band tailing and as a result the MI transition will be at a lower concentration.

The method used in our calculation for $\chi$, and effective mass was illuminated in part by the Chao and Berggren (CB) formulation for spin susceptibility in the shallow single-donor system Si:P in terms of the Gutzwiller variational treatment to finite temperature. Such formulation has led Ferreira da Silva to find a good scheme for $\chi$, which gives a satisfactory agreement between theory and experiment.

Following the CB scheme we may find the spin susceptibility at finite temperature $\chi(T)$ as

$$\chi(T) = \eta(T) \chi_0(T),$$

where $\chi_0(T)$ is the Pauli spin susceptibility and $\eta(T)$ is

![Image](image.png)

FIG. 1. Effective mass $m^*/m_0$ as a function of concentration $N$ at $T = 1.1$ K. Solid curves correspond to the present calculations. Solid circles correspond to observed values of Ref. 26.

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the enhancement factor

\[ \eta_s(T) = D(T)^{-1} \left( 1 - \frac{\chi_s(T) U [1 + U/2U_0(T)]}{2\mu_B^2 [1 + U/U_0(T)]} \right)^{-1} \]  

(2)

In Eq. (2) \( U \) is the intradonor Coulomb interaction or correlation energy, given by the experimental value \( U = 0.96E_B \) \( (E_B \) being the ionization energy of the system considered).\(^{22}\) \( \mu_B \) is the Bohr magnetron, \( U_0(T) \) is a critical correlation energy as a function of the free energy at \( U = 0 \), and \( D(T)^{-1} \) is identified as the effective mass.\(^{15,17}\)

\[ m^*/m_0 = D(T)^{-1} = [1 - (U/U_0(T))^2]^{-1} \]

(3)

where \( m_0 \) is the bare band mass.

The electronic effective mass will enhance \( \chi_s(T) \) as the MI is approached from the metallic side, with a dependence on the Hubbard \( U \).\(^{22}\) The quantities \( \chi_s(T) \) and \( U_0(T) \) are also dependent on the hopping energy.\(^{13}\) In our scheme we define the hopping integrals for doubly doped systems as \( T_{ij}^{\alpha,\beta} \), with adjacent sites \( i \) and \( j \) and screened parameters \( \alpha \) and \( \beta \). These latest parameters, \( \alpha \) and \( \beta \), are defined for two different kinds of donors, with differing values of the impurity binding energy, \( E_B \), i.e., \( \alpha = 1/a_s^* \) and \( \beta = 1/a_p^* \), where \( a_s^* = e^2/2\pi\epsilon\epsilon_0 E_B \) is the effective Bohr radius for a system like Si:X, with \( X = \text{Sb}, \text{P}, \text{or As} \). \( T_{ij}^{\alpha,\beta} \) are defined by

\[ T_{ij}^{\alpha,\beta} = \int \psi_i^* (r) H_1 \psi_j (r) d^3r \]

(4)

where \( H_1 \) is the one-particle Hamiltonian including the kinetic-energy operator and the electron-donor interaction. Here the wave function is written as\(^{6,9,11,23,24}\)

\[ \psi_i^*(r) = \frac{1}{\sqrt{V}} \sum_{l=1}^{\nu} F_{il}^*(r - R_l) \phi_l (r) \]

(5)

for the ground state associated with \( \nu \) equivalent conduction-band minima (\( \nu = 6 \) for Si). \( \phi_l \) is the Bloch function at the \( l \)th minima and \( F_{il} \) are the screened hydrogenic wave functions. Equation (4) can be scaled to the binding energy \( E_B \) of Si:P and written as

\[ S^{\alpha,\beta} = S^{\beta,\alpha} = \frac{8y^{5/2}}{(1 - y^2)^2} \left[ 1 + \exp(1 - y)R^* + \frac{1 - \exp(1 - y)R^*}{(1 - y^2)R^*} \right] \exp(-R^*) \]

(8)

and

\[ K^{\alpha,\beta} = \frac{4y^{1/2}}{(1 - y^2)} \left[ 1 + \frac{2[1 - \exp(1 - y)R^*]}{(1 - y^2)R^*} \right] \exp(-R^*) \]

(9)

and

\[ K^{\beta,\alpha} = \frac{4y^{1/2}}{(y^2 - 1)} \left[ 1 + \frac{2y[1 - \exp(y - 1)R]}{(y^2 - 1)R^*} \right] \exp(-R^*) \]

(10)

where \( y = a_s^*/a_p^* \) (i.e., the ratio of the different impurity binding energies), \( R^* = R/a_s^* \), and \( R^* = R/a_p^* \), \( R \) being the separation between donor states.

For \( y \to 1 \) Eqs. (8) and (9) reduce to the very well known Slater's integrals\(^{15}\) \( S = (1 + w + w^*/3) \exp(-w) \) and \( K = (1 + w) \exp(-w) \), where \( w = R/a_s^* \). Then the calculation turns out to be for a single-donor system like Si:P or Si:As.

The calculations are performed, for both Si:P,As and Si:P,Sb (as well as for Si:P) assuming an average in Eq. (6)
due to the oscillating term $I$, as well as the different arrangements of the donors and different types of hoppings (i.e., $T^{a,a}$, $T^{a,b}$, $T^{b,a}$, $T^{b,b}$). It is worth mentioning that the different binding energies introduced by a double-donor system give a different hopping energy when compared to a single-donor system, e.g., at a certain concentration the bandwidths are different and certainly will be the shape of the impurity bands for both systems, which lead to different $\chi(T)$, $m/m_0$, and $N_c$.

The results for the effective mass $m/m_0$ at $T = 1.1$ K are shown in Fig. 1 for different systems. The qualitative agreement between theory and experiment for Si:P is satisfactory. In Fig. 2 we show the spin susceptibility $\chi_s(T)$ for the same systems presented in Fig. 1. A good agreement with the existing data for $T = 1.1$ K is found for Si:P. The MI transitions take place at $N_c(Si:P) = 3.2 \times 10^{18}$ cm$^{-3}$, $N_c(Si:P) = 3.5 \times 10^{16}$ cm$^{-3}$, and $N_c(Si:P,As) = 4.5 \times 10^{18}$ cm$^{-3}$. The experimental values for the two latest $N_c$ are $3.7 \times 10^{18}$ cm$^{-3}$ and $5.1 \times 10^{18}$ cm$^{-3}$, respectively. In a Mott-Hubbard picture we found $3.4 \times 10^{18}$ cm$^{-3}$ and $4.6 \times 10^{18}$ cm$^{-3}$, respectively. These quantities lead to a transition in the following order: $N_c(Si:P,Sb) < N_c(Si:P) < N_c(Si:P,As)$. For $\chi_s$ and $m/m_0$ we also observe an enhancement around $N_c$ as $(m/m_0)(Si:P,Sb) < (m/m_0)(Si:P) < (m/m_0)(Si:P,As)$. The parameters used in the calculation were compiled from Refs. 6, 11, and 30. Further experimental and theoretical works on these doubly doped systems could be of interest to test the model.

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