Electron and impurity correlations in doped semiconductors

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The recent theory of Ferreira da Silva *et al.* for the specific heat of doped semiconductors, described by the Hubbard model with a random-transfer integral, has been studied in the presence of a magnetic field and impurity correlations, incorporated through a hard-core pair-correlation function. The low-temperature specific heat and the zero-temperature susceptibility of uncompensated phosphorus-doped silicon have been calculated as a function of the impurity concentration. It is found that both electron and impurity correlations enhance the susceptibility and quench the specific heat. The behavior of the relative change in the specific heat due to the magnetic field agrees qualitatively with the low-temperature experimental results.

It is well established that in the metal-nonmetal transition of doped semiconductors, both the electron correlations and the disorder play an essential role.[1] However, the degree of their interplay depends on the impurity concentration. For example, at very low concentrations in which impurities are isolated from each other, and at high concentrations in which all states are extended and the system behaves as a metal, electron correlations dominate over disorder.[2] At intermediate concentrations where the density of states at the Fermi level is finite but the system is nonmetallic because of the localization of the single-particle states, both the electron correlations and the disorder are equally important.[3,4] Theoretical treatments which take into account both the electron correlations and the disorder on an equal footing are based on the Mott-Hubbard model.[1,5] The recent theory of Ferreira da Silva *et al.*[3] for the specific heat, based on this model with a completely random distribution of impurities, agrees well with experiments at intermediate concentrations. In this paper we extend their study in the presence of a magnetic field and calculate the specific heat as well as the susceptibility of uncompensated phosphorus-doped silicon (Si:P), taking into account the impurity correlations neglected by them.

In the presence of a magnetic field H, the Hubbard Hamiltonian with random transfer integral can be written as[3]

$$\mathcal{H}=\sum_{ij\sigma}(V_{ij}-\sigma H\delta_{ij})a_{i\sigma}^{\dagger}a_{j\sigma}+\frac{U}{2}\sum_{i\sigma}n_{i\sigma}n_{i-\sigma} \quad . \tag{1}$$

All the symbols in Eq. (1) are the same as that of Ferreira da Silva *et al.*[3] For the Hamiltonian (1), the configurationally averaged single-particle Green's functions take the form

$$\langle G_{ii\sigma}^{\pm}(\omega)\rangle_{\text{av}}=\frac{n_{-\sigma}^{\pm}}{\omega^{\pm}+\sigma H}\zeta(\omega^{\pm}+\sigma H) \quad , \tag{2}$$

where $\zeta(\omega)$ is given by the self-consistent equation

$$\frac{1}{\zeta(\omega)}=1-\frac{N\zeta(\omega)}{8\pi^2\omega^2}\int\frac{V^2(\vec{k})\,d\vec{k}}{1-[N\zeta(\omega)/\omega^2]\,V(\vec{k})} \quad , \tag{3}$$

and $\omega^{\pm}=\omega-(U/2)(1\pm1)$, N is the impurity concentration, and the Fourier transform $V(\vec{k})$ is

$$V(\vec{k})=\int V(\vec{R})g(\vec{R})e^{i\vec{k}\cdot\vec{R}}\,d\vec{R} \quad . \tag{4}$$

Here $V(\vec{R})\equiv V(\vec{R}_{ij})\equiv V_{ij}$ and $g(\vec{R})$, the impurity pair-correlation function, takes into account the effect of the impurity correlations.[6] For a completely random distribution of the impurities, considered by Ferreira da Silva *et al.*,[3] $g(R)=1$. In our calculation we assume that the hard-core impurity pair correlation $g(R)$, is such that $g(R)=1$ for $R>R_0$ and zero for $R<R_0$, where R_0 is the hard-core radius.

The specific heat and the susceptibility can be expressed in terms of the density of states[3]

$$D_{\sigma}^{\pm}(\omega)=-\frac{N}{\pi}\text{Im}\langle G_{ii\sigma}^{\pm}(\omega)\rangle_{\text{av}} \quad , \tag{5}$$

which, from Eq. (2), can be rewritten as

$$D_{\sigma}^{\pm}(\omega)=n^{\pm}D_0(\omega^{\pm}+\sigma H)\pm\sigma m D_0(\omega^{\pm}+\sigma H) \quad , \tag{6}$$

where $D_0(\omega)$ is the noninteraction electron density of states

$$D_0(\omega)=-\frac{N}{\pi}\text{Im}\left[\frac{\zeta(\omega)}{\omega}\right] \quad , \tag{7}$$

$$m=\sum_{\sigma}\sigma n_{\sigma} \tag{8}$$

is proportional to the magnetic moment per impurity, and $n^{+}\equiv\frac{1}{2}\sum_{\sigma}n_{\sigma}$, $n^{-}=1-\frac{1}{2}\sum_{\sigma}n_{\sigma}$. The number of electron per impurity with spin σ, n_{σ} appearing in the expressions for m and $n^{\pm}$ can be obtained from the relation[3,7]

$$n_{\sigma}=\frac{1}{N}\int_{-\infty}^{\infty}[D_{\sigma}^{+}(\omega)+D_{\sigma}^{-}(\omega)]f(\omega)\,d\omega \quad , \tag{9}$$

where $f(\omega)$ is the Fermi distribution function. On substituting Eq. (9) in Eq. (8) and then using Eq. (6) for $D_\sigma^\pm(\omega)$, we get

$$m=\frac{(1/N)\sum_\sigma\sum_{p=\pm}\sigma n^p\int_{-\infty}^{\infty}D_0(\omega^p+\sigma H)f(\omega)\,d\omega}{1+(1/N)\sum_\sigma\sum_{p=\pm}p\int_{-\infty}^{\infty}D_0(\omega^p+\sigma H)f(\omega)\,d\omega} \tag{10}$$

which, on expanding as a function of the magnetic field H, gives the susceptibility

$$\chi=\lim_{H\to 0}\frac{N\mu_B m}{H}=\frac{2\mu_B\sum_p n^p\int_{-\infty}^{\infty}D_0'(\omega^p)f(\omega)\,d\omega}{1+(2/N)\sum_p p\int_{-\infty}^{\infty}D_0(\omega^p)f(\omega)\,d\omega}\ , \tag{11}$$

where the prime in $D_0(\omega^p)$ denotes the first derivation.

The specific heat is obtained from the configurationally averaged energy[13]

$$\bar{E}=\int_{-\infty}^{\infty}\left[\omega D(\omega)-\frac{U}{2}D^+(\omega)\right]f(\omega)\,d\omega\ , \tag{12}$$

where

$$D(\omega)=\sum_p D^p(\omega)=\sum_p\sum_\sigma D_\sigma^p(\omega)\ . \tag{13}$$

By expanding the energy (12) in power of temperature T, we get the low-temperature specific heat as

$$C_v\equiv\frac{d\bar{E}}{dT}=\gamma T\ , \tag{14}$$

where

$$\gamma=\frac{\pi^2k^2}{3}\left[D(\epsilon_F)-\frac{U}{2}\left(D^{+\prime}(\epsilon_F)-\frac{D^+(\epsilon_F)D'(\epsilon_F)}{D(\epsilon_F)}\right)\right]_{T\to 0}-\frac{6m_1}{\pi^2k^2}\sum_\sigma\sigma\int_{-\infty}^{\epsilon_F}\left[\omega\sum_p pD_0(\omega^p+\sigma H)-\frac{U}{2}D_0(\omega^++\sigma H)\right]d\omega \tag{15}$$

ϵ_F denotes the Fermi energy and the coefficient m_1 comes from the low-temperature expansion of m as

$$m=m(T=0)+m_1T^2 \tag{16}$$

with

$$m_1=\frac{(1/N)\sum_{\sigma p=\pm}\sigma n^pB_\sigma^p+(1/N)\sum_{\substack{\sigma p\\ \sigma' p'}}(p\sigma' n^{p'}-p'\sigma n^p)A_\sigma^pB_{\sigma'}^{p'}}{\left[1+(1/N)\sum_{\sigma p}pA_\sigma^p\right]^2}\ , \tag{17}$$

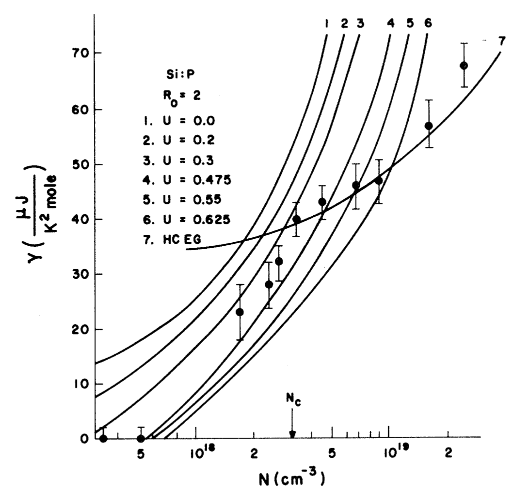

FIG. 1. Electronic specific-heat coefficient γ for Si:P as a function of the impurity concentration N for various values of electron correlation parameter U and hard-core radius $R_0=2$. Curve 7 (Ref. 10) is the HCEG calculation. The solid circles with error bars are the experimental data measured by Sasaki and co-workers (Ref. 8). N_c indicates the impurity critical concentrations.

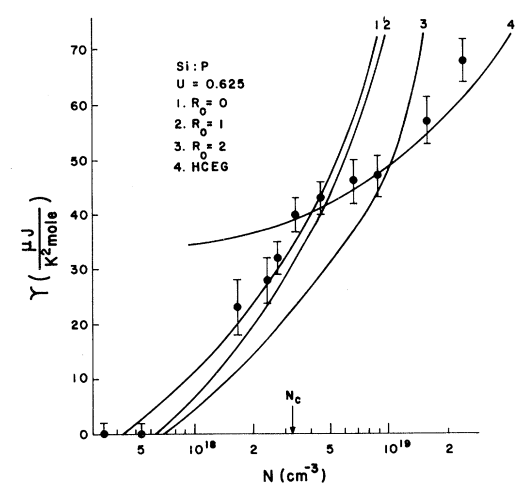

FIG. 2. Same as Fig. 1 for γ as a function of N for various values of R_0 and with a $U=0.625$.

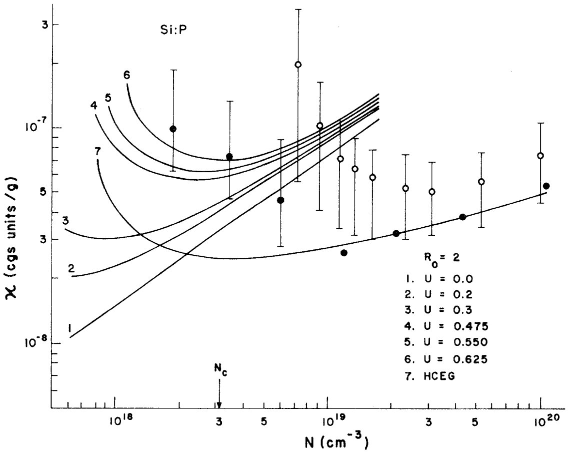

FIG. 3. Spin susceptibility χ of Si:P as function of the impurity concentration N for various values of U with $R_0=2$. Curve 7 (Ref. 11) and the open circles with error bars (Ref. 12) are the results from the HCEG model. The solid circles are the experimental data (Ref. 9) extrapolated to $T=0$ K.

where

$$A^p_\sigma = \int_{-\infty}^{\epsilon_F} D_0(\omega^p+\sigma H)\,d\omega \tag{18}$$

and

$$B^p = \frac{\pi^2 k^2}{6}\left[D_0'(\omega^p+\sigma H) - D_0(\omega^p+\sigma H)\left(\frac{D'(\epsilon_F)}{D(\epsilon_F)}\right)_{T=0}\right] . \tag{19}$$

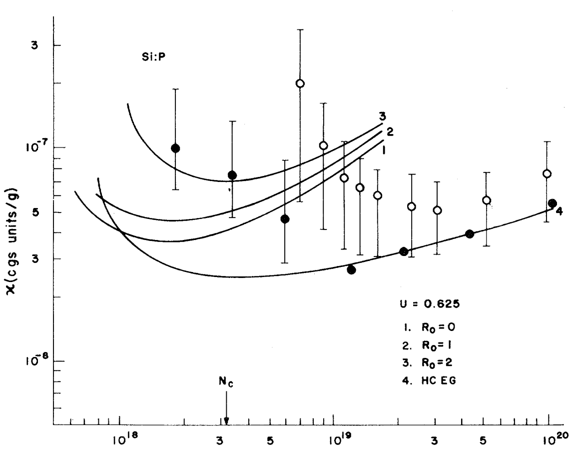

FIG. 4. Same as Fig. 3 for χ as a function of N for various values of R_0 with $U=0.625$.

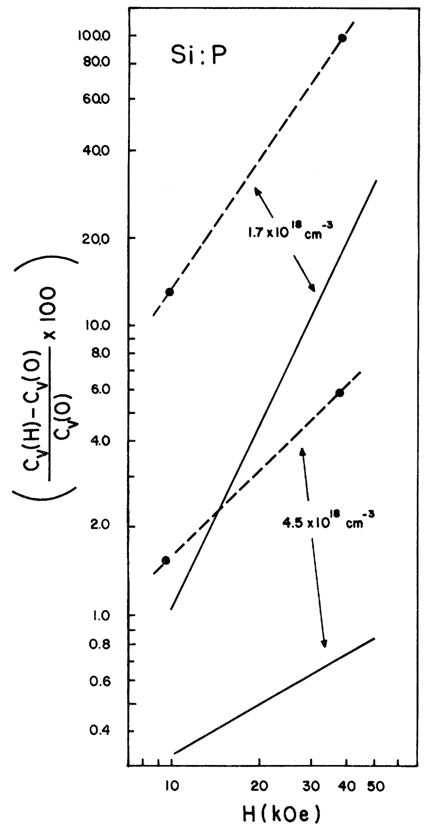

FIG. 5. Relative change in the specific heat of Si:P due to magnetic field for concentrations of 1.7×10^{18} and 4.5×10^{18} cm^{-3}. Solid circles are the experimental points of Kobayashi *et al.* (Ref. 13) at $T=1.6$ K.

We have calculated the zero-temperature susceptibility from Eq. (11) and γ from Eq. (15) together with Eqs. (16) and (17) in the absence of magnetic fields ($H=0$) as a function of the impurity concentration for various values of the electron correlation parameters U and the hard-core radius R_0. Figures 1 and 2 for the specific heat of Si:P show that both electron and impurity correlations have a tendency to reduce the specific heat for a given concentration. On the other hand, the susceptibility shown in Figs. 3 and 4 is enhanced by both of these correlations. Also, we should note that as the impurity concentration increases, the tendency of reduction in the specific heat increases while the tendency of enhancement of the susceptibility decreases. For the sake of comparison, we have also shown the experimental points[8,9] and the theoretical results of highly correlated electron gas (HCEG) model.[10–12] In Fig. 5, the relative changes in the specific heat due to magnetic field have been shown. Our calculations are in qualitative agreement with the low-temperature experimental results of Kobayashi *et al.*[13]

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