

IMPURITY SELF-SCREENING*

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In a mixed valence impurity system the distribution of impurity charges can be adjusted to minimize the Coulomb energy of inter-impurity interactions. In this paper we discuss the possibility of extending the methods of analytical evaluation of the pair correlation function for classical liquids to apply to a system with a built-in disorder, where the occupation probability is governed by the Fermi-Dirac statistics.

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In order to describe most of the correlation effects occurring in many body systems Monte Carlo simulations are necessary. In some cases, however, analytical approximations can be successfully used. In this way classical liquids of particles interacting via various types of potentials were studied [1]. In the case of correlated occupancy of mixed valence impurities in a semiconductor the classical approximation cannot be applied and the Fermi-Dirac statistics must be used. As a consequence, the higher order correlation functions cannot be easily approximated with the use of correlation functions of the lower order. In particular, for quantum statistics, the probability that an impurity center, with two other impurities in its neighborhood, is occupied cannot be expressed as a simple product of the pair correlation functions corresponding to the neighbors. Moreover, in the case of impurities which are fixed at random sites in the crystal matrix a complete ordering of the impurity charges is not possible. This built-in disorder must be taken into consideration [2].

In this paper we present introductory results of analytical evaluation of the pair correlation function for partially occupied donors. We present the basic equations. Next, the weak correlation approach is examined. Generally, the occupation probability can be expressed by the pair correlation function, $g(r)$:

$$g(r) = \frac{N_D}{n_{D+}} \int_{-\infty}^{\infty} \rho(E + V(r)) [1 - f(E)] dE, \quad (1)$$

where r is the distance from the charged donor, N_D is the donor concentration, n_{D+} is the ionized donor concentration, and ρ is the impurity density of states (DOS) distribution function. V is the mean value of the electrostatic potential given by

$$V(r) = \frac{e^2}{\epsilon r} \exp(-r/\lambda) + \frac{n_{D+} e^2}{\epsilon} \int [g(r + \mathbf{R}) - 1] \frac{\exp(-R/\lambda)}{R} d^3 R, \quad (2)$$

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where λ is the Thomas-Fermi screening radius induced by conduction electrons.

The set of Eqs. (1) and (2) cannot be solved as long as the distribution function of the density of states, $\rho(E, r)$, which is also distance-dependent, is not defined. Some parameters of the distribution, e.g., the mean energy values for occupied and empty states, could be determined from the pair correlation function [2]. To obtain higher moments of the distribution, however, higher order pair correlation functions are needed and they cannot be easily found.

One of the approaches to this problem is to make some assumptions concerning DOS. In the case of weak correlation, when the background fluctuations of the local potential or of the donor energy are much greater than the Coulomb potential fluctuations coming from the analyzed donors, one can assume a fixed, distance-independent DOS distribution. This allows to solve the set of Eqs. (1) and (2). The results for a Gaussian distribution of DOS, with a fixed second moment are presented below.

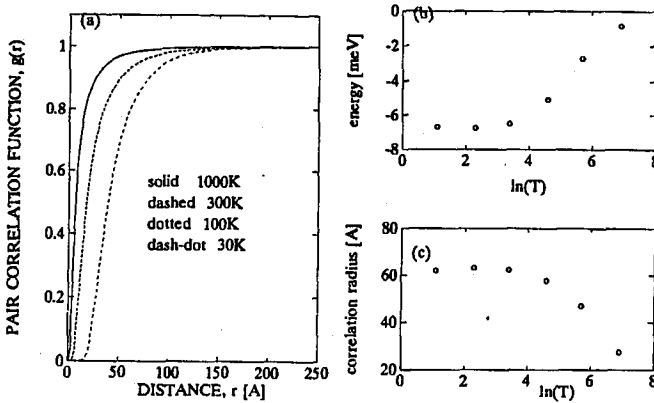


Fig. 1. The temperature dependence of the correlation for donor concentration $N_D = 10^{18} \text{ cm}^{-3}$, $\lambda = 60 \text{ \AA}$, $\sigma = 10 \text{ meV}$ and filling factor $f = 0.5$. (a) The pair correlation function for various temperatures. (b) Temperature dependence of the correlation energy, E_c . (c) Variation of the correlation radius, r_c .

Figure 1a shows the temperature variation of the pair correlation function for a fixed filling factor of the donor level, $f = n_{D+}/N = 1/2$. The value of λ was assumed to be equal to 60 \AA and built-in fluctuations $\sigma = 10 \text{ meV}$. Figure 1b presents the temperature dependence of the correlation energy (per charged impurity) defined as

$$E_c = \frac{n_{D+} e^2}{\epsilon} \int [g(r) - 1] \frac{\exp(-r/\lambda)}{r} d^3 r. \quad (3)$$

The temperature dependence of the correlation radius, r_c , which is defined by the volume in which the self-screening charge of impurities is distributed, is shown in Fig. 1c. The correlation radius and the screening charge, q_s , are given by the

equations

$$\frac{q_s}{n_{D+}} = \frac{4}{3}\pi r_c^3 = \int [g(r) - 1] d^3r. \quad (4)$$

There is no visible change of the correlation effects below 30 K. In this temperature range the integrated screening charge, q_s , is about $0.5e$. At increased temperatures a systematic weakening of the spatial correlation effects is seen. The correlation energy, E_c , correlation radius, r_c , and the screening charge, q_s , decrease. This behaviour corresponds to the results of the Monte Carlo simulation [3].

For low impurity concentrations, the pair correlation function weakly depends on the concentration, owing to the fact that in the potential $V(r)$ (Eq.(2)) the first term dominates. The correlation radius is almost constant and, in consequence, the screening charge is approximately proportional to the concentration. However, at high concentrations the screening charge saturates as it cannot exceed unity. But for high concentrations the weak correlation approach is no longer valid and the existence of the Coulomb gap in DOS cannot be omitted.

The proposed approach is a considerable improvement as compared to the simple step-like approach for the pair correlation function [4]. It allows us to analyze charge correlation at high temperatures. It is also much easier than numerical simulations and simple enough to study realistic cases where more than one type of impurities interact with each other.

References

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