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Density of states of systems with randomly distributed donor monovalent impurities in two dimensions: an analytical treatment

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Abstract. Analytical calculations are made for a two-dimensional (2D) disordered system in order to obtain the impurity density of states. It is shown that the impurity band is roughly symmetric and has no long low-energy tail, contrary to a three-dimensional system. The results are in agreement with the previous numerical calculations by Ferreira da Silva and Fabbri and are compared with other 2D models.

The problem of two-dimensional (2D) disordered systems is a subject of current interest, especially in connection with the study of the electronic properties where a change in the dimensionality (i.e. from three-dimensional (3D) to a 2D system) leads to the poorly understood metal-to-non-metal transition. A technique for investigating the problem of spatial disorder has been introduced by Matsubara and Toyozawa (MT) (1961), which has enabled calculations of the density of states and conductivity of doped semiconductors to be made utilising a Green function approach. Calculations were carried out analytically for 3D systems with sufficient merit to warrant closer inspection in 2D. Following their scheme, Debney (1976, 1977), using a 3D electron hopping energy integral V_{ij} , calculated numerically (Kikuchi 1974) and analytically the 2D density of states. Considering this type of pure off-diagonal disorder numerically, he found that an Anderson transition does take place at a critical concentration given by $N^{1/2}a_H = 0.364$ (N being the concentration and a_H the effective Bohr radius). The type of disorder that he found in his work has caused some discussion (Mott 1978, Thouless 1978). Weaire and Srivastava (1977), Economou and Antoniou (1977), Hoshino and Watanabe (1977), Tsujino *et al* (1979), Yonezawa (1980) and Fertis *et al* (1981) found that the pure off-diagonal disorder cannot localise states, e.g. at the centre of the band (Fabbri and Ferreira da Silva 1983a, b). It is by now clear that the discrepancy between the work of Debney and those cited above is due to the different types of hopping matrix element V_{ij} used.

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In this paper we perform an analytical calculation with a proper 2D V_{ij} and its Fourier transform in order to obtain the 2D density of states for disordered systems. The disorder is according to the MT scheme. We show that the 2D density of states does not present a long low-energy tail nor strong asymmetry, both of which appeared in Debney's calculation. The results obtained are in accord with our previous numerical calculation (Ferreira da Silva and Fabbri (1984), hereafter referred to as I) and we found some similarity to the results obtained by Puri and Odagaki (1981).

For doped semiconductors with monovalent impurities, the Hamiltonian in a random one-body tight-binding approximation is taken to be

$$H = \sum_i E_i a_i^\dagger a_i + \sum_{i \neq j} V_{ij} a_i^\dagger a_j = E_d \sum_i a_i^\dagger a_i + \sum_{i \neq j} V_{ij} a_i^\dagger a_j \quad (1)$$

for a single impurity band, where a_i^\dagger and a_i respectively, are the creation and the annihilation operators of an electron at the i th impurity site. In the absence of compensation, the diagonal matrix element $\{E_i\}$ can be assumed to be independent of i (Chao and Ferreira da Silva 1979, Ferreira da Silva 1980, Ferreira da Silva *et al* 1983). As measured from the host conduction band, it can be taken as $E_d = \varepsilon_1$ ($= -2.0$ effective Hartrees, in a 2D system (according to I), the ionisation energy of an isolated impurity. In this work, we take this as our energy origin. Each of the off-diagonal matrix elements V_{ij} depends mainly on the relative distance R_{ij} between the site i and the site j . The 2D V_{ij} between two hydrogenic 1s orbitals is obtained as (see I[†])

$$V_{ij} = -2V_0 R_{ij} K_1(2R_{ij}) = -8R_{ij} K_1(2R_{ij}) \quad (2)$$

where $V_0 = 2|E_d|$ and K_1 is the modified Bessel function of first order.

The density of states, as in the original MT scheme, is calculated from the Green functions, whose matrix elements in the site representation are defined as

$$G_{mn}^\pm(E) = \langle 0 | a_m (E - H \pm i\varepsilon)^{-1} a_n^\dagger | 0 \rangle \quad (3)$$

$$G_{mn}(E) = (i/2\pi)[G_{mn}^+(E) - G_{mn}^-(E)]. \quad (4)$$

It is convenient to define

$$\xi^\pm = w_\pm \overline{G_{mn}^\pm(E)} = (1 - \eta^\pm)^{-1} \quad (5)$$

where the bar indicates configuration averaging, and $w_\pm = E \pm i\varepsilon$. Here we shall drop the superscripts (\pm) as no confusion can arise, since the analysis is equally valid for either Green function. Then ξ satisfies the adapted original MT equation for two dimensions:

$$\eta = 1 - \frac{1}{\xi} = \frac{1}{(2\pi)^2} \frac{N\xi}{w^2} \int \frac{v(\mathbf{k})^2 d^2k}{1 - (N\xi/w)v(\mathbf{k})} \quad (6)$$

where N is the impurity concentration per square centimetre and $v(\mathbf{k})$ is the 2D Fourier transform of V_{ij} (equation (2)) obtained as (see I)

$$v(\mathbf{k}) = -64\pi V_0 a_{\text{H}}^2 / 4(4 + k^2 a_{\text{H}}^2)^2. \quad (7)$$

Equation (6) can be rewritten, in Hartree units, as

$$w - \frac{w}{\xi} = \frac{1}{(2\pi)^2} \int \frac{v(\mathbf{k}) d^2k}{1 - (N\xi/w)v(\mathbf{k})} + 1. \quad (8)$$

[†] In this previous work, because of a typing error, figures 1 and 4 should be in hartrees, and equations (5) and (11) should be compared with equations (2) and (7), respectively, in the present paper.

Defining

$$P = 16\pi N\alpha^{-2} \quad (9)$$

as the dimensionless impurity concentration, and

$$X = -P\xi/w \quad (10)$$

and using equation (7), in hartrees, as

$$v(\mathbf{k}) = -16\pi\alpha^2/(\alpha^2 + k^2)^2 \quad (11)$$

where $\alpha = 2/a_H$, we can rewrite equation (8) as

$$w = 1 - P/X - 4I(X) \quad (12)$$

where

$$I(X) = \int_0^\infty \frac{2k dk}{(1+k^2)^2 - X}. \quad (13)$$

By writing

$$X = X_0 \exp(i\theta) \quad (14)$$

where $0 < \theta < \pi$ for G_{ii}^+ and $-\pi < \theta < 0$ for G_{ii}^- , we easily obtain

$$I(X) = (1/2X^{1/2}) (\ln R_0 + i\varphi) \quad (15)$$

where

$$R_0 = \{[1 + X_0^{1/2} \cos(\theta/2)]^2 + X_0 \sin^2(\theta/2)\} / \{[1 - X_0^{1/2} \cos(\theta/2)]^2 + X_0 \sin^2(\theta/2)\}^{1/2} \quad (16)$$

$$\varphi = \varphi_F^+ + \varphi_F^- + \pi \quad (17)$$

and

$$\tan(\varphi_F^\pm) = -[1 \mp X_0^{1/2} \cos(\theta/2)] / X_0^{1/2} \sin(\theta/2). \quad (18)$$

Then, the self-consistent equation (12) is written as

$$w = 1 - (P/X_0)(\cos \theta - i \sin \theta) - (1/2X_0^{1/2})[\cos(\theta/2) - i \sin(\theta/2)](\ln R_0 + i\varphi). \quad (19)$$

From the real and imaginary parts we obtain the following equations:

$$w = 1 - (P/X_0) \cos \theta - (1/2X_0^{1/2})[\cos(\theta/2) \ln R_0 + \varphi \sin(\theta/2)] \quad (20)$$

and

$$(P/X_0) \sin \theta = (1/2X_0^{1/2})[\varphi \cos(\theta/2) - \ln R_0 \sin(\theta/2)]. \quad (21)$$

Varying θ , we obtain the X_0 -values which satisfy equation (21), for a given value of P and, from equation (20), we obtain the corresponding energies. The density of states is given by $D(E) = -(N/\pi) \text{Im}[G_{ii}^+]$ and is obtained as

$$D(E) = -(N/\pi) \text{Im}(\xi/E) = (N/P\pi) \text{Im} X = (1/4\pi^2 a_H^2) X_0 \sin \theta. \quad (22)$$

The results for the 2D impurity density of states are shown in figure 1, for $N^{1/2}a_H = 0.24$ and 0.12. As the impurity concentration decreases, the band becomes narrower and more symmetric, with no long-band tailing on the low-energy side as observed in

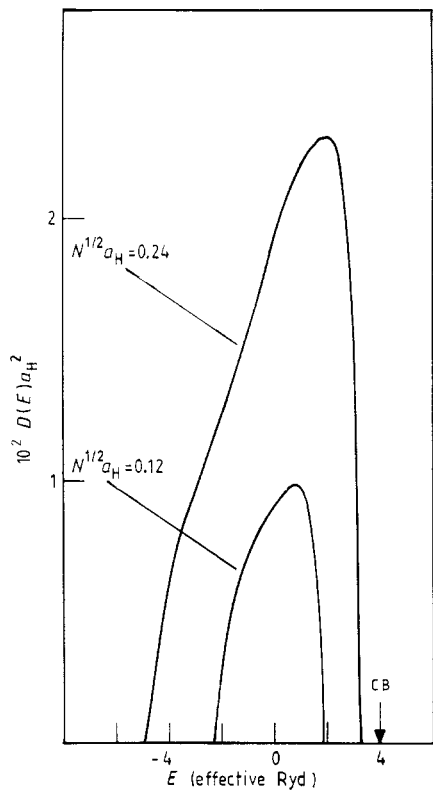


Figure 1. The 2D density of states for two values of $N^{1/2}a_H$. E_d is set at the origin. The bottom of the conduction band (CB) is set at 4.0 effective ryd.

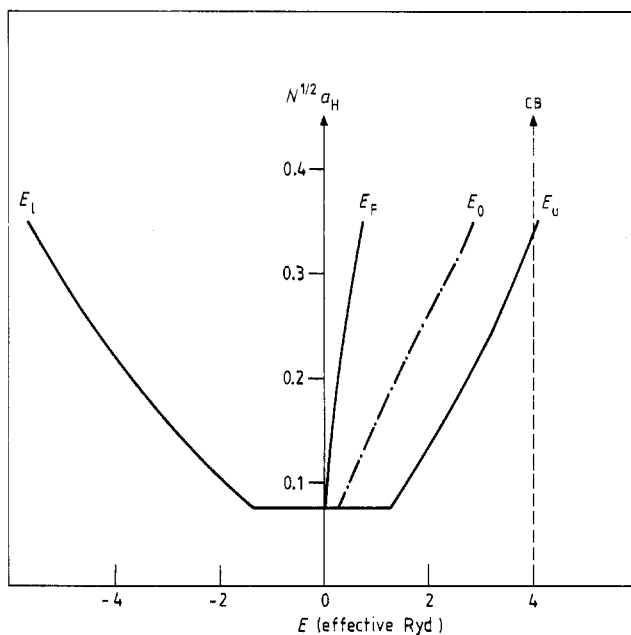


Figure 2. Dependence of band edges (E_l is the lower energy and E_u the upper energy), band centre E_0 and Fermi energy E_F on $N^{1/2}a_H$. The position of E_d is set at the origin. The bottom of the conduction band (CB) is set at 4.0 effective ryd.

the 3D density of states, as well as in Debney's work. These results are in accord with our previous cluster calculation (I). In I, $P = 12$ and 3 correspond properly to the $N^{1/2}a_H$ -values above. In figure 2 we show, as a function of $N^{1/2}a_H$, the band width, the Fermi energy E_F and the energy E_0 at which the density of states takes the maximum value. The energy is taken in effective rydbergs. It is worthwhile to point out that such behaviour, shown in both figures, was also obtained by Puri and Odagaki (1981) who used a homomorphic cluster coherent-potential approximation with a square lattice as an effective medium. For the criterion of localisation, they used a modified Hertz distribution which takes into account the V_{ij} as for a 3D system. For comparison, Fertis *et al* (1981) compared the $N_c^{1/3}a_H$ -value of about 0.19 at which the upper edge energy E_u in the 3D MT scheme crosses the conduction band with the very well known Mott (1974) criterion $N_c^{1/3}a_H \approx 0.26 \pm 0.05$ (Edwards and Sienko 1978) for the metal-to-non-metal transition in doped semiconductors and found that value very suggestive. In our 2D calculations, E_u crosses the conduction band at $N^{1/2}a_H = 0.34$. This result agrees very well with Debney's result.

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