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14. Abstract/Notes

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2-D IMPURITY STATES ASSOCIATED WITH INVERSION LAYERS

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ABSTRACT

We obtain the density of states for electrons at the inversion layer of a MOS structure due to Na^+ impurities located in the oxide. The impurity potential is assumed unscreened. We take account of disorder to obtain the configurational averaged Green's function starting from a tight binding Hamiltonian.

It is well known that bound states due to sodium ions in the proximity of the Si-SiO_2 interface of a MOSFET give rise to impurity bands at concentrations that vary between 10^{11} - 10^{12} cm^{-2}. Since the earlier calculation of these bound states by Stern and Howard (S-H)[1] using the effective mass theorem and considering a thickless inversion layer, many improvements have been achieved.

In this work we explore the possibility of an impurity band formation taking as single particle eigenstates those obtained by S-H corresponding to an unscreened Coulomb potential but assuming a finite distance from the impurity to the inversion layer. This distance is chosen to be equal to twice the effective Bohr radius. That is due to the separation between the peak on the charge density of the inversion-layer and the oxide-semiconductor interface.

We start with an Anderson Hamiltonian

$$H = \sum_{i,\sigma} E_o \, a^+_{i\sigma} a_{i\sigma} + \sum_{i,j\sigma} T_{ij} \, a^+_{i\sigma} \, a_{j\sigma} \qquad (1)$$

with $T_{ii} = 0$. We assume as our base the set of one particle functions $< \vec{r}|n >$ corresponding to a single impurity located at the site n and obeying the Schrödinger equation.

$$- \frac{\partial^2 P}{\partial r^2} - \{\frac{1}{4r^2} - \frac{2}{(d^2 + r^2)^{1/2}} - E_o\} \quad P(r) = 0 \qquad (2)$$

where d is the distance (in units of Bohr radius) from the impurity to the inversion layer, E_o is given in effective rydbergs (1 Ry* = 42 meV) and

$$P(r) = r^{1/2} < \vec{r}|m > . \qquad (3)$$

The matrix elements of the Hamiltonian are

$$< m|H|n > \simeq E_o \, \delta_{mn} + [E_o < m|n > + V_{mn}] \, . \, (1 - \delta_{mn}) \qquad (4)$$

where we have neglected two and three center integrals,

$$V_{mn} = \int d^2 r < m|\vec{r} > V(\vec{r} - \vec{R}_m) < \vec{r}|n > \qquad (5)$$

and $V(\vec{r} - \vec{R}_m)$ is the potential seen by an electron due to an impurity at $\vec{R}_m$.

The values of E_o as a function of d are easily obtained numerically from Eq. (2). The case d=0 corresponds to the 2-D hydrogen atom, $E_o = -4Ry^*$ and $\psi(r) = \sqrt{8/\pi} \; a_o^{-1} \exp(-2r/a_o)$.

The zero-temperature density of states is calculated by using the method of Matsubara-Toyozawa (M-T)[2] with the Green's function obtained according to a theory previonsly developed for impurity bands in a semiconductor[3]. The configurational average of the Green's function becomes.

$$< G_{ii\sigma}(\omega) > \frac{1}{2} \quad \frac{1}{\omega - E_o} \quad \xi(\omega - E_o), \tag{6}$$

where $\xi(\omega) = (1 - \eta/\omega)^{-1}$

and

$$\eta(\omega) = \frac{N_i \, \xi(\omega)}{4\pi^2\omega^2} \int \frac{V^2(\vec{k})\, d^2k}{1 - \dfrac{N_i \, \xi(\omega)}{\omega} V(\vec{k})} \; . \tag{7}$$

In the above equation N_i is the number of impurities per cm^2 and $V(\vec{k})$ is the Fourier transform of the hopping potential.

We perform the calculation considering the M-T expression for Eq. (4). Accordingly we obtain[4]

$$V(\vec{k}) = 128\pi \; (E_o - k^2) \; \phi^2(\vec{k}) \quad (a_o^2 \; Ry^*), \tag{8}$$

where $\phi(\vec{k})$ is the 2-D Fourier transform of $\psi(\vec{r})$. For d = 0 Eq. (8) reduces to

$$V(\vec{k}) = - \; 128\pi \; (4 + k^2)^{-2} \; (a_o^2 \; Ry^*). \tag{9}$$

The density of states obtained from Eq. (6) for the impurity concentrations $N_i = 1.55 \times 10^{11}$ cm^{-2} and $N_i = 3.10 \times 10^{11}$ cm^{-2} are shown in Figs. 1a and 1b for d=0, and Figs. 2a and 2b for d=2.

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FIGURE CAPTIONS

Fig. 1 - Density of states with d = 0 for $N_i = 1.55 \times 10^{11} cm^{-2}$ ($N_i a_o^2$ = = 0.0075) (a), and $N_i = 3.10 \times 10^{11}\ cm^{-2}$ ($N_i a_o^2 = 0.015$) (b).

Fig. 2 - Same as Fig. 1 for d = 2.

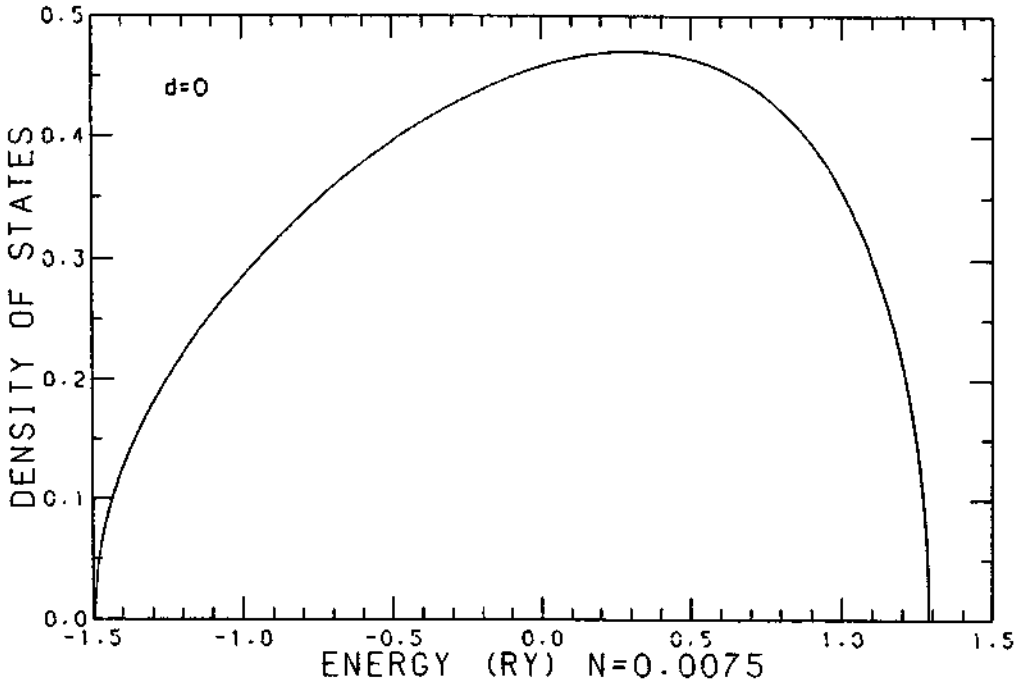
d=0
DENSITY OF STATES
0.0
0.1
0.2
0.3
0.4
0.5
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
ENERGY (RY) N=0.0075

Fig. 1a

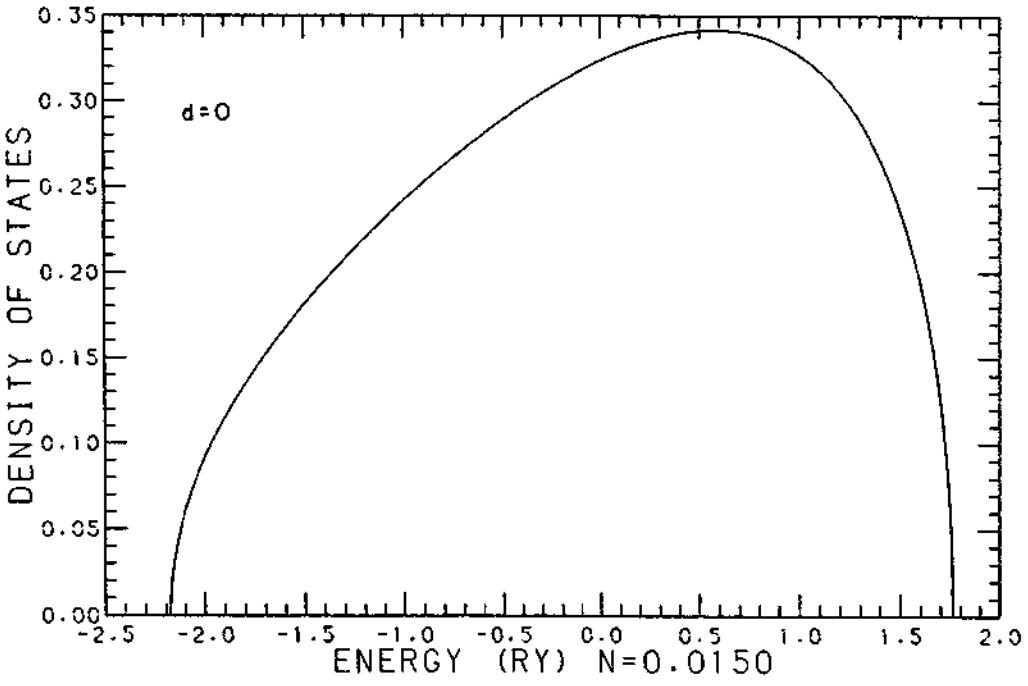
d=0
DENSITY OF STATES
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
ENERGY (RY) N=0.0150

Fig. 1b

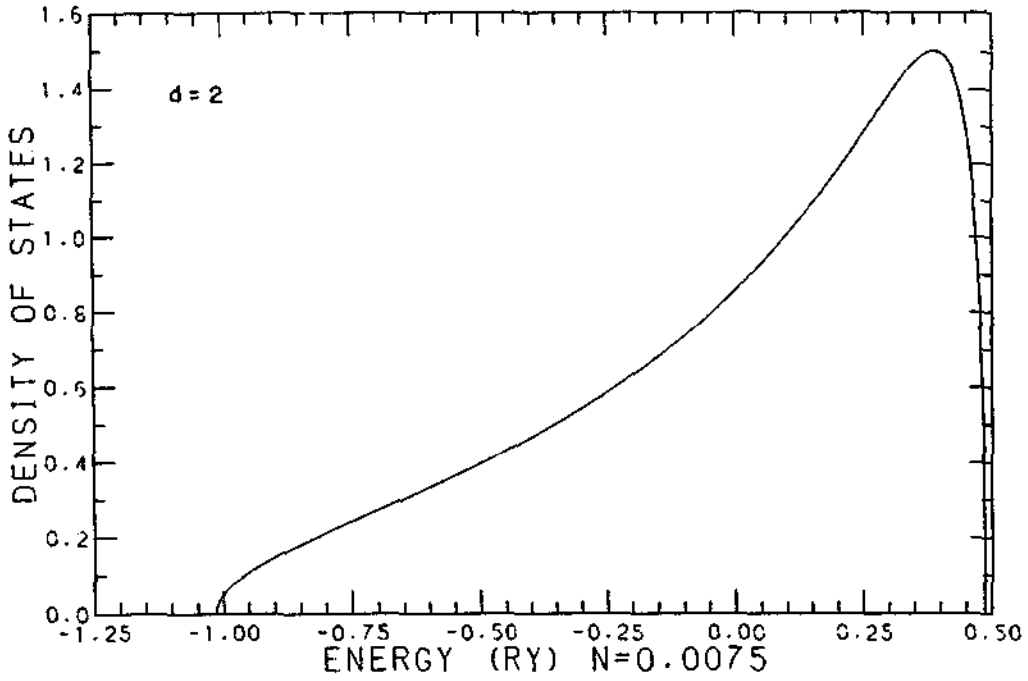
d = 2
DENSITY OF STATES
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-1.25
-1.00
-0.75
-0.50
-0.25
0.00
0.25
0.50
ENERGY (RY) N=0.0075

Fig. 2a

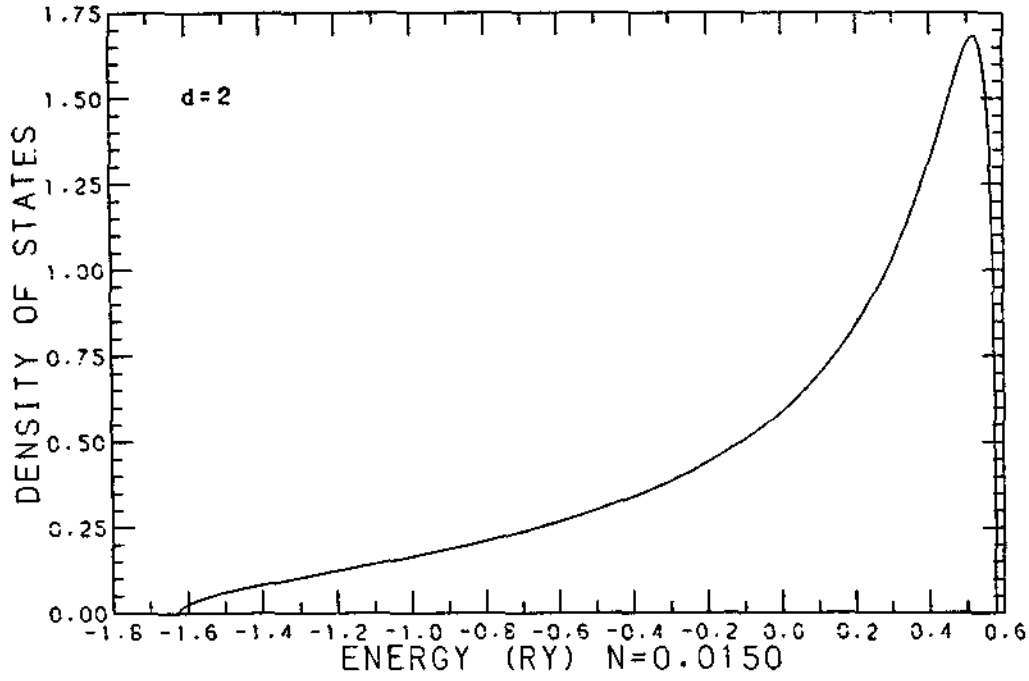
d = 2
DENSITY OF STATES
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
-1.8
-1.6
-1.4
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
0.2
0.4
0.6
ENERGY (RY) N=0.0150

Fig. 2b