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The Hubbard model for the disordered systems: An
application to the specific heat of the phosphorus doped silicon

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I. INTRODUCTION

Recently considerable attention has been given to the study of doped semiconductors because they provide a good model system where both disorder and electron correlations play their roles[1]. Thermodynamics and electrical properties of these systems show that the degree of interplay of electron correlations and disorder varies with the concentration of the impurities. However, the relative importance of these effects is still not fully understood.

At present, experimental results are reasonably well understood only for the impurity concentrations very much smaller or very much larger than the critical concentration N_c where semiconductors to metal (S-M) transition occurs. For example in the concentration region very much smaller than N_c, quantitative interpretation is possible in terms of electrons localized at the randomly distributed donor impurities. Here electron correlation plays the essential role. It is believed that it produces antiferromagnetic exchange to make the system as a prototype of amorphous antiferromagnet. However, no evidence of antiferromagnetic ordering has been found[2]. On the other hand, at concentration much larger than N_c, the properties of the metallic sample can be understood in terms of the rigid band model which assumes that the electrons occupy slightly modified conduction band of the host[2]. However, in the case of both amorphous antiferromagnet and metallic samples, the above mentioned models become unsatisfactory as the concentration approaches N_c.

At intermediate concentration, Mott[1] describes S-M transition as follows. For concentration very much smaller than N_c, there are two separated Hubbard bands[3], a lower band, consisting of D^0 states

(related to singly occupied impurities), and an upper band, consisting of D^- states (doubly occupied impurities). The energy gap between the two bands corresponds to the intraatomic Coulomb interaction of two electrons at the same impurity site, and the system behaves as a semiconductor. As the concentration increases, the Hubbard bands are broadened and eventually start overlapping. It the disorder due to random distribution of impurities is not sufficient to produce localized states at the bottom of the upper Hubbard band, S-M transition takes place at the concentration at which the two bands just start overlapping. On the otherhand, for sufficiently strong disorder which produces localized states in the bottom of the upper Hubbard band up to a mobility edge E_c, S-M transition takes place when the Fermi energy enters in the region of extended states above E_c. On further increase of concentration, the Fermi level enters the conduction band of the host and the property of the system can be described by assuming that the electrons move in the slightly modified host conduction band. According to this picture one should expect a Friedman anomaly in the Hall coefficient, p type thermopower on the semiconductor side of the transition, activation energy and N_c, sensitive to the compensation, and very strong enhancement of the specific heat. So far the first three effects have not been observed and the enhancement of specific heat is observed to be quite weak. To avoid these difficulties, Mott[1] suggested that the transition is purely Anderson type[4] due to the localization of electronic states caused by disorder at the Fermi energy as N_c is approached from above. However, Economou and Antoniou[5] found that the randomness of the off-diagonal disorder cannot produce localization in the middle of the band and thus raised doubts about completely disorder dominates

transition. Thus it shows that at least for uncompensated samples, the electron correlation and not the disorder plays a major role near the S-M transition. And for any theory of doped semiconductors to be valid in the whole range of concentration of impurities, both disorder and electron correlation should be taken into account.

We, in this paper, present such theory by considering that the disordered systems are described by the Hubbard Hamiltonian[3] with random transfer integral. In the past[6], this Hamiltonian has been studied to calculate density of states, and critical concentration using Hubbard's approximation[7] which, as shown by Edwards and Hewson[8], suffers from the difficulty that no sharp Fermi surface exist in the metallic region of a translationally invariant system.

Fedro and Wilson[9] developed a self-consistent many-body theory for the single-particle Green's function. Here we use the generalization proposed by Kishore[10] for any particle Green's function to obtain the equation of motion for the single particle Green's function. Also, we use an approximation which, in the case of translationally invariant systems, is equivalent to that of Ikeda et al[11] and is free from the defects of Hubbard's approximation[7]. The configuration average of these equations is performed according to the method of Matsubara and Toyozawa[12]. By considering the hydrogen like impurities, we calculate the specific heat of the uncompensated phosphorus doped silicon and compare with the experimental results of Sasaki and co-workers[13] and Marko et al[2], and the theoretical calculations based on the highly correlated electron gas (HCEG) model[14] and the Alternant-Molecular-Orbital method in the Matsubara-Toyozawa scheme (AMO-MT)[15].

In Sec. II, we describe the Hubbard Hamiltonian for the disordered

systems. After giving a brief outline of the self consistent many body theory, equations of motion of the single particle Green's functions are obtained and then Matsubara-Toyozawa theory is used to obtain the configurationally averaged Green's function. In Sec. III, the energy of the system and from that, the low temperature electronic specific heat is calculated. In Sec. IV, we discuss our numerical results for the specific heat of phosphorus doped silicon and give the concluding remarks.

II. GREEN'S FUNCTION FORMULATION

We consider a disordered system described by the Hubbard Hamiltonian[3]

$$H = \sum_{ij\sigma} V_{ij} \, a_{i\sigma}^{+} \, a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} \, n_{i-\sigma} \tag{1}$$

where $a_{i\sigma}^{+}$ and $a_{i\sigma}$ are the creation and the annihilation operators of an electron of spin σ at the site i, V_{ij} is the random transfer integral associated with the site i and j, U represents the intraatomic Coulomb interaction (or correlation) energy, and $n_{i\sigma} = a_{i\sigma}^{+} \, a_{i\sigma}$ is the number operator corresponding to the site i and spin σ. We shall apply above Hamiltonian for an n-type doped semiconductor with randomly distributed donor impurities. In this case, summation over sites in (1) should be considered as summation over the impurity sites. Also, we shall restrict ourselves to uncompensated samples in which V_{ii} can be considered a constant independent of the site i[16]. We shall define the energy scale such that $V_{ii} = 0$. The transfer integral V_{ij} and intraatomic interaction U will be calculated from hydrogen 1-s type wave functions.

The single particle Green's function is calculated by exploiting the self-consistent many body theory developed by Fedro and Wilson[9], and

Kishore[16] A brief outline of the theory is given as follows. An equation of motion for the Green's function[17]

$$G_{ij}(t) = i\theta(t) < [A_i, B_j(t)]_\eta > \; ; \; \eta = \pm \tag{2}$$

for any two sets of Heisenberg operators A_i and B_j, obeying the condition

$$< [A_i, B_j]_\eta > = < [A_i, B_j]_\eta > \delta_{ij} \tag{3}$$

is given as

$$-i \frac{\partial}{\partial t} G_{ij}(t) = < [A_i, B_i]_\eta > \delta_{ij} \delta(t) + i\theta(t) < [A_i, L B_j(t)]_\eta > \tag{4}$$

where for the Hamiltonian H and any operator X, the Liouville operator L is defined as

$$LX \equiv [H, X]_- \tag{5}$$

and the angular brackets <---> denote the grand canonical ensemble average. Now, the operator $B_j(t)$ is broken into two parts

$$B_j(t) \equiv P B_j(t) + (1 - P) B_j(t) \; . \tag{6}$$

The projection operator P is chosen such that

$$P \equiv \sum_j P_j \tag{7}$$

and

$$P_j X = \frac{B_j < [A_j, X]_\eta >}{< [A_j, B_j]_\eta >} \; . \tag{8}$$

By substituting the identity (6) in Eq. (4) and using the relation

$<|X,LY|_\eta> = -<[LX,Y]_\eta>$, obtained from the cyclic invariance of the trace implied in the ensemble average, we get

$$-i\frac{\partial}{\partial t} G_{ij}(t) = <[A_i,B_i]_\eta> \delta_{ij} \delta(t) + \sum_\ell \Omega_{i\ell} G_{\ell j}(t)$$
$$- i\Theta(t) <[L A_i, (1-P) B_j(t)]_\eta>, \tag{9}$$

where

$$\Omega_{i\ell} = \frac{<[A_i, L B_\ell]_\eta>}{<[A_\ell, B_\ell]_\eta>}. \tag{10}$$

From the solution of the equation of motion of the operator $(1-P)$ $\Theta(t)$ $B_j(t)$, it can be shown that[9,10]

$$(1-P)\Theta(t) B_j(t) = \sum_\ell \int_0^\infty dt\, e^{i\tau(1-P)L}(1-P)L\frac{B_\ell}{<[A_\ell, B_\ell]_\eta>} G_{\ell j}(t-\tau). \tag{11}$$

The substitution of Eq. (11) in Eq. (9) gives a closed equation for the Green's function

$$-i\frac{\partial}{\partial t} G_{ij}(t) = <[A_i,B_i]_\eta> \delta_{ij}\delta(t) + \sum_\ell \Omega_{i\ell} G_{\ell j}(t)$$
$$+ \sum_\ell \int_{-\infty}^\infty dt\, \gamma_{i\ell}(\tau) G_{\ell j}(t-\tau), \tag{12}$$

where

$$\gamma_{i\ell}(\tau) = \frac{-i\Theta(\tau)<[LA_i, e^{i\tau(1-P)L}(1-P)LB_\ell]_\eta>}{<[A_\ell, B_\ell]_\eta>}. \tag{13}$$

Eq. (12) can be easily solved by introducing the Fourier transform

$$E(t) = \frac{1}{2\pi}\int_{-\infty}^\infty d\omega\, e^{i\omega t} F(\omega) \tag{14}$$

where F represents either G or γ. We now take the Fourier transform of

(12) to find

$$\omega G_{ij}(\omega) = <[A_i, B_i]_\eta> \delta_{ij} + \sum_\ell \Omega_{i\ell} G_{\ell j}(\omega)$$

$$+ \sum_\ell \gamma_{i\ell}(\omega) G_{\ell j}(\omega), \tag{15}$$

which is the starting point of our present work. By chosing $A_i \equiv$

$\equiv a_{i\sigma} n^\pm_{i-\sigma}$, where $n^\pm_{i-\sigma} \equiv n_{i-\sigma}$ and $n^-_{i-\sigma} \equiv 1 - n_{i-\sigma}$; $B_i \equiv a^+_{i\sigma}$ and

$\eta = +$, Eq. (15) becomes.

$$\omega G^\pm_{ij\sigma}(\omega) = n^\pm_{-\sigma} \delta_{ij} + \sum_\ell \Omega^\pm_{i\ell\sigma} G_{\ell j\sigma}(\omega)$$

$$+ \sum_\ell \gamma^\pm_{i\ell}(\omega) G^\pm_{\ell j\sigma}(\omega) \tag{16}$$

where, for simplicity, $n^\pm_{-\sigma} \equiv <n^\pm_{i-\sigma}>$ is assumed to be independent of the site index in spite of the randomness of the system. The functions $G^\pm_{ij\sigma}(\omega)$ and $\gamma^\pm_{ij\sigma}(\omega)$ are the Fourier transform of

$$. G^\pm_{ij\sigma}(t) = i\Theta(t) <[a_{i\sigma} n^\pm_{i-\sigma}, a_{jc}]_+> \tag{17}$$

and

$$\gamma_{ij\sigma}(t) = \frac{-i\Theta(t) <[La_{i\sigma} n^\pm_{i-\sigma}, e^{it(1-P^\pm_\sigma)L}(1-P^\pm_\sigma)La^+_{j\sigma}]_+>}{n^\pm_{-\sigma}} \tag{18}$$

respectivily.

$$\Omega^\pm_{ij} = \frac{<[a_i n^\pm_{i-\sigma}, L a^+_{j\sigma}]_+>}{n^\pm_{-\sigma}} \tag{19}$$

and the projection operators $P^\pm_\sigma$ are defined as

$$P^\pm_\sigma \equiv \sum_j P^\pm_{j\sigma} \tag{20}$$

with

$$P_{j\sigma}^{\pm} \, \chi = \frac{a_{j\sigma}^{+} \, <[a_{j\sigma} \, n_{j-\sigma}^{\pm}, \, \chi]>}{n_{-\sigma}^{\pm}} \tag{21}$$

We are interested in the Fourier transform $G_{ij\sigma}(\omega)$ of the single particle Green's function

$$G_{ij\sigma}(t) = i \, \theta(t) \, <[a_{i\sigma}, \, a_{j\sigma}^{+}]> \, , \tag{22}$$

which is the sum of the Green's functions $G_{ij\sigma}^{+}(t)$ and $G_{ij\sigma}^{-}(t)$. The Green's function $G_{ij\sigma}(\omega) = G_{ij\sigma}^{+}(\omega) + G_{ij\sigma}^{-}(\omega)$ can be calculated from the solution of the equations of motion (16). In case of translationally invariant system, (16) can be solved by taking Fourier transform in momentum space. This case has been considered by Kishore et al[18]. In disordered systems, Eq. (16) should be averaged configurationally for all the random configurations before taking the Fourier transform in the momentum space. For configurational averaging, we shall use the method of Matsubara and Toyozawa[12]. Before applying their method of configurational averaging, we shall assume that $\gamma_{i\ell\sigma}^{\pm}(\omega)=0$. Within this approximation, by substituting

$$\Omega_{i\ell\sigma}^{\pm} = V_{i\ell} + \frac{U}{2} \, (1 \pm 1) \, \delta_{i\ell} \tag{23}$$

obtained from Eq. (19) for the Hubbard Hamiltonian (1), in Eq. (16), we get

$$(\omega - \epsilon^{\pm}) \, G_{ij\sigma}^{\pm}(\omega) = n_{-\sigma}^{\pm} \delta_{ij} + \sum_{\ell} V_{i\ell} \, G_{\ell j\sigma}^{\pm}(\omega) \tag{24}$$

where, $\epsilon^{+} = U$, and $\epsilon^{-} = 0$. In the case of translationally invariant systems, Eq. (24) gives the result of Ikeda et al[11]. Which is exact in both atomic and band limits and for small $\frac{U}{\Delta}$ (where Δ is the bandwidth) differs from Hartree-Fock theory only by an exponentially small quantity. Also it has sharp Fermi surface in the metallic region ($\frac{U}{\Delta} < 1$) and thus

removes the difficulties of the Hubbard's approximation.[7,8] For $\frac{U}{\Delta} > 1$, it

gives two separated Hubbard bands with local moment formation. The effects

of $\gamma_{ij\sigma}(\omega)$ have been considered by Kishore et al.[8] It was found that

for $\frac{U}{\Delta} > 1$, $\gamma_{ij\sigma}^{\pm}(\omega)$ gives spin dependent shifting and narrowing of the

bands. These effects make the ferromagnetic state more stable compared

to the paramagnetic state. We hope that for our paramagnetic system,

these effects may not alter the results very much.

Now we expand the Green's function $G_{ij\sigma}^{\pm}(\omega)$ in Eq. (24), in powers of

$1/(\omega-\epsilon)$ by making use of an iteration procedure, and get

$$G_{ij\sigma}^{\pm}(\omega) = \frac{n_{-\sigma}^{\pm}}{\omega-\epsilon^{\pm}} \left[\delta_{ij} + \frac{V_{ij}}{\omega-\epsilon^{\pm}} + \frac{\sum_{\ell} V_{i\ell} V_{\ell j}}{(\omega-\epsilon^{\pm})^2} + \cdots \right] \tag{25}$$

The configurationally averaged Green's function $\overline{G_{ij\sigma}^{\pm}(\omega)}$ can be obtained

by just taking the configurational average of the right band side of

(25) over the random destribution of the transfer integral. For this,

we use the diagramatic summation method of Matsubara and Toyozawa[12] and

obtain the configurationally averaged diagonal Green's functions.

$$\overline{G_{ii\sigma}^{\pm}(\omega)} = \frac{n_{-\sigma}^{\pm}}{\omega-\epsilon^{\pm}} \zeta(\omega-\epsilon^{\pm}) , \tag{26}$$

where

$$\zeta(\omega) = \frac{1}{1-\eta(\omega)} , \tag{27}$$

and

$$\eta(\omega) = \frac{N\zeta(\omega)}{8\pi^3\omega^2} \int \frac{V^2(\vec{k}) \, d\vec{k}}{1 - \frac{N\zeta(\omega)}{\omega^2} V(\vec{k})} . \tag{28}$$

N is the number of the impurity sites per unit volume and

$$V(\vec{k}) = \int V(\vec{R}) \, e^{i \, \vec{k} \cdot \vec{R}} \, d\vec{R} \, , \tag{29}$$

is the Fourier transform of

$$V_{ij} = -V_0 (1+\alpha | \vec{R}_i - R_j |) \, e^{-\alpha | \vec{R}_i - \vec{R}_j |} = V(| \vec{R}_i - \vec{R}_j |) . \tag{30}$$

Eq. (30) is obtained from the hydrogen like 1-s wave functions. Here, V_0 is equal to twice the ionization energy of the 1-s state and α^{-1} the radius of the 1-s orbit. The Matsubara-Toyozawa method[12] can also be applied to calculate the configurational average of the off-diagonal elements of the Green's functions. But for our purpose, we shall require only the diagonal element.

III. SPECIFIC HEAT

The calculation of the specific heat requires the energy of the system which can be expressed in terms of the single particle Green's function for the system described by the Hubbard Hamiltonian (1). The energy of the system is given as[19]

$$E = <H> = -\frac{1}{2\pi} \lim_{\varepsilon \to 0+} \sum_{ij\sigma} \int_{-\infty}^{\infty} (\omega \delta_{ij} + V_{ij}) \left[Im\{G_{ji\sigma}(\omega + i\varepsilon)\} \right] f(\omega) d\omega \tag{31}$$

where, $f(\omega)$ is the Fermi destribution function

$$f(\omega) = \frac{1}{e^{\beta(\omega - \varepsilon_F)} + 1} \, , \tag{32}$$

ε_F denotes the Fermi energy and $\beta = 1/kT$. Eq. (31) can be expressed

solely in terms of diagonal Green's function by using Eq. (24) which gives

$$(\omega-\varepsilon^{\pm}) \; Im \; \{G^{\pm}_{ii\sigma}(\omega+ i\varepsilon)\} = \sum_{j} V_{ij} \; Im \; \{G^{\pm}_{ji\sigma}(\omega+ i\varepsilon)\} \qquad (33)$$

By substituting Eq. (33) in Eq. (31), we get

$$E = - \frac{1}{2\pi} \lim_{\varepsilon \to 0+} \sum_{i\sigma} \int_{-\infty}^{\infty} (2\omega-\varepsilon^{\pm}) \; [Im \; \{G^{\pm}_{ii\sigma} (\omega+ i\varepsilon)\}] \; f(\omega) d\omega \qquad (34)$$

Since we are dealing with a disordered system, Eq. (34) must be averaged configurationally over all the random configuration. The configurational average of (34) gives us

$$\bar{E} = - \frac{N}{\pi} \lim_{\varepsilon \to 0+} \sum_{p\sigma} \int_{-\infty}^{\infty} (\omega-\varepsilon^{p}/2) [Im \; \overline{\{G^{p}_{ii\sigma}(\omega+ i\varepsilon)\}}] \; f(\omega) d\omega \qquad (35)$$

where, $p = \pm$.

Eq. (35) can be rewritten in terms of the density of states defined as

$$D(\omega) = \sum_{p} D^{p} (\omega), \qquad (36)$$

with

$$D^{p}(\omega) = - \frac{N}{\pi} \lim_{\varepsilon \to 0+} \sum_{\sigma} Im \; \overline{\{G^{p}_{ii\sigma}(\omega+ \varepsilon i)\}} , \qquad (37)$$

$D^{+}(\omega)$ and $D^{-}(\omega)$ correspond to the density of states of the upper and the lower Hubbard bands respectivily. From Eqs. (36) and (37), Eq. (35) becomes

$$\bar{E} = \int_{-\infty}^{\infty} \{\omega \; D(\omega) - \frac{U}{2} D^{+}(\omega)\} \; f(\omega) d\omega \qquad (38)$$

Because of the Fermi distribution function $f(\omega)$ in (38), the energy of the system E is a temperature dependent quantity. At low temperatures, we can express it in powers of temperature. This is done by using the low temperature expansion, for any arbitrary function $F(\omega)$ [20].

$$\int_{-\infty}^{\infty} F(\omega)\ f(\omega)\ d\omega = \int_{-\infty}^{\varepsilon_F} F(\omega)\ d\omega + \frac{(\pi kT)^2}{6}\ [F'(\varepsilon_F) - F(\varepsilon_F)\frac{D'(\varepsilon_F)}{D(\varepsilon_F)}]+\cdots$$

(39)

Here, ε_F is the Fermi energy at T=0, and

$$F'(\varepsilon_F) = \frac{d\ F(\omega)}{d\omega}\ \Big|_{\omega=\varepsilon_F}\ ,$$

(40)

and $\quad D'(\varepsilon_F) = \frac{d\ D(\omega)}{d\omega}\ \Big|_{\omega=\varepsilon_F}\ .$

By taking $F(\omega) = \omega D(\omega) - \frac{U}{2}\ D^+(\omega)$, Eq. (39) gives

$$\bar{E} = \int_{-\infty}^{\varepsilon} \{\omega\ D(\omega) - \frac{U}{2}\ D^+\ (\omega)\}\ d\omega$$

$$+ \frac{(\pi kT)^2}{6}\ \left[D\ (\varepsilon_F) - \frac{U}{2}\ \left\{ D^+\ (\varepsilon_F) - \frac{D^+(\varepsilon_F)\ D'(\varepsilon_F)}{D\ (\varepsilon_F)} \right\} \right]\ ,$$

(41)

which on differentiating with respect to T gives the low temperature specific heat

$$C_v = \frac{d\bar{E}}{dT} = \gamma\ T$$

(42)

with

$$\gamma = \frac{\pi^2 k^2}{3}\ \left[D(\varepsilon_F) - \frac{U}{2}\ \left\{ D^+\ (\varepsilon_F) - \frac{D^+(\varepsilon_F)\ D'(\varepsilon_F)}{D\ (\varepsilon_F)} \right\} \right]$$

(43)

Thus, the calculation of the specific heat requires the total and the upper Hubbard band density of states and their derivatives at the Fermi energy ε_F which can be calculated from the formula

$$nN = \int_{-\infty}^{\varepsilon_F} D(\omega) \, d\omega \qquad (44)$$

where $n = \sum_{p\sigma} n_\sigma^p$ is the total number of electrons per impurity. In the next section we shall discuss the results of numerical calculation of specific heat of uncompensated phosphorus doped silicon using Eq. (42) together with Eqs. (43), (37), (36) and (26) to (30).

IV. RESULTS AND DISCUSSIONS

In Fig. 1 we have plotted our numerical result of γ, curve 1, as a function of donor impurity concentration N for the uncompensated phosphorus doped silicon. The experimental critical concentration N_c, at which S-M transition occurs, is also shown. The experimental results of Sasaki and co-workers[13] are shown as dots with error bars. We see a very good agreement between our calculation and experiment over the entire semiconductor to the dilute metallic region $(N<5\times10^{18}cm^{-3})$. We have also shown the results of calculation based on HCEG model of Berggren and Sernelius[14] as curves 3 and 4, and AMO-MT method of Chao and Ferreira da Silva[15], as curve 2. HCEG model, based on the electron-hole droplets model[21] with immobile impurity ions playing the role of the mobile holes, although gives a good agreement with the experiment in the metallic region $N>N_c$, fails completely in the semiconductor region $N<N_c$. On the other hand AMO-MT method, which

takes into account the correlation effects in Matsubara-Toyozawa[12] theory, gives only a rough agreement in the intermediate region $(N-N_c)$. In Figs. 2, 3 and 4, we have plotted the specific heat C_V as a function of temperature for various concentrations of donor impurity together with the experimental results of Sasaki and co-workers[13] and Marko et al[2] and calculations based on the inhomogeneous model[2]. It should be noted that our results agree fairly well with the experiment and are better than the inhomogeneous model[2].

The shape of the density of states and the position of the Fermi level are shown in Fig. 5 for various concentrations of donor impurity. And in Fig. 6 the behavior of the top and the bottom edges of the Hubbard bands is shown. These figures show that the Hubbard bands start overlapping at a concentration much less than the critical concentration N_c. It shows that the electronic states near the bottom of the upper Hubbard band should be localized so that the S-M transition can occur when the Fermi level crosses the mobility edge, separating the regions of localized and extended states. The localization of the electronic states near the bottom of the upper Hubbard band has been shown by Aoki and Kamimura[6]. Thus, our theory supports Mott's description of S-M transition in the doped semi-conductor as described in Section I. It should be noted that the density of states in both the Hubbard bands, is tailed in the low energy side. It has been shown by Aoki and Kamimura[6] that the consideration of resonance broadening (dynamical motion of the electrons with spin), neglected by us, can give tailing in both low and high energy sides of the Hubbard bands. Recently, Ferreira da Silva et al[22] have shown that the impurity-impurity correlations can

also produce this high energy tailing.

In our theory, we have not taken into account the presence of the host conduction band which, we think, is necessary to get agreement with the experiment in the metallic region ($N>5\times10^{18}cm^{-3}$). Nonorthogonality corrections, resulting from the nonorthogonal nature of the 1-s wave functions, should also be incorporated in the theory. At present, we are studying these effects. To give a further support to our theory, we shall also calculate the conductivity and the susceptibility. The present theory can be improved by considering also resonance broadering corrections and impurity-impurity correlation.

- 16 -

FIGURE CAPTIONS

Fig. 1 - Electronic specific heat coefficient γ for Si:P as function of the impurity concentration N. Curve 1 is the present calculation. Curve 2 (Ref. 15) is the AMO-MT calculation. Curves 3 and 4 (Ref. 14) are the results from the higly correlated electron gas model. The dots with error bars are the experimental data measured by W. Sasaki and co-workers (Ref. 13). N_c indicates the impurity critical concentration.

Fig. 2 - The electronic specific heat of Si:P in units of $\mu J/°K$-Mole as a function of temperature of various impurity concentrations indicated by the numbers. Full drawn curves refer to the present calculation. Open triangle or solid triangle and solid circles are the experimental data by W. Sasaki and co-workers (Ref. 13).

Fig. 3 - The electronic specific heat of Si:P in units of $J/°K$- Mole as a function of temperature for impurity concentration $1.8 \times 10^{18} cm^{-3}$. Dashed line refers to the present calculation. Full line refers to the inhomogeneity model by Marko et al (Ref. 2). Solid circles correspond to the experimental data by Marko et al (Ref. 2).

Fig. 4 - The electronic specific heat of Si:P as a function of temperature for impurity concentration $2.4 \times 10^{18} cm^{-3}$. Dashed line is the present calculation. Solid line is the inhomogeneity model and solid circles are experimental data, both from Marko et al (Ref. 2).

Fig. 5 - Density of states of impurity Hubbard bands for various values of the normalized impurity concentration $P = 32\pi Na_0^3$. N is the true impurity concentration and a_0 (α^{-1}) is the Bohr radius of the impurity. The position of the Fermi energy is indicated by dashed lines and the bottom of the host conduction band by dotted line.

Fig. 6 - Top and bottom edges of the impurity Hubbard bands as function of the impurity concentration P. CB is the bottom of the conduction band at $E/V_0=0.5$. U/V_0 is the intraatomic correlation energy equal to 0.625. The arrow indicates the concentration where the bands start overlapping.

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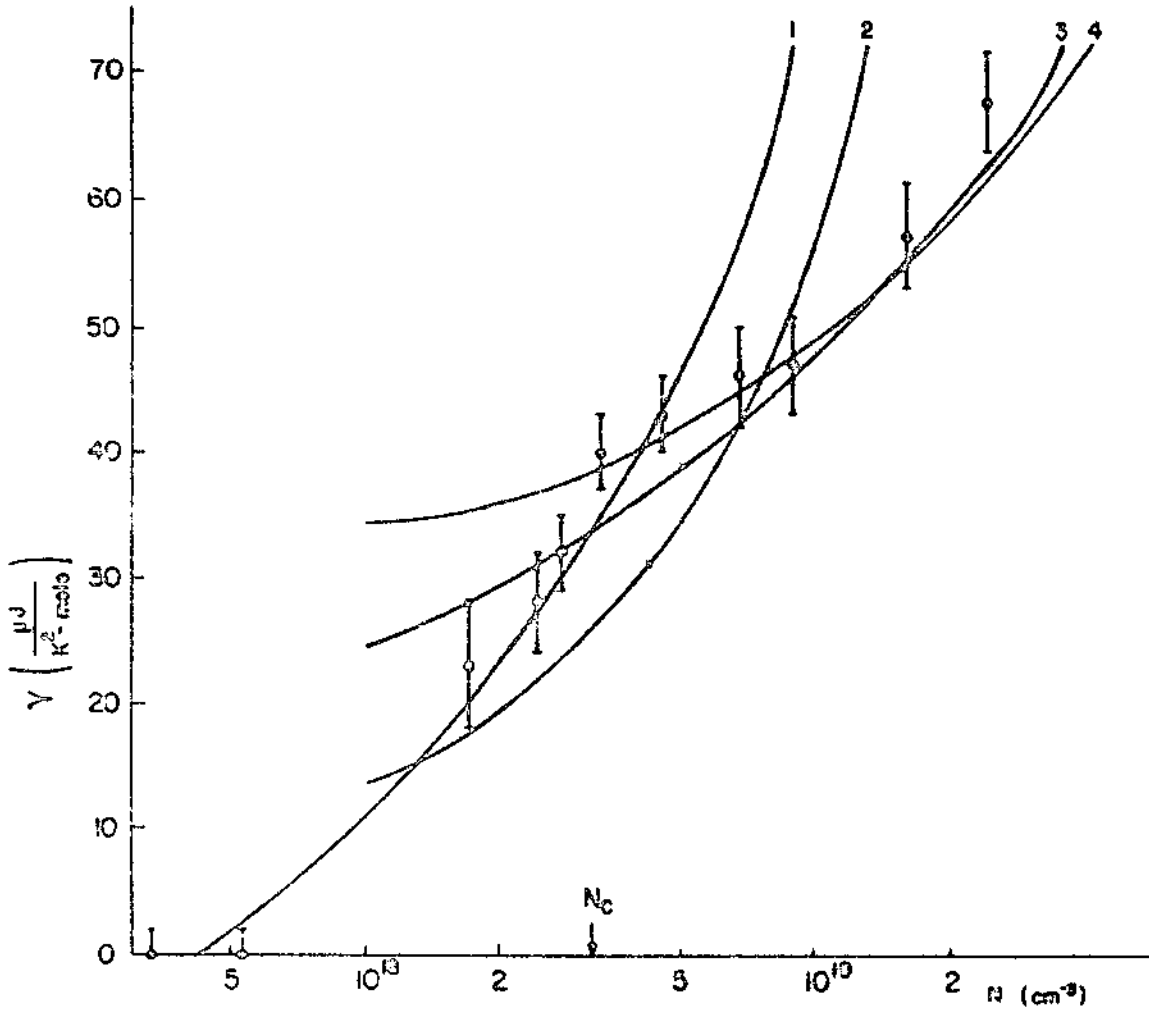
Fig.1 - A.Ferreira da Silva et al.
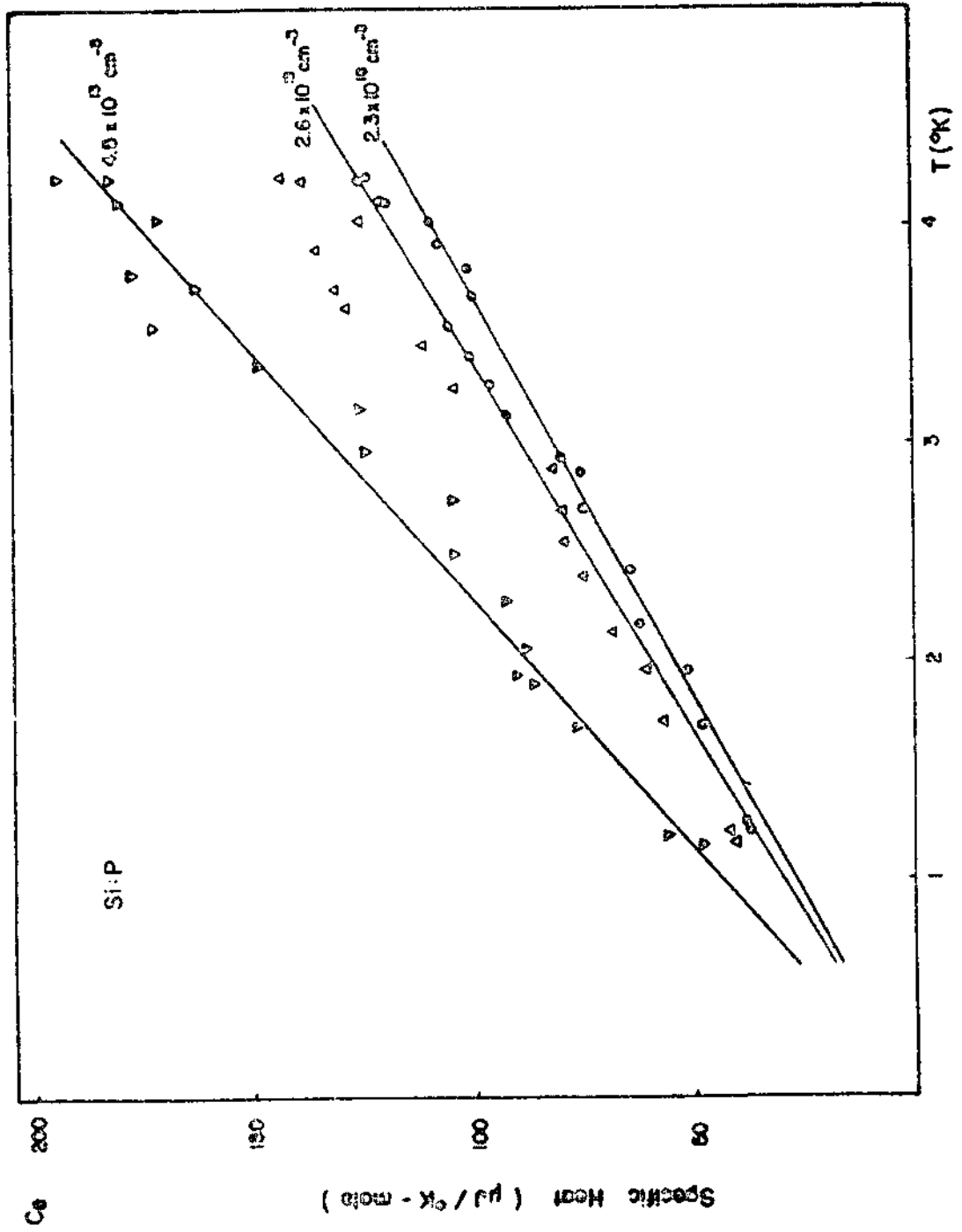
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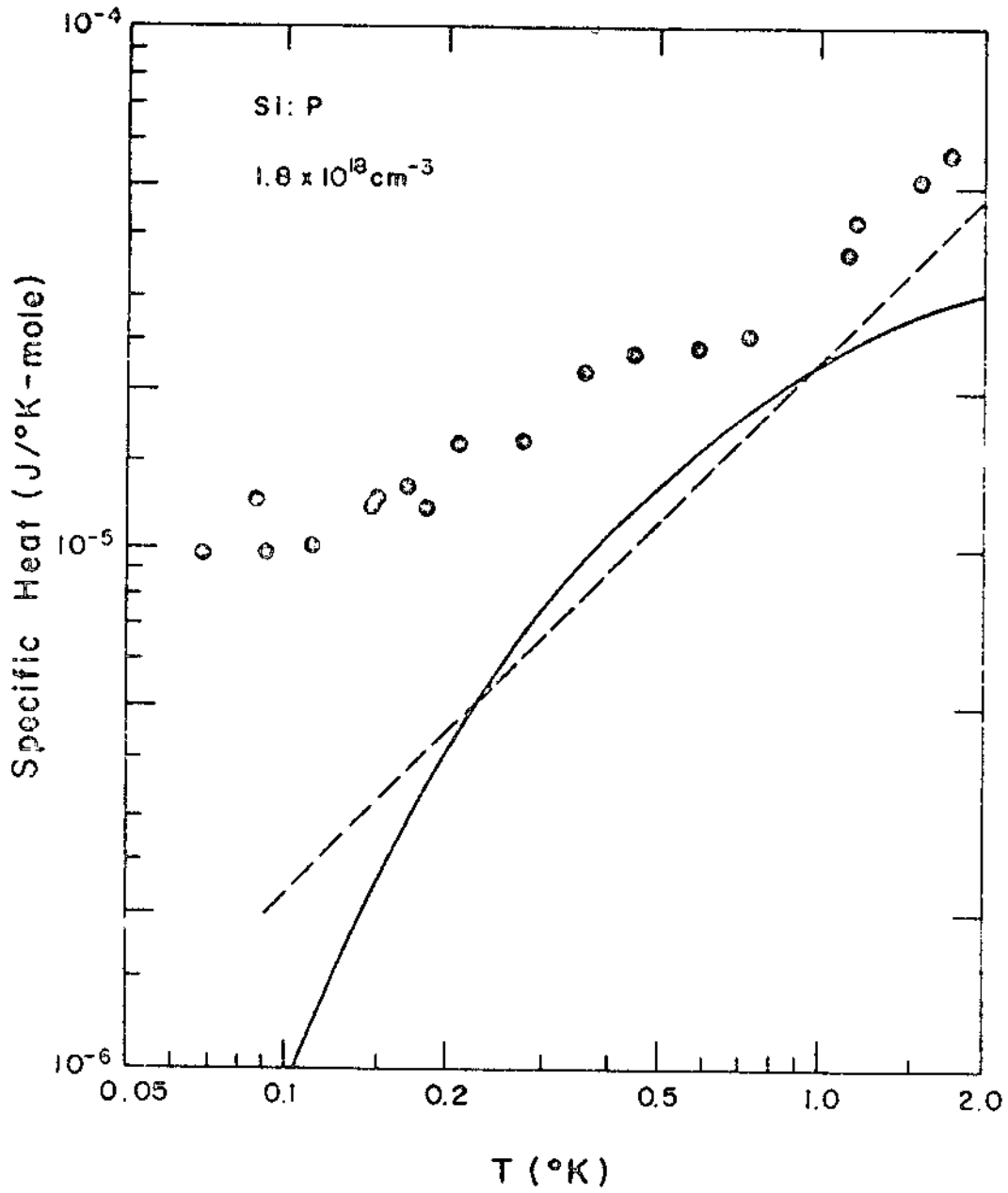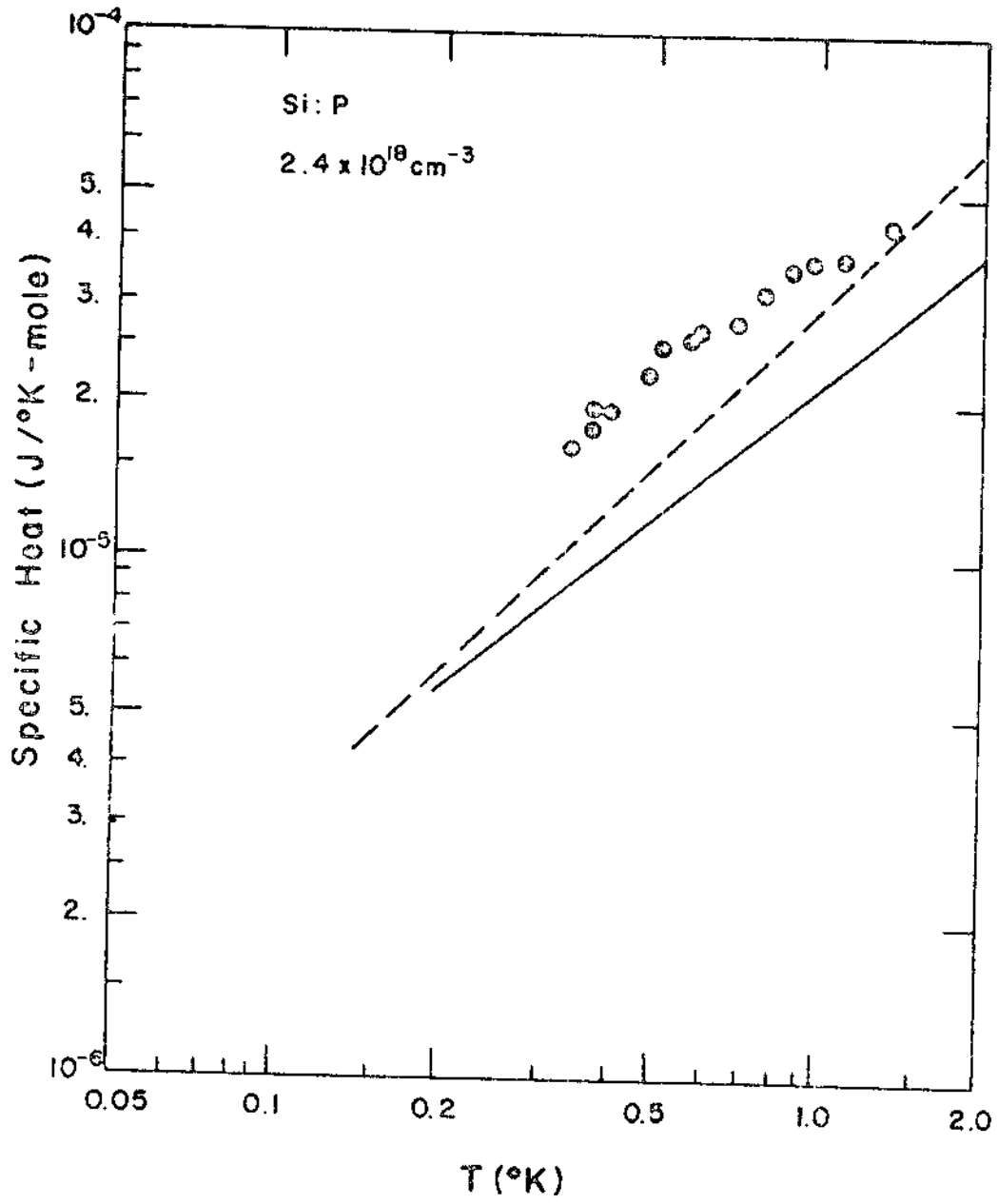
Fig.3 - A.Ferreira da Silva et al.
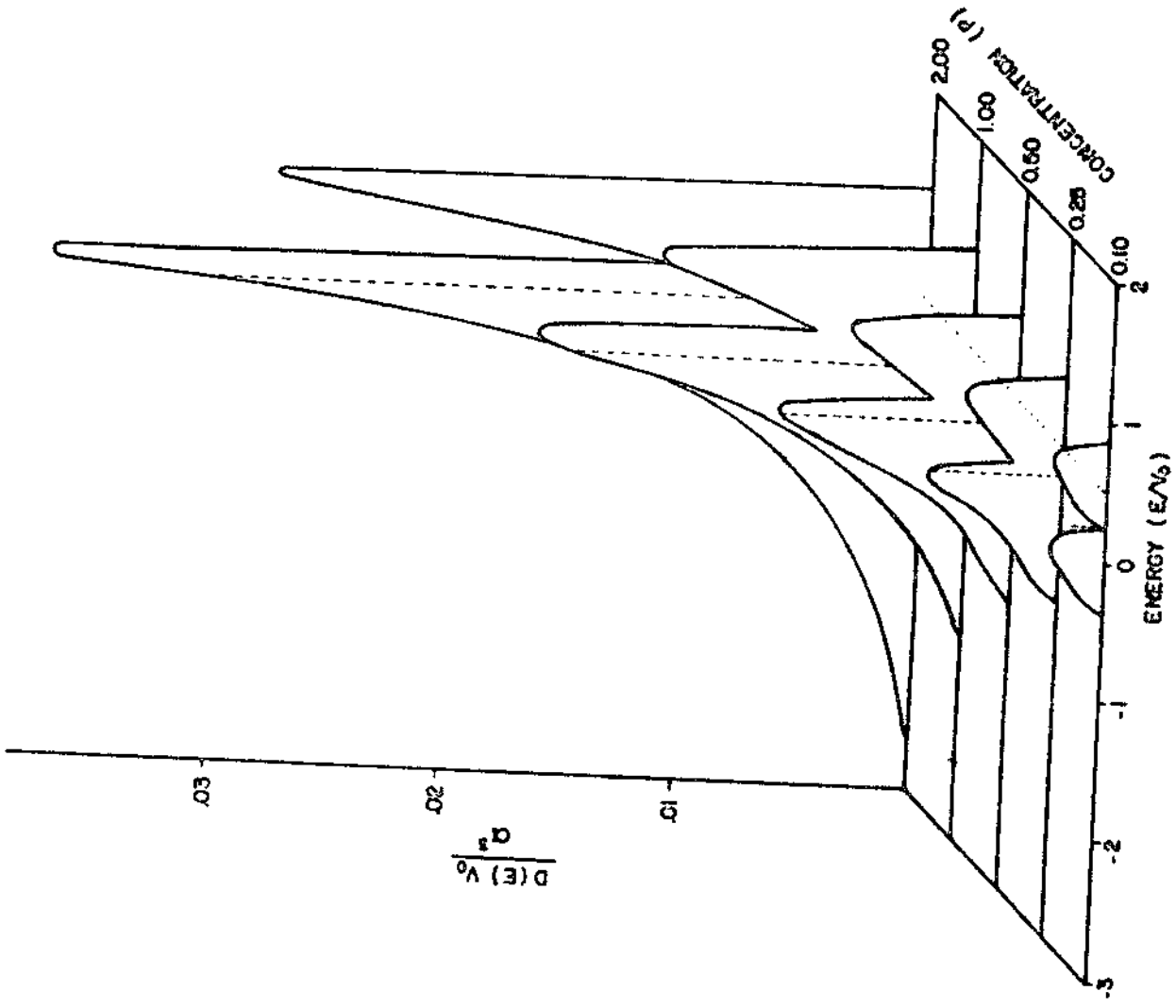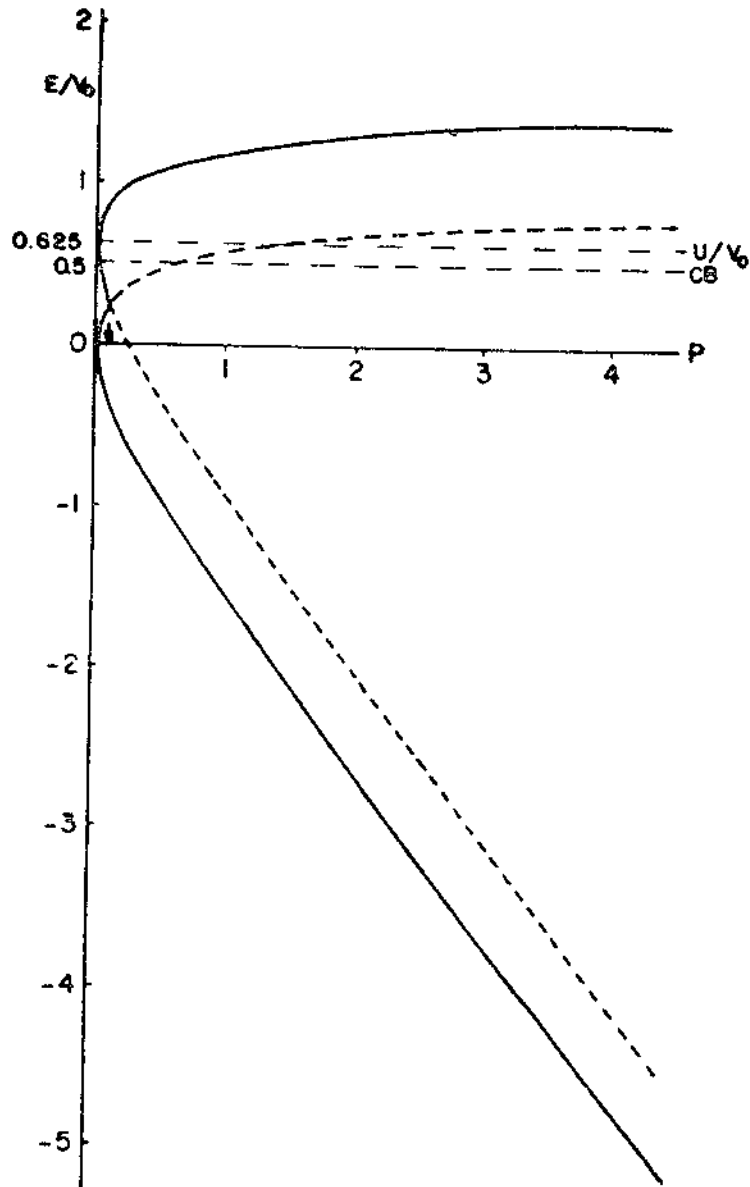
Fig.4 - A.Ferreira da Silva et al.

Fig. 5 - A.Ferreira da Silva et al.

Fig. 6 - A.Ferreira da Silva et al.