

REFERENCE

IC/76/72

INTERNATIONAL CENTRE FOR  
THEORETICAL PHYSICS



LOCALIZED STATES IN SEMICONDUCTORS -  
II: ARSENIC IN GERMANIUM

A. Q. Sarker



INTERNATIONAL  
ATOMIC ENERGY  
AGENCY



UNITED NATIONS  
EDUCATIONAL,  
SCIENTIFIC  
AND CULTURAL  
ORGANIZATION

1976 MIRAMARE-TRIESTE



International Atomic Energy Agency  
and  
United Nations Educational Scientific and Cultural Organization

## INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

## LOCALIZED STATES IN SEMICONDUCTORS -

## II: ARSENIC IN GERMANIUM \*

A.Q. Sarker \*\*

International Centre for Theoretical Physics, Trieste, Italy.

## ABSTRACT

The multi-valley effective mass formalism for the asymmetric energy surfaces developed in an earlier paper is extended for the calculations of the ground state energies of isocoric donors in Ge. The impurity potential is constructed from the  $k$ -dependent dielectric function of Ge and a variational trial wave function, belonging to an irreducible representation of the point group  $T_d$  of the Hamiltonian, is used. The calculated energy levels for the singlet  $A_1$  and the triplet  $T_2$  symmetries of the  $1s$  states for As in Ge is found to be of the same order (-9.6 to -12.8 meV) as observed experimentally; however, the predicted  $E(A_1) - E(T_2)$  splitting is rather too small ( $\sim -0.5$  to  $-0.7$  meV) compared with the observed value -4.23 meV.

MIRAMARE - TRIESTE

August 1976

\* To be submitted for publication.

\*\* Permanent address: Department of Physics, Dacca University, Dacca-2, Bangladesh.

## 1. INTRODUCTION

The single-valley effective mass theory, as given by Kittel and Mitchell (1954), Lampert (1954) and Kohn and Luttinger (1954), predicts for the  $1s$  donor states in Ge a four-fold degeneracy. On the other hand, experiments (Reuszer and Fisher, 1964) show that this degeneracy is lifted and the four  $1s$  states split into a singlet  $A_1$  (the lowest state) and a triplet  $T_2$ . For isocoric impurity such as Arsenic in Ge (and with which we shall be concerned in this paper), the experimental values of the energies  $E(A_1)$  and  $E(T_2)$  are -14.04 meV and -9.81 meV respectively. The experimentally measured transverse and longitudinal effective electron masses in Ge are  $m_t = 0.08152 \pm 0.00008 m_0$  and  $m_l = 1.588 \pm 0.005 m_0$  (Levinger and Frankl, 1961).

It was pointed out by Baldereschi (1970) that the degeneracies of the  $1s$  donor levels of Si and Ge can be lifted by the introduction of the valley orbit interactions into the effective mass theory. He considered a simple Coulomb impurity potential screened by the  $k$ -dependent dielectric function  $\epsilon(\vec{k})$  appropriate to the  $\Delta k$  value of valley separation in Ge, treated it by the perturbation method and obtained for the  $1s(A_1) - 1s(T_2)$  splitting a value -0.6 meV, compared with the experimental value -4.23 meV. The spherical effective mass approximation, as used by Pantelides and Sah (1974) for donors in Si, is not expected to be reliable for Ge, since the single-valley calculations for the latter show that the eccentricity  $q$  of the ellipsoidal orbit of the impurity electron is quite large ( $\sim 0.94$ ) and to replace it by zero (spherical orbit) is a rather poor approximation.

In an earlier paper (Sarker 1976), hereafter referred to as I, a multi-valley effective mass formalism for the asymmetric energy surfaces was developed for the calculations of the ground state energies of isocoric donors in Si. In this paper the technique is extended and is used to calculate the  $1s$  isocoric donor levels in Ge. In Si, the relevant six conduction band minima are situated on either transverse or longitudinal positions. In the case of Ge, there are four equivalent conduction band minima situated in the directions  $[111]$  and the angle  $\beta_0$  between any two of these is  $109^\circ.47$ . By making suitable rotations, wave functions, belonging to an irreducible representation of the tetrahedral point group  $T_d$  for the substitutional impurities in Ge and centred at each of the band minima, have been constructed. Moreover, because of the large eccentricity of the impurity electron orbit in Ge, the  $q^2$  expansion in calculating the inter-valley matrix elements needed to be suitably rearranged so as to obtain faster convergence than that of I. The predicted values of the energy levels  $E(A_1)$  and  $E(T_2)$  are of the same order as observed experimentally; however, the  $E(A_1) - E(T_2)$  is only

-0.5 to -0.7 meV, compared with the experimental result of -4.23 meV (which is about 43.25% of the single-valley result). This small splitting between the two 1s levels in Ge (as compared with the corresponding splitting of -11.6 meV, which is about 37.15% of the single valley result, for P in Si) is traced <sup>due</sup> mainly to the fact that the 1s impurity electron orbit in Ge, as calculated from the single-valley EMT, is much larger ( $D^{-1} = 41.12$  a.u.,  $B^{-1} = 117.40$  a.u.) compared with that in Si ( $D^{-1} = 25.71$  a.u.;  $B^{-1} = 44.76$  a.u.) for similar (isocoric) impurities, and the (almost) pure Coulomb impurity potential in the central cell region has then much smaller effects on the 1s states in Ge than in Si. Hence the prediction on the  $E(A_1) - E(T_2)$  splitting is so small in the case of Ge.

The plan of the paper is as follows. In Sec. 2 we derive the expressions for the envelope functions having the correct symmetry and give the expressions for the ground state energies for Arsenic in Ge. The impurity potential is discussed in Sec. 3. The results are presented and discussed in Sec. 4.

## 2. ENVELOPE FUNCTIONS AND ENERGY EXPRESSIONS

The impurity electron wave function for the 1s states of Ge, having  $A_1$  and  $T_2$  symmetries (denoted by  $\Gamma$ ), can be written as

$$\Psi_{\Gamma}(\vec{r}) = \sum_{i=1}^4 \alpha_i(\Gamma) F_i(\vec{r}) u_i(\vec{r}_i, \vec{r}) \text{Exp}(i\vec{k}_i \cdot \vec{r}), \quad (1)$$

where  $u_i(\vec{r}) e^{i\vec{k}_i \cdot \vec{r}}$  is the Bloch function and  $F_i(\vec{r})$  the hydrogen-like modulated envelope functions centred at the  $i^{\text{th}}$  band minima and  $\alpha_i(\Gamma)$  some numerical coefficients determined from the group  $T_d$  for substitutional impurities in Ge (Appel 1964). The envelope function  $F_i(\vec{r})$ , satisfies the eigenvalue Eq. (I.3) (referred to in I). To obtain the envelope functions  $F_i(\vec{r})$ , we consider the set of four equivalent  $L_1$  conduction band minima at

$$\frac{\pi}{a}(1,1,1)_1, \frac{\pi}{a}(1,-1,-1)_2, \frac{\pi}{a}(-1,1,-1)_3 \text{ and } \frac{\pi}{a}(-1,-1,1)_4.$$

Now by making a rotation of  $45^\circ$  around the  $k_x$  axis followed by a rotation of  $\alpha = \tan^{-1}\sqrt{2}$  around the  $k_z$  axis, the two minima 1 and 2 are brought into the  $k_x k_y$  plane, with the minima 1 lying along the  $k_x$  axis and minima 2 situated making an angle  $\beta_0 = -109^\circ.47$  with the  $k_x$  axis. (Fig. 1).

The envelope function  $F_1(\vec{r})$  can now easily be written down ( $x, y$  etc. replaced by  $x, y$  etc)

$$F_1(\vec{r}) = \left(\frac{B^2 D}{\pi}\right)^{1/2} \text{Exp} \left[ -\left\{ B^2 (y^2 + z^2) + D^2 x^2 \right\}^{1/2} \right], \quad (2)$$

having the kinetic energy term  $T_1(-i\vec{\nabla})$ ,

$$T_1(-i\vec{\nabla}) = -\left[ \frac{1}{2m_x} \left( \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{1}{2m_x} \frac{\partial^2}{\partial x^2} \right]. \quad (3)$$

The envelope function  $F_2(\vec{r})$  is then given by

$$F_2(\vec{r}) = \left(\frac{B^2 D}{\pi}\right)^{1/2} \text{Exp} \left[ -\left\{ B^2 (x \sin \beta_0 + y \cos \beta_0)^2 + B^2 z^2 + D^2 (x \cos \beta_0 - y \sin \beta_0)^2 \right\}^{1/2} \right]. \quad (4)$$

One can obtain the other two envelope functions  $F_3(\vec{r})$  and  $F_4(\vec{r})$  similarly or from (4) by symmetry considerations. We note that (4) gives the correct transverse valley envelope function for  $\beta_0 = \pi/2$  and the longitudinal valley envelope function for  $\beta_0 = \pi$ . As in I, we take for the impurity potential  $U(\vec{r})$  the same general screened Coulomb form

$$U(\vec{r}) = -\frac{e^2}{\epsilon r} \sum_{l=0}^L A_l e^{-\lambda_l r}, \quad (5)$$

and the energy eigenvalues  $E(\Gamma)$  are written down in the form

$$E(\Gamma) = \left[ T(\Gamma) + U(\Gamma) \right] / N(\Gamma), \quad (6)$$

where  $N(\Gamma)$  stands for normalization terms,  $T(\Gamma)$  the matrix elements of the kinetic energy terms, e.g. (3), and similarly other four terms, and  $U(\vec{r})$  those of the potential (5) taken between the envelope functions  $F_i(\vec{r})$ , as given by, e.g., (2) and (4) and similar terms:

$$N(\Gamma) = \sum_{i,j}^4 \alpha_j^*(\Gamma) \alpha_i(\Gamma) \langle F_j(\vec{r}) e^{i\vec{k}_j \cdot \vec{r}} | F_i(\vec{r}) e^{i\vec{k}_i \cdot \vec{r}} \rangle, \quad (7)$$

$$T(\Gamma) = \sum_{i,j}^4 \alpha_j^*(\Gamma) \alpha_i(\Gamma) \langle F_j(\vec{r}) | T_i(-i\vec{\nabla}) | F_i(\vec{r}) e^{i(\vec{R}_i - \vec{R}_j) \cdot \vec{r}} \rangle, \quad (8)$$

$$U(\Gamma) = \sum_{i,j}^4 \alpha_j^*(\Gamma) \alpha_i(\Gamma) \langle F_j(\vec{r}) | U(\vec{r}) | F_i(\vec{r}) e^{i(\vec{R}_i - \vec{R}_j) \cdot \vec{r}} \rangle. \quad (9)$$

The sums over the set of  $\alpha_i$  and  $\alpha_j$  can easily be carried out and the results are given in terms of the constants  $g_\beta(\Gamma)$ ,  $\beta = 0, 1$ .

$$\left. \begin{aligned} g_0(A_1) \\ g_0(T_2) \end{aligned} \right\} = 1, \quad \begin{aligned} g_1(A_1) &= 3, \\ g_1(T_2) &= -1, \end{aligned} \quad (10)$$

where we have used the subscript 0 for the intra-valley and the subscript 1 for the inter-valley terms.

Using the spheroidal co-ordinate system and  $q^2$  expansion for the inter-valley terms, the volume integrations in (7)-(9) can be carried out explicitly. We present the results in the following forms, similar to those of I.

We define

$$C = m_1/m_2, \quad (11)$$

$$\begin{aligned} q^2 &= 1 - B^2/D^2 \\ &= u^2(1+u^2)^{-1} \quad (< 1), \end{aligned} \quad (12)$$

$$b^* = B^2 + D^2/C, \quad (13)$$

$$\bar{b} = B^2 - D^2/C, \quad (14)$$

$$\delta_0 = 0, \quad \delta_1 = \frac{R_0}{D}; \quad (15)$$

$$S = \frac{u}{q}, \quad d_0 = 1, \quad d_1 = \frac{1}{2} + \frac{1}{2}S; \quad (16)$$

where  $k_0 = \frac{1}{\sqrt{2}} \frac{2\pi}{a}$ ,  $a$  being the lattice constant for Ge. We use the unit of length  $a_0 = \frac{\hbar^2 \epsilon}{m_t e^2} = 188.420$  a.u. and that of energy  $E_0 = \frac{m_t}{e^2} E_H = 9.40234$

meV for  $\epsilon = 15.36$ , unless otherwise stated.

The results are

$$N(\Gamma) = \sum_{\beta=0}^1 \frac{d_\beta g_\beta(\Gamma)}{(d_\beta^2 + \delta_\beta^2)^2} + g_1(\Gamma) \sum_{n=1}^{\infty} (q^2)^n R_n(\delta_1, S), \quad (17)$$

$$T(\Gamma) = \sum_{\beta=0}^1 g_\beta(\Gamma) T_\beta + g_1(\Gamma) \sum_{n=1}^{\infty} (q^2)^n K_n(\delta_1, b^*, S), \quad (18)$$

where

$$\begin{aligned} T_\beta &= \frac{1}{2} \left[ \frac{b^*}{d_\beta^2 + \delta_\beta^2} - \frac{d_\beta B^2}{(d_\beta^2 + \delta_\beta^2)^2} \right. \\ &\left. + \frac{\bar{b}}{\delta_\beta^2} \left\{ \frac{1}{d_\beta^2 + \delta_\beta^2} - \frac{d_\beta}{(d_\beta^2 + \delta_\beta^2)^2} + \frac{\tan^{-1}(\delta_\beta/d_\beta)}{\delta_\beta} - 1 \right\} \right]; \end{aligned} \quad (19)$$

$$U(\Gamma) = \sum_{\beta=0}^1 g_\beta \sum_{\lambda=0}^L (U_{\beta\lambda} + \bar{U}_{\beta\lambda}) + g_1(\Gamma) \sum_{\lambda=0}^L \sum_{n=1}^{\infty} (q^2)^n U'_{\lambda n}(\delta_1, B, S), \quad (20)$$

where

$$h_{\beta\lambda} = d_\beta^2 + \frac{\delta_\beta^2}{q^2} - \frac{\lambda^2}{4B^2}, \quad (21)$$

$$U_{\beta 1} = - \frac{B A_1}{q} \frac{\frac{\delta_0^2}{u} - \frac{q \lambda_1}{2B} (d_\beta + \frac{\lambda_1}{2D})}{h_{\beta 1} \left\{ (d_\beta + \frac{\lambda_1}{2D})^2 + \delta_0^2 \right\}} \quad (22)$$

$$\bar{U}_{\beta 1} = - \frac{B d_0 A_1}{q h_{\beta 1}^{3/2}} \tan^{-1} \left\{ \frac{2 h_{\beta 1}^{1/2} (d_\beta - \frac{\lambda_1}{2B}) \tan(u/2)}{h_{\beta 1} - \frac{\delta_0^2}{q^2} - (d_\beta - \frac{\lambda_1}{2B})^2 \tan^2(u/2)} \right\} \quad (23)$$

if  $h_{\beta 1} > 0$ ;

or if  $h_{\beta 1} < 0$

$$\bar{U}_{\beta 1} = + \frac{B d_0 A_1}{2q (-h_{\beta 1})^{1/2}} \times$$

$$\ln \left| \frac{\left\{ (d_\beta - \frac{\lambda_1}{2B})^2 \tan^2(u/2) + h_{\beta 1} + \frac{\delta_0^2}{q} \right\} - 4 h_{\beta 1} \frac{\delta_0^2}{q^2}}{\left[ \left\{ (d_\beta - \frac{\lambda_1}{2B})^2 \tan^2(u/2) + (-h_{\beta 1})^{1/2} \right\}^2 + \frac{\delta_0^2}{q^2} \right]^{1/2}} \right| \quad (24)$$

with

$$u = \tan^{-1} u \quad (25)$$

The last terms in (17), (18) and (20) are the correction terms arising from the  $q^2$  expansion of the envelope functions (4) in evaluating the inter-valley matrix elements. They are given as follows:

$$R_1(\delta_1, s) = - \frac{3}{2} \int_0^1 d\xi \operatorname{Re} \frac{s X_1(\xi)}{(d_1 + i \delta_1 \xi)^4} \quad (26a)$$

$$R_2(\delta_1, s) = - \frac{3}{2} \int_0^1 d\xi \left\{ \operatorname{Re} \frac{s V_1(\xi)}{(d_1 + i \delta_1 \xi)^4} - \operatorname{Re} \frac{s^2 X_2(\xi)}{(d_1 + i \delta_1 \xi)^5} \right\} \quad (26b)$$

etc.

$$K_1(\delta_1, b^+, s) = \int_0^1 d\xi \left\{ \operatorname{Re} \frac{\frac{1}{2} b^+ s X_1(\xi)}{(d_1 + i \delta_1 \xi)^3} - \operatorname{Re} \frac{b^+ \xi^2 s X_1(\xi)}{(d_1 + i \delta_1 \xi)^4} \right\} \quad (27a)$$

$$K_2(\delta_1, b^+, s) = \int_0^1 d\xi \left\{ \operatorname{Re} \frac{\frac{1}{2} b^+ s^2 V_1(\xi)}{(d_1 + i \delta_1 \xi)^3} + \operatorname{Re} \frac{\frac{3}{8} b^+ s^2 X_2(\xi) - b^+ \xi^2 s V_1(\xi)}{(d_1 + i \delta_1 \xi)^4} \right\} \quad (27b)$$

etc.

$$U'_{11}(\delta_1, B, s) = B \int_0^1 d\xi \frac{A_1}{(1 - q^2 \xi^2)^{1/2}} \operatorname{Re} \frac{s X_1(\xi)}{(a_1 + i b_1)^3} \quad (28a)$$

$$U'_{12}(\delta_1, B, s) = B \int_0^1 d\xi \frac{A_1}{(1 - q^2 \xi^2)^{1/2}} \times$$

$$\left\{ \operatorname{Re} \frac{s V_1(\xi)}{(a_1 + i b_1)^3} - \operatorname{Re} \frac{\frac{3}{8} s^2 X_2(\xi)}{(a_1 + i b_1)^3} \right\} \quad (28b)$$

etc.

where

$$b_1 = \delta_1 \xi \quad (29a)$$

$$a_s = d_1 + \frac{\lambda_L}{2B} (1 - q^2 \xi^2)^{1/2} \quad (29b)$$

$$X_1(\xi) = -\frac{1}{2} \left\{ s - \frac{1}{2} t \right\}, \quad (30)$$

$$X_2(\xi) = +\frac{1}{4} \left\{ s^2 - st + \frac{3}{8} t^2 + 2\omega \right\}, \quad (31)$$

$$V_1(\xi) = \frac{1}{2} (s-1) - \frac{1}{2} X_2(\xi), \quad (32)$$

$$X_3(\xi) = -\frac{1}{8} \left[ s^3 - \frac{3}{2} s^2 t + \frac{9}{8} s t^2 - \frac{5}{16} t^3 - \frac{9}{2} t \omega + 6s\omega \right] \quad (33)$$

$$V_2(\xi) = -\frac{1}{2} (s-1) X_1(\xi) - \frac{1}{2} X_3(\xi) - \frac{1}{2} \omega, \quad (34)$$

etc.

with

$$s = 1 + \xi^2 \sin^2 \beta_0, \quad (35)$$

$$t = (1 - \xi^2) \sin^2 \beta_0, \quad (36)$$

$$\omega = \xi^2 (1 - \xi^2) \sin^2 \beta_0 \cos^2 \beta_0. \quad (37)$$

In the actual calculations for Ge, terms upto  $q^8$  are taken into consideration, which is estimated to yield about 90% of the corrections for  $q$  as large as 0.92. We note that the term (37) vanishes both for the transverse ( $\beta_0 = \pi/2$ ) and the longitudinal ( $\beta_0 = \pi$ ) valleys. For the longitudinal valleys  $t$  is also zero and  $s$  is simply unity.

### 3. IMPURITY POTENTIAL

The impurity potential  $U(\vec{r})$  can be obtained from its Fourier transform  $U(\vec{k})$ , which is given in terms of the  $k$ -dependent dielectric function  $\epsilon(\vec{k})$  by:

$$U(\vec{r}) = \frac{U_b(\vec{r})}{\epsilon(\vec{r})}, \quad (38)$$

where

$$U_b(\vec{r}) = \frac{4\pi}{r^2} \quad (39)$$

and

$$U_b(\vec{r}) = -\frac{e^2}{r}, \quad (40)$$

in the point-charge model. The dielectric function  $\epsilon(\vec{k})$  for Ge has been calculated by a number of authors, e.g. Nara (1966), Srinivasan (1969), Walter and Cohen (1970), Vinsome and Jaros (1970) and Vinsome and Richardson (1971). In this work we shall be using  $\epsilon(\vec{k})$  as given by Walter and Cohen, and Vinsome and Richardson. The  $\epsilon(\vec{k})$  as given by Walter and Cohen can be fitted to the form (Fit I).

$$\frac{1}{\epsilon(\vec{r})} = \frac{A r^2}{r^2 + \alpha^2} + \frac{1}{\epsilon(0)} \frac{\beta^2}{r^2 + \beta^2} + \frac{(1-A) r^2}{r^2 + \gamma^2}, \quad (41a)$$

where

$$A_W = 1.0, \alpha_W = 0.79 \text{ a.u.}, \beta_W = 2.5 \text{ a.u.}, \gamma_W = 0, \quad (41b)$$

while that given by Vinsome and Richardson fits best to the form (Fit II),  $\chi^2 = 0.060$

$$\frac{1}{\epsilon(\vec{r})} = \frac{A r^2}{r^2 + \alpha^2} + \frac{\{(1-A) - 1/\epsilon(0)\} r^2}{r^2 + \beta^2} + \frac{1}{\epsilon(0)}, \quad (42a)$$

with

$$A_R = 0.9211, \alpha_R = 0.91266 \text{ a.u.}, \beta_R = 0.07076 \text{ a.u.} \quad (42b)$$

The quality of these fits is shown in Fig. 2. We point out that (42a) tends to give slightly larger values of  $\epsilon(\vec{k})$  for  $k > 0.4$  a.u. than the expression (41a). The function  $\epsilon(\vec{k})$  can also be suitably normalized at  $k = 0$  using the appropriate value of  $\epsilon(0)$  without affecting its values for  $k > 0.1$  a.u. significantly. Vinsome and Richardson obtained the value of  $\epsilon(0)$  to be 15.74, which is to be compared with the experimental value 16.0 for Ge. However, Walter and Cohen obtained only 14.0 for the value of  $\epsilon(0)$ . From a comparison of the experimental value of  $E(2P_{\frac{1}{2}}) - E(2P_0)$  with the single-valley calculations for Ge, Faulkner (1969) estimated that  $\epsilon(0)$  should have a value  $15.36 \pm 0.05$ . This also gives results for the excited acceptor states in Ge that agree quite well with experiments (Baldereschi and Lipari 1973). However, we have considered values of  $\epsilon(0)$  that lie between 14.0 and 16.0. Using (41) or (42) in (38) and taking the inverse Fourier transform of  $U(\vec{k})$  one obtains the impurity potential  $U(\vec{r})$  in the form

$$U(\vec{r}) = -\frac{e^2}{\epsilon r} \left[ 1 + A\epsilon e^{-\alpha r} + \{(1-A)\epsilon - 1\} e^{-\beta r} \right], \quad (43)$$

where the parameters  $A$ ,  $\alpha$  and  $\beta$  are given by (41b) for the case of Walter-Cohen  $\epsilon(\vec{k})$  or by (42b) for that of Vinsome and Richardson.

#### 4. RESULTS AND DISCUSSION

For a given set of the potential parameters of (43), the energy  $E(\Gamma)$  for each of the two  $A_1$  and  $T_2$  1s states for Arsenic donor in Ge is then determined from the expressions (6)-(38) by minimization varying  $B$  and  $u$ . These energy levels are calculated for a number of values of  $\epsilon(0)$  which are shown in Fig. 3. In the same figure, for comparison, the single-valley energy with the same Richardson and Vinsome potential parameters (42b) is also shown. We point out that the predicted values of the  $E(A_1) - E(T_2)$  splitting is only  $-(0.5-0)$  meV compared with experimental value  $-4.23$  meV. Detail contributions to these energy levels are given in Table I. Comparison of this table with Tables II and III of I clearly shows that the absolute values of the inter-valley energy terms for Ge are relatively much smaller than the corresponding energies in the case of Si. Although the symmetries are different and the positions of the band minima in Si are at  $k_0 = 0.85 k_{\max}$ , while that for Ge at the zone boundary, the small predicted value of  $E(A_1) - E(T_2)$  splitting in Ge compared with that in Si can easily be traced to the fact that the impurity electron orbit in Ge is much

larger than that in Si for similar impurities, already mentioned in the introduction, and the pure Coulomb potential in the central cell region is unable to produce large enough  $E(A_1) - E(T_2)$  splitting in Ge, as observed experimentally. With the present formalism a  $-4.00$  meV value of the  $E(A_1) - E(T_2)$  splitting for Ge can, however, be obtained if only  $\alpha_w$  in (41) is of the order of 0.4 a.u. This of course gives a very sharp fall of  $\epsilon(\vec{k})$  with  $k$  (Fig. 2), not at all close to the calculated values of  $\epsilon(\vec{k})$  by Walter and Cohen, and Vinsome and Richardson and others, which may also easily be ruled out by the form of  $\epsilon(\vec{k})$  necessary to provide an adequate fit to the phonon spectra. In the configuration space this corresponds to the slow rise of the Coulomb potential  $-e^2/r$  in the central cell region to the value  $-e^2/\epsilon r$  with the increase of  $r$  and hence gives the large  $-4.00$  meV  $E(A_1) - E(T_2)$  splitting.

The central cell corrections (not included) are similar to those for Si as worked out in I and would not alter the conclusion reached with the present formalism for the 1s isocoric donor states in Ge.

#### ACKNOWLEDGMENTS

The author would like to thank Professor A. Baldereschi for discussions and suggestions. He would also like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste.



REFERENCES

Appel, J. 1964, Phys. Rev. 133A, 280-7.  
 Baldereschi, A. 1970, Phys. Rev. E1, 4673-7.  
 Baldereschi, A. and Lipari, N.O. 1973, Phys. Rev. B8, 2697-709.  
 Faulkner, R.A. 1969, Phys. Rev. 125, 1560-7.  
 Kittel, C. and Mitchel, A.H. 1954, Phys. Rev. 96, 1488-93.  
 Kohn, W. and Luttinger, J.M. 1954, Phys. Rev. 97, 869-88.  
 Lampert, M. 1954, Phys. Rev. 97, 352-3.  
 Levinger, B.W. and Frankl, D.R. 1961, J. Phys. Chem. Solids 20, 281-  
 Pantelides, S.T. and Sah, C.T. 1974, Phys. Rev. E16, 621-58  
 Reuszer, J.H. and Fisher P. 1964, Phys. Rev. A135, 1125-32.  
 Sarker, A.Q. 1976, ICTP, Trieste, Preprint IC/76/58.  
 Vinsome, P.K.W. and Jaros, M. 1970, J.Phys. C3, 2140-5.  
 Vinsome P.K.W. and Richardson, D. 1971, J. Phys. C4, 2650-7.  
 Walter, J.P. and Cohen M.L. 1970, Phys. Rev. B2, 1821-6.

TABLE CAPTION

Table I The detail contributions to  $E(A_1)$  and  $E(T_2)$  for the Walter-Cohen (WC) potential parameters (41) and those of Vinsome-Richardson (42). The single-valley (SV) results are for the Vinsome-Richardson parameters only.  $\epsilon(q) = 15.36$ . All energies are in meV.

TABLE I

Energy level	Potential parameters	$D^{-1}$ (a.u.)	$q^2$	$T_0$	$T_1$	$U_0$	$U_1$	$E(\Gamma)_{th}$	$E(\Gamma)_{exp.}$
$A_1, T_2$ (Single-Valley)	VR	38.17	0.8786	11.23		-21.53		-10.29	
	VR	36.20	0.878	12.58	0.059	-22.89	0.191	-10.71	-14.04
$A_1$	WC	36.67	0.878	12.30	0.057	-22.39	-0.217	-10.57	
	VR	38.71	0.879	10.84	0.046	-21.12	-0.149	-10.17	
$T_2$	WC	39.66	0.879	10.33	0.042	-20.39	-0.162	-9.94	-9.81

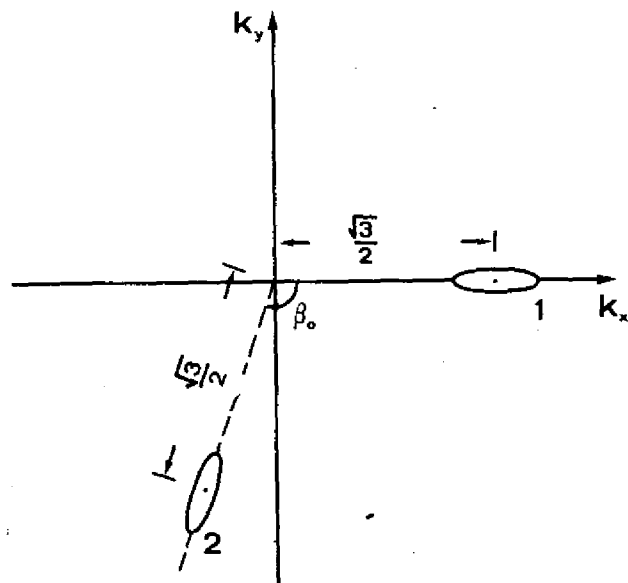


Fig. 1 Constant energy ellipsoids around the conduction band minima 1 and 2 after rotations discussed in the text. The units of  $k_x$  and  $k_y$  are  $\frac{2\pi}{a}$ ,  $a$  being the lattice constant.  $\beta_0 = 109^\circ.47$ .

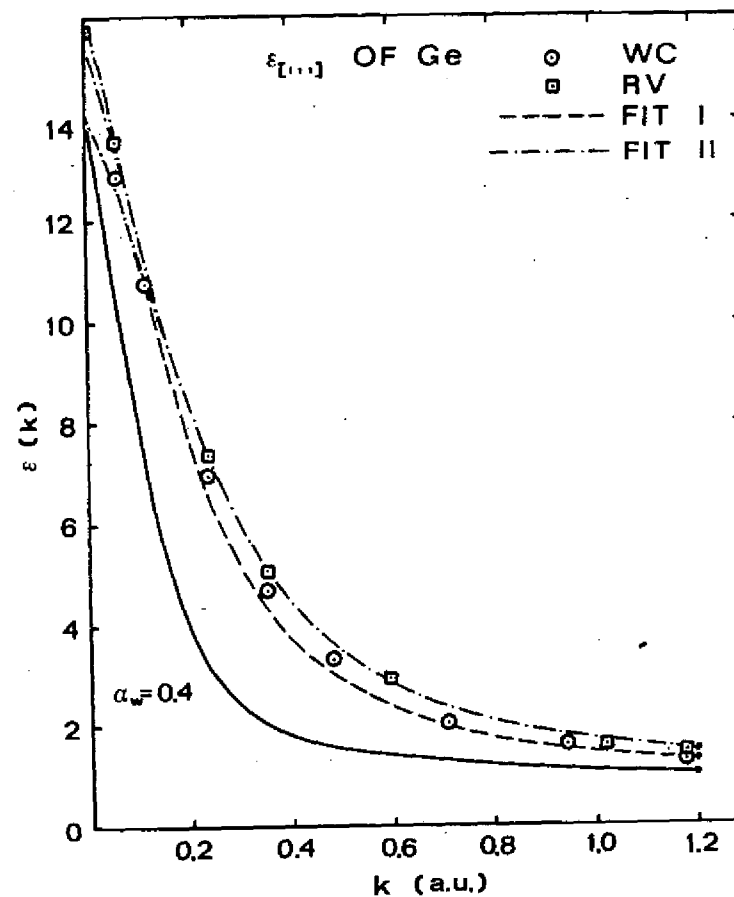


Fig. 2 The dielectric function  $\epsilon(\vec{k})$  of Ge as calculated by Walter and Cohen (WC) and Vinsome and Richardson (VR). Fit I is by the expression (41) and Fit II by (42)

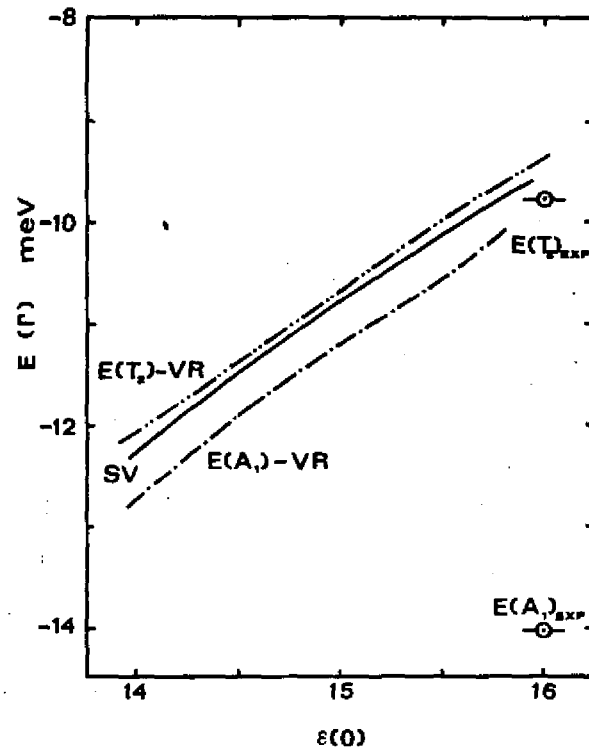


Fig. 3 The variation of the energies  $E(A_1)$ ,  $E(T_2)$  for the Vinsome-Richardson parameters (VR) (42) with respect to  $\epsilon(0)$ . SV shows the single-valley results for VR.

- IC/76/168 M. A. MARKOV: On possible non-locality of quantum field theories involving gravitation.
- IC/76/3 S. ALL, M. E. GRYPEOS and B. KARGAS: Calculation of the  $A$ -particle binding energy in nuclear matter with a simple functional variation method.
- IC/76/4\* D. H. SANCHEZ, M. C. G. PASSEGGI and T. E. HUBER: INT. REP. Empirical evidence for a spin glass state?
- IC/76/8\* J. G. BRANKOV and N. S. TONCHEV: On the relation between two models for superconductors with a structural distortion.
- IC/76/9 ABDUS SALAM and J. STRATHDEE: Black holes as solitons.
- IC/76/10\* M. N. MAHANTA: Generalized Bianchi identities INT. REP. and unification of gravitation and electrodynamics.
- IC/76/11 P. OSLAND and D. TRELEANI: Propagation and decay of resonances produced coherently on nuclei.
- IC/76/13\* ABDUS SALAM and J. STRATHDEE: The mass problem INT. REP. for tensor mesons.
- IC/76/14\* S. L. KALLA: Operators of fractional integration. INT. REP.
- IC/76/15\* M. AHMED and G. RICKAYZEN: On the effect of  $p$  wave scattering to the electrical conductivity of dilute magnetic alloys at high temperatures.
- IC/76/16 Y. UEDA: The pseudoscalar meson mixing problem, spectral function sum rules and chiral symmetry.
- IC/76/17 A. M. HARUN AR-RASHID: A simple derivation of Schwinger's sum rule for spin-dependent structure functions.
- IC/76/18 V. de ALFARO and G. FURLAN: Spontaneously broken conformal symmetry and the nucleon sigma model.
- IC/76/19\* D. KUMAR: Critical phenomena in discarded INT. REP. systems: A renormalization group approach.
- IC/76/20 L. FONDA: A critical discussion on the decay of quantum unstable systems.
- IC/76/21 ABDUS SALAM: The unconfined unstable quark (predictions from a unified gauge theory of unstable strong, weak and electromagnetic interactions).
- IC/76/22\* R. BANSAL, M. P. KHANNA and K. N. PATHAK: INT. REP. Fifth moment sum rule for the density response function.
- IC/76/23\* S. H. CHOH: Point charge approximation of INT. REP. tetragonal  $Yb^{3+}$  and  $Ce^{3+}$  centres in  $CaF_2$ .
- IC/76/24 P. BUDINI: Dynamical symmetry breaking for leptons.
- IC/76/25 H. D. DOEBNER and J.-E. WERTH: Local group actions and Lie algebra representations - I: Globalizations and integrability.
- IC/76/26 A. D. LINDE: Dynamical symmetry restoration and breaking and constraints on masses and coupling constants in gauge theories.
- IC/76/30\* A. OSMAN: Coloumb ( $^3He, n$ ) stripping reactions: INT. REP.
- IC/76/33\* A. D. Linde: Coloured monopoles and confinement of quarks.
- IC/76/34\* A. AMUSA and S. K. SHARMA: Modified Hartree-INT. REP. Fock calculations in  $O^{16}$  nucleus.
- IC/76/37\* N. KUMAR and V. S. KRISHAN: Upper mass limit for neutron star stability against black hole formation.

\* Internal Reports: Limited distribution.

THESE PREPRINTS ARE AVAILABLE FROM THE PUBLICATIONS OFFICE, ICTP, P. O. BOX 586, I-34100 TRIESTE, ITALY. IT IS NOT NECESSARY TO WRITE TO THE AUTHORS.

