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ISAS - INTERNATIONAL SCHOOL FOR ADVANCED STUDIES

THESIS FOR THE TITLE

OF

"MAGISTER PHILOSOPHIAE"

DIELECTRIC MATRIX IN SEMICONDUCTORS: A DIRECT APPROACH

Section: Physics of Condensed Matter

Supervisor: Prof. R. Resta

Candidate: Andrzej Fleszar

Academic Year: 1982/1983

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Contents

I. Introduction

Respons of a medium built up of charged particles to a weak external scalar potential can be described with the aid of a so called longitudinal dielectric function (or rather iverse of it). This function is non-local in space and time, and gives the following relation between external potential $V^{ext}_{(\bar{r},t)}$ and the total screened potential $V^{scr}_{(\bar{r},t)}$:

$$V^{ext}_{(\bar{r},t)} = \int d\bar{r}' \int dt' \, \epsilon(\bar{r}, \bar{r}', t-t') V^{scr}_{(\bar{r}',t')} \qquad \text{I-1}$$

where $V^{scr}_{(\bar{r},t)}$ is equal to the sum of $V^{ext}_{(\bar{r},t)}$ and $\delta V(\bar{r},t)$ -a potential due to rearrangements of particles of medium :

$$V^{scr}_{(\bar{r},t)} = V^{ext}_{(\bar{r},t)} + \delta V(\bar{r},t) \qquad \text{I-2}$$

Because of the homogeneity of the system with respect to translations in time, the dielectric function depends on the difference $t - t'$ .If a similar homogeneity with respect to space co-ordinates were, the dielectric function would depend as well on the difference $\bar{r} - \bar{r}'$,and the relation I-1 would have a simple form in the fourier representation:

$$V^{ext}_{(\bar{q},\omega)} = \epsilon(\bar{q},\omega) V^{scr}_{(\bar{q},\omega)} \qquad \text{I-3}$$

In what follows we shall deal only with the <u>electronic</u> longitudinal dielectric function in crystals (more precisely - in semiconductors) trating ions as rigidly staying in their positions in the lattice. Such a system of electrons instead of being fully homogeneous in space,

is invariant only with respect to discrete translations forming translation group of a given crystal. This fact reflects itself in the way the relation I-1 can be written in fourier representation:

$$V^{ext}(\bar{q}+\bar{G},\omega)=\sum_{\bar{G}'}\epsilon(\bar{q}+\bar{G},\bar{q}+\bar{G}';\omega)V^{sa}(\bar{q}+\bar{G}',\omega) \qquad I-4$$

where $\bar{q}$ is limited to be inside the Brillouin zone and $\bar{G}, \bar{G}'$ are reciprocal lattice vectors. The object $\epsilon(\bar{q}+\bar{G},\bar{q}+\bar{G}',\omega)$ is called the Dielectric Matrix (DM). The matrix indices are reciprocal lattice vectors.

It follows from the very efinition of DM that it is a fundamental quantity in solid state physics, knowledge of which is very important for understanding the physics of crystals. In different classes of phenomena however, and according to our need of accuracy, different levels of sophistication in the application of DM are used. There is a class of phenomena (optical mainly), where so called dynamic dielectric function ($\bar{q}=0$, $\bar{G}=\bar{G}'=0$, $\epsilon=\epsilon(\omega)$),if not only dielectric constant, is sufficient. On the other hand, if the purturbing potential doesn't depend on time, we need only to know the static DM $(\epsilon(\bar{q}+\bar{G},\bar{q}+\bar{G}',\omega=0)\equiv\epsilon(\bar{q}+\bar{G},\bar{q}+\bar{G}))$. For a need of some applications (in metals mostly), it is sufficient to have only diagonal part of DM, as if the system was homogeneous. There are some phenomena however, where the knowledge of full DM is necessary, and the diagonal approximation doesn't work at all. The most striking example are phonon calculations in insulators and semiconductors.(1)
Since first principles calculations of DM are extremely difficult, a number of models of DM appeared during last decade, which describe with a better or worsl success the above mentioned class of phenomena.(2-7)

The increase in computational possibilities last years encouraged solid state theorists to look at many phenomena in crystals from higher level of sophistications. This caused an increase of interests in DM.

Many papers appeared, whose authors try to calculate from first principles (i.e. starting from a realistic band structure of a solid) the DM'es.[8-13] These calculations turned out however to be so elaborate, that only in $\vec{q} \to 0$, $\omega = 0$ limits and for a few materials could be done, in other cases applied approximations shake their relyability.

Present work enters the class of works of first principle calculations of static DM'es. It has however a new feature with respect to previous calculations, a feature that makes the computations more easy and more effective, we belive. The method we apply is "direct" and "non-perturbative", as previous works used. The meaning of this and the idea of our computational method we shall explain in Sect.II. In Sect. III we shall present some computational details. The results and the comparision with already existing data will be given in Sect. IV. We present there DM'es calculated in RPA-approximation for silicon and gallium arsenide in X,L and partly in Γ points.Inprinciple this method allows to calculate DM'es also for points inside Brillouin zone. In that section we calculate also so called dielectric band structure[14] in X and L points. Conclusions and perspectives close our work.

II. Presentation of the Method

In this section we shall present our method of calculation of static electronic DM and we shall point out the differences detween this and previous mrthods.

In the presence of external static potential $V^{ext}_{(\bar{r})}$ electrons in a crystal rearrange themselves forming a new density $n(\bar{r})$ .The change in the electronic density $\Delta n(\bar{r})$,so the difference between this density and unpurturbed one $n^{\circ}(\bar{r})$

$$\Delta n(\bar{r}) = n(\bar{r}) - n^{\circ}(\bar{r}) \qquad \text{II-1}$$

is responsable for forming an additional potential $\delta V(\bar{r})$,that screens $V^{ext}_{(\bar{r})}$ according to the Poisson rule:

$$\delta V(\bar{r}) = V^{scr}_{(\bar{r})} - V^{ext}_{(\bar{r})} = e^2 \int d\bar{r}' \frac{\Delta n(\bar{r}')}{|\bar{r} - \bar{r}'|} \qquad \text{II-2}$$

If $V^{ext}_{(\bar{r})}$ is small,so also $V^{scr}_{(\bar{r})}$ is small,there must be a linear connection between $\Delta n(\bar{r})$ and $V^{scr}_{(\bar{r})}$:

$$\Delta n(\bar{r}) = \int d\bar{r}' \, \hat{\chi}(\bar{r}, \bar{r}') V^{scr}_{(\bar{r}')} \qquad \text{II-3}$$

Function $\hat{\chi}(\bar{r}, \bar{r}')$ is called proper polarisability.Combining II-2 and II-3 we get:

$$V^{ext}_{(\bar{r})} = \int d\bar{r}' \left[\delta(\bar{r} - \bar{r}') - e^2 \int d\bar{r}'' \frac{\hat{\chi}(\bar{r}'', \bar{r}')}{|\bar{r} - \bar{r}''|} \right] V^{scr}_{(\bar{r}')} \qquad \text{II-4}$$

Comparision with I-1 yields (written in compact form):

$$\hat{\epsilon} = \hat{1} - \hat{v}_c \hat{\chi} \qquad \text{II-5}$$

where $\hat{1} = \delta(\bar{r} - \bar{r}')$, $\hat{v}_c = \frac{e^2}{|\bar{r} - \bar{r}'|}$

Equation II-5 written in fourier space takes the form:

$$\epsilon(\bar{q}+\bar{G}, \bar{q}+\bar{G}') = \delta_{\bar{G}\bar{G}'} - \frac{4\pi e^2}{|\bar{q}+\bar{G}|^2} \hat{\chi}(\bar{q}+\bar{G}, \bar{q}+\bar{G}') \qquad \text{II-6}$$

To calculate DM in RPA approximation one starts from a self-consistent one-particle band equation:

$$\left[\frac{p^2}{2m} + V_{cr}(\bar{r}) \right] \psi_\alpha(\bar{r}) = E_\alpha \psi_\alpha(\bar{r}) \qquad \text{II-7}$$

When an external purturbing potential $V^{ext}_{(\bar{r})}$ is present, in the self-consistent equation (in Hartree scheme) $V^{scr}_{(\bar{r})}$ appears:

$$\left[\frac{p^2}{2m} + V_\alpha(\bar{r}) + V^{scr}(\bar{r}) \right] \psi_{\alpha'}(\bar{r}) = E_{\alpha'} \psi_{\alpha'}(\bar{r}) \qquad \text{II-8}$$

The next step is to calculate the change in electron density $\Delta n(\bar{r})$ from the relation:

$$\Delta n(\bar{r}) = n(\bar{r}) - n^\circ(\bar{r}) = \sum_{\alpha'} f_{\alpha'} |\psi_{\alpha'}(\bar{r})|^2 - \sum_{\alpha} f_\alpha |\psi_\alpha(\bar{r})|^2 \qquad \text{II-9}$$

where f_α is the occupation number.
If $V^{scr}_{(\bar{r})}$ is assumed small, equation II-8 can be solved perturbationally. In this way, one expresses the "purturbed" wave functions $\psi_{\alpha'}$ by "unpurturbed" ones ψ_α according to the formulas of perturbation theory and one gets $\hat{\chi}$ or trough II-6 $\hat{\epsilon}$ in a well known (Adler-Wiser)[15] expression:

$$\epsilon(\bar{q}+\bar{G}, \bar{q}+\bar{G}') = \delta_{\bar{G}\bar{G}'} - \frac{4\pi e^2}{|\bar{q}+\bar{G}|^2} \sum_{\bar{k}ll'} \frac{[f_{l'}(\bar{k}+\bar{q}, l') - f(\bar{k}l)] \langle \psi_{l\bar{k}} | e^{-i(\bar{q}+\bar{G})\bar{r}} | \psi_{l'\bar{k}+\bar{q}} \rangle \langle \psi_{l'\bar{k}+\bar{q}} | e^{i(\bar{q}+\bar{G}')\bar{r}} | \psi_{l\bar{k}} \rangle}{E_{\bar{k}+\bar{q}l'} - E_{\bar{k}l}}$$

II-10

Existing calculations of DM are all (according to our knowledge) based on equ. II-10 .There are two basic difficulties making these calculations elaborate: summation over Brillouin zone and summation over conduction bands.First can be overcomed with the aid of special points technique.[12,16,19] The second creates more troubles,since to get good convergence about 90 conduction bands are needed in the case of insulators and semiconductors [13] .The above facts make the first principles calculations of DM extremely time consuming.

Our method is based on the direct computation of the new electronic density $n(\bar{r})$,i.e. on solving equ. II - 8 exactly,without using perturbation theory.We start with a semiempirical pseudopotential band equation of Cohen-Bergstresser[17],to which we add a small monochromatic potential of a given chosen wave vector.The Cohen-Bergstresser potential plays a role of an unpurturbed self-consistent crystal potential in one-electron band equation.Additional small monochromatic potential simulates self-consistently screened external potential.Having solved the new equation we calculate electronic density summing over all occupied states.We subtruct from it the unpurturbed electronic density $n^{o}(\bar{r})$ and fourier analise the difference.The response to a perturbation of a wave vector $\bar{q}+\bar{G}$, $V^{scr}_{(\bar{q}+\bar{G})}$,must be of course of the form $\Delta n(\bar{q}+\bar{G}')$, where $\bar{G}$, $\bar{G}'$ are reciprocal lattice vectors.Dividing $\Delta n(\bar{q}+\bar{G}')$ by $V^{scr}(\bar{q}+\bar{G})$ we get $\hat{\chi}(\bar{q}+\bar{G},\bar{q}+\bar{G}')$.

There are however a few essential problems in this method.The Schrödinger equation with additional potential to be solvable should possess a discrete translational symmetry.The presence of $V^{scr}_{(\bar{r})}$ generally destroys the original translational symmetry of the lattice.This fact seriously limits the possibilities of application of this method to special $\bar{q}$ points in the Brillouin zone.If $\bar{q}$-vector of $V^{scr}_{(\bar{r})}$ is equal to $\bar{G}$ - a reciprocal lattice vector - the original lattice symmetry is not destroyed and the calculations do not differ much from those without perturbation.If $\bar{q}$ cannot be traced to the centre of BZ by a translation from the reciprocal lattice,the translational symmetry of our hamiltonian is changed.When $\bar{q}$-vector lies on the border of the Brillouin

zone (at points X or L for example),or can be join to such a point by a reciprocal lattice translation,we are able to solve the equation II-8 with the aid of supercell technique,we expand the elementary call twise in a relevant direction.Within present computational capabilities the Schrödinger equation II-8 can be solved when $\bar{q}$ lies in the midway from the zone centre to the border of BZ and even for smaller $\bar{q}$.
Another problem ceates the hermiticity of a hamiltonian with monochromatic potential.Since we are able to solve only hermitian Schrödinger equations,the potential should be real.This problem is easy to overcome.We solve the equ. II-8 separately with sin(qr) and cos(qr) as perturbations,and from them extract the relevant information.
Usually one defines $\bar{G}=0$, $\bar{G}'=0$ (or vice versa) elements of $\epsilon(\bar{q}+\bar{G},\bar{q}+\bar{G}')$ as "wings",and $\bar{G}\neq 0$, $\bar{G}'\neq 0$ as "body" of DM.The present method doesn't allow to compute $\epsilon(0,0)$ element of DM,neither the non-analitical elements in wings at $\bar{q}\longrightarrow 0$.At the centre of BZ we are able to calculate only "body" of DM,outside the centre however,we can compute the whole dielectric matrix.
The band equations we solve are the following:

$$\left[\frac{p^2}{2m} + V_a(\bar{r}) + c\sin[(\bar{q}+\bar{G})\bar{r}]\right]\psi_{\bar{k}n}(\bar{r}) = E_n(\bar{k})\psi_{\bar{k}n}(\bar{r})$$

$$\left[\frac{p^2}{2m} + V_a(\bar{r}) + c\cos[(\bar{q}+\bar{G})\bar{r}]\right]\psi_{\bar{k}n}(\bar{r}) = E_n(\bar{k})\psi_{\bar{k}n}(\bar{r}) \qquad \text{II-11}$$

Here c is the strength of a perturbation.We have performed preliminary studies with different strengths in order to be sure that we are in a "linear regime",i.e. the responce in the density $\Delta n(\bar{r})$ is proportional to c.We put cequal to 0.0001 Ry.
Next,we calculate in both cases the electronic density:

$$n^{\sin}_{\bar{q}+\bar{G}}(\bar{r}) = \sum_{\text{occ. bands}} \int_{BZ} \frac{d\bar{k}}{(2\pi)^3} \left|\psi_{\bar{k}n}(\bar{r})\right|^2 \qquad \text{II-12}$$

Similarly we get $n^{\cos}_{\bar{q}+\bar{G}}(\bar{r})$.

Δn is given by:

$$\Delta n^{sin}_{\bar{q}+\bar{G}}(\bar{r}) = n^{sin}_{\bar{q}+\bar{G}}(\bar{r}) - n^{o}(\bar{r})$$

$$\Delta n^{cos}_{\bar{q}+\bar{G}}(\bar{r}) = n^{cos}_{\bar{q}+\bar{G}}(\bar{r}) - n^{o}(\bar{r})$$

The unpurturbed density $n^{o}(\bar{r})$ we obtain of course from the solution of usual Cohen-Bergstresser band hamiltonian without any additional potential.

We have the following relations defining $\hat{\chi}(\bar{r},\bar{r}')$:

$$\Delta n^{sin}_{\bar{q}+\bar{G}}(\bar{r}) = \int d\bar{r}'\, \hat{\chi}(\bar{r},\bar{r}')\, c\, \sin[(\bar{q}+\bar{G})\bar{r}'] \qquad \text{II -13}$$

$$\Delta n^{cos}_{\bar{q}+\bar{G}}(\bar{r}) = \int d\bar{r}'\, \hat{\chi}(\bar{r},\bar{r}')\, c\, \cos[(\bar{q}+\bar{G})\bar{r}']$$

Writing these relations in fourier space yields:

$$\Delta n^{sin}_{\bar{q}+\bar{G}}(\bar{q}+\bar{G}') = \frac{c}{2i}\left[\hat{\chi}(\bar{q}+\bar{G}',\bar{q}+\bar{G}) - \hat{\chi}(\bar{q}+\bar{G}',-\bar{q}-\bar{G})\right] \qquad \text{II-14}$$

$$\Delta n^{cos}_{\bar{q}+\bar{G}}(\bar{q}+\bar{G}') = \frac{c}{2}\left[\hat{\chi}(\bar{q}+\bar{G}',\bar{q}+\bar{G}) + \hat{\chi}(\bar{q}+\bar{G}',-\bar{q}-\bar{G})\right]$$

Subtracting, we come to the final conclusion:

$$\hat{\chi}(\bar{q}+\bar{G},\bar{q}+\bar{G}') = \left[\Delta n^{cos}_{\bar{q}+\bar{G}'}(\bar{q}+\bar{G}) + i\,\Delta n^{sin}_{\bar{q}+\bar{G}'}(\bar{q}+\bar{G})\right]/c \qquad \text{II-15}$$

In the next section we give some details of the calculations.

III. Computational Details

We have calculated DM'es for Si and Ga-As in point Γ (the "body" elements),in X and L points.We have used in equ.s II-7 , II-8 original Cohen-Bergstresser[17] form factors of crystal potential.For these same potentials RPA calculations at the zone centre are available.As the basis of functions plane waves of $(\bar{q}+\bar{G})^2 \leq 21$ (in $\frac{2\pi}{a}$ units) were used.The whole matrix of hamiltonian in this basis was diagonalised,without applying Löwdin's perturbation method.We are convinced however,that in future work with larger supercells Löwdin's method will be unavoidable,since in that case both the time of computation of band structure and the number of independent elements of DM to be calculated increase strongly.

In the case of X and L points we have to solve equ.s II-11 with a supercell technique.To this end elementary cell should be expanded twice in a relevant direction in such a way, to make from vectors $\bar{q}_x$ or $\bar{q}_L$,the vectors of a new reciprocal lattice.In this way,the number of basis functions that are used to solve band hamiltonian increases about twice with respect to the number of functions that is in normal cell,and for X and L points it becoms equal to about 200.This fact is the origin of most difficulties.For points in the midway between the zone centre and its border,the number of basis functions would be of the order of 400.Within the present computational possibilities the direct diagonalisation of such a great matrix is excluded.As was already mentioned,Löwdin's perturbation method would be of great help in this case.Authors dealing with different problems within supercell geometry have found the Löwdin's technique very useful and accurate[18].

It was demonstrated in Sect.II that the basic quantity to be calculated is the electronic density.To have it in zero temperarure case,to which our work is limited,one must integrate the squere modulus of Bloch functions over the Brillouin zone and sum over all occupied bands (for Γ point this summation will include four valence bands, in the case of a supercell for X and L points.there will be eight

valence bands). The integration can be done with the aid of mean value points technique. From various possibilities of mean value points [16,19] we have chosen those of Monkhorst and Pack. With their technique the results of normal cell can be exactly reproduced in supercell. We have used (4,4,4) division of simple cubic cell underlaying the normal f.c.c. cell and the supercell (see Appendix A of [19]). In the case of normal f.c.c. lattice this choise is equivalent to using two mean value points of Chadi-Cohen. These two points of co-ordinates $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ and $(\frac{3}{4},\frac{1}{4},\frac{1}{4})$ remain really two only for completely symmetric functions, in other cases one has to rotate them obtaining 32 points (8 coming from $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$, 24 coming from $(\frac{3}{4},\frac{1}{4},\frac{1}{4})$). Their co-ordinates are the following:

$$\bar{k}_{1-8} = \frac{2\pi}{a}\left(\pm\frac{1}{4},\pm\frac{1}{4},\pm\frac{1}{4}\right) \qquad \bar{k}_{9-16} = \frac{2\pi}{a}\left(\pm\frac{3}{4},\pm\frac{1}{4},\pm\frac{1}{4}\right)$$

$$\bar{k}_{17-24} = \frac{2\pi}{a}\left(\pm\frac{1}{4},\pm\frac{3}{4},\pm\frac{1}{4}\right) \qquad \bar{k}_{25-32} = \frac{2\pi}{a}\left(\pm\frac{1}{4},\pm\frac{1}{4},\pm\frac{3}{4}\right) \qquad \text{III-1}$$

In the supercell, the number of non-equivalent points diminishes to 16, for some of them can be joined by supercell reciprocal lattice vectors. Because of time-reversal symmetry, we need to diagonalise supercell hamiltonians yet in smaller number of points (8-for X point, 10-for L point).

The calculations were performed for so called Hermitian Dielectric Matrix (HDM), which is defined as follows:

$$\tilde{\epsilon}(\bar{q}+\bar{G},\bar{q}+\bar{G}') = \frac{|\bar{q}+\bar{G}|}{|\bar{q}+\bar{G}'|}\epsilon(\bar{q}+\bar{G},\bar{q}+\bar{G}') \qquad \text{III-2}$$

The two objects ϵ and $\tilde{\epsilon}$ are equivalent, the advantage of working with HDM is that one needs to bother only about one "triangle" of HDM and one can compute easy the dielectric band structure.

We have computed only independent elements of HDM, i.e. these that can not be connected one to another by any symmetry operation. For

Γ point,if HDM is 113x113 matrix,there are 217 such elements (without non-analiticities at "wings"-there are 210 such elements). For X and L points,if HDM is 108x108 matrix,there are 468 and 598 such elements respectively.The advantage of our method is,that we need not to compute separately all those (217 or 468 or 598) elements. Since some of them delong to the same row,they are obtained in the same cycle of calculations.A cycle of calculations contains the solution of equ.s II-11 with a given,one,reciprocal lattice vector $\bar{G}$ in purturbing potential.In one cycle one can have the whole row of DM.We need to do as many cycles as are independent elements of HDM with right-hand site vectors different (i.e. with different purturbing potentials in equ.II-11). In the case of $\bar{q}=0$ HDM (210 independent elements !), there would be 9 cycles only.IN the case of X and L points,there will be 14 and 16 cycles respectively for 108x108 HDM.

In the next section we shall present our results.

IV. Results

In this section, the HDM's calculated for silicon and gallium-arsenide are presented. In Table I, some of "body" elements of HDM of Si in Γ point are shown. They are compared with previous results obtained by Baldereschi and Tosatti[12]. Both these results were got with the use of one mean-value point (Baldereschi point)[16]. Origin of reference is between atoms.

Table I. "Body" of HDM of Si for $\vec{q}=0$.

G	G'	Present work $\epsilon(\vec{G},\vec{G}')$	Previous results $\epsilon(\vec{G},\vec{G}')$
(1, 1, 1)	(1, 1, 1)	1.7109	1.711
($\bar{1}$, 1, 1)	(1, 1, 1)	-.0164	-.016
(2, 0, 0)	(1, 1, 1)	.0853	.085
(1, $\bar{1}$, 1)	($\bar{1}$, 1, 1)	-.0204	-.020
(1, $\bar{1}$, $\bar{1}$)	($\bar{1}$, 1, 1)	-.1127	-.113
(2, 0, 0)	($\bar{1}$, 1, 1)	.0079	.008
(2, 0, 0)	(2, 0, 0)	1.5290	1.529
($\bar{2}$, 0, 0)	(2, 0, 0)	-.0082	-.008
(0, 2, 0)	(2, 0, 0)	-.0245	-.025

In Table II, the same "body" elements of HDM at Γ point for Ga-As are shown, together with already existing data obtained by Resta and Baldereschi[13]. Origin of reference is between Ga and As atoms.

Table II. Some of "body" elements of HDM of Ga-As for $\tilde{q}=0$.

G	G'	Present work		Previous results	
		$\mathrm{Re}\epsilon(\tilde{G},\tilde{G}')$	$\mathrm{Im}\epsilon(\tilde{G},\tilde{G}')$	$\mathrm{Re}\epsilon(\tilde{G},\tilde{G}')$	$\mathrm{Im}\epsilon(\tilde{G},\tilde{G}')$
(1,1,1)	(1,1,1)	1.6889	.0000	1.6891	.0000
$(\bar{1},1,1)$	(1,1,1)	-.0035	-.0464	-.0036	-.0463
(2,0,0)	(1,1,1)	.1083	-.0391	.1085	-.0390
$(1,\bar{1},1)$	$(\bar{1},1,1)$	-.0096	.0000	-.0097	.0000
$(1,\bar{1},\bar{1})$	$(\bar{1},1,1)$	-.1071	.0714	-.1068	.0716
(2,0,0)	$(\bar{1},1,1)$	.0107	-.0079	.0105	-.0079
(2,0,0)	(2,0,0)	1.5150	.0000	1.5152	.0000
$(\bar{2},0,0)$	(2,0,0)	.0020	.0000	.0023	.0000
(0,2,0)	(2,0,0)	-.0037	.0000	-.0038	.0000

As it can be seen, in both cases the results are almost perfectly equal. The difference is less then 0.001, and can be traced to the finite value of the purturbing potential strength c. This value of c however, cannot be too small, not to submit the results to the influence of computational "noises" (coming mostly from the process of integrating over the Brillouin zone). The above results were computed in order to test our method and check its accuracy. New results - HDM'es of Si and Ga-As calculated in points X and L - are presented in Tables III-IV. These calculations were done with the technique of mean value points of Monkhorst and Pack. Origin of reference again

between atoms.

Table III. Some of HDM elements of Si and Ga-As in point X. $\vec{q}_x=(1,0,0)$

G	G'	Silicon	Gallium-Arsenide	
		$\epsilon(\vec{q}_L+\vec{G},\vec{q}_L+\vec{G}')$	$\mathrm{Re}\,\epsilon(\vec{q}_x+\vec{G},\vec{q}_x+\vec{G}')$	$\mathrm{Im}\,\epsilon(\vec{q}_x+\vec{G},\vec{q}_x+\vec{G}')$
(0,0,0)	(0,0,0)	2.9484	2.8921	.0000
$(\bar{2},0,0)$	(0,0,0)	.0000	.0000	.4504
$(\bar{1},1,\bar{1})$	(0,0,0)	.0829	.1266	-.0188
$(\bar{1},1,\bar{1})$	$(\bar{1},1,\bar{1})$	2.0860	2.0621	.0000
(0,0,2)	$(\bar{1},1,\bar{1})$	-.0022	-.0006	.0002
(1,1,1)	$(\bar{1},1,\bar{1})$	.0185	-.0010	.0039
(0,0,2)	(0,0,2)	1.4198	1.4032	.0000
$(0,0,\bar{2})$	(0,0,2)	-.0209	-.0212	.0000
(0,2,2)	(0,0,2)	-.0065	-.0038	.0167
$(1,\bar{1},1)$	$(1,\bar{1},1)$	1.3305	1.3178	.0000
(1,1,1)	$(1,\bar{1},1)$	-.0109	-.0067	.0192
(2,0,0)	$(1,\bar{1},1)$	.0532	.0585	.0181
(0,2,2)	(0,2,2)	1.1819	1.1796	.0000
(2,0,0)	(0,2,2)	.0146	.0129	.0048
$(\bar{2},\bar{2},\bar{2})$	(0,2,2)	-.0122	-.0076	.0094

Table IV. Some of HDM elements of Si and Ga-As in point L. $q_L = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

G	G'	Silicon	Gallium-Arsenide	
		$\epsilon(\bar{q}_L+\bar{G}, \bar{q}_L+\bar{G}')$	Re $\epsilon(\bar{q}_L+\bar{G}, \bar{q}_L+\bar{G}')$	Im $\epsilon(\bar{q}_L+\bar{G}, \bar{q}_L+\bar{G}')$
(0,0,0)	(0,0,0)	3.1683	3.0854	.0000
$(\bar{1},\bar{1},\bar{1})$	(0,0,0)	.7425	.6818	.4391
$(\bar{2},\bar{2},\bar{2})$	(0,0,0)	-.1393	-.1425	-.0198
$(\bar{1},1,\bar{1})$	$(\bar{1},1,\bar{1})$	1.7969	1.7871	.0000
$(\bar{2},0,0)$	$(\bar{1},1,\bar{1})$	.1095	.1443	-.0543
$(\bar{1},\bar{1},\bar{1})$	$(\bar{1},1,\bar{1})$	.0232	.0083	.0023
$(\bar{1},1,1)$	$(\bar{1},1,1)$	1.4290	1.4200	.0000
(0,0,2)	$(\bar{1},1,1)$	.0628	.0739	.0215
$(\bar{2},0,2)$	$(\bar{1};1;1)$	.0551	.0648	-.0181
(0,0,2)	(0,0,2)	1.2775	1.2737	.0000
(1,1,1)	(0,0,2)	.0532	.0617	.0185
$(\bar{1},\bar{1},\bar{3})$	(0,0,2)	-.0087	-.0018	-.0047
(1,1,1)	(1,1,1)	1.2711	1.2693	.0000
$(\bar{2},\bar{2},\bar{2})$	(1,1,1)	-.0197	-.0064	.0153
$(\bar{2},0,2)$	(1,1,1)	.0157	.0128	.0027

As a first immediate application of our DM'es, dielectric band structure in points X and L was calculated for Si and Ga-As. Dielectric band structure are called eigenvalues and eigenvectors of DM (or HDM) at a given vector $\bar{q}$:[14,17]

$$\sum_{\bar{G}'} \tilde{\varepsilon}(\bar{q}+\bar{G}, \bar{q}+\bar{G}')\, V(\bar{q}+\bar{G}') = \varepsilon(\bar{q})\, V(\bar{q}+\bar{G}) \qquad \text{IV-1}$$

In Tabl.V, the greatest eigenvalues of DM'es of Si and Ga-As in points X and L are shown.

Table V. The greatest eigenvalues of DM of Si and Ga-As in X and L points. Symmetry notation as in Bassani's book[20]

Silicon				Gallium-Arsenide			
Point X		Point L		Point X		Point L	
	$\varepsilon(\bar{q}_x)$		$\varepsilon(\bar{q}_L)$		$\varepsilon(\bar{q}_x)$		$\varepsilon(\bar{q}_L)$
X_1	3.060	L_1	4.066	M_1	3.471	L_1	4.095
X_4	2.393	L_1'	2.547	M_4	2.741	L_1	2.563
X_1	2.016	L_3'	2.010	M_5	2.401	L_3	2.110
X_3	1.554	L_1	1.966	M_4	2.004	L_1	1.979
X_2	1.552	L_3	1.860	M_1	1.905	L_3	1.748
X_4	1.527	L_1'	1.551	M_5	1.537	L_3	1.537

In [7], dielectric band structure of silicon resulting from some models of DM was calculated. In Fig.I we present the comparision of our results with those of [7]. The comparision is done for $\varepsilon^{-1}(q)$

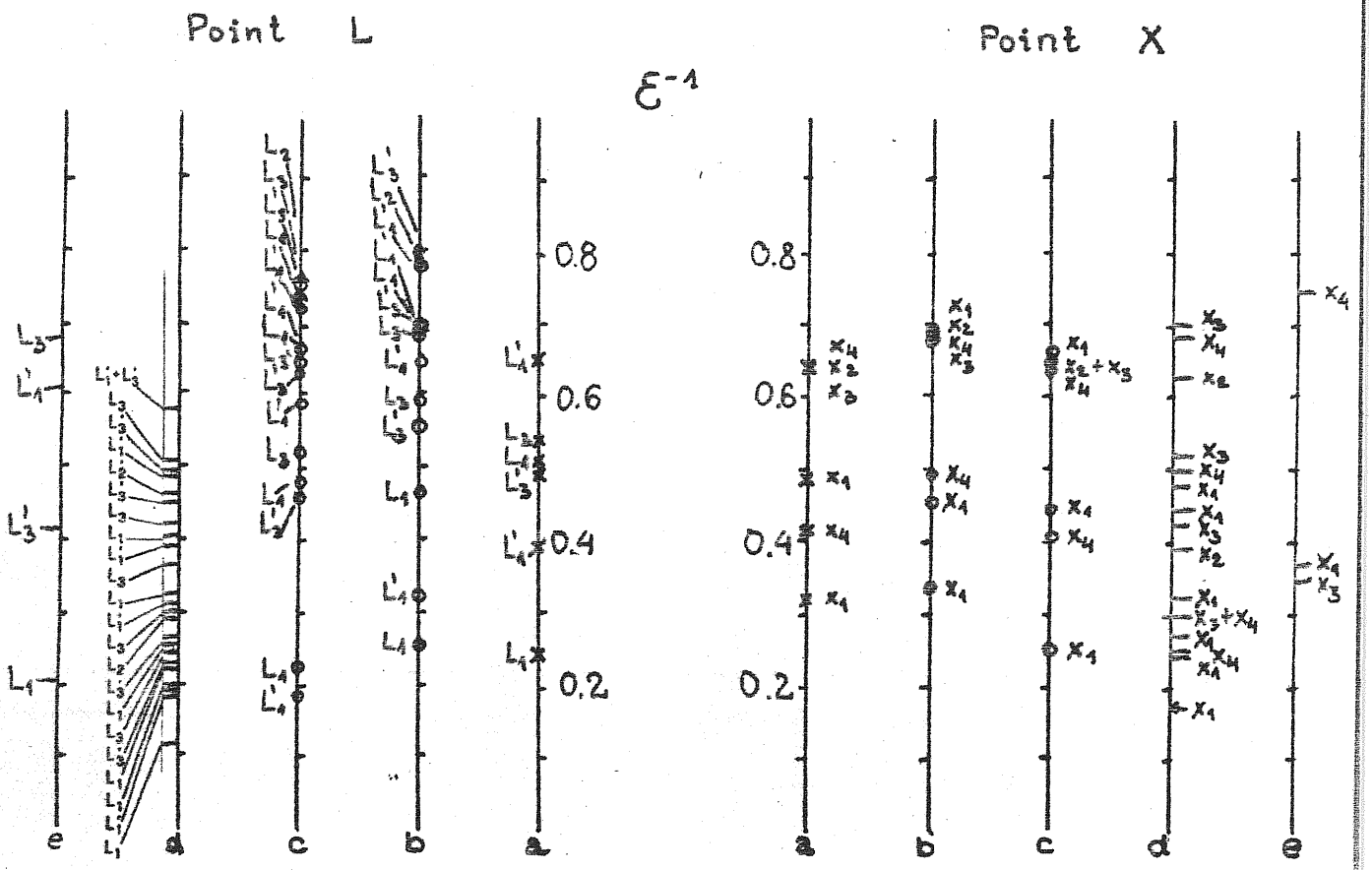

Fig. I. Dielectric band structure ($\varepsilon^{-1}(q)$ resulting from models and the present work: a-present work, b-Car-Selloni model, c-local density model, d-Johnson's model, e-Sinha's model

It can be seen, that the most similar results to ours Car-Selloni model gives (with partially different symmetry ordering however). A characteristic feature of the spectra of $\varepsilon^{-1}(q)$ is the gap $L_1 - L_1'$ which is "closed" in "empty lattice" dielectric band structure. Its value could serve then as a measure of the importance of local field effects. As can be seen from the picture, Sinha's model too much overestimates its value, Johnson's model and local density model too much underestimate it. These facts are in agreement with

general trends of these models,resulting from the basis they were established (too much ionic,or too much metallic). Car-Selloni model gives for this gap a value about two times smaller then our value is, which suggests that local field effects are underestimated in this model.

V . Conclusions and Perspectives

We have presented in this work a "direct" method of calculation of RPA dielectric matrices in semiconductors and insulators. "Direct"- means that equation II-8 is not solved perturbationally, but directly. We have calculated "body" elements of DM in point Γ and the whole DM'es in points X and L for silicon and galium-arsenide. The agreement with already existing results in Γ point is excellent.The small difference (less then .001) in results can be treated as the accuracy of calculation coming from a finite strength of perturbation c. When this strength goes to zero, our results should exactly reproduce previous ones. In the case of X and L points there are no available data to be copared with ours.
We have calculated the dielectric band structure of Si and Ga-As in points X and L . Comparision with the values given by different models approves the model of Car-Selloni with respect to other models.

In conclusion we can say, that our method of calculation of DM turned out to be very effective. We belive, with present computational possibilities we can compute DM'es also for pcints inside the Brillouin zone. For future work we plan to calculate DM'es for points in midway between the zone centre and X and the centre and point L respectively and also in 1/4 of these distances from point Γ .

The calculated DM'es can serve for many purposes. They can give a good frame of reference for a satisfactory model of DM for which there is a continous need.They can serve in phonon calculations. They can be used in so called - real space local field investigations,that is in computation of the change in electronic density due to a given perturbation.

VI. References

1. R.M.Pick,M.H.Cohen and R.M.Martin,Phys.Rev.B1 910 (1970)

2. C.M.Bertoni,V.Bortolani,C.Calandra and E.Tosatti,Phys. Rev. B9 1710 (1974)

3. S.K.Sinha,Phys.Rev. 177 1256 (1969)

4. S.K.Sinha,R.P.Gupta and D.L.Price,Phys.Rev. B9 2564,2573('74)

5. D.L.Johnsos,Phys.Rev. B9 4475 (1974)

6. R.Car and A.Selloni,Phys.Rev.Letters 40 1365 (1979)

7. For a review on DM models see: R.Car,E.Tosatti,S.Baroni and S.Leelaprute,Phys.Rev.B24, 985 (1981)

8. J.A.Van Vechten and R.M.Martin,Phys.Rev.Letters 28,446(1972)

9. W.Hanke and L.J.Sham,Phys.Rev.Letters 33,582 (1974)

10. S.G.Louie,J.R.Chelikowsky and M.L.Cohen,Phys.Rev.Letters 34,155 (1975)

11. J.T.DEVREESE,P.E. Van CAMP and V.E.Doren,Bull.Am.Phys.Soc. 23,224 (1978)

12. A.Baldereschi and E.Tosatti,Phys.Rev. B17, 4710 (1978)

13. R.Resta and A.Baldereschi,Phys.Rev. B23 ,6615, (1981) to overcome the summation over conduction bands,so-called "closure-approximation" was proposed:J.T.Devreese,P.E. Van Camp and V.E.Van Doren,Phys.Rev.Letters 42 1224 (1979)

14. A.Baldereschi and E.Tosatti,Solid State Commun.29,131,(1979)

15. S.L.Adler,Phys.Rev. 126,413(1962):N.Wiser,Phys.Rev.129. 62, (1963)

16. A.Baldereschi,Phys.Rev. B7,5215,(1973)· D.J.Chadi and M.L.Cohen,Phys.Rev. B 8, 5747 (1973)

17. M.L.Cohen and T.K.Bergstresser,Phys.Rev. 141,739 (1966)

18. K.Kunc and R.M.Martin in:"Ab initio calculation of phonon spectra",edited by J.T.Devreese (1983) p.65
R.M.Martin and K.Kunc, ibid p.49

19. M.J.Monkhorst and J.D.Pack,Phys.Rev. B13, 5188 (1976)

20. F.Bassani and G.Pastori parravicini: "Electronic States and Optical Transitions in Solids", Perg.Press (1975)