A Self-Consistent APW-k.p Energy Band Method*

I. C. DA CUNHA LIMA and NELSON J. PARADA*"

Instituto de Física "Gleb Wataghin", Universidade Estadual de Campinas, Campinas, S. P.*

It is shown that a self-consistent electronic APW energy band calculation can be simplified if the $\mathbf{k} \cdot$ p expansion is used for obtaining the Bloch functions. An expression for the spherically symmetric charge density is derived in the "muffin-tin" approximation for the crystalline potential. Some advantages in the computation time are pointed out.

Neste trabalho é mostrado como um calculo autoconsistente de faixas de energia pelo método APW pode ser simplificado se a expansão $\mathbf{k} \cdot$ p é utilizada para a obtenção das funções de Bloch. Uma expressão para a densidade de carga esfericamente simétrica é derivada na aproximação "Muffin-tin" para o potencial cristalino. Algumas vantagens no tempo de computação são apresentadas.

1. Introduction

In 1967, one of the authors[1] proposed a method to obtain the electronic energy bands in a general point $\mathbf{k}$ of the Brillouin zone, once the bands were known at a particular point $\mathbf{k}_0$ of the same zone. The method was based on the expansion of the band functions at $\mathbf{k}$ in terms of the Kohn-Luttinger complete set of functions[2], that is,

$$b_{n,i}^{\Gamma_\alpha(\mathbf{k})} (\mathbf{k}, \mathbf{r}) = \sum_{m,j} C_{n,i}^{m,j} (\mathbf{k} - \mathbf{k}_0) \, \chi_{m,j} (\mathbf{k} - \mathbf{k}_0, \mathbf{r}), \qquad (1.1)$$

where $b_{n,i}^{\Gamma_\alpha(\mathbf{k})} (\mathbf{k}, \mathbf{r})$ is a Bloch function belonging to the nth band and transforming like the ith partner of the $\Gamma_\alpha(\mathbf{k})$ irreducible representation of the group of the wavevector k.

The Kohn-Luttinger function $\chi_{m,j}(\mathbf{k} - \mathbf{k}_0,\mathbf{r})$ is defined in terms of the Bloch function $b_{m,j}^{\Gamma_\beta(\mathbf{k}_0)}(\mathbf{k}_0, \mathbf{r})$ by

$$\chi_{m,j}(\mathbf{k} - \mathbf{k}_0, \mathbf{r}) = \exp\left[i(\mathbf{k} - \mathbf{k}_0)\cdot \mathbf{r}\right]\, b_{m,j}^{\Gamma_\beta(\mathbf{k}_0)}(\mathbf{k}_0, \mathbf{r}). \tag{1.2}$$

With the above expansion, it is possible to get a simple expression for the Hamiltonian matrix elements which are written in terms of the matrix elements of momentum operator between two levels at $\mathbf{k}_0$. More explicitly, the problem of calculating the energy levels reduces to that of finding the solutions $E_n(\mathbf{k})$ of the secular equation

$$\det\left\{\left[\frac{\hbar^2}{2m_e}\mathbf{k}^2 + E_m(\mathbf{k}_0) - E_n(k)\right]\delta_{m'm}\,\delta_{ij} + \frac{h}{m}\mathbf{K}\cdot\mathbf{p}_{m,m'}^{i,j}\right\} = 0 \tag{1.3}$$

where

$$\mathbf{p}_{m,m'}^{i,j} = \int d^3\mathbf{r}\,\left[\psi_{m,i}^{\Gamma_\alpha(\mathbf{k}_0)}(\mathbf{k}_0, \mathbf{r})\right]^*\,\rho\,\psi_{m',j}^{\Gamma_\beta(\mathbf{k}_0)}(\mathbf{k}_0, \mathbf{r}),$$

and

$$\mathbf{K} = \mathbf{k} - \mathbf{k}_0.$$

The $\mathbf{k}\cdot$ p method provides good results[3-8] for the bands at any point in the Brillouin zone. However, if the traditional APW method is used for this purpose, an enormous and tedious work becomes necessary, mainly at low symmetry points. Such a difficulty becomes more evident when we try to make the calculation self-consistent. It is necessary to calculate the charge density point by point in the unitary cell and this implies knowing the Bloch functions for a great number of k-vectors in the Brillouin zone. As a consequence, there is an unavoidable compromise between the accuracy of the calculation and the time of computation which necessarily disfavors the former.

Nevertheless, the calculation by the $\mathbf{k}\cdot$ p method does not depend on the symmetry of the point in which it is made. The only compromise in accuracy refers to the number of levels used iriitially at the point $\mathbf{k}_0$. But the computation time for calculation for each vector k depends on this number almost entirely in the determination of the matrix elements of momentum, which is made only once per iteration. Therefore, there exists a much less restrictive compromise.

For that reason, the self-consistent calculation of bands by the $\mathbf{k}\cdot$ p expansion is a powerfull method, mainly when the "muffin-tin" approximation for the crystalline potential is assumed. From now on we shall use this approximation.

2. Charge Density

Matheiss *et al.*[9] presented an expression for the spherically symmetrical charge density in each "muffin-tin" sphere:

$$\sigma_s(r) = \int_{s \text{ sphere}} \sum_k \sum_\alpha \frac{r^2}{v_s} \, | \psi^\alpha(\mathbf{r} \,; \mathbf{k}) |^* \, \psi(\mathbf{r} \,; \mathbf{k}) \, d\Omega, \tag{2.1}$$

where the integral is taken in a solid angle about the center s of the sphere. The summations in a and k refer to all the occupied states. In Eq. (2.1), each term in the summations represents the contribution of state $\mathbf{k}$ in the band a to the charge density on the surface of radius $\mathbf{r}$. By substituting the expression of the Bloch function in terms of $APW's$, we obtain[9]

$$\sigma_s^{k,\alpha}(r) = \frac{r^2}{v_s} \int_{\text{sphere}} | \psi^\alpha(\mathbf{r} \,; \mathbf{k})^* \, \psi^\alpha(\mathbf{r} \,; \mathbf{k}) \, d\Omega =$$

$$= \frac{\tau}{v_s N_{k,\alpha}} \sum_i \sum_l \sum_j v^*(\mathbf{k}_i) \, v(\mathbf{k}_j) \, C_{ijl}^{\alpha(s)} \left[\frac{r \, u_l(\mathbf{r} \,; E)}{R_s u_l(R_s \,; E)} \right]^2 \tag{2.2}$$

Now let us use expansion (1.2) in order to obtain the charge density $\sigma_s^{k,\alpha}$:

$$\sigma_{s,n,i}^{k}(r) = \frac{r^2}{v_s} \int_{\text{sphere}} \{ \sum_{m',j'} C_{n,m'}^{i,j'}(\mathbf{k} - \mathbf{k}_0) \, e^{i(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{r}} \, b_{m',j'}^{\Gamma_\alpha(\mathbf{k}_0)}(\mathbf{k}_0, \mathbf{r}) \}^* \times$$

$$\times \{ \sum_{m,j} C_{n,m}^{i,j}(\mathbf{k} - \mathbf{k}_0) \, e^{i(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{r}} \, b_{m,j}^{\Gamma_\beta(\mathbf{k}_0)}(\mathbf{k}_0, \mathbf{r}) \} \times \sin \theta d\theta d\phi, \tag{2.3}$$

where we include the band subscription and the partner index. The above expression may be written as

$$\sigma_{s,n,i}^{k}(r) = \frac{r^2}{v_s} \sum_{m',j'} \{ C_{n,m'}^{i,j'}(\mathbf{k} - \mathbf{k}_0) \, C_{n,m}^{i,j}(\mathbf{k} - \mathbf{k}_0) \} \times$$

$$\times \left\{ \int_{\text{sphere}} b_{m',j'}^{\Gamma_\alpha(\mathbf{k}_0)*}(\mathbf{k}_0, \mathbf{r}) \, b_{m,j}^{\Gamma_\beta(\mathbf{k}_0)}(\mathbf{k}_0, \mathbf{r}) \sin \theta d\theta d\phi \right\}, \tag{2.4}$$

the summations being extended to all levels and partners, occupied or not.

421

The spherically symmetrical charge density (aniount of charge in a spherical shell of radius r and thickness dr) will be given by

$$\sigma_s(r) = \sum_{n,i} \frac{\tau}{(2\pi)^3} \int_{ZB} d^3k \; \sigma_{s,n,i}^k(r).$$

(2.5)

where the summations only involve the occupied states.

Nevertheless, an important simplification may be done. In **Eq.** (2.4), the integral

$$\int_{\text{spherea}} d\Omega \; b_{m',i}^{\Gamma_\alpha(k_0)} (\mathbf{k}_0, \mathbf{r})^* \cdot b_{m,j}^{\Gamma_\beta(k_0)} (\mathbf{k}_0, \mathbf{r})$$

(2.6)

is invariant under rotations of the coordinate system because it extends over the whole solid angle around the center s. Therefore it obeys the scalar product theorem

$$\langle f_{i,j}^\alpha | g_{k,l}^\beta \rangle = \delta_{\alpha\beta} \delta_{ik} \langle f_{i,i}^\alpha | g_{i,l}^\alpha \rangle$$

(2.7)

and **Eq.** (2.5) becomes

$$\sigma_{s,n,i}^k(r) = \frac{r^2}{v_s} \sum_{m',m,j}^\alpha \{ C_{n,m'}^{i,j*} (\mathbf{k} - \mathbf{k}_0) \; C_{n,m}^{i,j} (\mathbf{k} - \mathbf{k}_0) \} \times$$

$$\int_{\text{spheres}} \sin\theta d\theta d\phi \; b_{m',j}^{\Gamma_\alpha(k_0)*}(\mathbf{k}_0, \mathbf{r}) \cdot b_{m,j}^{\Gamma_\alpha(k_0)} (\mathbf{k}_0, \mathbf{r}),$$

(2.8)

the summations being performed by taking into account only terms whose wavefunctions for different levels transforrn as the same partner of the same irreducible representation of the group of $\mathbf{k}_0$.
Finally by substituting (2.8) into (2.5) we obtain

$$\sigma_s(r) = \frac{r^2}{v_s} \sum_{m,m',j}^\alpha \left\{ \left[\sum_{n,i} \frac{\tau}{(2\pi)^3} \int_{ZB} d^3k \; C_{n,m'}^{i,j} (\mathbf{k} - \mathbf{k}_0)^* \; C_{n,m}^{i,j} (\mathbf{k} - \mathbf{k}_0) \right] \times \right.$$

$$\times \int_{\text{sphere}} \sin\theta d\theta d\phi \; b_{m',j}^{\Gamma_\alpha(k_0)} (\mathbf{k}_0, \mathbf{r}) \cdot b_{m,j}^{\Gamma_\alpha(k_0)} (\mathbf{k}_0, \mathbf{r}) \cdot$$

(2.9)

After obtaining the energy levels and the wavelùnctions at point $\mathbf{k}_0$, the integrals in solid angles can be evaluated immediately. Then, we make the expansion $\mathbf{k} \cdot p$ which gives directly, at every point k, the values of the Kohn-Luttinger functions coefficierits $C_{n,m}^{i,j}(\mathbf{k} - \mathbf{k}_0)$ which

allows us to calculate the integral in reciprocal space, provided that a sufficiently large number of points is taken into account.

The self-consistency is then established by using the charge density $\sigma_s(r)$ in Poisson's equation for the crystalline potential.

3. Conclusion

We can conclude that the use of $\mathbf{k} \cdot \mathbf{p}$ method for calculating the self-consistent charge density allows a considerable simplification, which comes from the fact that we only have contributions coming from states with the same symmetry, and a great reduction in computation time, because the coefficients $C_{n,m}^{i,j}(\mathbf{k} - \mathbf{k}_0)$ are quickly obtained even at general points of the Brillouin zone.

In a later work, we will present applications of this method to semiconductors of the group 111-V, particularly $GaAs$ and GaP, and give information about the computation time required for each iteration as well as others inherents to the calculation.

References

1. G. W. Pratt Jr. and N. J. Parada, Int. J. Quant. Chemistry 1S, 189 (1967).
2. W. Kohn and L. Luttinger, Phys. Rev. 140, **A1133** (1965).
3. N. J. Parada, Phys. Kev. **B3,** 2042 (1971).
4. I. C. da Cunha Lima, M. Sc. thesis presented to the *Instituto de Fisica* "Gleb Wataghin': UNICAMP (unpublished).
5. N. P. Ahmad, M. Sc. thesis presented to the *Instituto de Física* "Gleb Wataghin", UNICAMP (unpublished).
6. L. M. Brescansin, M. Sc. thesis presented to the *Instituto de Física* "Gleb Wataghin", UNICAMP (unpublished).
7. T. T. Sans, M. Sc. thesis presented to the *Instituto de Fisica* "Gleb Wataghin", UNICAMP (unpublished).
8. D. D. Bus and N. J. Parada, Phys. Rev. B1, 2692 (1970).
9. L. F. Matheiss, J. H. Wood and C. Switendick, *The Augmented Plane Wave Method in Methods on Computational Physics,* vol. 8 (1968). Academic Press.
10. see, e.g., J. F. Cornwell, *Group Theory and Electronic Energy Bands in Solids,* North Holland, Amsterdam, 1969.