BLOCH AND WANNIER FUNCTIONS IN MOMENTUM SPACE

Jean-Louis CALAIS

Quantum Chemistry Group, University of Upsala, Box 518, S-75120-Upsala, Sweden

Dedicated to Dr R. Zahradník on the occasion of his 60th birthday.

Direct calculations of wave functions in momentum space require a study of the formal properties of such functions. Here we discuss the momentum space counterparts of Bloch and Wannier functions, both in general and for two extreme kinds of basis set expansions: plane waves and atomic orbitals.

Although I was well aware of Rudolf Zahradník's name from the literature it was not until 1981 that I had the pleasure of meeting him personally. That was one of those rare occasions when one knows immediately that — to make an understatement — our "personal chemistries" were compatible. Our later encounters have only confirmed and strengthened those first impressions.

When the Löwdin lectureship at the University of Upsala was established Rudolf Zahradník was invited to become the first Löwdin lecturer. In the best Löwdin tradition he analyzed the connections between chemistry, physics and biology.

"Chemistry is about the distribution of electrons in atoms, molecules, molecular fragments and aggregates", as claimed by Cook[1], is one possible characterization of chemistry. The title of Platt's article in Handbuch der Physik, "The Chemical Bond and the Distribution of Electrons in Molecules"[2] also emphasizes the importance of the electron density. A theoretical support for that view is provided by the Hohenberg–Kohn theorem[3], which has opened up the study of electronic structure, particularly for solids, to density functional methods[4,5].

In basic quantum mechanics we learn however that position and momentum are complementary. One usually works with wave functions in position space, which give among other things the "ordinary" density $\varrho(r)$. But we can equally well work with wave functions in momentum space, i.e. the Fourier transforms of the positions space functions:

$$\phi(\boldsymbol{p}) = (8\pi^3)^{-1/2} \int \mathrm{d}v\, \phi(\boldsymbol{r})\, \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}. \tag{1}$$

The information content of $\phi(\boldsymbol{p})$ is exactly the same as that of $\phi(\boldsymbol{r})$. The momentum distribution (or density), $\sigma(\boldsymbol{p})$, is easily obtained from the wave function in mo-

mentum space, but can equally well be calculated from the wave function in position space.

Experimental progress in Compton scattering as well as in other methods for determining momentum distributions[6,7] has encouraged theorists to investigate various aspects of momentum space[5,6,8−10]. Wave functions in position space have been used to calculate measurable momentum space properties, primarily Compton profiles.

Density matrices[5,11] provide a connection between momentum space and position space[5,12]. For an electronic system with at most two-particle interactions the second order density matrix contains all information that is needed. The first order density matrix can be obtained from the second order matrix by integration. The density is the diagonal part of the first order density matrix. There is more information in the first order density matrix, though, which is also accessible experimentally through the momentum density[5,6,9],

$$\sigma(\boldsymbol{p}) = (8\pi^3)^{-1} \int dv \, dv' \, \gamma(\boldsymbol{r}|\boldsymbol{r}') \, e^{-i\boldsymbol{p}.(\boldsymbol{r}-\boldsymbol{r}')}. \qquad (2)$$

Here $\gamma(\boldsymbol{r}|\boldsymbol{r}')$ is the spatial part of the first order density matrix. The diagonal part of γ gives the position density

$$\varrho(\boldsymbol{r}) = \gamma(\boldsymbol{r}|\boldsymbol{r}) \,, \qquad (3)$$

and the non-diagonal part the momentum density (see Eq. (2)).

Thus from the point of view of density matrix theory it would seem that the second order density matrix is the fundamental quantity needed for both chemistry and physics. To begin with we need however both the diagonal *and* the non-diagonal parts of the first order density matrix, or expressed in another way we need both the position space density and the momentum distribution. The connection between density functional theory and the density matrix perspective is far from clear (for an interesting discussion see Ref.[5], in particular the paper by Harriman).

March[13] has recently drawn attention to the importance of studying momentum distributions theoretically both for small molecules and polymers. There are at least two ways of approaching that problem. The traditional one is to use position space wave functions to get the density matrix $\gamma(\boldsymbol{r}|\boldsymbol{r}')$ which then yields the momentum density via Eq. (2). An alternative approach is to calculate wave functions directly in momentum space, as proposed by Navaza and Tsoucaris[14]. Defranceschi and collaborators[15,16] have done that both for H_3 and for an infinite chain of hydrogen atoms.

It is also of interest to study wave functions in momentum space from a *formal* point of view. Both for molecules and solids a number of properties of wave functions in position space are well known. For their counterparts in momentum space the situation is rather different, however. For regular solids two kinds of orbitals

are commonly used: Bloch functions which have a well defined crystal momentum but are delocalized throughout the solid, and Wannier functions which are associated with the unit cells of the direct lattice and are more or less localized there. In the present paper we study the properties of their counterparts in momentum space. We introduce a suitable notation and summarize their properties in direct (position) space. Then we study momentum space Bloch functions and the momentum space counterparts of the Wannier functions. In addition to the properties of general Bloch and Wannier functions we discuss plane wave and LCAO expansions.

Basic Properties in Direct Space

We recall some of the basic properties of Bloch and Wannier functions and at the same time introduce a consistent notation. A Bloch function (BF) is labeled by a wave vector $\boldsymbol{k}$ in reciprocal space which can be quasi-continuous or continuous. It is an eigenfunction of any of the translations associated with the direct lattice,

$$\psi\big(\boldsymbol{k}, \boldsymbol{r} - \boldsymbol{m}\big) = \mathrm{e}^{-\,\mathrm{i}\boldsymbol{k}.\boldsymbol{m}}\,\psi(\boldsymbol{k}, \boldsymbol{r})\,. \tag{4}$$

Here

$$\boldsymbol{m} = \boldsymbol{a}_1\mu_1 + \boldsymbol{a}_2\mu_2 + \boldsymbol{a}_3\mu_3\,; \quad -G/2 \leqq \mu_i < G/2\,, \tag{5}$$

is a direct lattice vector and the condition for the integers μ_i defines the Born–Karman (BK) region, which thus contains $N = G^3$ lattice sites or unit cells of volume $V_{\mathrm{oa}} = \boldsymbol{a}_1 . (\boldsymbol{a}_2 \wedge \boldsymbol{a}_3)$. The very large integer G characterizes the periodic boundary conditions satisfied by the Bloch functions:

$$\psi\big(\boldsymbol{k}, \boldsymbol{r} - G\boldsymbol{a}_i\big) = \psi(\boldsymbol{k}, \boldsymbol{r})\,; \quad i = 1, 2, 3\,. \tag{6}$$

The wave vector $\boldsymbol{k}$ is defined by

$$\boldsymbol{k} = 2\pi G^{-1}\big(\boldsymbol{b}_1\kappa_1 + \boldsymbol{b}_2\kappa_2 + \boldsymbol{b}_3\kappa_3\big) = \boldsymbol{b}_1 k_1 + \boldsymbol{b}_2 k_2 + \boldsymbol{b}_3 k_3\,, \tag{7}$$

where the basis vectors $\boldsymbol{b}_j$ of the reciprocal lattice satisfy

$$\boldsymbol{a}_i . \boldsymbol{b}_j = \delta_{ij}\,; \quad i, j = 1, 2, 3\,. \tag{8}$$

The κ_i are integers. The first Brillouin zone (BZ) is defined by

$$-G/2 \leqq \kappa_i < G/2\,; \quad i = 1, 2, 3\,, \tag{9}$$

when $\boldsymbol{k}$ is quasi-continuous. BZ then contains $G^3 = N$ wave vectors $\boldsymbol{k}$. When $\boldsymbol{k}$ is

continuous BZ is defined by

$$-\pi \leqq k_i < \pi ; \quad i = 1, 2, 3 . \tag{10}$$

Reciprocal lattice vectors are linear combinations of the basis vectors $\boldsymbol{b}_i$ with coefficients of the form $2\pi \times$ integer; they are denoted $\boldsymbol{K}$.

The Bloch condition (4) can also be expressed as a factorization of the Bloch function in a plane wave (PW) and a function which has the periodicity of the lattice:

$$\psi(\boldsymbol{k}, \boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u(\boldsymbol{k}, \boldsymbol{r}) ; \quad u(\boldsymbol{k}, \boldsymbol{r} - \boldsymbol{m}) = u(\boldsymbol{k}, \boldsymbol{r}) . \tag{11}$$

Given a set of Bloch functions

$$\Psi = \left[\ldots \psi(\boldsymbol{k}, \boldsymbol{r}) \ldots \right] , \tag{12}$$

for all $\boldsymbol{k}$ in BZ, which correspond to a single band isolated from all other bands, we can define a set of Wannier functions (WF),

$$\boldsymbol{W} = \left[\ldots W(\boldsymbol{m}, \boldsymbol{r}) \ldots \right] , \tag{13}$$

one for each unit cell in the direct lattice, by means of the unitary transformation

$$\boldsymbol{W} = \Psi \boldsymbol{U}^+ . \tag{14}$$

Here the unitary matrix $\boldsymbol{U}$ consists of the elements

$$U(\boldsymbol{m}, \boldsymbol{k}) = N^{-1/2} e^{i\boldsymbol{k}\cdot\boldsymbol{m}} , \quad \boldsymbol{m} \in \mathrm{BK} ; \quad \boldsymbol{k} \in \mathrm{BZ} . \tag{15}$$

The WF associated with the unit cell $\boldsymbol{m} = \boldsymbol{0}$, is just the sum of all the BF in BZ:

$$W(\boldsymbol{r}) = W(\boldsymbol{0}, \boldsymbol{r}) = N^{-1/2} \sum_{\boldsymbol{k}}^{\mathrm{BZ}} \psi(\boldsymbol{k}, \boldsymbol{r}) . \tag{16}$$

The other WF are obtained from Eq. (16) by translation:

$$W(\boldsymbol{m}, \boldsymbol{r}) = W(\boldsymbol{r} - \boldsymbol{m}) . \tag{17}$$

WF associated with different unit cells are orthonormal,

$$\int \mathrm{d}v \, W^*(\boldsymbol{m}, \boldsymbol{r}) \, W(\boldsymbol{n}, \boldsymbol{r}) = \delta(\boldsymbol{m}, \boldsymbol{n}) , \tag{18}$$

and BF associated with different wave vectors are also orthonormal,

$$\int \mathrm{d}v \, \psi^*(\boldsymbol{k}', \boldsymbol{r}) \, \psi(\boldsymbol{k}, \boldsymbol{r}) = \delta(\boldsymbol{k}', \boldsymbol{k}) . \tag{19}$$

When several bands are connected an extension of this procedure is necessary[17-22]. In the present paper we will only discuss the single band case and we will therefore suppress the band index on both BF and WF.

The term "Bloch function" by no means provides an exhaustive characterization of the function. The Bloch functions vary from crystal to crystal and for a given crystal from band to band. Further different approximation procedures yield different types of Bloch functions. The purpose of the present paper is just to study how Bloch and Wannier functions obtained by different methods are represented in momentum space.

Effective one electron equations for solids are usually solved by variational calculations. Different methods are then primarily characterized by the basis sets. We can distinguish between two extreme types of basis sets: delocalized and localized ones. The prototype for the delocalized kind is the plane wave (PW),

$$\eta(\mathbf{k}, \mathbf{r}) = V^{-1/2} e^{i\mathbf{k}\cdot\mathbf{r}} \,. \tag{20a}$$

Here $\mathbf{k}$ is a wave vector *anywhere in reciprocal space* and V is the volume of BK, which means that the PW are normalized in that region of space. When $\mathbf{k}$ is continuous and BK is infinite we use instead of $(20a)$

$$\eta(\mathbf{k}, \mathbf{r}) = (8\pi^3)^{-1/2} e^{i\mathbf{k}\cdot\mathbf{r}} \,. \tag{20b}$$

The PW form a complete set of functions since

$$\sum_{\mathbf{k}}^{\text{all}} \eta(\mathbf{k}, \mathbf{r}) \, \eta^*(\mathbf{k}, \mathbf{r}') \rightarrow (8\pi^3)^{-1} \int d\mathbf{k} \, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \delta(\mathbf{r} - \mathbf{r}') \,. \tag{21}$$

In an expansion of a Bloch function $\psi(\mathbf{k}, \mathbf{r})$ with $\mathbf{k} \in$ BZ we only need PW with wave vectors $\mathbf{k} + \mathbf{K}$, however,

$$\psi(\mathbf{k}, \mathbf{r}) = \int dv' \, \delta(\mathbf{r} - \mathbf{r}') \, \psi(\mathbf{k}, \mathbf{r}') = \sum_{\mathbf{k}} \eta(\mathbf{k} + \mathbf{K}, \mathbf{r}) \, A(\mathbf{k} + \mathbf{K}) \,, \tag{22}$$

since $\psi(\mathbf{k}, \mathbf{r})$ is orthogonal to all other PW.

The WF corresponding to a set of PW is, according to Eq. (16)

$$W_{\mathbf{k}}(\mathbf{r}) = N^{-1/2} \sum_{\mathbf{k}}^{\text{BZ}} \eta(\mathbf{k} + \mathbf{K}, \mathbf{r}) = V_{0a}^{-1/2} f(\mathbf{r}) \, e^{i\mathbf{K}\cdot\mathbf{r}} \,, \tag{23}$$

with

$$f(\mathbf{r}) = N^{-1} \sum_{\mathbf{k}}^{\text{BZ}} e^{i\mathbf{k}\cdot\mathbf{r}} = \prod_{j=1}^{3} (\pi r_j)^{-1} \sin \pi r_j \,. \tag{24}$$

Each factor in this product is thus an oscillatory decreasing function which reaches its largest value at $r_j = 0$.

The general Bloch function (22) then corresponds to the Wannier function

$$W(r) = N^{-1/2} \sum_{k}^{BZ} \psi(k, r) = N^{-1/2} \sum_{k}^{all} \eta(k + K, r) A(k + K) . \qquad (25)$$

If all the coefficients $A(k + K)$ are independent of k, we have

$$W(r) = N^{1/2} f(r) u(r) , \qquad (26)$$

where $u(r)$ is the (then) k-independent periodic factor of the Bloch function.

The other "extreme" kind of Bloch function is the LCAO expansion.

$$\psi(k, r) = \sum_{\mu} \chi_{\mu}(k, r) c_{\mu}(k) , \qquad (27)$$

where $\chi_{\mu}(k, r)$ is a Bloch sum

$$\chi_{\mu}(k, r) = N^{-1/2} \sum_{m}^{BK} \varphi_{\mu}(m, r) e^{ik.m} . \qquad (28)$$

If the basis functions $\varphi_{\mu}(m, r)$ are completely orthonormal atomic orbitals (OAO), that sum is normalized[23-26]. The set of AO is in principle complete but great care is needed because of possible linear dependencies[23,27].

The WF corresponding to *one* Bloch sum $\chi_{\mu}(k, r)$ is the OAO φ_{μ} itself. The WF corresponding to the Bloch function (27) is in general

$$W(m, r) = N^{-1} \sum_{\mu}^{BK} \sum_{n} \varphi_{\mu}(n, r) \left[\sum_{k}^{BZ} c_{\mu}(k) e^{ik.(n-m)} \right] . \qquad (29)$$

The coefficients $c_{\mu}(k)$ depend on k via a phase factor[28].

Bloch Functions in Momentum Space

The momentum space counterpart of a function which satisfies periodic boundary conditions in position space vanishes except at a quasi-continuous set of the type (7) (ref.[29]). Thus if $\phi(r)$ satisfies Eq. (6) we have for its counterpart in momentum space

$$\phi(p) = (8\pi^3)^{-1/2} \int dv \, \phi(r) \, e^{-ip.r} = \phi_G(p) \, 8\pi^3 V_{0a}^{-1} \sum \delta(Gp - K) , \qquad (30)$$

where

$$\phi_G(p) = (8\pi^3)^{-1/2} \int_{BK} dv \, \phi(r) \, e^{ip.r} . \qquad (31)$$

Thus a finite Born–Karman region leads to a discretization of the argument for these momentum space functions to values of the type

$$p = 2\pi G^{-1}(b_1 v_1 + b_2 v_2 + b_3 v_3) ; \quad v_i \text{ integer} . \tag{32}$$

For "allowed" values of p the value of $\phi(p)$ is obtained from Eq. (31).

For a Bloch function $\psi(k, p)$ there is a further restriction for the argument p. Combining the basic transformation rule (1) with the Bloch condition (4) we get

$$\psi(k, p) = e^{i(k-p)\cdot m} \psi(k, p) , \tag{33}$$

for any direct latice vector m. This implies that $\psi(k, p)$ vanishes unless $k - p$ is a reciprocal lattice vector K. Thus for a given k in BZ $\psi(k, p)$ vanishes except for $p = k + K$, i.e. at wave vectors equivalent to k. The momentum space counterpart of the periodic factor (11) of a Bloch function can be written

$$u(k, p) = \psi(k, k + p) , \tag{34}$$

which implies that $u(k, p)$ vanishes unless p is a reciprocal lattice vector K.

A Bloch function does not have the periodicity of the direct lattice — it "only" changes its phase in passing from one cell to the next one. That can be used to "concentrate" the information content of the Bloch function counterpart in momentum space. Combining Eqs (4) and (31) we get

$$\psi_G(k, p) = (8\pi^3)^{-1/2} \int_{BK} dv \, \psi(k, r) \, e^{-ip\cdot r} = \psi_{cell}(k, p) \sum e^{i(k-p)\cdot m} , \tag{35}$$

with

$$\psi_{cell}(k, p) = (8\pi^3)^{-1/2} \int_{cell} dv \, \psi(k, r) \, e^{-ip\cdot r} . \tag{36}$$

The sum in Eq. (35) implies that $\psi_G(k, p)$ vanishes unless $k - p$ is a reciprocal lattice vector K. Thus any function in momentum space whose counterpart in position space satisfies periodic (Born–Karman) boundary conditions, vanishes except at the quasi-continuous set of values (32) for its argument p. If that function is also a Bloch function labeled by a wave vector k in BZ, the values of p where the momentum space Bloch function is different from zero, are further restricted to $k + K$.

It is interesting to compare $\psi(k, p)$, $\psi_G(k, p)$ and $\psi_{cell}(k, p)$ for a PW, where these functions can be obtained in different ways. Using Eqs (30), (31) and (35) we get with Eq. $(20a)$, remembering that both p and $k' = k + K$ are quasi-continuous

$$\eta(k', p) = (8\pi^3 V^{-1})^{1/2} \delta(k' - p) ; \tag{37}$$

$$\eta_G(k', p) = (V(8\pi^3)^{-1})^{1/2} \, \delta_{k',p} \tag{38}$$

$$\eta_{cell}(k', k') = (V_{0a}(8\pi^3 N)^{-1})^{1/2} \, . \tag{39}$$

Using the PW expansion (22) we then get for an arbitrary Bloch function

$$\psi(k, p) = (8\pi^3 N V_{0a}^{-1})^{1/2} \sum \delta_{k+K,p} \sum \delta(Gp - K') \, A(k + K) \, . \tag{40}$$

This means that the function $\psi(k, p)$ vanishes except for $p = k + K$, where it equals

$$(8\pi^3 N V_{0a}^{-1})^{1/2} \, A(k + K) \, . \tag{41}$$

In order to get the momentum space counterpart of an LCAO Bloch sum (28) we need $[\varphi_\mu(r) = \varphi_\mu(0, r)]$,

$$\varphi_\mu(p) = (8\pi^3)^{-1/2} \int dv \, \varphi_\mu(r) \, e^{-ip \cdot r} \, , \tag{42}$$

which gives

$$\chi_{\mu,G}(k, p) = N^{1/2} \, \varphi_\mu(k + K) \, \delta_{p,k+K} \, . \tag{43}$$

This expression shows one of the advantages of working in momentum space: all the information needed is "concentrated" in the function $\varphi_\mu(p)$. If, as is often the case,

$$\varphi_\mu(r) = R_\mu(r) \, Y_{lm}(\vartheta, \varphi) \, , \tag{44}$$

we get using the partial wave expansion for $e^{-ip \cdot r}$,

$$\varphi_\mu(p) = (-i)^l \, (2\pi)^{-1/2} \, Y_{lm}(\vartheta_p, \varphi_p) \int R_\mu(r) \, j_l(pr) \, r^2 \, dr \, . \tag{45}$$

The momentum space counterpart of an arbitrary Bloch function in an LCAO representation can then be written (cf. ref.[30])

$$\psi_G(k, p) = \sum_\mu \chi_{\mu,G}(k, p) \, c_\mu(k) = N^{1/2} \, \delta_{p,k+K} \sum_\mu \varphi_\mu(k + K) \, c_\mu(k) \, . \tag{46}$$

Wannier Functions in Momentum Space

First of all we notice that a translation in direct space corresponds to a phase factor in momentum space. With

$$\phi(p) = (8\pi^3)^{-1/2} \int dv \, \phi(r) \, e^{-ip \cdot r} \, , \tag{47}$$

the function $\phi(m, r) = \phi(r - m)$ corresponds to

$$(8\pi^3)^{-1/2} \int dv \, \phi(m, r) \, e^{-ip \cdot r} = e^{-ip \cdot m} \, \phi(p) = \phi(m, p) \, . \tag{48}$$

A many centre function

$$\varphi(r) = \sum \phi(m, r) \, c(m) \,, \qquad (49)$$

consequently corresponds to

$$\varphi(p) = \phi(p) \sum c(m) \, e^{-ip.m} = \phi(p) \, d(p) \,. \qquad (50)$$

In other words the rather complicated transformation from ϕ to φ, Eq. (49), in momentum space just corresponds to multiplication of the momentum space counterpart of ϕ by a function of p. An important example of this procedure is symmetric orthonormalization[23-26] which is more easily carried out in momentum space.

Because of Eq. (48) it is sufficient to calculate the momentum space Wannier function "at the origin". Using Eq. (16) we get

$$W(p) = (8\pi^3)^{-1/2} \int dv \, W(r) \, e^{-ip.r} = N^{-1/2} \sum_{k}^{BZ} \psi(k, p) \,. \qquad (51)$$

The property given by Eq. (33) for the Bloch functions in momentum space implies[29]

$$\sum_{m}^{BK} \psi(k, p) = N \, \psi(k, p) = \psi(k, p) \sum_{m}^{BK} e^{i(k-p).m} =$$

$$= 8\pi^3 V_{0a}^{-1} \, \psi(k, p) \sum_{K} \delta(k - p + K) \,. \qquad (52)$$

Combining Eqs (51) and (52) we get

$$W(p) = N^{-1/2} \, \psi(p - K', p) \,, \qquad (53)$$

where K' is that reciprocal lattice vector which brings $p - K'$ to BZ. In analogy with the functions ψ, ψ_G, and ψ_{cell} we get W, W_G, and W_{cell}.

Thus the momentum space counterpart to the PW Wannier function (23) is

$$W_{K,G}(p) = N^{-1/2} \, \eta_{K,G}(p - K', p) = \sqrt{[V_{0a}(8\pi^3)^{-1}]} \, \delta_{K',K} \,. \qquad (54)$$

Each reciprocal lattice vector K corresponds to a Brillouin zone. Throughout the zone characterized by K, $W_{K,G}(p)$ is a constant for all "allowed" values of p (in the sense of Eqs (30) and (32)). Outside that zone $W_{K,G}(p)$ vanishes.

As a consequence an arbitrary Wannier function in momentum space is essentially the coefficient in the PW expansion of the direct space Bloch function (22):

$$W_G(p) = \sqrt{[V_{0a}(8\pi^3)^{-1}]} \, A(p) \,. \qquad (55)$$

Conversely one can say that the coefficients in the PW expansion of an arbitrary Bloch function are the coresponding Wannier functions in momentum space:

$$\psi(\boldsymbol{k}, \boldsymbol{r}) = \sqrt{(8\pi^3 V_{0a}^{-1})} \sum_{\boldsymbol{K}} \eta(\boldsymbol{k} + \boldsymbol{K}, \boldsymbol{r}) \, W_G(\boldsymbol{k} + \boldsymbol{K}) \,. \tag{56}$$

The momentum space counterpart of the Wannier function corresponding to an LCAO Bloch sum (28) is with (43) and (48)

$$W_{\mu,G}(\boldsymbol{p}) = \varphi_{\mu,G}(\boldsymbol{p}) \,. \tag{57}$$

This is what could be expected since with one Bloch sum of orthonormalized atomic orbitals these are identical to the Wannier function. With several such Bloch functions we get using Eqs (46) and (53),

$$W_G(\boldsymbol{p}) = \delta_{\boldsymbol{p}, \boldsymbol{k}+\boldsymbol{K}'} \sum_{\mu} \varphi_\mu(\boldsymbol{p}) \, c_\mu(\boldsymbol{k}) \,. \tag{58}$$

CONCLUSION

Strictly speaking wave functions have no direct physical or chemical interpretation. The various properties that are calculated by means of wave functions are however more or less influenced by various features of the wave functions. The very common habit of chemists and physicists of thinking in terms of wave functions can therefore be defended. Because of the dominance of independent and quasi independent particle models most of the visualizations in this connection are associated with orbitals — one electron functions. What is visualized is however nearly always a function in (or rather of) position space. Despite certain overinterpretations it can hardly be denied that such attempts at visualization and interpretation have been helpful for filling abstract ideas with more concrete content.

Compared to such conceptions in position space the corresponding visualizations and interpretations in momentum space seem to be situated at a higher level of abstraction. That feeling may at least partially be due to the fact that we are much less accustomed to think in terms of wave functions in momentum space. That situation ought to be changed, though. Because of the inherent complementarity it is difficult to avoid the conclusion that by not taking full advantage of momentum space we deprive ourselves of important pieces of information. One way to remedy that situation leads to a systematic study of momentum space wave functions. That means to begin with to study the counterparts of well known properties in position space. Conversely it will be interesting to investigate what characteristic properties in momentum space mean in position space.

It is understandable that most work connected with momentum space has been focused on the momentum distribution and its Fourier transform (the reciprocal form factor)[6,10,30-38]. One of the few exceptions is a paper by Harthoorn and Mijnarends[39], in which they study the symmetry properties of Bloch functions in momentum space. More detailed investigations of both symmetry properties and other characteristics of Bloch and Wannier functions in momentum space are desirable, though. The relations summarized in the present paper may serve as a starting point for such investigations.

REFERENCES

1. Cook D. B.: *Structures and Approximations for Electrons in Molecules*. Ellis Horwood, Chichester 1978.
2. Platt J. R. in: *Handbuch der Physik*, Band XXXVII/2 (S. Flügge, Ed.), p. 173. Springer, Berlin 1961.
3. Hohenberg P., Kohn W.: Phys. Rev. *136*, B864 (1964).
4. Callaway J., March N. H.: Solid State Phys. *38*, 136 (1984).
5. Erdahl R., Smith V. H., jr (Eds): *Density Matrices and Density Functionals*. Reidel, Dordrecht 1987.
6. Williams B. G. (Ed.): *Compton Scattering*. McGraw Hill, New York 1977.
7. Bonham R. A., Lee J. S., Kennerly R., John W. S.: Adv. Quantum Chem. *11*, 1 (1978).
8. Lindner P.: Phys. Scr. *15*, 112 (1977).
9. Kaijser P., Smith V. H., jr.: Adv. Quantum Chem. *10*, 37 (1977).
10. Mijnarends P. in: *Positron Solid-State Physics* (W. Brandt and A. Dupasquier, Eds), p. 146. North-Holland, Amsterdam 1983.
11. Löwdin P.-O.: Phys. Rev. *97*, 1474 (1955).
12. Calais J.-L.: J. Chim. Phys. *84*, 601 (1987).
13. March N. H.: Int. J. Quantum Chem., Symp. *19*, 719 (1986); *20*, 367 (1986).
14. Navaza J., Tsoucaris G.: Phys. Rev., A *24*, 683 (1981).
15. Defranceschi M., Suard M., Berthier G.: C. R. Acad. Sci. *296*, 1301 (1983).
16. Defranceschi M., Delhalle J.: C. R. Acad. Sci. *301*, 1405 (1985); Phys. Rev., B *34*, 5862 (1986).
17. Kohn W.: Phys. Rev. *115*, 809 (1959).
18. Bulyanitsa D. S., Svetlov Y. E.: Sov. Phys. — Solid State *4*, 981 (1962).
19. des Cloizeaux J.: Phys. Rev. *129*, 554 (1963); Phys. Rev. *135*, A685, A698 (1964).
20. Teichler H.: Phys. Status Solidi B *43*, 1189 (1971).
21. Lix B.: Phys. Status Solidi B *44*, 411 (1971).
22. Kögel G.: Phys. Status Solidi B *44*, 577 (1971).
23. Löwdin P.-O.: Adv. Phys. *5*, 1 (1956); Adv. Quantum Chem. *5*, 185 (1970).
24. Aikala O.: J. Phys., C *16*, 2217 (1983).
25. von Boehm J., Calais J.-L.: J. Phys., C *17*, 249 (1984).
26. Calais J.-L.: Int. J. Quantum Chem., Symp. *19*, 655 (1986).

27. Ahlenius T., Calais J.-L., Löwdin P.-O.: J. Phys., C *6*, 1896 (1973).
28. von Boehm J., Calais J.-L.: J. Phys., C *12*, 3661 (1979).
29. Calais J.-L., Weyrich W.: Unpublished results.
30. Causa M., Dovesi R., Pisani C., Roetti C.: Phys. Rev., B *32*, 1196 (1985).
31. Weyrich W.: Ber. Bunsenges. Phys. Chem. *83*, 797 (1979).
32. Weyrich W., Pattison P., Williams B. G.: Chem. Phys. *41*, 271 (1979).
33. Pattison P.. Weyrich W.: J. Phys. Chem. Solids *40*, 213 (1979).
34. Pattison P., Schneider J. R.: Acta Crystallogr., A *36*, 390 (1980).
35. Pattison P., Hansen N. K., Schneider J. R.: Acta Crystallogr., B *40*, 38 (1984); Chem. Phys. *59*, 231 (1981); Z. Phys., B *46*, 285 (1982).
36. Podloucky R., Redinger J.: J. Phys., C *16*, 6955 (1984).
37. Bauer G. E. W., Schneider J. R.: Solid State Commun. *47*, 673 (1983); Z. Phys., B *54*, 17 (1983); J. Phys. Chem. Solids *45*, 675 (1984); Phys. Rev. Lett. *52*, 2061 (1984); Phys. Rev., B *31*, 681 (1985).
38. Bauer G. E. W.: Phys. Rev., B *30*, 101 (1984).
39. Harthoorn R., Mijnarends P. E.: J. Phys., F *8*, 1147 (1978).