Energy Bands and Projection Operators in a Crystal: Analytic and Asymptotic Properties

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In an n-dimensional crystal, an energy band is usually made of several branches which are connected with each other. Accordingly, the Bloch states of wave vector **K** which are eigenfunctions of a one-electron Hamiltonian $H=-\Delta+V$ and which belong to a given band $\mathcal{B}$, define a subspace $\mathcal{S}(\mathbf{K})$ of finite dimensionality. For a large class of potentials, two properties concerning the subspaces $\mathcal{S}(\mathbf{K})$ which are associated with a fixed band $\mathcal{B}$ have been proved for n-dimensional crystals. (1) The projection operator $P(\mathbf{K})$ on $\mathcal{S}(\mathbf{K})$ can be defined for complex values of **K**, and its matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ are analytic in a strip of the complex **K** space; this strip is centered on the real **K** space and is independent of **r** and **r**′. (2) The projection operator $P=\int d^h\mathbf{K}P(\mathbf{K})$ (integration on the Brillouin zone) has matrix elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$ which decrease exponentially when the length $|\mathbf{r}-\mathbf{r}'|$ goes to infinity.

I. INTRODUCTION

In an insulating crystal, the electrons form a kind of bound state and it is generally recognized that, for this reason, a local disturbance has only short-range effects. This phenomenon appears even in the independent-particle approximation. It comes from the fact that, in an ideal crystal, at zero temperature, the lower bands are completely filled, whereas the upper bands are empty. If a band is full, each Bloch state is occupied by an electron but we may say also that each Wannier function of this band is occupied by an electron. Kohn[1] has shown, for a linear crystal with a center of symmetry, that it is always possible to build properly localized Wannier functions by starting from Bloch waves which are analytic functions of the wave number K in a strip of the complex K plane containing the real axis; as a consequence, the corresponding Wannier functions have exponentially decreasing tails. Thus, the electrons of an insulator can be considered as really localized; at least, this point of view which is common among chemists can be established for linear crystals.

Here, we want to derive closely related properties of the energy bands but our proofs are also valid for n-dimensional crystals. As a direct generalization of Kohn's results presents special difficulties, the problem is not examined here. However, we plan to use our results later on, to show that in n-dimensional crystals, it is often possible to build really localized Wannier functions, i.e., functions which decrease exponentially at infinity.

The motion of the electrons in an infinite crystal can be described in first approximation, by using a one-electron Hamiltonian of the form $H=-\Delta+V$. The eigenvalues of H form continuous bands and we consider here a given band $\mathcal{B}$. This band is simple or complex but, by definition, it does not touch any other band; it is isolated. The Bloch waves of wave vector **K** which belong to $\mathcal{B}$ define a subspace $\mathcal{S}(\mathbf{K})$. For real values of **K**, this subspace can be characterized by the projection operator $P(\mathbf{K})$ on $\mathcal{S}(\mathbf{K})$, which is a periodic function of **K**. General conditions of regularity are assumed for the potential; they are used to show that $P(\mathbf{K})$ can be defined for complex values of $\mathbf{K}=\mathbf{K}'+i\mathbf{K}''$ and that its matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ are analytic with respect to **K**, in a strip of the complex **K** space; this domain is defined by an inequality of the form $|\mathbf{K}''|<A$ where A is a positive constant which depends on the band but not on **r** and **r**′. For linear crystals, this result is trivial; the operator $P(\mathbf{K})$ can be expressed directly in terms of Bloch waves and Kohn has shown the existence, in linear crystals, of Bloch waves which are analytic in a strip of the complex K plane. However, our result is valid also, in n-dimensional crystals, for simple or complex bands. In this case, the Bloch waves may have branch points for real values of **K** and therefore, in general, they are not analytic in a strip defined by an inequality of the form $|\mathbf{K}''|<A$.

On the other hand, the operator P of projection on the space formed by the set of all the subspaces $\mathcal{S}(\mathbf{K})$ which belong to $\mathcal{B}$, is defined as an integral of $P(\mathbf{K})$ on the Brillouin zone. It is shown that, when $|\mathbf{r}-\mathbf{r}'|$ increases, the modulus of the matrix elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$ decreases faster than $\exp[-\epsilon A|\mathbf{r}-\mathbf{r}'|]$, where ϵ is any positive number smaller than one. This result is a direct consequence of the analyticity of the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ in the strip $|\mathbf{K}''|<A$. It shows clearly the localization of the electrons in an insulator.

In Sec. II, we prove the analyticity of the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ with respect to **K** and their continuity with respect to **r** and **r**′. Sections IIA, IIB, and IIC contain definitions and general remarks. Our assumptions concerning the regularity of the potential V are given in Sec. IID. These requirements are not very restrictive: They are fulfilled for $n=1$ by δ potentials for $n=3$ by screened Coulomb potentials. In Sec. IIE, we prove the uniform convergence of all the series which appear in the following. Section IIF forms the central part of the proof. An operator $Q(\mathbf{K})$ proportional to $P(\mathbf{K})$ is introduced and we prove the analyticity of this operator in a special representation, for a small domain of the **K** space. Finally, in Sec. IIG, we prove the

[1] W. Kohn, Phys. Rev. **115**, 809 (1959).

analyticity of the matrix elements $\langle \mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ in a larger domain $|\mathbf{K}''|<A$, by using the results of Secs. IIE and IIF. In Sec. III, it is shown that the matrix elements $\langle \mathbf{r}|P|\mathbf{r}'\rangle$ exist and decrease exponentially at infinity. Section IIIA contains definitions. A preliminary theorem is given in Sec. IIIB and the final result is obtained in Sec. IIIC.

The results which are established here are certainly very general and, for instance, they should remain valid for spin-dependent Hamiltonians. But instead of considering here, all possible cases, it seemed better to treat more rigorously a restricted problem. For this reason, special attention has been paid to convergence problems which are essential for the validity of the proofs. However, if the reader is interested only by the general method, he may very well skip Secs. IIE and IIF which deal with these problems. A few assumptions have been used in the proofs; they concern mainly the existence of bands and the completeness[2] of the Hamiltonian H.

II. DEFINITION AND ANALYTICITY PROPERTIES OF THE PROJECTION OPERATORS $P(\mathbf{K})$ ASSOCIATED WITH AN ENERGY BAND $\mathcal{B}$

A. Elementary Definition of $P(\mathbf{K})$ for K Real

In an n-dimensional crystal, an energy band is usually made of several branches which are connected with each other. By definition, if two branches touch each other for a real value of the wave vector $\mathbf{K}$, they are parts of the same band. The number of Bloch states of wave vector $\mathbf{K}$ which belong to a band $\mathcal{B}$ is a characteristic constant d of the band; for a simple band $d=1$, for a complex band $d>1$ (see Fig. 1). One-dimensional crystals have (in general) only simple bands.

The Bloch states of wave vector $\mathbf{K}$ can be labeled by an index l. It is convenient to assume that the energy $E(l,\mathbf{K})$ associated with the Bloch state $|\varphi(l,\mathbf{K})\rangle$ is a nondecreasing function of the index l which is an integer running from a given value l_0 to $+\infty$. By choosing l_0 properly, we can always label the states belonging to $\mathcal{B}$ by values of l running from 1 to d.

In an infinite crystal, the Dirac type of normalization must be used for the Bloch waves,

$$\langle\varphi(l,\mathbf{K})|\varphi(l',\mathbf{K}')\rangle=\delta_{ll'}\delta_c(\mathbf{K}-\mathbf{K}'). \tag{1}$$

The distribution $\delta_c(\mathbf{K}-\mathbf{K}')$ is defined by

$$\delta_c(\mathbf{K}-\mathbf{K}')=\sum_{\mathbf{u}}\delta(\mathbf{K}-\mathbf{K}'+\mathbf{u}), \tag{2}$$

where the summation is made for all the translations $\mathbf{u}$ of the reciprocal lattice.

However, if we remain inside the subspace $\mathcal{S}(\mathbf{K})$ of wave vector $\mathbf{K}$, we can perform the integrations on a unit cell only. In the following, this kind of normalization is indicated by round brackets. We put

$$|\varphi(l,\mathbf{K}))=v^{-1/2}|\varphi(l,\mathbf{K})\rangle, \tag{3}$$

where v is the volume of the unit cell. Thus, the normalization condition can be written also

$$(\varphi(l,\mathbf{K})|\varphi(l',\mathbf{K}'))=\delta_{ll'}. \tag{4}$$

With these notations, we can define the operator $P(\mathbf{K})$ for real values of $\mathbf{K}$ by

$$P(\mathbf{K})=\sum_{l=1}^{l=d}|\varphi(l,\mathbf{K})\rangle\langle\varphi(l,\mathbf{K})|. \tag{5}$$

In general, this operator is determined by its matrix elements, for instance, the functions $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$,

$$\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle=\sum_{l=1}^{l=d}\langle\mathbf{r}|\varphi(l,\mathbf{K})\rangle\langle\varphi(l,\mathbf{K})|\mathbf{r}'\rangle. \tag{6}$$

The term $\langle\mathbf{r}|\varphi(l,\mathbf{K})\rangle$ is just a Bloch function. As $P(\mathbf{K})$ is a projection operator, it satisfies the relations

$$P(\mathbf{K})P(\mathbf{K}')=\delta_c(\mathbf{K}-\mathbf{K}')P(\mathbf{K}), \tag{7}$$

$$\int_V\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}\rangle d^n\mathbf{r}=vd. \tag{8}$$

In the last equation, the domain of integration is a unit cell of the crystal.

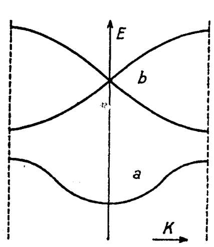

FIG. 1. Simple band (a) and complex band (b) in an n-dimensional crystal.

B. Definition of $P(\mathbf{K})$ for Complex Values of K

Let us introduce new states by putting

$$\langle\mathbf{r}|l,\mathbf{K}\rangle=\exp[-i\mathbf{K}\cdot\mathbf{r}]\langle\mathbf{r}|\varphi(l,\mathbf{K})\rangle. \tag{9}$$

These states are periodical and normalized

$$(l,\mathbf{K}|l',\mathbf{K})=\delta_{l'l}. \tag{10}$$

They are solutions of equations obtained by transforming the Schrödinger equation

$$H|\varphi(l,\mathbf{K})\rangle=E(l,\mathbf{K})|\varphi(l,\mathbf{K})\rangle. \tag{11}$$

By putting

$$\mathrm{H}(\mathbf{K})=e^{-i\mathbf{K}\mathbf{r}}He^{i\mathbf{K}\mathbf{r}}, \tag{12}$$

we get immediately

$$\mathrm{H}(\mathbf{K})|l,\mathbf{K})=E(l,\mathbf{K})|l,\mathbf{K}). \tag{13}$$

[2] E. Titchmarsh has shown how to tackle some of these problems in his book *Eigenfunctions Expansions Associated With Second-Order Differential Equations* (Clarendon Press, Oxford, 1958). However, the theorems which are given there are not very general; for instance, they are valid only for bounded potentials.

Now, the Hamiltonian depends on **K** but the solutions must always be periodical; therefore for a given value of **K**, the spectrum of H(**K**) is discrete. If **K** is real, H(**K**) is Hermitian because transformation (12) is unitary in this case. On the contrary, if **K** is complex, this property does not remain true because

$$\mathrm{H}^{\dagger}(\mathbf{K})=\mathrm{H}(\mathbf{K}^*). \tag{14}$$

When **K** is complex, Eq. (13) may still have solutions but the eigenstates are not orthogonal to each other anymore. However, by using Eq. (14), it is easy to show that the eigenstates of $H(\mathbf{K})$ can be orthonormalized as follows:

$$(l,\mathbf{K}^*|l',\mathbf{K})=\delta_{ll'}, \tag{15}$$

which is a generalization of Eq. (10). Thus, the states $|\varphi(l,\mathbf{K})\rangle$ can be defined, for complex values of **K**, by Eq. (9). We have in this case

$$(\varphi(l,\mathbf{K}^*)|\varphi(l,\mathbf{K}))=\delta_{ll'}. \tag{16}$$

Kohn's work on one-dimensional crystals implies that for sufficiently small values of the imaginary part of **K**, it is possible to follow by continuity the eigenstates which belong to a band. A general derivation of this result ($n\geq 1$) is given in the following sections.

Consequently, for $\mathbf{K}=\mathbf{K}'+i\mathbf{K}''$ and small values of $|\mathbf{K}''|$, we can define $P(\mathbf{K})$ by putting

$$P(\mathbf{K})=\sum_{l=1}^{l=d}|\varphi(l,\mathbf{K})\rangle\langle\varphi(l,\mathbf{K}^*)|, \tag{17}$$

or more explicitly,

$$\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle=\sum_{l=1}^{l=d}\exp[i\mathbf{K}\cdot(\mathbf{r}-\mathbf{r}')]\langle\mathbf{r}|l,\mathbf{K}\rangle\langle l,\mathbf{K}^*|\mathbf{r}'\rangle. \tag{18}$$

By looking at this expression, we see immediately that in spite of a formal appearance, $P(\mathbf{K})$ depends really on **K** not on $\mathbf{K}^*$. In fact, it will be shown in the following sections that its matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ are analytic functions of **K**.

C. Remarks on the Analyticity Properties of Operators

In the following sections, the analyticity properties of $P(\mathbf{K})$ will be investigated but, first, we should like to make a few remarks about analytic operators. By definition, a matrix is analytic with respect to a complex variable z when all its matrix elements are analytic functions of z. Now, it is clear that any finite matrix which is analytic with respect to z is changed by a unitary transformation into another analytic matrix. Therefore, if an operator is defined in a space with a finite number of dimensions, it is analytic by definition if one of its matrix representations is analytic. However, a unitary transformation in an Hilbert space does not always conserve the analyticity of a matrix with respect to a variable z. The analyticity of an operator acting in such a space is defined for some kind of representation only. For instance, the projection operator $P(\mathbf{K})$ for free electrons has matrix elements in the ordinary space

$$\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle=\exp[i\mathbf{K}\cdot(\mathbf{r}-\mathbf{r}')], \tag{19}$$

which are obviously analytic with respect to **K**. However, the representation of $P(\mathbf{K})$ in the reciprocal space is singular (the matrix elements contain δ functions). In the following, the analyticity of $P(\mathbf{K})$ will be proved in this restricted sense. Our aim is really to derive the analyticity of the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$.

On the other hand, the fact that all the functions which we consider are analytical functions of several variables does not bring additional difficulties: Hartog's theorem[3] indicates that a function which is analytic with respect to each variable separately can be expanded in convergent Taylor series with respect to all variables and conversely.

D. Nature of the Hamiltonian and Eigenfunctions

The analyticity properties of the operator $P(\mathbf{K})$ depend, of course, of the nature of the Hamiltonian. Really general and rigorous proofs concerning these properties require great care. In fact, in a complete theory, the existence of energy bands should not be assumed *a priori* but proved for a certain class of Hamiltonians.

On the other hand, in order to derive the analyticity properties of $P(\mathbf{K})$, it is convenient to define this operator by expansions and several vector bases will be used. But, as we noticed above, the analyticity properties of an operator depend on its representation. The analyticity properties of the sum of a series depend not only on the analyticity properties of each term but also on the convergence of the series. Again, the convergence of our expansions depends on the nature of the Hamiltonian.

Consequently, the Hamiltonian of the problem must belong to a well-defined type. In the following, for reasons of simplicity, it will be assumed that H has the form

$$H=-\Delta+V(\mathbf{r}). \tag{20}$$

However, as the reader will realize, the method can be generalized and similar results could be derived for other types of Hamiltonian.

The operator $H(\mathbf{K})$ corresponding to this Hamiltonian is very simple;

$$\mathrm{H}(\mathbf{K})=e^{-i\mathbf{K}\mathbf{r}}He^{i\mathbf{K}\mathbf{r}}=(-i\nabla+\mathbf{K})^2+V. \tag{21}$$

The eigenfunctions $\langle\mathbf{r}|l,\mathbf{K}\rangle$ of $H(\mathbf{K})$ are periodical and the square of their modulus is integrable; therefore, they are vectors of an Hilbert space which can be

[3] S. Bochner and W. T. Martin, *Several Complex Variables* (Princeton University Press, Princeton, New Jersey, 1948).

spanned by the states $|\mathbf{p}\rangle$ defined by

$$\langle\mathbf{r}|\mathbf{p}\rangle=\exp(i\mathbf{pr}), \tag{22}$$

$$|\mathbf{p})=v^{-1/2}|\mathbf{p}\rangle, \tag{23}$$

where the vectors $\mathbf{p}$ are reciprocal lattice vectors. The state $|l,\mathbf{K})$ can be defined by its matrix elements $(\mathbf{p}|l,\mathbf{K})$ which are finite (at least for $\mathbf{K}$ real). The operator $H(\mathbf{K})$ can be represented in this basis. The potential $V(\mathbf{r})$ is assumed to be integrable, and, therefore, we can calculate its Fourier series,

$$V(\mathbf{r})=v^{-1}\sum \mathrm{V}(\mathbf{p})\exp(i\mathbf{pr}). \tag{24}$$

The coefficients $\mathrm{V}(\mathbf{p})$ are bounded:

$$|\mathrm{V}(\mathbf{p})|<\infty. \tag{25}$$

The operator $H(\mathbf{K})$ can be represented explicitly in the reciprocal space by its matrix elements

$$(\mathbf{p}|H(\mathbf{K})|\mathbf{p})=(\mathbf{p}+\mathbf{K})^2\delta_{\mathbf{p},\mathbf{q}}+\mathrm{V}(\mathbf{p}-\mathbf{q}). \tag{26}$$

If the potential $V(\mathbf{r})$ is smooth, its Fourier transform decreases rapidly for large values of $\mathbf{p}$. More precisely, it will be assumed, in the following, that for an n-dimensional crystal, our potential V satisfies the condition

$$p^{n-1}|\mathrm{V}(\mathbf{p})|<\infty. \tag{27}$$

This condition is not very restrictive, it does not even imply the convergence of the series given by Eq. (24). In fact, for $n=1$, a potential made of δ functions satisfy Eqs. (24) and (26). On the other hand, for $n>1$, potentials of the form e^{-ar}/r obey also these conditions.

Now, as we shall see, these bounding inequalities imply a kind of smoothness of the Bloch waves which is characterized by the asymptotic behavior of the coefficients $(\mathbf{p}|l,\mathbf{K})$.

As the wave function must be normalized, we have

$$(l,\mathbf{K}^*|l,\mathbf{K})\equiv\sum_{\mathbf{p}}(l,\mathbf{K}^*|\mathbf{p})(\mathbf{p}|l,\mathbf{K})=1. \tag{28}$$

Therefore, the coefficients $(\mathbf{p}|l,\mathbf{K})$ must be bounded (at least for $\mathbf{K}$ real):

$$|(\mathbf{p}|l,\mathbf{K})|<\infty. \tag{29}$$

Moreover, for large values of $\mathbf{p}$, these coefficients decrease, and as a consequence of Eqs. (27) and (29), we have

$$p^{n+1}|(\mathbf{p}|l,\mathbf{K})|<\infty. \tag{30}$$

This result can be derived by inspection of the Schrödinger equation which can be written

$$[E(l,\mathbf{K})-(\mathbf{K}+\mathbf{p})^2](\mathbf{p}|l,\mathbf{K})=\sum_{\mathbf{q}}\mathrm{V}(\mathbf{p}-\mathbf{q})(\mathbf{q}|l,\mathbf{K}). \tag{31}$$

First, let us assume that the sum $\sum_{\mathbf{p}}|(\mathbf{p}|l,\mathbf{K})|$ is convergent. In this case, it is clear that the main contribution in the sum $\sum_{\mathbf{q}}\mathrm{V}(\mathbf{p}-\mathbf{q})(\mathbf{q}|l,\mathbf{K})$ comes from terms of small $\mathbf{q}$; accordingly, the asymptotic properties of this sum depend on the behavior of $\mathrm{V}(\mathbf{p})$ for large values of $\mathbf{p}$. If, in agreement with Eq. (26), $\mathrm{V}(\mathbf{p})$ contains terms of the order $p^{-(n-1)}$ or less, then the sum is also of the order $p^{-(n-1)}$. Thus the coefficients $(\mathbf{p}|l,\mathbf{K})$ which appear in the left-hand side of the Schrödinger equation must be at most of the order $p^{-(n+1)}$ at condition (29) holds. Conversely, if this condition is valid, then the sum $\sum_{\mathbf{p}}|(\mathbf{p}|l,\mathbf{K})|$ converges. Therefore it is consistent to assume that the coefficients $(\mathbf{p}|l,\mathbf{K})$ are at most of the order of $p^{-(n+1)}$. It is clear that such a result would be obtained by perturbation methods.

In Appendix I, a more rigourous proof of this result is given for real values of $\mathbf{K}$ and more stringent bounding inequalities are obtained.

$$|(\mathbf{p}|l,\mathbf{K})|\leq C \quad (C=1 \text{ for } \mathbf{K} \text{ real}), \tag{32}$$

$$p^{n+1-\epsilon}|(\mathbf{p}|l,\mathbf{K})|<C(\epsilon,E_0), \tag{33}$$

for $E(l,\mathbf{K})\leq E_0$ and $|K|<R$. Here ϵ is an arbitrary small positive value and $C(\epsilon,E_0)$ is a positive constant. The fact that $C(\epsilon,E_0)$ does not depend on $\mathbf{K}$ is very important and will be used extensively in the following.

The proof remains valid for complex values of $\mathbf{K}$ in the regions where the modulus of the state $|l,\mathbf{K})$ remains bounded.

$$(l,\mathbf{K}|l,\mathbf{K})=\sum_{\mathbf{p}}(l,\mathbf{K}|\mathbf{p})(\mathbf{p}|l,\mathbf{K})<C_0, \tag{34}$$

where C_0 is a constant independent of $\mathbf{K}$. However, for special values of $\mathbf{K}=\mathbf{K}'+i\mathbf{K}''$, the states $|l,\mathbf{K})$ and $|l,\mathbf{K}^*)$ may become orthogonal to each other. In this case, since the normalization condition (28) remains valid for this states, their modulus must become infinite. In the vicinity of a point of degeneracy defined by a real wave vector $\mathbf{K}_0$ (for instance, the center of the Brillouin zone for the complex band of Fig. 1) this situation may occur even for very small values of $|\mathbf{K}-\mathbf{K}_0|$. Strictly speaking, for such points $P(\mathbf{K})$ cannot be defined by Eq. (17). However, it is not difficult to verify on examples, and we shall prove later on, that the matrix elements of $P(\mathbf{K})$ remain quite regular at these anomalous points because cancellations occur in the right-hand side of Eq. (17). Therefore, the difficulties introduced by this anomaly are spurious and in the following, we shall not pay much attention to them.

E. Change of Representation and Problems of Convergence

Until now, the states $|l,\mathbf{K})$ have been defined by their components $(\mathbf{p}|l,\mathbf{K})$, but it is useful to consider also other representations. The components of $|l,\mathbf{K})$ in a new basis are given by series in terms of the coefficients $(\mathbf{p}|l,\mathbf{K})$. We shall examine here the convergence of such series. This question is important because, in order to derive the analytic properties of $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$, we have to use several representations of $P(\mathbf{K})$; therefore, it is necessary to prove that the series which are introduced by a change of representation, are uniformly convergent with respect to $\mathbf{K}$.

For instance, the wave function $\langle\mathbf{r}|l,\mathbf{K}\rangle$ is given by

$$\langle\mathbf{r}|l,\mathbf{K}\rangle=v^{-1}\lim_{p_0\to\infty}\sum_{p<p_0}\langle\mathbf{r}|\mathbf{p}\rangle(\mathbf{p}|l,\mathbf{K})$$
$$=v^{-1}\lim_{p_0\to\infty}\sum_{p<p_0}\exp(i\mathbf{p}\cdot\mathbf{r})(\mathbf{p}|l,\mathbf{K}). \quad (35)$$

This series can be majorized,

$$\sum_{p<p_0}|\langle\mathbf{r}|\mathbf{p}\rangle(\mathbf{p}|l,\mathbf{K})|<\sum_{p<p_0}|(\mathbf{p}|l,\mathbf{K})|. \quad (36)$$

According to Eq. (33) when p_0 goes to infinity, the series of Eq. (36) converge uniformly with respect to $\mathbf{K}$. Therefore the series of Eq. (34) converges absolutely and uniformly with respect to $\mathbf{K}$. The sum, which defines $\langle\mathbf{r}|l,\mathbf{K}\rangle$, is a continuous function of $\mathbf{r}$.

In the following, it will be convenient to use also as a basis, the set of eigenstates of $H(\mathbf{K})$ which correspond to a given real value $\mathbf{K}_0$. The reasons of such a choice will become clear in the next section. It is assumed that this set of states is complete; this condition can be written explicitly,

$$\sum_m(\mathbf{p}|m\mathbf{K}_0)(m\mathbf{K}_0|\mathbf{q})=(\mathbf{p}|\mathbf{q})=\delta_{\mathbf{pq}}. \quad (37)$$

Now the component $(\mathbf{p}|l,\mathbf{K})$ can be expressed in terms of the coefficients $(m\mathbf{K}_0|l,\mathbf{K})$ by a formal series,

$$(\mathbf{p}|l,\mathbf{K})\doteqdot\sum_m(\mathbf{p}|m\mathbf{K}_0)(m\mathbf{K}_0|l,\mathbf{K}). \quad (38)$$

The terms $(m\mathbf{K}_0|l,\mathbf{K})$ can be defined explicitly by

$$(m\mathbf{K}_0|l,\mathbf{K})=\sum_{\mathbf{q}}(m\mathbf{K}_0|\mathbf{q})(\mathbf{q}|m\mathbf{K}_0), \quad (39)$$

and according to Eqs. (32) and (33), these Hermitian products exist and are bounded.

Our purpose is to show that the formal series (38) converges to $(\mathbf{p}|l,\mathbf{K})$ uniformly. This task is performed in Appendix V (at least for real values of $\mathbf{K}$). A study of the convergence of the formal series (38) shows that the sum of the series is $(\mathbf{p}|l,\mathbf{K})$. Moreover, it is proved that the series converges to $(\mathbf{p}|l,\mathbf{K})$ uniformly with respect to $\mathbf{K}$. This statement can be expressed more explicitly. We say that it is possible to associate with each positive number ϵ, a finite number $E_0(\epsilon)$ possessing the following properties: (1) $E_0(\epsilon)$ is independent of $\mathbf{K}$ [but $E(m,\mathbf{K})$ is assumed to be bounded]. (2) For any value E bigger than $E_0(\epsilon)$, we have

$$\Big|(\mathbf{p}|l,\mathbf{K})-\sum_{\substack{E(m,\mathbf{K}_0)<E\\ E>E_0(\epsilon)}}(\mathbf{p}|m,\mathbf{K}_0)(m,\mathbf{K}_0|l,\mathbf{K})\Big|<\epsilon. \quad (40)$$

This important result will be used in Sec. IIG to derive the analyticity properties of the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$.

F. Definition and Analyticity of the Matrix Elements $(m,\mathbf{K}_0|Q(\mathbf{K})|m',\mathbf{K}_0)$

Our aim is to redefine the operator $P(\mathbf{K})$ of a band $\mathcal{B}$ for complex values $\mathbf{K}=\mathbf{K}'+i\mathbf{K}''$ and to show that its matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ are analytic functions of $\mathbf{K}$ in a region of the complex $\mathbf{K}$ space, defined by an inequality of the form $|\mathbf{K}''|<A$; here, A is a positive constant independent of $\mathbf{K}$, $\mathbf{r}$, and $\mathbf{r}'$. However, these properties are difficult to establish directly.

It is convenient to introduce an auxiliary operator $Q(\mathbf{K})$. This operator is defined rigorously in the following and turns out to be

$$Q(\mathbf{K})=\sum_{l=1}^{l=d}|l,\mathbf{K})(l,\mathbf{K}^*|. \quad (41)$$

In the space of the periodical functions and for real values of $\mathbf{K}$, $Q(\mathbf{K})$ is an ordinary projection operator. This operator is very closely related to $P(\mathbf{K})$ since according to Eqs. (17) and (2), we have

$$\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$$
$$=v\exp[i\mathbf{K}(\mathbf{r}-\mathbf{r}')]\langle\mathbf{r}|Q(\mathbf{K})|\mathbf{r}'\rangle$$
$$=\exp[i\mathbf{K}(\mathbf{r}-\mathbf{r}')]\sum_{\mathbf{p},\mathbf{p}'}\langle\mathbf{r}|\mathbf{p}\rangle(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')\langle\mathbf{p}'|\mathbf{r}'\rangle. \quad (42)$$

Now let $\mathbf{K}_0$ be a real value of $\mathbf{K}$; the states $|m,\mathbf{K}_0)$ which are eigenstates of $H(\mathbf{K}_0)$ form an orthogonal basis of the space of the periodic functions. In this section, we want to prove the analyticity of $Q(\mathbf{K})$ in this basis, for small values of $(\mathbf{K}-\mathbf{K}_0)$. This result is derived by using the general properties of the Hamiltonian H. It is generalized in the next section in order to prove the analyticity of the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ in a strip of the complex $\mathbf{K}$ space. The problem is rather delicate because the validity of the proof depends very much on the nature of the Hamiltonian H. In particular, the matrix elements $(m,\mathbf{K}|Q(\mathbf{K})|m'\mathbf{K})$ and $\langle\mathbf{r}|P(\mathbf{K})\mathbf{r}'\rangle$ are given by expansions and, for this reason, it is quite necessary to prove the uniform convergence of these series. Therefore, for the sake of simplicity, it is assumed that the Hamiltonian is of the form $H=-\Delta+V$ and that the potential satisfies the general conditions listed in Sec. IID.

In the basis formed by the states $|m,\mathbf{K}_0)$, $H(\mathbf{K}_0)$ and $Q(\mathbf{K}_0)$ are diagonal. On the other hand, the states $|l,\mathbf{K})$ are eigenstates of $H(\mathbf{K})$ and therefore for small values of $|\mathbf{K}-\mathbf{K}_0|$, the operator $[H(\mathbf{K})-H(\mathbf{K}_0)]$ can be considered as a perturbation. In fact, according to Eq. (21), we have

$$H(\mathbf{K})-H(\mathbf{K}_0)=-2(\mathbf{K}-\mathbf{K}_0)i\nabla+(\mathbf{K}^2-\mathbf{K}_0^2). \quad (43)$$

In order to give a direct definition of $Q(\mathbf{K})$ and to derive the analyticity properties of the matrix elements $(m,\mathbf{K}_0|Q(\mathbf{K})|m',\mathbf{K}_0)$, we introduce the resolvant

$$R(E\ \mathbf{K})=1/(E-H(\mathbf{K})). \quad (44)$$

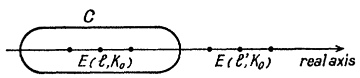

FIG. 2. Contour c in the complex energy plane. The points which are inside the contour correspond to eigenvalues of H belonging to $\mathfrak{B}$. The points which are outside are due to other bands.

We consider $\mathbf{K}_0$ as fixed, and in the complex energy plane, we draw a closed contour c, in the following way: all the points which correspond to eigenvalues $E(l,\mathbf{K}_0)$ belonging to $\mathfrak{B}(l=1\cdots d)$ lie inside the contour, all the points associated with the other eigenvalues $E(l',\mathbf{K}_0)$ remain outside (see Fig. 2). We can define $Q(\mathbf{K})$ for small real or complex values of $(\mathbf{K}-\mathbf{K}_0)$ by integrating $R(E,\mathbf{K})$ on this contour

$$Q(\mathbf{K})\equiv\frac{1}{2\pi i}\int_c\frac{dE}{E-H(\mathbf{K})}. \tag{45}$$

For small values of $(\mathbf{K}-\mathbf{K}_0)$, this definition coincides with the definition given above by Eq. (35); this fact can be verified immediately, if we assume the continuity of the eigenvalues $E(l,\mathbf{K})$ in the vicinity of $\mathbf{K}_0$. We have

$$\begin{aligned} Q(\mathbf{K})|l,\mathbf{K})&=E(l,\mathbf{K})|l,\mathbf{K}), \quad && E(l,\mathbf{K})\in\mathfrak{B}\\ &=0, && E(l,\mathbf{K})\notin\mathfrak{B}. \end{aligned} \tag{46}$$

These relations are direct consequences of Eq. (45) and are also completely equivalent to definition (41) because the states $|l,\mathbf{K})$ are normalized by Eq. (15). In the real $\mathbf{K}$ space, it is, of course, necessary to assume the continuity of the eigenvalues $E(l,\mathbf{K})$; otherwise it would be impossible to define energy bands. Thus, we know that for real values of $\mathbf{K}$, the definition (41) of $Q(\mathbf{K})$ must be valid. Therefore, for $\mathbf{K}$ real, the definition (42) of $P(\mathbf{K})$ in terms of $Q(\mathbf{K})$ coincides always with the elementary definition (5) of Sec. IIA, and this is just what we want. On the contrary, for complex values of $\mathbf{K}$, we do not need any continuity assumptions; the analyticity properties of $Q(\mathbf{K})$ remain defined by Eq. (42).

Now, let us show that for small values of $(\mathbf{K}-\mathbf{K}_0)$ definition (45) is meaningful for complex values of $\mathbf{K}$. [We do not assume the continuity of the eigenvalues $E(l,\mathbf{K})$.] The operator $R(E,\mathbf{K})$ can be written as follows:

$$R(E,\mathbf{K})=\frac{1}{E-H(\mathbf{K}_0)}\times\frac{1}{1-[H(\mathbf{K})-H(\mathbf{K}_0)][E-H(\mathbf{K}_0)]^{-1}}. \tag{47}$$

Thus, $R(E,\mathbf{K})$ can be expanded in a formal way in terms of the operator $[H(\mathbf{K})-H(\mathbf{K}_0)][E-H(\mathbf{K}_0)]^{-1}$. As $H(\mathbf{K})$ is a polynomial function of $\mathbf{K}$, the analyticity properties of the matrix elements of $R(E,\mathbf{K})$ can be derived easily by using this expansion, but first we have to show the validity of this operation for small values of $(\mathbf{K}-\mathbf{K}_0)$. More precisely, we must prove that in a small domain of the complex $\mathbf{K}$ space around the point $\mathbf{K}_0$, the upper bound of the modulus of the operator $[H(\mathbf{K})-H(\mathbf{K}_0)][E-H(\mathbf{K}_0)]^{-1}$ remains smaller than one.

Neither $H(\mathbf{K}_0)$ nor $(i\boldsymbol{\nabla})$ which appear in $[H(\mathbf{K})-H(\mathbf{K}_0)]$ are bounded operators. However, the operator $(i\boldsymbol{\nabla})$ is bounded with respect to $H(\mathbf{K}_0)$. More explicitly, we show in Appendix III that for any periodic normalizable state

$$(f|-\Delta|f)<A(f|H(\mathbf{K}_0)|f)+B(f|f), \tag{48}$$

where A and B are positive constants independent of $|f)$. We may write, also,

$$(f|-\Delta|f)<A|(f|[E-H(\mathbf{K}_0)]|f)+(f|f), \tag{49}$$

where E is the affix of any point of the contour c. The coefficients A and c are positive constants which depend only on $\mathbf{K}_0$ and c.

Now let $|g)$ be an arbitrary state. We can define another state $|f)$ by putting

$$|f)=[E-H(\mathbf{K}_0)]^{-1}|g). \tag{50}$$

In general, the operator $[E-H(\mathbf{K}_0)]^{-1}$ is not Hermitian but its eigenvectors are orthogonal. On Fig. 2, it appears immediately that the affix E of any point of the contour c always satisfies the inequality

$$|E-E(l,\mathbf{K}_0)|\geq L; \tag{51}$$

where L is the isolation length of the contour. Accordingly, the state $|f)$ introduced above satisfies the condition

$$(f|f)\equiv(g|[E^*-H(\mathbf{K}_0)]^{-1}\times[E-H(\mathbf{K}_0)]^{-1}|g)<L^{-2}(g|g). \tag{52}$$

Therefore, if E belongs to the contour, the state $|f)$ exists and Eq. (49) can be applied:

$$\begin{aligned} |(g|[E^*-H(\mathbf{K}_0)]^{-1}(-\Delta)[E-H(\mathbf{K}_0)]^{-1}|g)\\ \leq A|(g|[E^*-H(\mathbf{K}_0)]^{-1}|g)|\\ +C(g|[E^*-H(\mathbf{K}_0)]^{-1}[E-H(\mathbf{K}_0)]^{-1}|g)\\ \leq(AL^{-1}+BL^{-2})(g|g). \end{aligned} \tag{53}$$

On the other hand, any operator $\mathbf{U}$ satisfies the inequality

$$|(f|\mathbf{U}|f)|^2\leq(f|f)(f|\mathbf{U}^\dagger\mathbf{U}|f), \tag{54}$$

which is a trivial consequence of the fact that for any complex constant vector $\boldsymbol{\lambda}$, we have

$$(f|(\mathbf{U}^\dagger+\boldsymbol{\lambda}^*)(\mathbf{U}+\boldsymbol{\lambda})|f)\geq0. \tag{55}$$

By putting

$$\mathbf{U}=(i\boldsymbol{\Delta})[E-H(\mathbf{K}_0)] \tag{56}$$

in Eq. (54) and by using Eq. (53), we get

$$|(g|(i\boldsymbol{\nabla})[E-H(\mathbf{K}_0)]^{-1}|g)<D(g|g), \tag{57}$$

where D is a constant independent of E. Finally, we obtain the majorization [see Eq. (43)]

$$|(g|[H(\mathbf{K})-H(\mathbf{K}_0)][E-H(\mathbf{K}_0)]^{-1}|g)| < [2D|\mathbf{K}-\mathbf{K}_0|+L^{-1}|\mathbf{K}^2-\mathbf{K}_0^2|](g|g). \quad (58)$$

If $C(\mathbf{K}_0)$ is small enough, the condition

$$|\mathbf{K}-\mathbf{K}_0|\leq C(\mathbf{K}_0) \quad (59)$$

implies

$$|(g|[H(\mathbf{K})-H(\mathbf{K}_0)][E-H(\mathbf{K}_0)]^{-1}|g)<(g|g) \quad (60)$$

for all values of E belonging to c. Therefore the resolvant $R(E,\mathbf{K})$ can be expanded in an absolutely convergent series [see Eq. (47)]

$$R(E,\mathbf{K})=\frac{1}{E-H(\mathbf{K}_0)}+\frac{1}{E-H(\mathbf{K}_0)} \times[H(\mathbf{K})-H(\mathbf{K}_0)]\frac{1}{E-H(\mathbf{K}_0)}+\cdots. \quad (61)$$

As each term is an analytic function of $\mathbf{K}$, $R(E,\mathbf{K})$ is also an analytic function of $\mathbf{K}$, the series can be integrated on the contour c and as it converges uniformly with respect to $\mathbf{K}$, the operator $Q(\mathbf{K})$ which is proportional to the sum of the integrated series is also an analytic operator. More precisely, we state that the matrix elements $(m,\mathbf{K}_0|Q(\mathbf{K})|m',\mathbf{K}_0)$ are analytic functions of $\mathbf{K}$ for $|\mathbf{K}-\mathbf{K}_0|<C(\mathbf{K}_0)$.

In Sec. IID, we described anomalies connected with the fact that $|l,\mathbf{K})$ and $|l,\mathbf{K}^*)$ may become orthogonal to each other even for arbitrary small values of $\mathbf{K}''$. This phenomenon occurs in the neighborhood of the real branch points of the Bloch functions. We see now that these anomalies have no influence whatsoever on the analyticity properties of the matrix elements of $Q(\mathbf{K})$ in the basis formed by the states $|m,\mathbf{K}_0)$.

G. Analyticity of the Matrix Elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$

The operator $P(\mathbf{K})$ is given in terms of $Q(\mathbf{K})$ by Eq. (42) and the analyticity of $Q(\mathbf{K})$ for $|\mathbf{K}-\mathbf{K}_0|<C(\mathbf{K}_0)$ in the basis of the states $|m,\mathbf{K}_0)$ can be used now to prove the analyticity of the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$. But, for this purpose, $Q(\mathbf{K})$ must be expressed in other representations.

The matrix elements $(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')$ can be defined by

$$(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')=\lim_{E\to\infty}\sum_{E(m,\mathbf{K}_0)\leqslant E}\sum_{E(m',\mathbf{K}_0)\leqslant E}(\mathbf{p}|m,\mathbf{K}_0) \times(m,\mathbf{K}_0|Q(\mathbf{K})|m',\mathbf{K}_0)(m',\mathbf{K}_0|\mathbf{p}') \quad (62)$$

(sum over m and m'). Each term of this series is analytic with respect to $\mathbf{K}$. Therefore the sum is also analytic for $|\mathbf{K}-\mathbf{K}_0|<C(\mathbf{K}_0)$, if the series converges uniformly with respect to $\mathbf{K}$. But according to Eq. (50), $(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')$ can be written in a more explicit way (at least for $\mathbf{K}$ real):

$$(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')=\sum_l\sum_m\sum_{m'}(\mathbf{p}|m,\mathbf{K}_0) \times(m,\mathbf{K}_0|l,\mathbf{K})(l,\mathbf{K}^*|m',\mathbf{K}_0)(m',\mathbf{K}_0|\mathbf{p}'). \quad (63)$$

We proved in Sec. IID that the series giving $(\mathbf{p}|l,\mathbf{K})$ in terms of the components $(m,\mathbf{K}_0|l,\mathbf{K})$ [see Eq. (40)] converges to $(\mathbf{p}|l,\mathbf{K})$ uniformly with respect to $\mathbf{K}$ when E goes to infinity. Therefore, for real values of $\mathbf{K}$, the double sum of Eq. (62) converges uniformly to the value of $(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')$ which correspond to the elementary definition (41). The same method can be applied for complex values of $\mathbf{K}$; however, it is not really valid for the anomalous points because, in this case, definition (41) becomes meaningless. However, the difficulty is not a very serious one; we saw before that the matrix elements $(m,\mathbf{K}_0|Q(\mathbf{K})|m',\mathbf{K}_0)$ remain well defined and analytic at these points. In any case, we can define the matrix elements $(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')$ without ambiguity by using Eq. (62). The nature of the convergence of the series giving $(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')$ depends on the behavior of high-energy terms and not on low-energy effects related to degeneracies. Therefore, we can assume safely that the double sum of Eq. (71) is uniformly convergent with respect to $\mathbf{K}$ for real or complex values of $\mathbf{K}$. Thus, the matrix elements $(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')$ must be analytic for $|\mathbf{K}-\mathbf{K}_0|<C(\mathbf{K}_0)$.

The same method can be used to derive the analyticity of the matrix elements $\langle\mathbf{r}|Q(\mathbf{K})|\mathbf{r}'\rangle$ in the domain defined by $|\mathbf{K}-\mathbf{K}_0|<C(\mathbf{K}_0)$. These matrix elements must be defined by [see Eq. (22) and (23)]

$$\langle\mathbf{r}|Q(\mathbf{K})|\mathbf{r}'\rangle=v^{-1}\lim_{p_0\to\infty}\sum_{p<p_0}\sum_{p'<p_0}\langle\mathbf{r}|p\rangle(\mathbf{p}|Q(\mathbf{K})|\mathbf{p}')\langle\mathbf{p}'|\mathbf{r}\rangle. \quad (64)$$

Each term of this series is analytic with respect to $\mathbf{K}$. Again we can write explicitly $\langle\mathbf{r}|Q(\mathbf{K})|\mathbf{r}'\rangle$ in terms of the states $|l,\mathbf{K})$ by replacing the operator $Q(\mathbf{K})$ in the right-hand side of (64) by its expansion (41). In this way, we can show that the double series of Eq. (64) converges uniformly with respect to $\mathbf{K}$. This result is obtained by comparison with Eq. (35) which gives the function $\langle\mathbf{r}|l,\mathbf{K}\rangle$ in terms of the components $(\mathbf{p}|l,\mathbf{K})$; in fact, we proved in Sec. IIE that this series converges uniformly with respect to $\mathbf{K}$ when p_0 goes to infinity. The matrix elements $\langle\mathbf{r}|Q(\mathbf{K})|\mathbf{r}'\rangle$ are defined by a series which converges in the same way; therefore they are analytic with respect to $\mathbf{K}$ for $|\mathbf{K}-\mathbf{K}_0|<C(\mathbf{K}_0)$.

Now, we can extend the domain of analyticity of these matrix elements $\langle\mathbf{r}|Q(\mathbf{K})|\mathbf{r}'\rangle$. In the real $\mathbf{K}$ space, we consider a closed spherical domain containing the Brillouin zone and defined by $|\mathbf{K}|\leq R$. Each point of this domain is determined by a value $\mathbf{K}_0$ of $\mathbf{K}$ and is the center of an analyticity sphere of radius $C(\mathbf{K}_0)$. Borel-Lebesgue theorem indicates that the whole domain can be covered by a finite number of these spheres. Therefore the matrix elements $\langle\mathbf{r}|Q(\mathbf{K})|\mathbf{r}'\rangle$ remain analytic in a domain defined by the equations $|\mathbf{K}'|\leq R$, $|K''|\leq A$ where A is a positive constant.

According to Eq.(51), the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ are analytic in the same domain. Furthermore, by definition, they are periodic with respect to $\mathbf{K}$ for real values of $\mathbf{K}$; consequently they are also periodic for $\mathbf{K}$ complex and with the same periods. This result comes from the fact that two analytic functions which have the same values on a segment are identical. This final remark permits to formulate the fundamental result of this section: When the Hamiltonian H satisfies proper regularity conditions, the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ of the operators $P(\mathbf{K})$ associated with a given band $\mathfrak{B}$, are analytic functions of $\mathbf{K}=\mathbf{K}'+i\mathbf{K}''$ in a domain defined by a condition $|\mathbf{K}''|<A$ where A is a positive constant which depends only on the characteristics of the band. In practice, the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ remain analytic in larger domains; for instance, in tubes defined by inequalities of the form $|\mathbf{K}''|<A(\hat{K}'')$ where $A(\hat{K}'')$ is a positive function of the direction of $\mathbf{K}''$.

III. DEFINITION AND ASYMPTOTIC PROPERTIES OF THE OPERATOR ASSOCIATED WITH AN ENERGY BAND P

A. Definition of P

By definition, P is the operator of projection on the set of all the eigenstates which belong to a band $\mathfrak{B}$. It can be expressed as an integral of $P(\mathbf{K})$ on the Brillouin zone

$$\langle\mathbf{r}|P|\mathbf{r}'\rangle=\int_{\mathrm{B.Z.}} d^n\mathbf{K}\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle. \tag{65}$$

As the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ are analytic with respect to $\mathbf{K}$ for real values of $\mathbf{K}$ and in the neighborhood, the matrix elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$ are well defined and when the potential V fulfill the requirements of Sec. IID, they are continuous with respect to $\mathbf{r}$ and $\mathbf{r}'$. They are also periodic in the following sense:

$$\langle\mathbf{r}+\mathbf{t}|P|\mathbf{r}'+\mathbf{t}\rangle=\langle\mathbf{r}|P|\mathbf{r}'\rangle. \tag{66}$$

Here $\mathbf{t}$ is a translation of the crystal. On the other hand, the fact that P is a projection operator appears clearly in the identity

$$P^2=P, \tag{67}$$

which is a direct consequence of Eq. (7).

Our aim is to show that the matrix elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$ decrease exponentially when $|\mathbf{r}-\mathbf{r}'|$ goes to infinity. This behavior is directly related to the localizability properties of the electrons in insulators; this correlation is, in fact, the reason of our interest in this matter and can be demonstrated easily. For instance, if the space of the eigenfunctions of H which belong to $\mathfrak{B}$ can be spanned[4] by a set of Wannier functions $\langle\mathbf{r}|M_j\rangle$, it is possible to express P in the form

$$\langle\mathbf{r}|P|\mathbf{r}'\rangle=\sum_{M,j}\langle\mathbf{r}|M_j\rangle\langle M_j|\mathbf{r}'\rangle. \tag{68}$$

Here the points M are the nodes of a lattice; the index j is used to label the Wannier function which are associated with the same site M. We see immediately, in this case, that, if the modulus of the Wannier functions decrease exponentially at infinity, the same property remains true for the matrix elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$ when $\mathbf{r}$ or $\mathbf{r}'$ goes to infinity.

In fact, the asymptotic properties of the matrix elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$ can be related directly to the analyticity of $P(\mathbf{K})$ in a strip of the complex $\mathbf{K}$ plane, but to show this connection, we need a theorem which is given in the next section.

B. Analyticity of Periodic Functions and Asymptotic Properties of Their Fourier Coefficients

The following theorem appears under different forms in the literature. Its proof which is very simple is given here for the sake of completeness.

Theorem: Let $f(\mathbf{K})$ be an n-periodical function of the n-dimensional complex vector $\mathbf{K}=\mathbf{K}'+i\mathbf{K}''$, admitting real vectors $\mathbf{K}_j$ $(j=1\cdots n)$ as periods. Thus $f(\mathbf{K}+\mathbf{K}_j)=f(\mathbf{K})$. On the other hand, let $\mathbf{t}$ be the translation vectors of the reciprocal lattice. This lattice is defined by the reciprocal vectors $\mathbf{t}_l$ $(l=1\cdots n)$ and we have

$$\mathbf{K}_j\cdot\mathbf{t}_l=2\pi\delta_{jl}, \tag{69}$$

$$\mathbf{t}=\sum_l \nu_l\mathbf{t}_l \quad (\nu_l=\text{integer}). \tag{70}$$

Then, if $f(\mathbf{K})$ is an analytic function of $\mathbf{K}$ in a domain defined by $|\mathbf{K}''|<A$, it can be expanded in a convergent Fourier series in this domain:

$$f(\mathbf{K})=\sum_{\mathbf{t}} e^{i\mathbf{K}\mathbf{t}}g(\mathbf{t}), \tag{71}$$

and the Fourier coefficients $g(\mathbf{t})$ satisfy the condition

$$\lim_{t\to\infty} e^{\epsilon At}g(\mathbf{t})=0. \tag{72}$$

Conversely, if the coefficients $g(\mathbf{t})$ of a Fourier series have this asymptotic behavior, the series converges in the region $|\mathbf{K}'|<A$ and its sum is an analytic function of $\mathbf{K}$ in this domain.

Proof: As $f(\mathbf{K})$ is analytic in the domain $|\mathbf{K}''|<A$, it can be expanded in Fourier series for $\mathbf{K}$ real.

$$f(\mathbf{K})=\sum_{\mathbf{t}} e^{i\mathbf{K}\mathbf{t}}g(\mathbf{t}). \tag{73}$$

For $|\mathbf{K}''|<A$, we can make an analytic continuation

[4] This question has been discussed previously. J. des Cloizeaux, Phys. Rev. **129**, 554 (1963).

of this formula. We have

$$f(\mathbf{K}'+i\mathbf{K}'')=\sum_{\mathbf{t}} e^{i\mathbf{K}'\mathbf{t}-\mathbf{K}''\mathbf{t}}g(\mathbf{t}). \tag{74}$$

We consider here $f(\mathbf{K}'+i\mathbf{K}'')$ as a periodical function of $\mathbf{K}'$; the Fourier coefficients of this function are $e^{-\mathbf{K}''\mathbf{t}}g(\mathbf{t})$. But the function $f(K'+iK'')$ is an analytic function of K' for real values of $\mathbf{K}'$. Therefore, according to a well-known theorem, the coefficients go to zero when $|\mathbf{t}|$ becomes infinite. By putting

$$\mathbf{K}''=-\epsilon A\hat{t} \quad (0<\epsilon<1) \quad (\hat{t}=\mathbf{t}/|\mathbf{t}|), \tag{75}$$

we get immediately

$$\lim_{t\to\infty} e^{\epsilon At}g(\mathbf{t})=0. \tag{76}$$

Conversely, if this relation is valid for any value of ϵ smaller than one, the Fourier series which is built with the coefficients $g(\mathbf{t})$ converges uniformly in any domain $|\mathbf{K}''|\leq\epsilon A$ with $0<\epsilon<1$. Therefore, the sum of the series defines a function $f(\mathbf{K})$ which is analytic in the domain $|\mathbf{K}''|A$.

Remark: The preceding results can be generalized without difficulty. For instance, we can assume that $f(\mathbf{K})$ is analytic in a domain $\mathfrak{D}$ defined by $|\mathbf{K}''|<A(\hat{K}'')$ where $A(\hat{K}'')$ is a positive function of the direction of $\mathbf{K}''$. Let $B(\hat{r})$ be the upper limit of the scalar products $(\mathbf{K}''\cdot\hat{r})$ when $\mathbf{K}''$ belongs to $\mathfrak{D}$. Then it is trivial to show that

$$\lim_{t\to 0} \exp[\epsilon tB(\hat{t})]g(\mathbf{t})=0. \tag{77}$$

Conversely, if this relation holds for the coefficients of a Fourier series, the series defines a function $f(\mathbf{K})$ which is analytic in the domain $\mathfrak{D}$.

C. Asymptotic Properties of the Matrix Elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$

The analyticity of the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ in a domain given by an inequality of the form $|\mathbf{K}''|<A$, has been proved in Sec. II, for a large class of Hamiltonians. This result can be used now to derive, with the help of the preceding theorem, the asymptotic properties of the matrix elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$. More precisely, it will be shown that when $\mathbf{r}$ and $\mathbf{r}'$ remain fixed, we have:

$$\lim_{t\to\infty} e^{\epsilon At}\langle\mathbf{r}|P|\mathbf{r}'+\mathbf{t}\rangle=0. \tag{78}$$

Definition (65) implies:

$$\langle\mathbf{r}|P|\mathbf{r}'+\mathbf{t}\rangle=\int_{\mathrm{B.Z.}} d^n\mathbf{K}\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'+\mathbf{t}\rangle. \tag{79}$$

But $P(\mathbf{K})$ can be expressed in terms of Bloch waves as in Eq. (5). By definition

$$\langle\mathbf{r}+\mathbf{t}|\varphi(l,\mathbf{K})\rangle=e^{i\mathbf{K}\mathbf{t}}\langle\mathbf{r}|\varphi(l,\mathbf{K})\rangle, \tag{80}$$

therefore, we have also

$$\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'+\mathbf{t}\rangle=e^{-i\mathbf{K}\mathbf{t}}\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle. \tag{81}$$

By using this result in Eq. (79), we get

$$\langle\mathbf{r}|P|\mathbf{r}'+\mathbf{t}\rangle=\int_{B.Z.} d^n\mathbf{K}e^{-i\mathbf{K}\mathbf{t}}\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle. \tag{82}$$

On the other hand, as the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ are analytic with respect to $\mathbf{K}$ and periodic, they can be expanded in convergent Fourier series. The periods are the vectors which define the reciprocal lattice. Thus, the terms of the series are of the form $e^{i\mathbf{K}\mathbf{t}}$. Equation (91) shows immediately that the terms $\langle\mathbf{r}|P|\mathbf{r}'+\mathbf{t}\rangle$ are proportional to the Fourier coefficients. Finally, we may write

$$\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle=\Omega^{-1}\sum_{\mathbf{t}} e^{i\mathbf{K}\mathbf{t}}\langle\mathbf{r}|P|\mathbf{r}'+\mathbf{t}\rangle, \tag{83}$$

where Ω is the volume of the Brillouin zone.

Now, we can apply the theorem of Sec. II. We see immediately that the property (78) is a direct consequence of the analyticity of $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ in the domain $|\mathbf{K}''|<A$. The remark of Sec. IIB shows that this property can be generalized, if the matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ remain analytic in a strip of the complex $\mathbf{K}$ plane defined by an inequality of the form $|\mathbf{K}''|<A(\hat{K}'')$ where $A(\hat{K}'')$ is a positive function of the direction of $\mathbf{K}''$.

IV. CONCLUSION

In the previous sections, general assumptions concerning the regularity of a one-electron Hamiltonian $H=T+V$ and its completeness have been used to show that the projection operator $P(\mathbf{K})$ which can be associated with a given band $\mathfrak{B}$ has matrix elements $\langle\mathbf{r}|P(\mathbf{K})|\mathbf{r}'\rangle$ which are continuous with respect to $\mathbf{r}$ and $\mathbf{r}'$ and analytic with respect to $\mathbf{K}$ in a strip of the complex $\mathbf{K}$ space defined by $|\mathbf{K}''|<A$, where A is a positive constant. On the other hand, as a consequence of this analyticity property, it was shown that for large values of $|\mathbf{r}-\mathbf{r}'|$, the matrix elements $\langle\mathbf{r}|P|\mathbf{r}'\rangle$ have exponential tails

$$\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty} \exp[\epsilon A|\mathbf{r}-\mathbf{r}'|]\langle\mathbf{r}|P|\mathbf{r}'\rangle=0 \quad 0<\epsilon<1. \tag{84}$$

In the case of insulators, a physical interpretation of this result can be given in terms of electronic correlation functions at zero temperature. For each value of $\mathbf{K}$, we can introduce the operator $P_\perp(\mathbf{K})$ which is the sum of all the operators $P(\mathbf{K})$ which correspond to filled bands. For real values of $\mathbf{K}$, this operator is analytic. The domain of analyticity of $P(\mathbf{K})$ must be the same, in general, as the domain of analyticity of the operator $P(\mathbf{K})$ related to the valence band; it may be even larger. Thus, the corresponding operator $P_\perp$ satisfies a relation of the form (84). Its matrix elements are just equal to the one-electron correlation function as it is easy to verify

$$\langle\mathbf{r}|P_{\perp}|\mathbf{r}'\rangle=\langle\omega|C_{\mathbf{r}}^{+}C_{\mathbf{r}'}|\omega\rangle\equiv G(\mathbf{r},\mathbf{r}'). \tag{85}$$

Here $|\omega\rangle$ is the ground state obtained by filling all the lower bands. $C_{\mathbf{r}}^{+}$ and $C_{\mathbf{r}}$ are the creation and annihilation operators of an electron at the point of coordinate $\mathbf{r}$.

Thus, in the independent-electron approximation, the one-particle correlation function $G(\mathbf{r},\mathbf{r}')$ decrease exponentially when the distance $|\mathbf{r}-\mathbf{r}'|$ increases. This result remain probably valid also when there are interactions. It is likely to be true also for other correlation functions. These projection operators have the advantage of being completely independent of the phase factors of the Bloch waves. In general, difficulties are introduced by the determination of the individual phases of these waves. On the other hand, these phase factors seem devoid of any physical meaning. Apparently, many problems of solid-state physics could be treated properly without introducing Bloch waves in a specific way, but, instead, by using projection operators which are more simple objects. It is hoped that by emphasizing this fact, this study may help to the solution of these problems.

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APPENDIX I

Derivation of the bounding condition $|\mathbf{p}|^{n+1-\epsilon}|(\mathbf{p}|l,\mathbf{K})<C$ where C is a constant independent of $\mathbf{K}$ (for $\mathbf{K}$ real)

In the reciprocal space, the Schrödinger equation can be written

$$[E(l,\mathbf{K})-(\mathbf{K}+\mathbf{p})^2](\mathbf{p}|l,\mathbf{K})=\sum_{\mathbf{q}}\mathrm{V}(\mathbf{p}-\mathbf{q})(\mathbf{q}|l,\mathbf{K}). \tag{AI.1}$$

Let us consider the solutions which are associated with a given band $\mathcal{B}$. For these eigenstates, we have

$$|E(l,\mathbf{K})|<E_0, \tag{AI.2}$$

where E_0 is a constant which depends on the band. We want to show that the corresponding coefficients $(\mathbf{p}|l,\mathbf{K})$ satisfy an inequality of the form

$$p^{n+1-\epsilon}|(\mathbf{p}|l,\mathbf{K})|<C, \tag{AI.3}$$

where C is a constant independent of $\mathbf{K}$ and l; n is the number of space coordinates and ϵ an arbitrary positive constant. It is clear that the asymptotic properties of $(\mathbf{p}|l,\mathbf{K})$ for large values of $\mathbf{p}$ depend on the behavior of the following sum:

$$F(l,\mathbf{K},\mathbf{p})=\sum_{\mathbf{p}}\mathrm{V}(\mathbf{p}-\mathbf{q})(\mathbf{q}|l,\mathbf{K}). \tag{AI.4}$$

Let us derive first a weaker condition which implies the absolute convergence of $F(\mathbf{p})$,

$$p^2|(\mathbf{p}|l,\mathbf{K})|<C'. \tag{AI.5}$$

This condition can be established by showing that $|F(l,\mathbf{K},\mathbf{p})|$ has an upper bound independent of $\mathbf{p}$ and $\mathbf{K}$. The sum $|F(l,\mathbf{K},\mathbf{p})|$ can be considered as a scalar product and Schwartz inequality can be applied:

$$|F(l,\mathbf{K},\mathbf{p})|=|\sum_{\mathbf{q}}\mathrm{V}(\mathbf{p}-\mathbf{q})(\mathbf{q}|l,\mathbf{K})| \\ \leq[\sum_{\mathbf{q}}|\mathrm{V}(\mathbf{q})|^2\sum_{\mathbf{q}'}|(\mathbf{q}'|l,\mathbf{K})|^2]^{1/2}. \tag{AI.6}$$

The wave function is assumed to be normalized. Therefore, if $\mathbf{K}$ is real, we have

$$\sum_{\mathbf{q}}|(\mathbf{q}|l,\mathbf{K})|^2=1. \tag{AI.7}$$

On the other hand, the sum $\sum|\mathrm{V}(q)|^2$ converges if the square of the potential is integrable and, for instance, if we have

$$|\mathbf{p}|^{n+\frac{1}{2}}|\mathrm{V}(\mathbf{p})|^2<\infty, \tag{AI.8}$$

since the vectors $\mathbf{p}$ are associated with the points of a lattice in the reciprocal space. For $n\geq 3$, condition (AI.8) is weaker than the assumption of Eq. (26) which can be written

$$|\mathbf{p}|^{2n-2}|\mathrm{V}(\mathbf{p})|^2<\infty. \tag{AI.9}$$

For $n=1$ and $n=2$, this latter condition is not sufficient to insure the convergence of the series $\sum|\mathrm{V}(\mathbf{q})|^2$. However, even in this case, we can find an upper bound for $|F(l,\mathbf{K},\mathbf{p})|$ by assuming the uniform convergence of the mean value of the kinetic energy for the states under consideration

$$\sum p^2|(\mathbf{p}|l,K)|^2<C''. \tag{AI.10}$$

This assumption is highly reasonable since the eigenvalues $E(l,\mathbf{K})$ have an upper bound E_0. It is proved rigorously for real in Appendix IV by using the results of Appendices II and III. In this case, Schwartz inequality can be applied differently:

$$|F(l,\mathbf{K},\mathbf{p})|=|\sum_{\mathbf{q}}\mathrm{V}(\mathbf{p}-\mathbf{q})(\mathbf{q}|l,\mathbf{K})| \\ \leq\left[\sum_{\mathbf{q}}\frac{\mathrm{V}(\mathbf{p}-\mathbf{q})}{(q+a)^2}\sum_{\mathbf{q}'}(q'+a)^2|(\mathbf{q}'|l,\mathbf{K})|^2\right], \tag{AI.11}$$

where a is an arbitrary positive constant.

According to (AI.7)

$$\sum_{\mathbf{q}}(q+a)^2|(\mathbf{q}|l,\mathbf{K})|^2 \\ <4\sum_{\mathbf{q}}(q^2+a^2)|(\mathbf{q}|l,\mathbf{K})|^2<4(c''+a^2). \tag{AI.12}$$

On the other hand, if condition (AI.8) is realized, we can find for $|\mathrm{V}(\mathbf{q})|$ an upper bound of the form

$$|\mathrm{V}(\mathbf{q})|<A/(q^{n-1}+B), \tag{AI.13}$$

where A and B are positive constants. Consequently, we have

$$\sum_{\mathbf{q}} \frac{|\mathrm{V}(\mathbf{p}-\mathbf{q})|^2}{(q+a)^2} < \sum_{\mathbf{q}} \frac{A^2}{(|\mathbf{p}-\mathbf{q}|^{n-1}+B)^2(q+a)^2}. \quad \text{(AI.14)}$$

The sum in the right-hand side of this inequality converges and for $n=1$ and $n=2$, it is trivial to show that it has upper band independent of $\mathbf{p}$. Therefore, condition (AI.5) is established for any value of n.

For $n=1$, this condition (AI.5) implies Eq. (AI.3). Now, let us derive (AI.3) for $n>1$. We assume that for a number S, $(1<S\leq n)$ the following condition holds for any real values of $\mathbf{K}$:

$$p^S|(\mathbf{p}|l,\mathbf{K})|<\Gamma(S), \quad \text{(AI.15)}$$

where $\Gamma(S)$ is a constant independent of $\mathbf{K}$, and we want to show that a condition of this nature holds also if we replace S by $(S+1)$. Condition (AI.15) implies the absolute convergence of $F(\mathbf{p})$ and we can try to majorize this sum. As we have

$$|(\mathbf{p}|l,\mathbf{K})|<1, \quad \text{(AI.16)}$$

we can find an upper bound for $|(\mathbf{p}|l,\mathbf{K})|$ by using (AI.15)

$$|(\mathbf{p}|l,\mathbf{K})|<C(S)/(p^S+D(S)), \quad \text{(AI.17)}$$

where $C(S)$ and $D(S)$ are positive constants. For instance, we may choose $D(S)$ in an arbitrary way, and put

$$C(S)=\Gamma(S)+D(S). \quad \text{(AI.18)}$$

By using (AI.13) and (AI.18), we find an upper bound of $|F(\mathbf{p})|$:

$$|F(l,\mathbf{K},\mathbf{p})|<\sum_{\mathbf{q}}|\mathrm{V}(\mathbf{p}-\mathbf{q})|\,|(\mathbf{q}|l,\mathbf{K})|$$

$$<\sum_{\mathbf{q}} AC(S)/([|\mathbf{p}-\mathbf{q}|^{n-1}+B][q^S+D]). \quad \text{(AI.19)}$$

For $1<S<n$, it is easy to see that the sum on the right-hand side of (AI.19) converges and that the main contributions to this sum come from regions where $|\mathbf{q}|$ is of the order of $|\mathbf{p}|$. Therefore, for large values of $\mathbf{p}$

$$\sum \frac{1}{[|\mathbf{p}-\mathbf{q}|^{n-1}+B][q^S+D(S)]} \sim \frac{1}{\Omega}\int \frac{d^n\mathbf{q}}{[|\mathbf{p}-\mathbf{q}|^{n-1}][q^S+D(S)]}, \quad \text{(AI.20)}$$

where Ω is the volume of the Brillouin zone. But, we have also:

$$\int \frac{d^n\mathbf{q}}{[|\mathbf{p}-\mathbf{q}|^{n-1}+B][q^S+D(S)]} < \int \frac{d^n\mathbf{q}}{|\mathbf{p}-\mathbf{q}|^{n-1}q^S} = \frac{G(S)}{p^{S-1}}, \quad \text{(AI.21)}$$

where $G(S)$ is a positive constant. Therefore, from Eqs. (AI.19), (AI.20), and (AI.21), we deduce

$$p^{S-1}|F(l,\mathbf{K},\mathbf{p})|<\varphi(S), \quad \text{(AI.22)}$$

where $\varphi(S)$ is a positive constant independent of l and $\mathbf{K}$. Note that the whole argument breaks down if the condition $1<S<n$ is not fulfilled; in this case, the sums cannot be replaced by convergent integrals. Now, Schrödinger Eq. (AI.1), Eq. (AI.4), and Eq. (AI.22) imply the existence of an inequality of the form

$$p^{S+1}|(\mathbf{p}|l,\mathbf{K})|<C(S+1) \quad (1<S<n). \quad \text{(AI.23)}$$

But Eq. (AI.5) tells us that Eq. (AI.15) holds for $1<S<2$. According to (AI.23), it must hold also for $1<S<n+1$. Therefore (AI.3) is proved also for $n>1$.

APPENDIX II

Proof of the bounding inequality

$$|(f|V|f)|<\epsilon(f|-\Delta|f)+C(\epsilon)(f|f)$$

for any state $|f)$ having the same periodicity as V (ϵ= arbitrary positive constant)

Let V be a periodic potential and $\mathrm{V}(\mathbf{p})$ its Fourier coefficients

$$V(\mathbf{r})=\sum_{\mathbf{p}} e^{i\mathbf{p}\mathbf{r}}\,\mathrm{V}(\mathbf{p}). \quad \text{(AII.1)}$$

It is assumed that these coefficients $\mathrm{V}(\mathbf{p})$ are bounded and satisfy Eq. (26)

$$\mathrm{V}(\mathbf{p})<\infty, \quad \text{(AII.2)}$$

$$p^{n-1}|\mathrm{V}(\mathbf{p})|<\infty. \quad \text{(AII.3)}$$

In an equivalent way, these conditions imply the existence of two positive numbers A and B for which we have

$$|\mathrm{V}(\mathbf{p})|<A/(p^{n-1}+B). \quad \text{(AII.4)}$$

Now let ϵ be an arbitrary positive number and $|f)$ a normalized periodic state; we want to show that this state satisfies always an inequality of the form

$$|(f|V|f)|<\epsilon(f|-\Delta|f)+C(\epsilon)(f|f), \quad \text{(AII.5)}$$

where $C(\epsilon)$ is a constant independent of $|f)$. The function $\langle\mathbf{r}|f\rangle$ can be expanded in Fourier series

$$\langle\mathbf{r}|f\rangle=v^{-1/2}\sum_{\mathbf{q}}(\mathbf{q}|f)e^{i\mathbf{q}\mathbf{r}}, \quad \text{(AII.6)}$$

where v is the volume of the crystal cell. We have

$$(f|f)=\sum_{\mathbf{q}}|(\mathbf{q}|f)|^2, \quad \text{(AII.7)}$$

$$(f|-\Delta|f)=\sum_{\mathbf{q}} q^2|(\mathbf{q}|f)|^2, \quad \text{(AII.8)}$$

$$(f|V|f)=\sum_{\mathbf{p}\mathbf{q}}(f|\mathbf{p})(\mathbf{q}|f)\,\mathrm{V}(\mathbf{p}-\mathbf{q}). \quad \text{(AII.9)}$$

The modulus of the mean value of V can be majorized by using Schwartz inequality

$$|(f|V|f)|\leq\sum_{\mathbf{p}}|\mathrm{V}(\mathbf{p})|\sum_{\mathbf{q}}|(f|\mathbf{p}+\mathbf{q})||(\mathbf{q}|f)|$$
$$\leq\{\sum_{\mathbf{p}'}|\mathrm{V}(\mathbf{p}')(p'+a)^2|$$
$$\times\sum_{\mathbf{pq}}|(\mathbf{p}+\mathbf{q}|f)|^2|(\mathbf{q}|f)|^2\}^{1/2}, \quad \text{(AII.10)}$$

where a is an arbitrary positive constant which is introduced in order to get convergent sums. In fact, according to Eq. (AII.4), the sum $\sum_{\mathbf{p}}|\mathrm{V}(\mathbf{p})|(p+a)^{-2}$ converges to a constant value. On the other hand, we have

$$\sum_{\mathbf{pq}}(p+a)^2|(\mathbf{p}+\mathbf{q}|f)|^2|(\mathbf{q}|f)|^2$$
$$=\sum_{\mathbf{pq}}(|\mathbf{p}-\mathbf{q}|^2+a^2)|(\mathbf{p}|f)|^2|(\mathbf{q}|f)|^2$$
$$\leq\sum_{\mathbf{pq}}(4p^2+4q^2+a^2)|(\mathbf{p}|f)|^2|(\mathbf{q}|f)|^2. \quad \text{(AII.11)}$$

Finally, by comparing (AII.10), (AII.7), (AII.8), and (AII.11), we obtain: ($\alpha,\beta=$positive constants)

$$|(f|V|f)|^2\leq(f|f)[\alpha(f|-\Delta|f)+B(f|f)]. \quad \text{(AII.12)}$$

Let $C(\epsilon)$ be a positive number for which we have

$$C(\epsilon)\geq\alpha/2\epsilon \quad C\geq B. \quad \text{(AII.13)}$$

We verify immediately:

$$|(f|V|f)|<\epsilon(f|-\Delta|f)+C(\epsilon)(f|f). \quad \text{(AII.14)}$$

APPENDIX III

Proof of the bounding inequality $(f|-\Delta|f)<A(f|H(\mathbf{K})|f)+B(f|f)$ for any periodic normalizable state $|f)$ (A and B are positive constants independent of $|f)$).

According to the definition of $H(\mathbf{K})$ [see Eq. (21)], we have

$$(f|H(\mathbf{K})|f)=(f|(-i\nabla+\mathbf{K})^2|f)$$
$$+(f|V|f)>(f|(-\Delta+K^2)|f)$$
$$-2|(f|i\mathbf{K}\cdot\nabla|f)|-|(f|V|f). \quad \text{(AIII.1)}$$

We can majorize the last two terms of this inequality. We write

$$|(f|-i\nabla|f)|^2\leq(f|f)(f|-\Delta|f). \quad \text{(AIII.2)}$$

This equation implies

$$|(f|i\nabla|f)|\leq\tfrac{1}{2}\epsilon'(f|-\Delta|f)+(1/\epsilon')(f|f), \quad \text{(AIII.3)}$$

where ϵ' is an arbitrary positive constant.

On the other hand, we can use the results of Appendix II,

$$|(f|V|f)|<\epsilon''(f|-\Delta|f)+C(\epsilon'')(f|f), \quad \text{(AIII.4)}$$

where ϵ'' is an arbitrary positive constant. Therefore, by using Eqs. (AIII.1), (AIII.3), and (AIII.4), we obtain

$$(f|H(\mathbf{K})|f)>(1-\epsilon'-\epsilon'')(f|-\Delta|f)$$
$$+[K^2-(2/\epsilon')-C(\epsilon'')](f|f). \quad \text{(AIII.5)}$$

We put

$$A=\frac{1}{1-\epsilon'-\epsilon''} \quad B=\frac{1}{1-\epsilon'-\epsilon''}\left[\frac{2}{\epsilon'}+C(\epsilon'')\right], \quad \text{(AIII.6)}$$

and we choose small values of ϵ' and ϵ'' in order to have

$$A>0.$$

The final result is

$$(f|-\Delta|f)<A(f|H(\mathbf{K})|f)+B(f|f). \quad \text{(AIII.7)}$$

APPENDIX IV

Upper bound of the sum $\sum p^2|(\mathbf{p}|l,\mathbf{K})|^2$.

For an eigenstate $|l,\mathbf{K})$ of $H(\mathbf{K})$, the mean value of the kinetic energy is given by

$$T(l,\mathbf{K})=(l,\mathbf{K}|-\Delta|l,\mathbf{K})=\sum p^2|(\mathbf{p}|l,\mathbf{K})|^2. \quad \text{(AIV.1)}$$

We assume that $\mathbf{K}$ is real and we want to show that, if the state belongs to a given band $\mathcal{B}$, then the kinetic energy is bounded

$$T(l,\mathbf{K})<T, \quad \text{(AIV.2)}$$

where T is a constant independent of $\mathbf{K}$ and l. The eigenvalues $E(l,\mathbf{K})$ are given by

$$E(l,\mathbf{K})=(l,\mathbf{K}|H(\mathbf{K})|l,\mathbf{K}). \quad \text{(AIV.3)}$$

We assume that the energies $E(l,\mathbf{K})$ associated with $\mathcal{B}$ are bounded,

$$E(l,\mathbf{K})<E_0, \quad \text{(AIV.4)}$$

and we can use this fact by applying the results of Appendix III.

$$T(l,\mathbf{K})=(l,\mathbf{K}|-\Delta|l,\mathbf{K})<A(l,\mathbf{K}|H(\mathbf{K})|l,\mathbf{K})$$
$$+B(l,\mathbf{K}|l,\mathbf{K})=AE(l,\mathbf{K})+B.$$

By taking account of (AIV.4), we obtain

$$T(l,\mathbf{K})<AE_0+B\equiv T. \quad \text{(AIV.5)}$$

APPENDIX V

Proof of the existence of a finite number $E_0(\epsilon)$ independent of $\mathbf{K}$ and such that for any value of E larger than $E_0(\epsilon)$, we may write:

$$|(\mathbf{p}|l,\mathbf{K})-\sum_{E(m,\mathbf{K}_0)<E}(\mathbf{p}|m,\mathbf{K}_0)(m,\mathbf{K}_0|l,\mathbf{K})|<\epsilon$$

[*the sum is over m and it is assumed that $E(l,\mathbf{K})$ remains bounded when $\mathbf{K}$ varies*].

The eigenfunctions of $H(\mathbf{K}_0)$ form an orthonormal set of states $|m,\mathbf{K}_0)$ which can be defined by their components $(\mathbf{p}|m,\mathbf{K}_0)$. This set is assumed to be complete.

In the following, we use simplified notations:

$$\sum_{\mathbf{p}}\cdots\equiv\lim_{p_0\to\infty}\sum_{|\mathbf{p}|<p_0}\cdots, \quad \text{(AV.1)}$$

$$\sum_{m}\cdots\equiv\lim_{E\to\infty}\sum_{E(m,\mathbf{K}_0)<E}. \quad \text{(AV.2)}$$

Consequently, the orthonormalization conditions can be written

$$\sum_{\mathbf{p}}(m',\mathbf{K}_0|\mathbf{p})(\mathbf{p}|m,\mathbf{K}_0)=\delta_{mm'}, \quad \text{(AV.3)}$$

and the completeness assumption is equivalent to the relations

$$\sum_{m}(\mathbf{p}|m,\mathbf{K}_0)(m,\mathbf{K}_0|\mathbf{q})=\delta_{\mathbf{pq}}. \quad \text{(AV.4)}$$

On the other hand, we consider states $|l,\mathbf{K})$ which are eigengunctions of $H(\mathbf{K})$. The energies $E(l,\mathbf{K})$ are assumed to be bounded. The states $|l,\mathbf{K})$ are determined by their components $(\mathbf{p}|l,\mathbf{K})$ and, by definition, these components satisfy the conditions of Sec. IID and Appendix I, namely:

$$|(\mathbf{p}|l,\mathbf{K})|<C \quad \text{(AV.5)}$$

$$p^{n+1-\eta}|(\mathbf{p}|l,\mathbf{K})|<C(\eta) \quad 1>\eta>0. \quad \text{(AV.6)}$$

We want to show that it is possible to associate with each arbitrary positive number ϵ a finite number $E_0(\epsilon)$ independent of l and $\mathbf{K}$ possessing the following properties: for any number E bigger than $E_0(\epsilon)$, we have

$$|(\mathbf{p}|l,\mathbf{K})-\sum_{E(m,\mathbf{K}_0)<E}(\mathbf{p}|m,\mathbf{K}_0)(m,\mathbf{K}_0|l,\mathbf{K})|<\epsilon. \quad \text{(AV.7)}$$

First, we can prove the weaker relation,

$$(\mathbf{p}|l,\mathbf{K})=\sum_{m}(\mathbf{p}|m,\mathbf{K}_0)(m,\mathbf{K}_0|l,\mathbf{K}). \quad \text{(AV.8)}$$

By definition we have

$$\sum_{m}(\mathbf{p}|m,\mathbf{K}_0)(m,\mathbf{K}_0|l,\mathbf{K}) \equiv\sum_{m}(\mathbf{p}|m,\mathbf{K}_0)\sum_{\mathbf{q}}(m,\mathbf{K}_0|\mathbf{q})(\mathbf{q}|l,\mathbf{K}). \quad \text{(AV.9)}$$

By changing the order of summation, and by taking Eq. (AV.4) into account, we get

$$\begin{aligned}\sum_{m}(\mathbf{p}|m,\mathbf{K}_0)(m,\mathbf{K}_0|l,\mathbf{K}) &=\sum_{\mathbf{q}}(\mathbf{q}|l,\mathbf{K})\sum_{m}(\mathbf{p}|m,\mathbf{K}_0)(m,\mathbf{K}_0|\mathbf{q})\\ &=\sum_{\mathbf{q}}\delta_{\mathbf{pq}}(\mathbf{q}|l,\mathbf{K})=(\mathbf{p}|l,\mathbf{K}). \quad \text{(AV.10)}\end{aligned}$$

This is the result which we want to prove but we have to establish the validity of the change in the order of summation, by showing that the double sum on the right-hand side of Eq. (AV.9) is absolutely convergent. By using the Schwartz inequality, we can write

$$\begin{aligned}\sum_{m\mathbf{q}}|(\mathbf{p}|m,\mathbf{K}_0)||(m,\mathbf{K}_0|\mathbf{q})||(\mathbf{q}|l,\mathbf{K})| &\leq[\sum_{m\mathbf{q}}|(m,\mathbf{K}_0|\mathbf{q})|^2(q+a)^{-(n+\frac{1}{2})}\\ &\times\sum_{m'}|(\mathbf{p}|m',\mathbf{K}_0)|^2\sum_{\mathbf{q}'}|(\mathbf{q}'|l,\mathbf{K})|^2(q'+a)^{n+\frac{1}{2}}]^{1/2}. \quad \text{(AV.11)}\end{aligned}$$

Let us show that the terms which appear in the right-hand side are bounded; here a is just an arbitrary positive constant which is introduced to insure the convergence of the sums for small values of $|\mathbf{q}|$,

$$\sum_{m\mathbf{q}}|(m,\mathbf{K}_0|\mathbf{q})|^2(q+a)^{-(n+\frac{1}{2})} =\sum_{\mathbf{q}}(q+a)^{-(n+\frac{1}{2})}=\text{constant}, \quad \text{(AV.12)}$$

$$\sum_{m}|(\mathbf{p}|m,\mathbf{K}_0)|^2=1, \quad \text{(AV.13)}$$

$$\sum_{\mathbf{q}}|(\mathbf{q}|l,\mathbf{K})|^2q^{n+\frac{1}{2}}<D, \quad \text{(AV.14)}$$

where D is a constant independent of $\mathbf{K}$ [see Eq. (AV.6)]. Thus, the double sum of Eq. (AV.11) is bounded and for this reason converges. The double sum of Eq. (AV.9) converges absolutely and therefore the change in the order of the summations is valid. This remark completes the proof of Eq. (AV.7).

Moreover, as $E(l,\mathbf{K})$ remain bounded, by definition, it is easy to show that the convergence of the sum which appears in Eq. (AV.8) is uniform with respect to $\mathbf{K}$. More precisely, we have to establish the validity of Eq. (AV.7). This result can be obtained by majorizing the rest of the series which appears in this inequality; it is sufficient to prove

$$\sum_{\mathbf{q},E(m,\mathbf{K}_0)>E_0(\epsilon)}|(\mathbf{p}|m,\mathbf{K}_0)| \times|(m,\mathbf{K}_0|\mathbf{q})||(\mathbf{q}|l,\mathbf{K})|<\epsilon. \quad \text{(AV.15)}$$

Schwartz inequality can be used as above. The term (AV.14) is the only one which contains $\mathbf{K}$ and its upper bound is independent of $\mathbf{K}$. In the other series (AV.12) and (AV.13), the summations are restricted to the terms for which we have $E(m,\mathbf{K}_0)>E_0$; the corresponding sums converges to zero when E_0 becomes infinite. Therefore, it is always possible to find a number $E_0(\epsilon)$ for which (AV.15) is satisfied. Thus the condition $E>E_0(\epsilon)$ implies the validity of (AV.7).