Dynamics of band electrons in electric and magnetic fields: rigorous justification of the effective Hamiltonians

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Results concerning the rigorous justification of the effective Hamiltonians for band electrons in the presence of weak homogeneous electric and magnetic fields are reviewed. In the electric-field case the existence, in the sense of spectral concentration, of the Stark-Wannier resonances is proved. In the magnetic-field case, the existence of exponentially localized magnetic Wannier functions is established. As a consequence the Peierls-Onsager effective Hamiltonian is obtained.

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CONTENTS

I. Introduction	91
II. Resumé and Discussion of the Results	93
A. Generalities	93
B. The zero-field Hamiltonian	93
C. The electric-field case	94
D. The Stark-Wannier ladder controversy	96
E. The magnetic-field case	98
III. The Zero-Field Hamiltonian	99
IV. The Electric-Field Case	107
A. The deformed-band subspaces	107
B. The one-band Hamiltonian	109
V. The Magnetic-Field Case	112
A. The stability of the spectrum	112
B. The one-band Hamiltonian	114
VI. Other Approaches	121
A. The Stark-Wannier states	121
B. The Peierls-Onsager effective Hamiltonian	122
C. The semiclassical approach	123
D. The Harper equation	123
Appendix	124
References	126

I. INTRODUCTION

The problem of the dynamics of Bloch electrons in the presence of slowly varying external perturbations is as old as the quantum theory of solids. The literature on the subject is enormous, and even at present the subject is very much alive. The reasons are obvious: On the one hand it is very hard to overestimate the importance of the subject for the theory of metals (see, for example, Lifshitz, Azbel, and Kaganov, 1971). Even more, with the advance of modern technologies, more subtle aspects of the physics involved are coming to light experimentally, such as the confirmation of the Stark-Wannier levels in superlattice devices (Voisin *et al.*, 1988) and the proposal to use the "Bloch-Zener oscillator" as a source of terahertz electromagnetic radiation (Esaki and Tsu, 1970; Roblin and Muller, 1986). On the other hand, due to the fact that the perturbation created by a homogeneous electric or magnetic field is a singular one, the problem is subtle from the mathematical point of view. Accordingly, rigorous results are hard to come by, and if the matter is not handled with sufficient care unclear or even erroneous statements arise. This explains why some central points of the theory, such as the justification of the "Peierls-Onsager effective Hamiltonian" and the existence of the Stark-Wannier states, have remained unsettled and debated until very recently.

The simplest way to deal with the dynamics of Bloch electrons in the presence of external electromagnetic fields is to use the heuristics of the "generalized effective mass approximation." The basic assumption is that, in the presence of weak and slowly varying external fields, the electrons in crystals behave like free electrons but have their inertial properties changed by the presence of the periodic crystal potential. This amounts to the replacement of the usual parabolic relation between the momentum and the energy by the energy band $\lambda(\mathbf{p})$ of the crystal considered. If the external fields are described by the vector and scalar potentials $\mathbf{A}(\mathbf{x})$ and $\phi(\mathbf{x})$, respectively, then the classical Hamiltonian, according to the usual rules, is

$$\lambda\left[\mathbf{p}-\frac{e}{c}\mathbf{A}\right]+e\phi\ . \tag{1.1}$$

For the homogeneous magnetic-field case, $\phi\equiv 0$, $\mathbf{A}(\mathbf{x})==B\wedge\mathbf{x}/2$, the Hamiltonian (1.1) known as the Peierls-Onsager effective Hamiltonian, properly quantized and used in the weak-field limit, has met with fabulous success in describing the properties of metals in the presence of magnetic fields (Lifshitz *et al.*, 1971). The use of Eq. (1.1) in the homogeneous electric field case $\mathbf{A}=0$, $\phi(\mathbf{x})=\mathbf{E}\cdot\mathbf{x}$ leads to somewhat paradoxical, at least at first glance, behavior of the Bloch electrons (oscillatory rather than uniformly accelerated motion), and this triggered a long-term debate about the validity of Eq. (1.1) in this case. The point is that the Hamiltonian (1.1) is at best an approximation, whose justification and range of validity need to be carefully studied.

At a more basic level the quantum-mechanical Hamiltonian of the problem is

$$\frac{1}{2m}\left[\mathbf{P}-\frac{e}{c}\mathbf{A}(\mathbf{x})\right]^2+V(\mathbf{x})+e\phi(\mathbf{x})\ , \tag{1.2}$$

where as before $\mathbf{A}(\mathbf{x})$, $\phi(\mathbf{x})$ stand for the potentials of the external fields and $V(\mathbf{x})$ stands for the crystal potential.

At this point the following remark is in order. We shall describe many rigorous results concerning (1.2) and use the word "rigorous" advisedly. One should keep in mind that the whole theory is based on the one-electron approximation; in this approximation the medium appears as a static potential and, in particular, there is no electron-phonon interaction. The word "rigorous" is to be understood in terms of this theoretical framework.

From the theoretical point of view the main problem is to relate Eqs. (1.1) and (1.2) or, in others words, to decide to what extent and under what conditions (1.1) is a reasonable approximation of (1.2). It is quite difficult to give a complete list of all relevant papers dealing with the problem of deriving (1.1) from (1.2). For the early period we just mention a few reviews (Wannier, 1962; Blount, 1962a; Zak, 1972; Fischbeck, 1977) where complete lists of references as well as extended discussions on the subject can be found. In spite of all this considerable effort, mainly due to the mathematical difficulties, the justification of the Peierls-Onsager Hamiltonian

$$\lambda\left[\mathbf{P}-\frac{e}{c}\mathbf{A}\right]$$

was considered even recently (Obermair and Schellenhuber, 1981) "one of the few unsolved problems of one-particle quantum mechanics." Similarly the main consequence of Eq. (1.1) in the electric-field case, namely, the existence of the Stark-Wannier ladder of states, has been debated over a period of almost three decades and even now there is a constant flow of papers on this very topic.

The aim of this paper is to review some of the rigorous results concerning the spectral properties of Eq. (1.2) obtained during the last decade, leading to a rigorous justification of Eq. (1.1) under appropriate conditions. Since in most cases of physical interest the external fields are much smaller than the internal fields, the natural approach to a study of the spectral properties of (1.2) is the use of perturbation theory. One should stress, however, that there are some very important phenomena, such as the quantum Hall effect, electric and magnetic breakdown, etc., which are beyond the reach of perturbation theory and consequently will be not covered by the theory presented in this review.

Unfortunately, as already mentioned above, the perturbations created by homogeneous fields are singular, and the naive perturbation theory cannot be used. For a better understanding let us consider the situation for the simpler case of the atomic Stark and Zeeman effects. Although the Stark and Zeeman effects were the first examples of quantum-mechanical perturbation theory, it has taken half a century to develop a satisfactory mathematical description (see the references in Hunziker, 1980, 1988, Herbst, 1981, and Nenciu, 1981). Actually, asymptotic perturbation theory, as beautifully reviewed in Hunziker (1988), has been largely motivated by the Stark and Zeeman effects in atomic physics (the other major source was the anharmonic oscillator). Unfortunately, as it stands, the theory in Hunziker (1988) can be applied only to finitely degenerate isolated eigenvalues having localized eigenfunctions, while for the problem at hand a theory powerful enough to cope with infinite-dimensional subspaces corresponding to energy bands and spanned by delocalized Bloch functions is needed. In this context Howland (1981) posed the question whether the theory of spectral concentration could be generalized to cover the analog of the Stark effect in solid-state physics (see also the discussion about the "physical stability" of the bands in Avron and Zak, 1974). The theory in Nenciu (1981) gives a positive answer to this question. Concerning the magnetic field it should also be mentioned that even for the most basic questions, such as the stability of matter, it adds one more level of difficulty (Fröhlich, Lieb, and Loss, 1986; Lieb and Loss, 1986; Loss and Yau, 1986).

Let us make a little more precise the meaning of the "effective band Hamiltonian" as it will be used in the present review. Let H be the "true" Hamiltonian at hand [(1.2) in our case] acting in the Hilbert space $\mathcal{H}$. Suppose there exists a subspace $\mathcal{K}\subset\mathcal{H}$ invariant under H (i.e., H is block diagonal with respect to the decomposition $\mathcal{H}=\mathcal{K}\oplus\mathcal{K}^{\perp}$) such that, if P is the orthogonal projection on the states in $\mathcal{K}$, PHP is the unitary equivalent with a simpler Hamiltonian in another space $\mathcal{L}$, i.e., there exist $U:\mathcal{K}\rightarrow\mathcal{L}$ such that $UPHPU^{-1}:\mathcal{L}\rightarrow\mathcal{L}$ is either exactly soluble or at least, from the physical point of view, has a simple and transparent, form amenable to a detailed analytical or numerical study. Then $UPHPU^{-1}$ is called an effective Hamiltonian. In solid-state physics the name "one-band effective Hamiltonian" is used due to the fact that $\mathcal{K}$ is usually related to the subspace of states corresponding to an isolated energy band of the zero-field Hamiltonian. Unfortunately such an exact reduction is very rarely possible, and some kind of perturbation scheme needs to be used in which the true Hamiltonian H_ε depends on a small parameter ε (the magnitudes of the external fields in our case), $\mathcal{K}_\varepsilon$ can also depend on ε, and H_ε is not exactly block diagonal but the off-diagonal part $P_\varepsilon H_\varepsilon(1-P_\varepsilon)+\mathrm{H.c.}$ of H_ε is sufficiently small as $\varepsilon\rightarrow 0$. Of course the last requirement needs to be made precise in specific cases. Let us point out that the use of "effective Hamiltonians" in the sense described above is not specific to solid-state physics. Other famous examples are the Born-Oppenheimer approximation in atomic physics and the Bohr-Mottelson collective Hamiltonian in nuclear physics. While a rigorous justification of the Born-Oppenheimer vibrational-rotational Hamiltonian for biatomic molecules has been achieved during the last two decades (Combes *et al.*, 1981; Hagedorn, 1988), the similar problem of the Bohr-Mottelson Hamiltonian seems to be open.

For the problem at hand the first choice for $\mathcal{K}$ was the band subspace corresponding to an isolated energy band of the zero-field Hamiltonian. It was soon realized that this choice was not appropriate. Indeed, for the electric-field case the neglected off-diagonal matrix elements are linear in the field strength, i.e., of the same magnitude as the spacing between the Stark-Wannier levels. As for the magnetic-field case, the matrix elements of Eq. (1.2) restricted to the zero-field band subspace do not have the right structure to produce an effective Hamiltonian resembling (1.1). The problems to be solved are the following (ε stands for the external field strength):

(E1) The identification of the "band subspace" $\mathcal{K}_\varepsilon$.

(E2) The estimation of the off-diagonal term $P_\varepsilon H_\varepsilon(1-P_\varepsilon)+\mathrm{H.c.}$.

(E3) The identification of $\mathcal{L}$ (which *should not* depend on ε) and U_ε.

(E4) The computation of $H_{\varepsilon,\mathrm{eff}}$.

(E5). The spectral analysis of $H_{\varepsilon,\mathrm{eff}}$.

In this review we shall describe rigorous results, obtained during the last decade, concerning problems (E1)–(E5) above the case in which the "true" Hamiltonian is Eq. (1.2). The results below are proved for the case in which only electric *or* magnetic fields are present. Rigorous results when *both* electric and magnetic fields are present have not been obtained (to the best of our knowledge) so far. The starting point for almost all rigorous results and their proofs is the heuristics put forward in the physical literature on the subject. This review is in some sense the updated rigorous counterpart of the beautiful review by Wannier (1962) embodying earlier ideas of Peierls (1933), Luttinger (1951), Adams (1957), Onsager (1952), Kohn (1959b), and Wannier (1937, 1960), to name only a few. For (E1) and (E2) the periodicity of $V(\mathbf{x})$ is not used, so the results obtained are valid for nonperiodic systems as well.

The content of the paper is as follows. For readers not interested in the mathematical aspects, we give in Sec. II a resumé of the main results. In the same section we also discuss the controversy over the existence of the Stark-Wannier ladders of states (see also Avron, 1982; Krieger and Iafrate, 1988). The topic is still in a confused state; unclear or even erroneous claims appear, and sometimes it is concluded that the whole matter ought to be thoroughly reviewed (Churchill and Holmstrom, 1983). Section III contains proofs of some results on the zero-field Hamiltonian $H_0=\mathbf{P}^2+V(\mathbf{x})$. The main result is the existence of exponentially localized Wannier functions. There are two reasons for a full-scale discussion of this topic. The first is that the Wannier functions played a central role in most earlier attempts to derive the effective Hamiltonians [recall that the textbook presentation of the subject (Lifshitz *et al.*, 1971; Ziman, 1964) is via the "Wannier theorem" and that the first rigorous proof of the existence of the exponentially localized Wannier functions (Kohn, 1959a) for one-dimensional systems was an explicit attempt to provide justification for the Peierls-Onsager Hamiltonian (Kohn, 1959b), and the same Wannier functions are central to the recent rigorous developments (Béllissard, 1987, 1988; Nenciu, 1989; Helffer and Sjostrand, 1989a, 1989b). The second reason is that, contrary to the superficial widespread impression, the matter is far from being trivial and has never been reviewed thoroughly. Section IV contains the derivation of the effective Hamiltonian for the electric field case. Section V treats the magnetic field case.

As stated above, the literature on the dynamics of Bloch electrons in external fields is enormous. Moreover, due to the mathematical difficulties, many techniques have been used. As a consequence it seems almost impossible to cover in detail all the significant results. However, in Sec. VI we shall comment briefly on other approaches. A few important technical points of more general character are given in the Appendix.

II. RESUMÉ AND DISCUSSION OF THE RESULTS

A. Generalities

As already mentioned in the Introduction we shall give here a nontechnical resumé of the main results. We shall consider only one- and three-dimensional systems, so that in what follows $n\leq 3$. To simplify notation, the system of units in which $\hbar=2m=c=1$ is used. Moreover, the electron charge will be absorbed in the definition of the field strength. If not explicitly stated $V(\mathbf{x})$ will not be supposed to be periodic. The only technical condition (besides its reality) on $V(\mathbf{x})$ is that

$$\sup_{\mathbf{x}_0\in\mathbb{R}^n}\int_{|\mathbf{x}-\mathbf{x}_0|\leq 1}|V(\mathbf{x})|^2 d\mathbf{x}<\infty \ . \tag{2.1}$$

Concerning the zero-field Hamiltonian $H_0=-\Delta+V(\mathbf{x})$, we assume, as is crucial for all that follows, that it has a bounded isolated energy band σ_0. In what follows $\mathcal{K}_0$ stands for the band subspace corresponding to σ_0 and P_0 for the orthogonal projection on $\mathcal{K}_0$. In order not to obscure the main ideas, in this section we shall confine ourselves to some particular cases: one-dimensional systems in the electric case and simple bands in the magnetic case.

B. The zero-field Hamiltonian

As stressed above the answers to problems (E1) and (E2) in the Introduction depend on the existence of the energy gaps and not on the periodicity of the potential. Usually the existence of the energy gaps is related to the periodicity of the potential. While for completely disordered systems one cannot expect to have forbidden gaps, they still can exist if short-range order is present. The following result (Nenciu and Nenciu, 1981a) gives an example. Suppose H_0, with $V(\mathbf{x})$ periodic, has an energy gap. Let $\mathbf{y}(\mathbf{x})=\mathbf{x}+\delta\mathbf{h}(\mathbf{x})$ where $\mathbf{h}(\mathbf{x})$ is a vector-valued function with bounded partial derivatives up to the order 3. Then for δ positive and sufficiently small $-\Delta+V(\mathbf{y}(\mathbf{x}))$ still has an energy gap.

The steps (E3)–(E5) in obtaining and analyzing the effective Hamiltonians depend on the periodicity of $V(\mathbf{x})$. Suppose that $V(\mathbf{x})$ is periodic with respect to a Bravais lattice Γ. Let σ_0 be a simple band: $\sigma_0=\{\lambda_0(\mathbf{k})\}$ where

$\lambda_0(\mathbf{k})$ is a nondegenerate (for all $\mathbf{k}$) eigenvalue of H_0. Let $\psi_{0,\mathbf{k}}(\mathbf{x})$ be the Bloch functions corresponding to the band σ_0. The Wannier functions $w_{\mathbf{a}}(\mathbf{x})$ are defined as the Fourier coefficients of $\psi_{0,\mathbf{k}}(\mathbf{x})$ (for a more complete elementary discussion see Weinreich, 1965):

$$w_{\mathbf{a}}(\mathbf{x})=\int \psi_{0,\mathbf{k}}(\mathbf{x})\exp(-i\mathbf{k}\cdot\mathbf{a})d\mathbf{k} ,$$

where the integration extends over the Brillouin zone. Due to the orthonormalization of the Bloch functions and the fact that

$$\psi_{0,\mathbf{k}}(\mathbf{x}-\mathbf{a})=\psi_{0,\mathbf{k}}(\mathbf{x})\exp(-i\mathbf{k}\cdot\mathbf{a}) ,$$

one can verify at once that (as long as $w_{\mathbf{a}}$ are normalizable)

$$w_{\mathbf{a}}(\mathbf{x})=w_0(\mathbf{x}-\mathbf{a}) , \quad \int_{\mathbb{R}^n}\overline{w_{\mathbf{a}}(\mathbf{x})}w_{\mathbf{b}}(\mathbf{x})d\mathbf{x}=\delta_{\alpha,\beta} .$$

Suppose now that $\psi_{0,\mathbf{k}}$ are *differentiable and periodic* as functions of $\mathbf{k}$. Then by integration by parts, from the very definition, it follows that as $|\mathbf{a}|\to\infty$

$$w_{\mathbf{a}}(\mathbf{x})=w_0(\mathbf{x}-\mathbf{a})\sim 1/|\mathbf{a}|^n$$

for any natural number n, which means that $w_0(\mathbf{x})$ falls off faster than any power of $1/|\mathbf{x}|$. Moreover, if $\psi_{0,\mathbf{k}}(\mathbf{x})$ are analytic and periodic in $\mathbf{k}$ in a complex neighborhood of $\mathbb{R}^n$, then by a famous theorem of Paley and Wiener (see, e.g., des Cloizeaux, 1964) $w_0(\mathbf{x})$ falls off exponentially. At first sight one can believe that the existence of smooth and periodic Bloch functions is an easy matter. Unfortunately this is not so, and the difficulties are of the topological origin. The basic fact we shall prove in Sec. III is the existence of Bloch functions analytic and periodic with respect to $\mathbf{k}$ in a complex neighborhood of $\mathbb{R}^n$. As a consequence the corresponding Wannier functions are exponentially localized and form an orthonormal basis in the band subspace corresponding to σ_0. Note that $w_0(\mathbf{x})$ is not uniquely defined due to the fact that the analyticity and periodicity requirements fix $\psi_{0,\mathbf{k}}(\mathbf{x})$ only up to an analytic and periodic phase factor. The Wannier functions constructed in Sec. III are real and if the crystal has a center of inversion then, in addition, $w_0(-\mathbf{x})=\pm w_0(\mathbf{x}-\mathbf{a}_0)$ for an appropriately chosen $\mathbf{a}_0\in\Gamma$. Actually one can show that, without restricting the generality, one can consider only the case $\mathbf{a}_0=0$. By a direct computation one can see that, in the Wannier basis $\{w_{\mathbf{a}}\}_{\mathbf{a}\in\Gamma}$, H_0 takes a "tight-binding-approximation" form

$$H_0 w_{\mathbf{a}}=\sum_{\mathbf{b}\in\Gamma} h_0(\mathbf{a}-\mathbf{b})w_{\mathbf{b}} ,$$

where $h_0(\mathbf{a})$ are the Fourier coefficients of $\lambda_0(\mathbf{k})$. This leads to the fact that H_0, restricted to the band subspace corresponding to σ_0, is unitary equivalent to the following operator in $l^2(\Gamma)$:

$$H_{0,\mathrm{eff}}f(\mathbf{a})=\sum_{\mathbf{b}\in\Gamma} h_0(\mathbf{b}-\mathbf{a})f(\mathbf{b}) . \tag{2.2}$$

C. The electric-field case

As already said, we consider here only one-dimensional systems and homogeneous fields. The field strength (with the electron charge absorbed) is denoted by F. For the available electric fields F is very small: $F<10^{-12}$ J m^{-1}. The Hamiltonian is

$$H_F=-d^2/dx^2+V(x)+Fx\equiv H_0+FX_0 .$$

In spite of the smallness of F, the electric potential FX_0 diverges as $|x|\to\infty$ so that one cannot consider FX_0 as a small perturbation in the usual sense: we have to deal with a *singular* perturbation. The singularity of the perturbation manifests itself in the fact that it completely changes the spectrum of H_0: as far as $F\to 0$ the spectrum of H_F is absolutely continuous and fills the entire real axis (Avron *et al.* 1977; Reed and Simon 1978). Let us stress that absolute continuity of spectrum has a clear cut mathematical meaning; in particular, it excludes the existence of eigenvalues with square integrable eigenfunctions. In other words, all the eigenstates of H_F are extended. The fact that there are no gaps in the spectrum of H_F makes the identification of the band subspace for nonzero fields a difficult matter. At the heuristic level the way out from this difficulty was indicated a long time ago by Adams (1957), Kane (1959), and especially by Wannier (1960): in the presence of the electric field, the band subspace $\mathcal{K}_0$ corresponding to the band σ_0 of the zero-field Hamiltonian is slightly "deformed" to a field-dependent band subspace $\mathcal{K}_\varepsilon$, which is to be found by some perturbation scheme. Note that according to this heuristics, while the behavior of the spectrum is pathological in the limit $F\to 0$, the behavior of the band subspaces is smooth. The result below (Nenciu and Nenciu 1981b) substantiates these ideas.

Consider the off-diagonal part of H_ε with respect to the decomposition $\mathcal{K}_0\oplus\mathcal{K}_0^\perp$

$$FB_0\equiv P_0H_F(1-P_0)+\mathrm{H.c.}=FP_0X_0(1-P_0)+\mathrm{H.c.}$$
$$=F(1-2P_0)[X_0,P_0] .$$

Under the provision that B_0 is bounded, consider

$$H_1=H_0+FB_0 . \tag{2.3}$$

For sufficiently small F, H_1 still has an isolated energy band σ_1 which coincides with σ_0 in the limit $F\to 0$. $\mathcal{K}_1$ and P_1 stand for the energy band subspace and the spectral projection of H_1 corresponding to σ_1. Define

$$X_1=X_0-B_0 . \tag{2.4}$$

By construction

$$H_F=H_1+FX_1 , \quad [H_F-FB_0,P_0]=0 .$$

Continue the procedure by defining

$$B_1=(1-2P_1)[X_1,P_1] , \tag{2.5}$$

etc. At the qth step

$$B_q=(1-2P_q)[X_q,P_q] , \tag{2.6}$$

$$H_{q+1}=H_q+FB_q , \quad X_{q+1}=X_q-B_q . \tag{2.7}$$

Note that since FB_q is the nondiagonal part of H_F with respect to the band subspaces of H_q,

$$[H_F-FB_q,P_q]=0 . \tag{2.8}$$

The main fact about this recurrent construction is that B_q are of order F^q. More exactly, *for every* $q=1,2,\ldots$ *there exists* $b_q<\infty$, $F_q>0$ *such that*

$$\|B_q\|\le F^q b_q \quad \text{for } 0<F<F_q . \tag{2.9}$$

In other words, with respect to the decomposition $\mathcal{K}_q\oplus\mathcal{K}_q^{\perp}$, the off-diagonal part of H_F is of order F^{q+1}. From the physical point of view, in order to decide whether or not an effect can be seen experimentally, estimations of F_q, b_q are necessary. The proof in Nenciu and Nenciu (1981b) gives the means to estimate F_q and b_q. For example, the estimations (Nenciu, 1987) for the case when the potential $V(\mathbf{x})$ satisfies $|V(\mathbf{x})|\le 200$ eV, and the width of the energy gap is 4 eV, lead to

$$\begin{aligned} &b_0=3\times10^{-9}\ \mathrm{m}\ (\simeq 10^2 a_H) \text{ independently of } F ,\\ &E_1=e^{-1}F_1=6\times10^8\ \mathrm{V\,m^{-1}} ,\\ &b_1=80\ \mathrm{m^2J^{-1}}\ (\simeq 10^5 a_H^2/R_\infty) ,\\ &E_2=e^{-1}F_2=3\times10^7\ \mathrm{V\,m^{-1}} ,\\ &b_2=5\times10^{12}\ \mathrm{m^3J^{-2}}\ (\simeq 10^8 a_H^3/R_\infty^2) . \end{aligned} \tag{2.10}$$

We shall use these estimations when discussing the existence of the Stark-Wannier levels in the next subsection. As the limit $q\to\infty$ is concerned, due to the singularity of the perturbation, the recurrence procedure given above is not convergent but only asymptotic. More exactly, as $q\to\infty$, $F_q\to0$ and b_q diverges (probably as $q!$). So one cannot take the limit $q\to\infty$ and obtain for $F\neq0$ a "closed"-band subspace (i.e., a band subspace with respect to which the off-diagonal part of H_F is rigorously zero).

The next step is to analyze the one-band Hamiltonian of order q, defined as

$$H^q_{F,\mathrm{ob}}=P_qH_FP_q . \tag{2.11}$$

Consider first the periodic case $[V,T_a]=0$, where T_a is the translation operator. In this case

$$[H_q,T_a]=0 , \ [X_q,T_a]=aT_a \tag{2.12}$$

and moreover the spectral properties of H_q are similar to those of H_0. In particular, $\sigma_q=\{\lambda^q_F(k)\}$ where $\lambda^q_F(k)$ has an analytic and periodic extension to a complex neighborhood of the real axis. Moreover the phase factor in the Bloch functions $\psi^q_{F,k}$ corresponding to $\lambda^q(k)$ can be chosen as to make $\psi^q_{F,k}$ analytic and periodic in a complex neighborhood of the real axis. Writing $H^q_{F,\mathrm{ob}}$ in the basis $\psi^q_{F,k}$ one obtains the following form of the effective one-band Hamiltonian:

$$\mathcal{L}=L^2[\tfrac12,\tfrac12]=\left\{f(k)\,\middle|\,\int_{-1/2}^{1/2}|f(k)|^2dk\le\infty\right\} \tag{2.13}$$

and $H^q_{F,\mathrm{ob}}$ is unitary equivalent to

$$H^q_{F,\mathrm{eff}}=(-iFa_1/2\pi)(d/dk)_{\mathrm{per}}+Y^q_F(k) , \tag{2.14}$$

acting on functions $f(k)\in\mathcal{L}$ satisfying

$$(d/dk)f(k)\in\mathcal{L} \quad\text{and}\quad f(-\tfrac12)=f(\tfrac12) .$$

The function $Y^q_F(k)$ is the restriction to $[-\frac12,\frac12]$ of a function analytic and periodic with period 1 in a complex neighborhood of the real axis.

By Fourier representation, one can obtain the "Wannier representation" of the one-band Hamiltonian (Haker and Obermair, 1970). In this case

$$\mathcal{L}=l^2(\Gamma)=\left\{f_a\,\middle|\,\sum_{a\in\Gamma}|f_a|^2<\infty\right\} \tag{2.15}$$

and $H^q_{F,\mathrm{ob}}$ is unitary equivalent to

$$(H^{q,W}_{F,\mathrm{eff}}f)_a=\sum_{b\in\Gamma}\lambda^q_{F,a-b}f_b+Faf_a , \tag{2.16}$$

where $\lambda^q_{F,a}$ are the Fourier coefficients of $\lambda^q_F(k)$

The Hamiltonian (2.14) is "exactly soluble." Actually, via the "gauge transformation" (Avron, 1979)

$$(Gf)(k)=\exp\left[\frac{-iF2\pi}{a_1}\int_{-1/2}^{k}[Y^q_F(h)-c^q_F]dh\right] , \tag{2.17}$$

where

$$c^q_F=\int_{-1/2}^{1/2}Y^q_F(h)dh ,$$

(2.14) is unitary equivalent to

$$(-iFa_1/2\pi)(d/dk)_{\mathrm{per}}+c^q_F ; \tag{2.18}$$

i.e., up to an additive constant, (2.14) is unitary equivalent with the free motion on a circle with radius $1/2\pi$. It follows that the motion is periodic in time with the period $T=2\pi/Fa_1$, and the spectrum of $H^q_{F,\mathrm{ob}}$ is

$$\sigma(H^q_{F,\mathrm{ob}})=\{nFa_1+c^q_F\} , \quad n=0,\pm1,\pm2,\ldots . \tag{2.19}$$

The eigenfunctions $\psi^q_{F,n}$ of H^q_F are exponentially localized (Haker and Obermair, 1970; Nenciu and Nenciu, 1982). The spectrum (2.19) is the famous Stark-Wannier ladder. Note that the spectra of $H^q_{F,\mathrm{ob}}$, for different q, are the same up to a q-dependent shift.

As is well known (Lifshitz *et al.*, 1971; Blound, 1962a), the Wannier representation (2.16) is related to (1.1). More exactly, it is assumed that f_a is a "smooth" function of a and then f_a can be interpolated by a sufficiently smooth function $f(\mathbf{x})$. Then, since at the formal level

$$f(a-b)=[\exp(-iPb)f](a) ,$$

one obtains from (2.16) the following expression:

$$[\lambda^q_F(P)f](\mathbf{x})+Fxf(x) \tag{2.20}$$

which is nothing but (1.1) with $\mathbf{A}(\mathbf{x})=0$. Note that the passage from (2.16) to (2.20) is largely uncontrolled. First of all the Hilbert space has been changed and, in addition, the error introduced by the interpolation of the wave function and of the electric potential can be large. Actually, by a Fourier and a gauge transformation, (2.20) is unitary equivalent to $-iF(d/dk)$ on the whole real axis, whose spectrum is the whole real axis instead of (2.19). So, although reasonable at the first sight, the interpolation scheme leads to qualitative differences.

The results above about $H^q_{F,\mathrm{ob}}$ rely heavily on the periodicity of $V(\mathbf{x})$. It is a natural question what can be said in the general nonperiodic case. The answer is that (Soukoulis *et al.*, 1983; Delyon *et al.*, 1984; José *et al.*, 1985; Bentosela *et al.*, 1985; Bentosela *et al.*, 1983; Cota *et al.*, 1986; Nenciu and Nenciu, 1989) for a large class of nonperiodic systems the spectrum of $H^q_{F,\mathrm{ob}}$ is discrete, i.e., consists of at most finitely degenerate eigenvalues accumulating only at $\pm\infty$.

D. The Stark-Wannier ladder controversy

It was realized very early that the use of the effective Hamiltonian (1.1) in the case of homogeneous electric field leads to an oscillatory motion in the $\mathbf{x}$ space (Zener, 1943; Lifshitz *et al.*, 1959). Moreover, if λ belongs to the spectrum of H_F, then due to the commutation relation $[H_F,T_a]=FaT_a$, $\lambda+Fan, n=0,\pm1,\pm2,\ldots$, also belong to the spectrum of H_F. In other words the spectrum of H_F has a ladder structure. The real story started with the remark by Wannier (1960, 1962) that if H_F has closed-band subspaces then H_F has ladders of eigenvalues with square integrable eigenfunctions. Callaway (1963) wrote down the Stark-Wannier ladders in the approximation that the transitions between different zero-field band subspaces are neglected and suggested that the ladder structure can be seen experimentally in direct optical transitions. Since the only approximation in the Callaway computation was the neglect of the interband transitions, apart from some misunderstandings of purely technical character, the real controversial point was whether the Stark-Wannier ladder survives with the inclusion of the interband matrix elements. The survival of the ladder structure was questioned mainly by Zak (1968, 1969, 1972) (see also Rabinovitch and Zak, 1972). The doubt is well founded since *both* the spacing between levels and the neglected matrix elements are linear in the field strength F. So, as Wannier clearly pointed out, "the central problem is the status of the interband matrix elements." It has been argued by Wannier and Fredkin (1962) and by Wannier (1962) that actually the interband transitions are "nonessential" in the following sense: the band subspaces themselves are deformed by the electric field, and with respect to these field-dependent band subspaces the interband transitions vanish *exactly*. Unfortunately, as pointed out by Zak (1968), there is a subtle error in the Wannier-Fredkin argument. Actually, it is easy to prove by reduction *ad absurdum* that closed band subspaces cannot exist (Zak, 1972; Nenciu and Nenciu, 1981a, 1981b). In short, the existence of closed band subspaces would imply the existence of eigenvalues of H_F with square-integrable eigenfunctions, which contradicts the rigorous results by Avron *et al.* (1977) that all the states of H_F are extended. [Let us stress that this result applies to bounded potentials. For δ-like potentials there is convincing evidence, both analytic and numerical (Berezhkovski and Ovchinnicov, 1976; Bentosela, Grecchi, and Zironi, 1985), that at low fields the eigenstates of H_F are localized.] Let us mention that there are recent claims by Emin and Hart (1987, 1988) that closed band subspaces exist and, even more, that they are easily identified. It is not hard to see that their argument contains an error. Then, as already recognized by Wannier (1969), due to the nonexistence of exactly decoupled bands, Stark-Wannier ladders of eigenvalues do not exist. However, the results presented in the previous subsection lead to the existence of ladders of well defined *resonances.* A word of caution is in order here. As is well known, a unique and precise definition of resonances in quantum mechanics does not exist. Therefore, the existence of the Stark-Wannier resonances should be understood in the sense given below. We shall adopt the attitude that a resonance means a long-lived state.

Let $\lambda^q_{F,n}$ and $\psi^q_{F,n}$ be an eigenvalue and its corresponding eigenfunction of $H^q_{F,\mathrm{ob}}$ [see (2.19) above]. Then, from (2.9) and the time-dependent Schrödinger equation,

$$|(\psi^q_{F,n},\exp(-iH_Ft)\psi^q_{F,n})|\geq 1-b_qF^{q+1}|t| \ , \qquad (2.21)$$

which shows that at low fields $\psi^q_{F,n}$ is a metastable state. If the oscillatory motion is to be observed experimentally, the lifetime of $\psi^q_{F,n}$ must be at least a few times larger than the period $T=2\pi/Fa_1$. This imposes the condition

$$b_qF^{q+1}T=(2\pi/a_1)b_qF^q \ll 1 \ . \qquad (2.22)$$

From (2.10), for a lattice constant $a_1=5\times10^{-10}$ m, one obtains for $q=1$

$$(2\pi/a_1)b_2F^2<10^{12}\ F\,\mathrm{m/J} \ , \qquad (2.23)$$

which shows that the lifetime of $\psi^q_{F,n}$ is larger than T, at least up to fields of order 10^6 V/m. This is really important from the experimental point of view since one expects to observe the ladder structure only at rather high fields; at low fields the period of the oscillatory motion is larger than the lifetime, due to the scattering on phonons, impurities etc., so that the ladder structure is washed out by effects not considered in the present theory. Actually, the situation is much better in semiconductor superlattices, where a_1 is much larger, so that the period T of the oscillatory motion is much smaller. This explains why recently the Stark-Wannier states have been seen in semiconductor superlattices (Voisin *et al.*, 1988).

Alternatively, if following Avron *et al.* (1975) we take

$$\gamma^2=\langle(H_F-\lambda^q_{F,n})\psi^q_{F,n},(H_F-\lambda^q_{F,n})\psi^q_{F,n})\rangle$$

as the measure of the width of the resonance, then, due to

(2.8), (2.9), and (2.10), for $q=1$

$$\gamma \le b_1 F^2 < 80F^2 ,$$

which is smaller than the spacing $a_1 F$ up to the fields of order 10^6 V/m.

The rest of this subsection is devoted to the discussion of some other aspects of the dynamics of the Bloch electrons in electric fields related to the Stark-Wannier ladder controversy. Let us start with the questions related to the use of the vector potential to describe the electric field (Kittel, 1964; Nenciu and Nenciu, 1980; Krieger and Iafrate, 1986, 1988; Zak, 1968). The first remark is that the use of the time-dependent vector potential leads to an easy proof of the acceleration theorem (Kittel, 1964; Nenciu and Nenciu, 1980). For another nice proof of the acceleration theorem using the kq representation, see Zak (1972). Consider the subspaces

$$\mathcal{H}_k = \{ f(x) | f(x) = \exp(ik\cdot x) u(x) , \quad u(x) = u(x+a) \} .$$

[Actually $\mathcal{H}_k$ are not bona fide subspaces, but fibers in a direct integral decomposition of $L^2(\mathbb{R}^3)$ (Reed and Simon, 1978)]. As is well known, $\mathcal{H}_k = \mathcal{H}_l$ for $|k-l| = 2\pi/a_1$. Consider the evolution $f_t = \exp(-iH_F t) f$ with $f \in \mathcal{H}_k$. Also consider the gauge transformation

$$G(t) = \exp(iFxt) \tag{2.24}$$

and denote $\tilde{f}_t = G(t) f_t$. By a routine calculation (Kittel, 1964),

$$(id/dt)\tilde{f}_t = [(P-Ft)^2 + V(x)]\tilde{f}_t , \quad P = -id/dx . \tag{2.25}$$

As $[(P-Ft)^2 + V, T_a] = 0$, $\tilde{f}_t \in \mathcal{H}_k$ for all t, and one can write

$$(id/dt)\tilde{f}_t = H_{0,k}(Ft)\tilde{f}_t \tag{2.26}$$

where $H_{0,k}(Ft)$ is the restriction of $(P-Ft)^2 + V$ to $\mathcal{H}_k$. Now from the fact that $\tilde{f}_t \in \mathcal{H}_k$, it follows that

$$f_t = \exp(-iFxt)\tilde{f}_t = \exp[i(k-Ft)x] u_t(x) \in \mathcal{H}_{k-Ft} ,$$

which is nothing but the exponentiated form of the acceleration theorem.

The evolution (2.26) has exactly the form to which one can apply the adiabatic theorem of quantum mechanics (Messiah, 1969). Note that the singular term due to the electric-field potential disappeared at the expense of (slow) time dependence. Let $\lambda_j(k)$ be the eigenvalues of $H_{0,k}$, and $\psi_{j,k} = \exp(ikx) u_{j,k}(x)$ the corresponding Bloch functions with some fixed (see the previous subsection) phase factor. The eigenvalues and the eigenvectors of $H_{0,k}(Ft)$ are $\lambda_j(k-Ft)$ and $\exp(ikx) u_{j,k-Ft}(x)$. Let $\{\lambda_0(k)\}$ be an isolated band of H_0 and suppose that, at $t=0$, $f_0 = \psi_{0,k}$. Then, by the adiabatic theorem of quantum mechanics, in the limit of weak fields

$$\tilde{f}_t = \exp\left[-i \int_0^t \lambda_0(k-Fs) ds \right] \times \exp[-i\phi(t)] \exp(ikx) u_{0,k-Ft}(x) + O(F + F^2 t) ,$$

whereof

$$f_t = \exp\left[-i \int_0^t \lambda_0(k-Fs) ds \right] \exp[-i\phi(t)] \psi_{0,k-Ft} + O(F + F^2 t) . \tag{2.27}$$

The phase factor $\phi(t)$ (Berry's phase) is fixed by the condition (Kato, 1950, Simon, 1983)

$$\langle \exp[-i\phi(t)]\psi_{0,k-Ft'}(d/dt)\exp[-i\phi(t)]\psi_{0,k-Ft} \rangle = 0 ,$$

which gives

$$\phi(t) = iF \int_0^t \langle u_{k-Fs'}(d/ds) u_{k-Fs} \rangle ds . \tag{2.28}$$

The evolution f_t with $\phi(t)$ given by (2.28) is nothing but the famous Huston function (Huston, 1940) with the correct phase factor as given by Fritsche (1966) and Zak (1972). Note that the Huston function (2.27) represents accurately the evolution on intervals of time of order F^{-2}. Recent refinements of the adiabatic theorem (Nenciu and Rasche, 1989) provide "deformed" Huston functions that accurately describe the evolution f_t on intervals of time of order F^{-q}, provided F is sufficiently small.

The next remark concerns the free-electron limit (Churchill and Holmstrom, 1981). At the heuristic level the main point was emphasized long ago by Lifshitz and Kaganov (1959): in the free-electron limit the interband transitions become important so that the one-band approximation with all its consequences breaks down. This fact is clearly reflected in the behavior of the constants b_q in the free-electron limit. The dependence of b_q on the width d of the energy gap is $b_q \sim d^{-q}$ (Nenciu, 1987) so that b_q blows up in the free-electron limit, and the control on the interband transitions is lost.

Let us consider now the weak-field limit, $F \to 0$. Strictly speaking, as emphasized many times (Churchill and Holmstrom, 1983; Krieger and Iafrate, 1986), the limit is singular. However, from the physical point of view, nothing pathological happens in this limit. Note that in this limit the period of the oscillatory motion and the spatial extent of the eigenfunctions of the one-band Hamiltonian tend to infinity. On bounded intervals of time and regions in space (which are the interesting ones from the physical point of view) the dynamics at low fields converges smoothly to the zero-field dynamics [see, e.g., Eq. (2.27)].

The rigorous results described in the previous subsection, as well as other rigorous results described in Sec. VI, are obtained for infinite systems. The reason is that on the one hand the methods of modern mathematical physics are powerful enough to cope with continuous spectra, singular perturbations etc., and on the other hand the infinite systems avoid the complications due to the boundary conditions. Let us stress that these complications are especially severe for the problem at hand, due to the fact that the electric-field energy diverges as $|\mathbf{x}| \to \infty$. Actually, a significant part of the Stark-Wannier ladder controversy originates in such technical difficulties (see, e.g., Krieger and Iafrate, 1986, 1988;

Zak, 1968; Churchill and Holmstrom, 1981, 1983).

The motion of Bloch electrons in weak fields is often considered to be "semiclassical." A word of caution is in order here: the use of the word "semiclassical" in this context does not mean $h \to 0$ as usual. Rather (see Sec. VI.C), it indicates that the methods of the semiclassical limit are applied, with the strength of the field in the role of the Planck constant.

To summarize, for bounded potentials the situation is as follows.

(i) Closed bands or equivalently Stark-Wannier eigenvalues do not exist.

(ii) Stark-Wannier resonances do exist for weak fields, provided the zero-field Hamiltonian has isolated bands.

(iii) Generically the existence of the Stark-Wannier resonances does not depend on the periodicity of the potential.

(iv) Recent experiments confirm the existence of the Stark-Wannier states.

For δ-like potentials, the existence of Stark-Wannier eigenvalues is not ruled out.

E. The magnetic-field case

The Hamiltonian is

$$H_B = (P - \mathbf{B} \wedge \mathbf{x}/2)^2 + V(\mathbf{x}) , \quad \mathbf{B} = B\mathbf{n} \tag{2.29}$$

where B stands for the magnetic field strength, $\mathbf{n}$ for the direction of the magnetic field, and $\wedge$ denotes the vector product.

The first major step towards the rigorous justification of the Peierls-Onsager effective Hamiltonian is the proof of the stability of the spectrum. It has been proved (Avron and Simon, 1985; Nenciu, 1986; Helffer and Sjöstrand, 1989a, 1989b) that the perturbation given by an extended magnetic field is not very singular as far as the *location* of the spectrum is concerned: the boundaries of the energy gaps depend continuously on the strength of the magnetic field. As has been proved in Nenciu (1986), this result is of a very general genre: it does not depend on the periodicity of $V(\mathbf{x})$ and the homogeneity of the magnetic field. In particular, if the zero-field Hamiltonian has an isolated energy band σ_0, the Hamiltonian (2.29) has, for sufficiently weak fields, an isolated band $\sigma_{\mathbf{B}}$. Then it is natural to define $\mathcal{H}_{\mathbf{B}}$ as the band subspace corresponding to $\sigma_{\mathbf{B}}$. Let $P_{\mathbf{B}}$ be the orthogonal projection on $\mathcal{H}_{\mathbf{B}}$. Since by definition $P_{\mathbf{B}} H_{\mathbf{B}}(1-P_{\mathbf{B}})=0$, the problem of the one-band Hamiltonian, as far as its very existence is concerned, is solved by taking

$$H_{\mathrm{ob},\mathbf{B}} = P_{\mathbf{B}} H_{\mathbf{B}} P_{\mathbf{B}} : \mathcal{H}_{\mathbf{B}} \to \mathcal{H}_{\mathbf{B}} . \tag{2.30}$$

To find out an explicit form of $H_{\mathrm{ob},\mathbf{B}}$ we have to restrict consideration to periodic potentials and homogeneous fields. Moreover, we suppose the band σ_0 to be simple. The limit $B \to 0$ of $P_{\mathbf{B}}$ is quite pathological. More exactly,

$$\lim_{B \to 0} \| P_{\mathbf{B}} - P_0 \| = 1 . \tag{2.31}$$

This means in particular that for *arbitrarily* small B there are states in $\mathcal{H}_{\mathbf{B}}$ almost orthogonal to *all* states in $\mathcal{H}_0$. This pathology is a manifestation of the singularity of the perturbation, combined with the fact that the states in $\mathcal{H}_0$ are extended (in the atomic case $\lim_{B \to 0} \| P_{\mathbf{B}} - P_0 \| = 0$).

The way out of this difficulty was indicated long ago by Peierls (1933) in the tight-binding approximation, by Luttinger (1951), and especially by Wannier (1962) in the general case: take, as the "zero-order approximation" for $\mathcal{H}_{\mathbf{B}}$, instead of $\mathcal{H}_0$ the subspace $\mathcal{N}_{\mathbf{B}}$ generated by $\{v_{\mathbf{B},\mathbf{a}}\}_{\mathbf{a}\in\Gamma}$, where $v_{\mathbf{B},\mathbf{a}}$ are obtained by applying the "magnetic translations" (Zak, 1964) to the Wannier function $w(\mathbf{x})$ corresponding to $\mathcal{H}_0$:

$$v_{\mathbf{B},\mathbf{a}}(\mathbf{x}) = (T_{\mathbf{B},\mathbf{a}} w)(\mathbf{x}) = \exp[-i(\mathbf{B} \wedge \mathbf{x}) \cdot a/2] w(\mathbf{x}-\mathbf{a}) . \tag{2.32}$$

Let $Q_{\mathbf{B}}$ be the orthogonal projection on $\mathcal{N}_{\mathbf{B}}$. Note that $[T_{\mathbf{B},\mathbf{a}}, P_{\mathbf{B}}] = [T_{\mathbf{B},\mathbf{a}}, Q_{\mathbf{B}}] = 0$ while $[T_{\mathbf{B},\mathbf{a}}, P_0] \neq 0$. It has been shown at the heuristic level (Wannier, 1962) that the matrix elements $\langle v_{\mathbf{B},\mathbf{a}}, H_{\mathbf{B}} v_{\mathbf{B},\mathbf{a}} \rangle$ have the right structure to produce an effective Hamiltonian. At the rigorous level, there are two problems to be solved. The first one is that the set $\{v_{\mathbf{B},\mathbf{a}}\}_{\mathbf{a}\in\Gamma}$ is not orthonormal, so it is not clear whether $\{v_{\mathbf{B},\mathbf{a}}\}_{\mathbf{a}\in\Gamma}$ is a basis in $\mathcal{N}_{\mathbf{B}}$ (i.e., every $\psi \in \mathcal{N}_{\mathbf{B}}$ can be uniquely written as $\psi = \sum_{\mathbf{a}\in\Gamma} \psi_{\mathbf{a}} v_{\mathbf{B},\mathbf{a}}$). We shall prove that for weak fields $\{v_{\mathbf{B},\mathbf{a}}\}_{\mathbf{a}\in\Gamma}$ is indeed a basis in $\mathcal{N}_B$, and, moreover, we shall construct an *orthonormal* basis $\{\chi_{\mathbf{a}}\}_{\mathbf{a}\in\Gamma}$ in $\mathcal{N}_{\mathbf{B}}$ such that $\langle \chi_{\mathbf{a}}, H_{\mathbf{B}} \chi_{\mathbf{b}} \rangle$ still have the right structure to produce a Peierls-Onsager effective Hamiltonian. The second problem is the relation between $Q_{\mathbf{B}} H_{\mathbf{B}} Q_{\mathbf{B}}$ and $P_{\mathbf{B}} H_{\mathbf{B}} P_{\mathbf{B}}$. We shall prove that one can apply the regular perturbation theory around $Q_{\mathbf{B}} H_{\mathbf{B}} Q_{\mathbf{B}}$. In particular, $\lim_{B \to 0} \| P_{\mathbf{B}} - Q_{\mathbf{B}} \| = 0$.

The final result is that the description of $H_{\mathrm{ob},\mathbf{B}}$ is very similar to the description of $P_0 H_0 P_0$: one has only to replace the usual translations with the magnetic translations (2.32). More exactly, there exists $B_0 > 0$ such that, for $0 \le B \le B_0$, (i) there exists $w_{\mathbf{B}}(\mathbf{x})$, $\alpha > 0$, such that $\exp(\alpha|\mathbf{x}|) w_{\mathbf{B}}(\mathbf{x}) \in L^2(\mathbb{R}^3)$ and $\{w_{\mathbf{a},\mathbf{B}} \equiv T_{\mathbf{a},\mathbf{B}} w_{\mathbf{B}}\}_{\mathbf{a}\in\Gamma}$ is an orthonormal basis in $P_{\mathbf{B}} L^2(\mathbb{R}^3)$. Moreover,

$$\overline{w_{\mathbf{B}}(\mathbf{x})} = w_{-\mathbf{B}}(\mathbf{x}) , \tag{2.33}$$

and if the crystal has a center of inversion,

$$w_{\mathbf{a},\mathbf{B}}(-\mathbf{x}) = \pm w_{-\mathbf{a},\mathbf{B}}(\mathbf{x}) . \tag{2.34}$$

This result settles an old question concerning the existence of orthonormal and exponentially localized magnetic Wannier functions (Brown, 1964; Dana and Zak, 1983). Note, however, that the result holds true only for the whole band: if, for $\mathbf{B} \neq 0$, σ_0 splits into magnetic subbands, nothing is said about the existence of the Wannier functions for each subband; actually there are strong arguments that, in general, they do not exist.

(ii)

$$H_{\mathrm{ob},\mathbf{B}} w_{\mathbf{a},\mathbf{B}} = \sum_{\mathbf{b}\in\Gamma} \exp[i\mathbf{B}\cdot(\mathbf{a} \wedge \mathbf{b})/2] h_{\mathbf{B}}(\mathbf{a}-\mathbf{b}) w_{\mathbf{b},\mathbf{B}} , \tag{2.35}$$

where

$$h_{\mathbf{B}}(\mathbf{a})=\langle H_{\mathbf{B}}w_{\mathbf{B}},w_{\mathbf{a},\mathbf{B}}\rangle \ . \tag{2.36}$$

There exists $\beta>0$ such that $\sup_{\mathbf{a}\in\Gamma}\exp(\beta|\mathbf{a}|)|h_{\mathbf{B}}(\mathbf{a})|<\infty$,

$$\overline{h_{\mathbf{B}}(\mathbf{a})}=h_{-\mathbf{B}}(\mathbf{a}), \quad \overline{h_{\mathbf{B}}(\mathbf{a})}=h_{\mathbf{B}}(-\mathbf{a}) \ , \tag{2.37}$$

and if the crystal has a center of inversion,

$$h_{\mathbf{B}}(\mathbf{a})=h_{-\mathbf{B}}(\mathbf{a}) \ . \tag{2.38}$$

(iii) $h_B(\mathbf{a})$ has an asymptotic expansion in $\mathbf{B}$,

$$h_{\mathbf{B}}(\mathbf{a})=h_0(\mathbf{a})+\mathbf{B}\cdot\mathbf{h}_1(\mathbf{a})+\cdots \ , \tag{2.39}$$

where

$$\mathbf{h}_1(\mathbf{a})=\langle(\mathbf{P}\wedge\mathbf{x}+\mathbf{x}\wedge P)w,w_{\mathbf{a}}\rangle \\ -i\sum_{\mathbf{b}\in\Gamma}\langle w_{\mathbf{b}},(\mathbf{x}\wedge\mathbf{b})w_a\rangle h_0(\mathbf{b}) \ .$$

(iv) $H_{\mathrm{ob},\mathbf{B}}$ is unitary equivalent to the following operator in $l^2(\Gamma)$:

$$H_{\mathrm{eff},B}f(\mathbf{a})=\sum_{\mathbf{b}\in\Gamma}\exp[i\mathbf{B}\cdot(\mathbf{b}\wedge\mathbf{a})/2]h_{\mathbf{B}}(\mathbf{b}-\mathbf{a})f(\mathbf{b}) \\ =\sum_{\mathbf{c}\in\Gamma}\exp[-i\mathbf{B}\cdot(\mathbf{a}\wedge\mathbf{c})/2]h_{\mathbf{B}}(\mathbf{c})f(\mathbf{a}+\mathbf{c}) \ . \tag{2.40}$$

Note the similarity between (2.2) and (2.40). However, one should not take this similarity too seriously: while $H_{0,\mathrm{eff}}$ is a very simple operator [by inverse Fourier transformation it becomes multiplication with $\lambda(\mathbf{k}_0)$], $H_{\mathbf{B},\mathrm{eff}}$ is everything but a simple object, and its spectral analysis poses a very difficult problem. A detailed presentation of the results concerning the spectral properties of $H_{\mathbf{B},\mathrm{eff}}$ is outside the scope of this review (see Béllissard, 1987, 1988; Helffer and Sjöstrand, 1989a, 1987b, and references therein).

The zeroth-order term in (2.40) [i.e., in (2.40) $h_{\mathbf{B}}(\mathbf{a})$ is replaced by $h_0(\mathbf{a})$] is related to the famous Peierls-Onsager effective Hamiltonian. Indeed, at the formal level, writing

$$\exp[-i\mathbf{B}\cdot(\mathbf{a}\wedge\mathbf{c})/2]f(\mathbf{a}+\mathbf{c})=\exp[i(\mathbf{P}-\mathbf{B}\wedge\mathbf{a}/2)\cdot\mathbf{c}]f(\mathbf{a})$$

one obtains

$$H^{(0)}_{\mathrm{eff},\mathbf{B}}=\sum_{\mathbf{b}\in\Gamma}h_0(\mathbf{b})\exp[i(\mathbf{P}-\mathbf{B}\wedge\mathbf{a}/2)\cdot\mathbf{b}] \ . \tag{2.41}$$

By an interpolation argument similar to the one used in the electric-field case (see the discussion at the end of Sec. II.C) one "extends" (2.41) to $L^2(\mathbb{R}^3)$,

$$H_{\mathrm{PO}}f(\mathbf{x})=\sum_{\mathbf{c}\in\Gamma}h_0(\mathbf{c})\exp[i(\mathbf{P}-\mathbf{B}\wedge\mathbf{x}/2)\cdot\mathbf{c}]f(\mathbf{x}) \ , \tag{2.42}$$

which is nothing but the famous Peierls-Onsager effective Hamiltonian in the Fourier representation. Note that (2.42) coincides with

$$\lambda_0(\mathbf{P}-\mathbf{B}\wedge\mathbf{x}/2) \ , \tag{2.43}$$

where (2.43) is understood as the Weyl quantization of the symbol $\lambda_0(\mathbf{k})$.

As in the electric-field case, uncontrolled approximations are involved in passing from (2.41) to (2.42), and this leads to doubts concerning the validity of (2.42) (Zak, 1986). Fortunately, in this case, by a result of Helffer and Sjöstrand (1989b), the spectra of (2.41) as an operator in $l^2(\Gamma)$ coincide (as a set) with the spectra of (2.42) as an operator in $L^2(\mathbb{R}^3)$. In Sec. V we shall give an easy proof of this fact. Let us stress that, while the spectra of (2.41) and (2.42) coincide as sets, the degeneracies of the spectra are quite different (see also Obermair and Schellnhuber, 1980, 1981).

III. THE ZERO-FIELD HAMILTONIAN

In this section we shall recall, in a suitable form, some properties of the unperturbed Hamiltonian

$$H_0=-\Delta+V(\mathbf{x}) \ , \quad \mathbf{x}\in\mathbb{R}^n \ , \ n\le 3 \ , \tag{3.1}$$

where V is real and $-\Delta$ bounded with relative bound 0:

$$\lim_{a\to\infty}\|V(-\Delta+a)^{-1}\|=0 \ . \tag{3.2}$$

This is not a restrictive condition: by Theorem XIII 96 in Reed and Simon (1978), the condition (3.2) is implied by (2.1) for $n\le 3$. As a consequence of (3.2), H_0 is self-adjoint on the domain of $-\Delta$.

Definition 3.1. *A bounded set $\sigma_0\subset\mathbb{R}$ is an isolated band of H_0 if*

$$\sigma(H_0)=\sigma_0\cup\sigma_1 \ , \quad \mathrm{dist}(\sigma_0,\sigma_1)=d>0 \ , \tag{3.3}$$

where $\sigma(H_0)$ denotes the spectrum of H_0.

For an isolated band σ_0 of H_0, P_0 denotes the spectral projection of H_0 corresponding to σ_0. Usually the existence of isolated bands, or in other words the existence of energy gaps, is associated with long-range order, i.e., with the periodicity of V. The problem of the existence of the energy gaps in the spectrum of electrons in systems without long-range order is an old one (Lieb and Mattis, 1966; Mott and Davis, 1979). While for completely disordered systems one cannot expect to have forbidden gaps, the general belief is that the existence of the energy gaps depends to a great degree on the short-range order. For one-dimensional systems this belief has been substantiated by a result of Borland (1961). The Borland result, considered to be one of the basic results in the theory of the disordered systems (Lieb and Mattis, 1966), was proved by using methods of ordinary differential equations not available in higher dimensions. A proof for arbitrary dimensions was given in Nenciu and Nenciu (1981a). The surprising fact is that the proof is quite simple, almost trivial. The basic idea of the proof, which at the heuristic level goes back to Gubanov (1954, 1955) is to "shift" the disorder from the potential energy to the kinetic energy. [For another nice application of a similar technique, see Hunziker (1986).]

Let V be a periodic function and $\mathbf{h}(\mathbf{x})$ be a C^3 vector-valued function with the property that all the partial derivatives up to order 3 of its components are uniformly bounded by 1. We shall represent disordered systems by the following type of Hamiltonian:

$$H_\delta = -\Delta + V[\mathbf{x}+\delta\mathbf{h}(x)] \equiv K + V_\delta , \tag{3.4}$$

where δ is a small positive number. The periodic system is recovered for $\delta=0$. For small δ there is still a short-range order, but the long-range order is lost, the characteristic length being of order a/δ, where a is the linear dimension of the unit cell.

Theorem 3.1. *Suppose that* $[\alpha,\beta]\subset\mathbb{R}$ *is in the resolvent set of* H_0, *i.e.,* $[\alpha,\beta]\subset\rho(H_0)$. *Then for sufficiently small* δ, *there exist* $\alpha\le\alpha_\delta<\beta_\delta\le\beta$ *such that* $[\alpha_\delta,\beta_\delta]\subset\rho(H_\delta)$. *Moreover,*

$$\lim_{\delta\to 0}\alpha_\delta=\alpha , \quad \lim_{\delta\to 0}\beta_\delta=\beta . \tag{3.5}$$

Proof. The difficulty is due to the fact that the problem does not have a small parameter on which a perturbation approach could be based. In the first step we shall shift the disorder, by a change of variable, from the potential energy to the kinetic energy. In the new representation the kinetic energy can be written as the sum of the usual term $-\Delta$ and a perturbation. The second step is to show that the perturbation can be controlled.

There exists $\delta_0>0$ such that, for $0<\delta\le\delta_0$,

$$J_\delta(\mathbf{x})=\det|\partial[\mathbf{x}+\delta\mathbf{h}(\mathbf{x})]_i/\partial\mathbf{x}_j|\ge\tfrac{1}{2} . \tag{3.6}$$

Then one can define the unitary operator

$$Y_\delta : L^2(\mathbb{R}^3)\to L^2(\mathbb{R}^3) ,$$

$$Y_\delta f(\mathbf{x})=[J_\delta(\mathbf{x})]^{1/2} f(\mathbf{x}+\delta\mathbf{h}(\mathbf{x})) .$$

Consider

$$\tilde{H}_\delta = Y_\delta H_\delta Y_\delta^* = Y_\delta K Y_\delta^* + Y_\delta V_\delta Y_\delta^* .$$

By direct computation,

$$Y_\delta V_\delta Y_\delta^* f(\mathbf{x}) = V(\mathbf{x})f(\mathbf{x}) , \quad Y_\delta K Y_\delta^* = K+\delta D_\delta , \tag{3.7}$$

where D_δ has the form

$$D_\delta = \sum_{i,j=1}^{3} A_{i,j}(\mathbf{x})\partial^2/\partial x_i\partial x_j + \sum_{j=1}^{3} B_j(\mathbf{x})\partial/\partial x_j + C(\mathbf{x}) , \tag{3.8}$$

and all the coefficients appearing in (3.8) are uniformly bounded with respect to $\mathbf{x}\in\mathbb{R}^3$ and $\delta\in(0,\delta_0)$.

From functional calculus, one has, for $z\in R_d=\{z\in\mathbb{C}|\mathrm{Re}z\le -d<0\}$,

$$\begin{aligned} &\|(\partial^2/\partial x_i\partial x_j)(K-z)^{-1}\|\le 1 , \\ &\|(\partial/\partial x_i)(K-z)^{-1}\|\le(4d)^{-1} . \end{aligned} \tag{3.9}$$

From (3.8) and (3.9) it follows that, for $0\le\delta\le\delta_0$ and $z\in R_d$,

$$\|D_\delta(K-z)^{-1}\|\le c(d) .$$

The condition (3.2) assures the existence of $d_0<\infty$ such that, for $z\in R_{d_0}$,

$$\|V(K-z)^{-1}\|\le\tfrac{1}{2} .$$

Then using the identity

$$(K+V-z)^{-1}=(K-z)^{-1}[1+V(K-z)^{-1}]^{-1} ,$$

one obtains, for $0\le\delta\le\delta_0$, $z\in R_{d_0}$,

$$\|D_\delta(K+V-z)^{-1}\|\le 2c(d_0) ;$$

and the use of Theorem VI 5.12 from Kato's book (1966) finishes the proof of the theorem.■

A detailed description of the spectral properties of H_0 is available if $V(\mathbf{x})$ is periodic, i.e., there exists a Bravais lattice Γ in $\mathbb{R}^n$ such that $V(\mathbf{x}+\mathbf{a})=V(\mathbf{x})$ for $\mathbf{a}\in\Gamma$. Let $\{\mathbf{a}_i\}_i^n$ be a basis in Γ, $\{\mathbf{g}_j\}_1^n$ the dual basis

$$\mathbf{a}_i\mathbf{g}_j=2\pi\delta_{ij} , \tag{3.10}$$

and $\hat{\Gamma}=\{\mathbf{g}|\mathbf{g}=\sum_1^n m_j\mathbf{g}_j,\ m_j \text{ integers}\}$. If $\mathbf{x},\mathbf{k}\in\mathbb{R}^n$, $(x_1,\dots,x_n)$, $(k_1,\dots,k_n)$ denote their coordinates in the bases $\{\mathbf{a}_i\}$ and $\{\mathbf{g}_j\}$, respectively:

$$\mathbf{x}=\sum_1^n x_i a_i , \quad \mathbf{k}=\sum_1^n k_i\mathbf{g}_i \tag{3.11}$$

The basic period cells corresponding to $\{\mathbf{a}_i\}$ and $\{\mathbf{g}_j\}$ are denoted by Q and B, respectively:

$$Q=\{\mathbf{x}\in\mathbb{R}^n|-\tfrac{1}{2}\le x_i<\tfrac{1}{2}) ,$$

$$B=\{\mathbf{k}\in\mathbb{R}^n|-\tfrac{1}{2}\le k_i<\tfrac{1}{2}\} .$$

Sometimes $\mathbf{k}$ will be regarded as complex, $\mathbf{k}\in\mathbb{C}^n$; i.e., in (3.11) $k_i\in\mathbb{C}$.

Theorem 3.2. *Let*

$$\mathcal{M}=l^2(\hat{\Gamma})=\left\{\psi_g\,\Big|\,\sum_{g\in\hat{\Gamma}}|\psi_g|^2<\infty\right\} ,$$

$$\mathcal{H}=\int_B^\oplus \mathcal{M}\,d\mathbf{k}=\left\{f_g(k)\,\Big|\,\int_B d\mathbf{k}\sum_{\mathbf{g}}|f_g(\mathbf{k})|^2<\infty\right\} ,$$

and

$$\hat{V}_g=(\mathrm{vol}Q)^{-1}\int_Q \exp(-i\mathbf{g}\cdot\mathbf{x})V(\mathbf{x})d\mathbf{x} .$$

For $\mathbf{k}\in\mathbb{C}^n$ *define* $H_0(\mathbf{k})$ *in* $\mathcal{M}$ *by*

$$[H_0(\mathbf{k})\psi]_{\mathbf{g}}=(\mathbf{k}+\mathbf{g})^2\psi_{\mathbf{g}}+\sum_{\mathbf{h}\in\hat{\Gamma}}\psi_{\mathbf{h}}\hat{V}_{\mathbf{g}-\mathbf{h}} \tag{3.12}$$

with the domain

$$\mathcal{D}(H_0(\mathbf{k}))=\mathcal{D}_0=\left\{\psi\in\mathcal{M}\,\Big|\,\sum_{\hat{\Gamma}}|\mathbf{g}^4|\,|\psi_{\mathbf{g}}^2|<\infty\right\} .$$

Then

i. *For* $\mathbf{k}\in\mathbb{R}^n$, $H_0(\mathbf{k})$ *is self-adjoint;*

ii. $H_0(\mathbf{k})$ *is an entire analytic family of type A;*

iii. *for* $\mathbf{k}\in\mathbb{C}^n$, $H_0(\mathbf{k})$ *has compact resolvent;*

iv. *let* $S{:}L^2(\mathbb{R}^n,d\mathbf{x})\rightarrow\mathcal{H}$ *be given by*

$$(Sf)_{\mathbf{g}}(\mathbf{k})=\hat{f}(\mathbf{k}+\mathbf{g}) , \tag{3.13}$$

where $\hat{f}$ *denotes the Fourier transform of* f. *The operator* S *is unitary and*

$$SH_0S^*=\int_B^{\oplus}H_0(\mathbf{k})d\mathbf{k} . \tag{3.14}$$

[i.e., $(SH_0S^*f)_{\mathbf{g}}(\mathbf{k})=(\mathbf{k}+\mathbf{g})^2+\sum_{\hat{\Gamma}}f_{\mathbf{h}}(\mathbf{k})\hat{V}_{\mathbf{g}-\mathbf{h}}$*].*

Proof. See Reed and Simon (1978) and references therein. The formula (3.14) is nothing but the Bloch theorem in the momentum representation.■

Although $H_0(\mathbf{k})$ has nice analyticity properties, it is not periodic in $\mathbf{k}$, so we need another representation in order to discuss the periodicity properties of the eigenvalues and eigenfunctions of $H_0(\mathbf{k})$. Consider the following shift operator in $\mathcal{M}$:

$$(W_j\psi)_{\mathbf{g}}=\psi_{\mathbf{g}-\mathbf{g}_j} . \tag{3.15}$$

The operators W_j are unitary, and since -1 is not an eigenvalue of W_j there exist unique self-adjoint operators C_j such that $\|C_j\|\leq\pi$ and

$$W_j=\exp(iC_j) . \tag{3.16}$$

Consider now the bounded operator-valued function (note that C_j commute)

$$W(\mathbf{k})=\prod_1^n\exp(ik_jC_j)=\exp\left[i\sum_1^n k_jC_j\right] . \tag{3.17}$$

Obviously $W(\mathbf{k})$ is an entire function of the n complex variables, $k_1,k_2,\ldots,k_n$ and

$$W^*(k_1,\ldots,k_n)=W^{-1}(\bar{k}_1,\ldots,\bar{k}_n) .$$

Lemma 3.1. *Let* $\tilde{H}_0(\mathbf{k})$ *be given by*

$$\tilde{H}_0(\mathbf{k})=W(\mathbf{k})H_0(\mathbf{k})W^{-1}(\mathbf{k}) . \tag{3.18}$$

Then for all $\mathbf{g}\in\hat{\Gamma},\mathbf{k}\in\mathbb{C}^n$,

$$\tilde{H}_0(\mathbf{k})=\tilde{H}_0(\mathbf{k}+\mathbf{g}) . \tag{3.19}$$

Proof. It is sufficient to verify (3.19) for $\mathbf{g}=\mathbf{g}_j$, $j=1,2,\ldots,n$;

$$\tilde{H}_0(\mathbf{k}+\mathbf{g}_j)=W(\mathbf{k})W_jH_0(\mathbf{k}+\mathbf{g}_j)W_j^{-1}W^{-1}(\mathbf{k}) ,$$

and the only thing to do is to verify that

$$W_jH_0(\mathbf{k}+g_j)W_j^{-1}=H_0(\mathbf{k})$$

which is routine computation.■

Note that $\tilde{H}_0(\mathbf{k})$ is *not* an analytic family of type A since its domain is $\mathbf{k}$ dependent due to the fact that $W(\mathbf{k})$ does not leave $\mathcal{D}_0$ invariant. The representations $\int_B^{\oplus}H_0(\mathbf{k})d\mathbf{k}$ and $\int_B^{\oplus}\tilde{H}_0(\mathbf{k})d\mathbf{k}$ of H_0 complement each other: the first is suited for discussing the analyticity properties while the second is suited for discussing the periodicity properties.

Let us exploit now the reality of $V(\mathbf{x})$, or in other words the time-reversal invariance. Consider the following (antiunitary) involution $\vartheta{:}\mathcal{M}\rightarrow\mathcal{M}$:

$$(\vartheta\psi)_{\mathbf{g}}=\bar{\psi}_{-\mathbf{g}} . \tag{3.20}$$

Lemma 3.2. *For* $\mathbf{k}\in\mathbb{R}^n$,

$$\vartheta H_0(\mathbf{k})\vartheta=H_0(-\mathbf{k}) , \tag{3.21}$$

$$\vartheta W(\mathbf{k})\vartheta=W(-\mathbf{k}) . \tag{3.22}$$

Proof. Noting that the reality of V implies $\bar{\hat{V}}_{\mathbf{g}}=\hat{V}_{-\mathbf{g}}$, (3.21) follows from (3.12) by routine computation. From the definitions of ϑ and W_j,

$$\vartheta W_j\vartheta=W_j^{-1}=\exp(-iC_j) . \tag{3.23}$$

On the other hand,

$$\vartheta W_j\vartheta=\vartheta\exp(iC_j)\vartheta=\exp(-i\vartheta C_j\vartheta) . \tag{3.24}$$

From (3.23) and (3.24) and from the uniqueness of C_j, one obtains

$$\vartheta C_j\vartheta=C_j ,$$

which implies (3.22).

Suppose now that the crystal has a center of inversion, i.e., $V(\mathbf{x})=V(-\mathbf{x})$, that is equivalent to $\hat{V}_{\mathbf{g}}=\hat{V}_{-\mathbf{g}}$. Consider the following involution in $\mathcal{M}$:

$$(I\psi)_{\mathbf{g}}=\psi_{-\mathbf{g}} .$$

An argument similar to the one in the proof of Lemma 3.2 gives

$$IH_0(\mathbf{k})I=H_0(-\mathbf{k}) , \tag{3.25}$$

$$IW(\mathbf{k})I=W(-\mathbf{k}).\blacksquare \tag{3.26}$$

If $J=\vartheta I$, then by combining Lemma 3.1 with (3.25) and (3.26),one obtains the following.

Lemma 3.3.

$$JW(\mathbf{k})J=W(\mathbf{k})$$

and, if $V(\mathbf{x})=V(-\mathbf{x})$, *then in addition*

$$JH_0(\mathbf{k})J=H_0(\mathbf{k}) .$$

As a consequence of Theorem 3.2.iii, at fixed $\mathbf{k}$, $\sigma(\mathbf{k})\equiv\sigma_0(H(\mathbf{k}))$ is discrete; and as a consequence of Lemma 3.1, $\sigma(\mathbf{k})$ is periodic as a set:

$$\sigma(\mathbf{k})=\sigma(\mathbf{k}+\mathbf{g}) . \tag{3.27}$$

Definition 3.2. *A nonvoid part* $\sigma_0(\mathbf{k})$ *of* $\sigma(\mathbf{k})$, $\mathbf{k}\in\mathbb{R}^n$, *is said to be a direct isolated band of* $H_0(\mathbf{k})$ *if there exist continuous periodic functions* $f_i(\mathbf{k}){:}\mathbb{R}^n\rightarrow\mathbb{R}$, $f_i(\mathbf{k})$

$=f_i(\mathbf{k}+\mathbf{g})$, $\mathbf{g}\in\hat{\Gamma}$, $i=1,2$, *and a positive constant* $d>0$ *such that* $f_1(\mathbf{k})<f_2(\mathbf{k})$ *and*

$$\sigma_0(\mathbf{k})\subset[f_1(\mathbf{k}),f_2(\mathbf{k})]\ ,$$

$$\sigma(\mathbf{k})\cap[f_i(\mathbf{k})-d/2,f_i(\mathbf{k})+d/2]=\varnothing\ ,\quad i=1,2\ .$$

Let $P_0(\mathbf{k})$ be the spectral projection of $H_0(\mathbf{k})$ corresponding to a direct isolated band $\sigma_0(\mathbf{k})$, and

$$\tilde{P}_0(\mathbf{k})=W(\mathbf{k})P_0(\mathbf{k})W(\mathbf{k})^{-1}\ . \tag{3.28}$$

In a slightly different form the following result goes back to des Cloizeaux (1964a, 1964b).

Theorem 3.3. *There exists* $a>0$ *such that* $\tilde{P}_0(\mathbf{k})$ *is the restriction to* $\mathbb{R}^n$ *of a bounded projection-valued function analytic to*

$$\mathcal{J}_a^n=\{\mathbf{k}\in\mathbb{C}^n|\ |\mathrm{Im}\mathbf{k}|<a\}$$

satisfying

$$\tilde{P}_0(\mathbf{k})=\tilde{P}_0(\mathbf{k}+\mathbf{g})\ ,\quad \mathbf{k}\in\mathcal{J}_a^n\ ,\quad \mathbf{g}\in\hat{\Gamma}\ , \tag{3.29}$$

$$\vartheta\tilde{P}_0(\mathbf{k})\vartheta=\tilde{P}_0(-\mathbf{k})\ . \tag{3.30}$$

Moreover, if the crystal has a center of inversion then

$$I\tilde{P}_0(\mathbf{k})I=\tilde{P}_0(-\mathbf{k})\ . \tag{3.31}$$

Proof. The analyticity of $P_0(\mathbf{k})$ is a direct consequence of the theory of analytic perturbations (Reed and Simon, 1978; see also Bentosela, 1979). Then the analyticity of $\tilde{P}_0(\mathbf{k})$ follows from this and from the fact that $W(\mathbf{k})$ and $W(\mathbf{k})^{-1}$ are entire functions. Now (3.29)–(3.31) follow from Lemmas 3.1 and 3.2, via the Riesz formula for the spectra projection

$$\tilde{P}_0(\mathbf{k})=(2\pi i)^{-1}\int_C(\tilde{H}_0(\mathbf{k})-\zeta)^{-1}d\zeta\ ,$$

where C is a contour enclosing $\sigma_0(\mathbf{k})$. ■

From Theorem 3.3 it follows in particular that $m\equiv\dim\tilde{P}_0(\mathbf{k})$ does not depend on $\mathbf{k}$, and due to Theorem 3.2.iii, $m<\infty$. An isolated band is said to be simple if $\dim\tilde{P}_0(\mathbf{k})=1$ and complex otherwise.

We are going to discuss now the analyticity and periodicity properties of the eigenvalues and eigenfunctions corresponding to a direct isolated band. We shall consider first simple bands: $\sigma_0=\{\lambda_0(\mathbf{k})\}$. There are no problems for $\lambda_0(\mathbf{k})$: since $\lambda_0(\mathbf{k})$ is isolated for all $\mathbf{k}$, the analytic perturbation theory for isolated eigenvalues and (3.27) lead to the following.

Theorem 3.4. *For simple direct isolated bands,* $\lambda_0(\mathbf{k})$ *is analytic in* $\mathcal{J}_a^n$ *and*

$$\lambda_0(\mathbf{k}+\mathbf{g})=\lambda_0(\mathbf{k})\quad\text{for all }\mathbf{k}\in\mathcal{J}_a^n\ ,\ \mathbf{g}\in\hat{\Gamma}\ .$$

Note that this result does not depend on the reality of the Hamiltonian: in particular, it holds true if magnetic interactions are present.

For the eigenfunctions, the situation is much more involved. Let $\chi_0(\mathbf{k})$ be the normalized eigenvector of $H_0(\mathbf{k})$ corresponding to $\lambda_0(\mathbf{k})$ (unique up to a $\mathbf{k}$-dependent phase factor). At first sight, due to (3.29), one can believe that it is a trivial matter to choose the arbitrary phase factor to make

$$\tilde{\chi}_0(\mathbf{k})=W(\mathbf{k})\chi_0(\mathbf{k}) \tag{3.32}$$

analytic and periodic. Unfortunately this is not so. Indeed, the analytic perturbation theory provides $\chi_0(\mathbf{k})$ analytic in $\mathcal{J}_a^n$ and normalized in $\mathbb{R}^n$, but one cannot guarantee that $\tilde{\chi}(\mathbf{k})_0$ is periodic. On the other hand, one can make the "consistent" choice of the phase factor by which $\tilde{\chi}_0(\mathbf{k})$ coincide whenever $\tilde{H}_0(\mathbf{k})$ coincide. But now one cannot guarantee that such a $\chi_0(\mathbf{k})$ can be made analytic. The point is that the phase factor in $\chi_0(\mathbf{k})$ is fixed by analytic continuation, which is a local procedure, and may not fulfill the periodicity condition, which is of global nature. Actually, it turns out that if the magnetic field is present and consequently (3.21) does not hold true, analytic and periodic $\tilde{\chi}_0(\mathbf{k})$ in general do not exist [this accounts for the fact that some vector bundles over the three-dimensional torus are nontrivial; see, e.g., Dubrovin and Novicov (1980), Novicov (1981), Lyskova (1985)].

The main technical result of this section is contained in the following.

Theorem 3.5. *Suppose that* σ_0 *is a simple direct isolated band. There exists* $\chi_0(\mathbf{k})$ *analytic in* $\mathcal{J}_a^n$, *normalized in* $\mathbb{R}^n$ *such that*

$$H_0(\mathbf{k})\chi_0(\mathbf{k})=\lambda_0(\mathbf{k})\chi_0(\mathbf{k})\ , \tag{3.33}$$

$$W(\mathbf{k})\chi_0(\mathbf{k})=W(\mathbf{k}+\mathbf{g})\chi_0(\mathbf{k}+\mathbf{g})\ ,\quad \mathbf{g}\in\hat{\Gamma}\ , \tag{3.34}$$

$$\vartheta\chi_0(\mathbf{k})=\chi_0(-\mathbf{k})\ , \tag{3.35}$$

Moreover, for crystals with a center of inversion,

$$I\chi_0(\mathbf{k})=\pm\exp(i\mathbf{a}_0\cdot\mathbf{k})\chi_0(-\mathbf{k})\quad\text{for some }\mathbf{a}_0\in\Gamma\ . \tag{3.36}$$

Remark. The first proof of the existence of analytic and periodic Bloch functions for one-dimensional systems was given by Kohn (1959a) using methods of the theory of ordinary differential equations. His proof does not generalize to higher dimensions. The next major step forward was made by des Cloizeaux (1964), who proved Theorem 3.5 for crystals with a center of inversion. The restriction to the crystals with a center of inversion was removed by Nenciu (1983). A more elementary proof of Theorem 3.5 has been given recently by Helffer and Sjöstrand (1988b), but it seems that their proof gives a strip of analyticity for the Bloch functions narrower than the strip of analyticity of $P_0(\mathbf{k})$. Theorem 3.5 [without (3.35) and (3.36)] and even more general results can be proved starting from the results in Theorem 3.4 by using some significant results in the theory of analytic functions of several complex variables concerning the second Cousin problem (see, e.g., Range, 1986, Chap. VI and references therein). Actually, by "Oka's principle" it is sufficient to prove that there are no obstructions at the topological level, and this follows in a variety of cases from the reality of the Hamiltonian by using the theory of characteristic classes.

Before giving the proof of the Theorem 3.5, let us discuss the general case of complex bands. Consider a direct isolated band σ_0, of dimension m. Then $\sigma_0=\{\lambda_r(\mathbf{k})\}_1^m$. The labeling of the eigenvalues $\lambda_r(\mathbf{k})$ is a matter of convention. The generally accepted convention (Herring, 1937; Weinreich, 1965), is $\lambda_r(\mathbf{k})\le\lambda_{r+1}(\mathbf{k})$, $r=1,2,\ldots,m-1$. This labeling has the advantage that each $\lambda_r(\mathbf{k})$ is periodic. Unfortunately [we exclude the trivial case when $\lambda_r(\mathbf{k})$ do not touch each other] $\lambda_r(\mathbf{k})$ given by this convention are not analytic; at the intersection points they are not even differentiable. The problem occurs whenever it is possible to label the eigenvalues in such a way that all of them together with their corresponding eigenvectors are analytic in some complex neighborhood of $\mathbb{R}^n$. The answer seems to be negative in more than one dimension. The reason is that analytic matrices of more than one complex variable can have nonanalytic eigenvalues and eigenvectors, as can be seen from the following simple example (Kato, 1966):

$$T(k_1,k_2)=\begin{bmatrix} k_1 & k_2 \\ k_2 & -k_1 \end{bmatrix} ,$$

whose eigenvalues $\lambda_\pm(k_1,k_2)=\pm\sqrt{k_1^2+k_2^2}$ are nonanalytic at $k_1=k_2=0$. Concerning the eigenvectors, one can still question whether there exist m linear combinations of the eigenvectors of $H_0(\mathbf{k})$ corresponding to σ_0 with appropriate analyticity and periodicity properties. The same question applies to the case of an orthonormal basis $\{\chi_r(k)\}_1^m$ in $P_0(\mathbf{k})\mathcal{M}$ such that all $\chi_r(\mathbf{k})$ are analytic and periodic. The functions $\chi_r(\mathbf{k})$ in the "$\mathbf{x}$ representation" are named quasi-Bloch functions (des Cloizeaux, 1964).

A complete solution to the above questions can be obtained for the case when all but one of the variables k_j are kept fixed. More exactly, consider the properties of $H_0(\mathbf{k})$ as a function of k_1 at $k_\perp\equiv(k_2,k_3,\ldots,k_n)$ fixed. In order to emphasize this we shall write $H_0(k_1,k_\perp)\equiv H_{0,k_\perp}(k_1)$, and moreover when no confusion is possible we shall omit $k_\perp$ and write k for k_1. Obviously, $\tilde{H}_{0,k_\perp}(k_1)=W(k_1,k_\perp)H_{0,k_\perp}(k_1)W(k_1,k_\perp)^{-1}$ is entire and periodic [in the sense that both $H_{0,k_\perp}(k_1)$ and $W(k_1,k_\perp)$ are entire; note, however, that the domain of $\tilde{H}_{0,k_\perp}(k_1)$ depends on k_1] i.e., the analyticity and periodicity of $H_{0,k_\perp}(k_1)$ are the same as in the one-dimensional case. However, while in the one-dimensional case the bands are simple, the bands of $H_{0,k_\perp}(k_1)$ are generically complex.

Theorem 3.6. *Let $\sigma_0(k)$ be a direct isolated band of $H_0(k)$, $P_0(k)$ its corresponding spectral projection, and $\mathcal{J}_a^1$ the analyticity strip of $P_0(k)$.*

i. *There exist positive integers m, p; $p\le m$; functions $\lambda_j(k)$, $j=1,2,\ldots,p$ analytic in the strip $\mathcal{J}_b^1$ for some $b>0$ and real for $k\in\mathbb{R}$; positive integers $r_1, r_2,\ldots, r_p$ satisfying $\sum_1^p r_j=m$, such that $\sigma_0(k)=\{\lambda_j(k)\}_1^p$, each $\lambda_j(k)$ having the multiplicity r_j [i.e., $\lambda_j(k)$ are eigenvalues of $H_0(k)$ of multiplicity r_j; at the points where some λ_j coincide, the total multiplicity is $\sum_{\lambda_j(k)=\lambda}r_j$]. The functions $\lambda_j(k)$ are periodic with periods $p_j\le p$. The spectral projections $P_{0,j}(k)$ corresponding to $\lambda_j(k)$ are analytic in $\mathcal{J}_b^1$ and periodic with periods p_j.*

ii. *There exists an orthonormal basis in $P_{0,j}(k)\mathcal{M}$, $\{\psi_{j,s}\}_{s=1}^{r_j}$, such that $\psi_{j,s}(k)$ are restrictions to $\mathbb{R}$ of functions analytic in $\mathcal{J}_b^1$ and satisfy*

$$W(k)\psi_{j,s}(k)=W(k+p_j)\psi_{j,s}(k+p_j) .$$

iii. *There exists an orthonormal basis $\{\chi_i(\mathbf{k})\}_1^m$ in $P_0(k)\mathcal{M}$ such that all $\chi_i(k)$ are restrictions to $\mathbb{R}$ of functions analytic in $\mathcal{J}_a^1$ and satisfy*

$$W(k)\chi_i(k)=W(k+1)\chi_i(k+1) .$$

Remark. Theorem 3.6.ii implies that, in the "one-dimensional" case, analytic and periodic Bloch functions exist even for complex bands. Note, however, that the analyticity strip of the Bloch functions can be by far narrower than the analyticity strip of $P_0(k)$. Moreover, while the theory gives the means to estimate a it does not give any information about b.

Proof of Theorem 3.6.i. The existence of $\lambda_i(k)$ as well as their analyticity properties follows from the standard theory of perturbations for analytic families of type A (Kato, 1966; Reed and Simon, 1978). In particular, the analyticity of $\lambda_i(k)$ at the degeneracy points follows from the famous Rellich theorem. Consider next the periodicity properties. Due to (3.27), $\sigma_0(k)$ is a periodic set. Since, because of the analyticity, the number of points at which two or more $\lambda_i(k)$ coincide is finite in every compact, one can assume without loss of generality that the origin is not an intersection point. If t_i is the smallest integer for which $\lambda_i(t_i)=\lambda_i(0)$, then the period of $\lambda_i(k)$ is t_i. Since for all integers t the set $\sigma_0(t)$ does not depend on t and contains p points, it follows that $t_i\le p$. Consider now $P_{0,j}(k)$. Again by the Rellich theorem, $P_{0,j}(k)$ are analytic in $\mathcal{J}_b^1$, and due to the Reisz formula and (3.19), $W(k)P_{0,j}(k)W(k)^{-1}$ are periodic with periods p_j.■

Theorems 3.5, 3.6.ii, and 3.6.iii are corollaries to the existence of solutions of the following abstract problem concerning projection valued functions.

Problem C. *Let $\mathcal{H}$ be a separable Hilbert space, s be a positive integer, and $Q(z):\mathcal{H}\to\mathcal{H}$ be a projection-valued function analytic in $\mathcal{J}_a^s$ satisfying*

$$Q(z)=Q(z)^* \quad \text{for } z\in\mathbb{R}^s , \tag{3.37}$$

$$Q(z)=Q(z+\mathbf{p}) , \quad \mathbf{p}\in\mathbb{Z}^s . \tag{3.38}$$

Find a bounded, and with bounded inverse, operator-valued function $A(z):\mathcal{H}\to\mathcal{H}$ analytic in $\mathcal{J}_a^s$ satisfying

$$A^{-1}(z)=A(z)^* \quad \text{for } z\in\mathbb{R}^s , \tag{3.39}$$

$$Q(z)=A(z)Q(0)A(z)^{-1} , \quad A(0)=1 , \tag{3.40}$$

$$A(z)Q(0)=A(z+\mathbf{p})Q(0) , \quad z\in\mathcal{J}_a^s, \ \mathbf{p}\in\mathbb{Z}^s . \tag{3.41}$$

In general, because of topological obstructions. Problem C does not have solutions. However, the existence of solutions can be proved under additional conditions.

Theorem C.i. *In the cases below, Problem C has solutions:*

a. $\sup_{z\in\mathcal{J}_a^s}\|Q(\mathbf{z})-Q(\mathbf{0})\|<1;$ (3.42)

b. $s=1$*;*

c. $\dim Q(\mathbf{z})=1$ *and there exists an antiunitary involution* $\vartheta:\mathcal{H}\to\mathcal{H}$ *such that*

$$\vartheta Q(z)\vartheta=Q(-z) \quad \text{for } z\in\mathbb{R}^s . \tag{3.43}$$

ii. *If (3.43) is fulfilled then solutions satisfying*

$$\vartheta A(z)\vartheta Q(\mathbf{0})=A(-z)Q(\mathbf{0}) \text{ for } \mathbf{z}\in\mathbb{R}^s \tag{3.44}$$

exist. If in addition there exists unitary involution $I:\mathcal{H}\to\mathcal{H}$ *such that*

$$IQ(z)I=Q(-z) , \tag{3.45}$$

then solutions satisfying

$$IA(z)IQ(\mathbf{0})=\pm\exp\left[i\pi\sum_1^s\beta_j z_j\right]A(-z)Q(\mathbf{0}) , \quad \beta_j=0,1 . \tag{3.46}$$

exist.

Proof i.a. In this case a solution is given by the Sz-Nagy formula (Kato, 1966; Chap. II, 4.6)

$$A(z)=\{1-[Q(z)-Q(\mathbf{0})]^2\}^{-1/2} \times\{Q(\mathbf{z})Q(\mathbf{0})+[1-Q(\mathbf{z})][1-Q(\mathbf{0})]\} . \tag{3.47}$$

i.b. Consider $B(z)$ given by

$$i(d/dz)B(z)=K(z)B(z) ,$$
$$K(z)=i[1-2Q(z)](d/dz)Q(z) ;$$
$$B(0)=1 . \tag{3.48}$$

Then (Kato, 1966; see also the Appendix) $B(z)$ is analytic and invertible in $\mathcal{J}_a^s$ and satisfies (3.39) and (3.40) [but not (3.41)]. Consider

$$T=B(\tfrac{1}{2})B(-\tfrac{1}{2})^{-1} . \tag{3.49}$$

From (3.40) and (3.38) one obtains

$$[T,Q(-1/2)]=0 , \tag{3.50}$$

i.e., $T=T_1\oplus T_2$, where the orthogonal sum is according to the decomposition $\mathcal{H}=Q(-\frac{1}{2})\mathcal{H}\oplus[1-Q(-\frac{1}{2})]\mathcal{H}$. Since T_i are unitary, one can take the logarithm; i.e., there exist bounded self-adjoint operators D_i such that $\|D_i\|\le\pi$ and

$$T=\exp(iD) , \quad D=D_1\oplus D_2 .$$

Now $[D,Q(-\frac{1}{2})]=0$, and then

$$[Q(-\tfrac{1}{2}),\exp(izD)]=0 . \tag{3.51}$$

We claim that

$$A(z)=B(z)\exp(-izD) \tag{3.52}$$

satisfies all the required conditions. The analyticity and the invertibility are obvious. From the fact that $B(z)$ satisfies (3.40) and (3.51), one obtains (3.40) for $A(z)$. Using (3.51), the differential equation for $B(z)$ and the fact that $K(z)$ is self-adjoint, one can verify recurrently that

$$(d^n/dz^n)A(z)|_{z=-1/2}=(d^n/dz^n)A(z)|_{z=1/2} ,$$

which implies the periodicity of $A(z)$. Finally, since $B(z)$ is unitary for real z and D is self-adjoint, $A(z)$ is unitary for real z.

i.c. Let $B(z)$ be constructed as in the one-dimensional case with respect to z_s $[\mathbf{z}=(z_1,z_2,\ldots,z_s)]$ at $\mathbf{z}^{s-1}=(z_1,z_2,\ldots,z_{s-1})$.

Suppose that (3.43) holds true. Then for real $\mathbf{z}$

$$\vartheta K(\mathbf{z})\vartheta=K(-\mathbf{z})$$

which, via the differential equation for $B(\mathbf{z})$ implies

$$\vartheta B(\mathbf{z})\vartheta=B(-\mathbf{z}) , \quad \mathbf{z}\in\mathbb{R}^s . \tag{3.53}$$

In a similar way, if (3.45) holds true, one obtains

$$IB(\mathbf{z})I=B(-\mathbf{z}) . \tag{3.54}$$

Define

$$T(\mathbf{z}^{s-1})=B(\mathbf{z}^{s-1},\tfrac{1}{2})B(\mathbf{z}^{s-1},-\tfrac{1}{2})^{-1} . \tag{3.55}$$

Clearly $T(\mathbf{z}^{s-1})$ is analytic, invertible, and periodic in $\mathcal{J}_a^{s-1}$, but unfortunately we do not know whether $T(z^{s-1})$ admits an analytic and periodic logarithm. Since $[T(\mathbf{z}^{s-1}),Q(\mathbf{z}^{s-1},\frac{1}{2})]=0$, for $f\in Q(\mathbf{z}^{s-1},\frac{1}{2})\mathcal{H}$

$$T(\mathbf{z}^{s-1})f=\lambda(\mathbf{z}^{s-1})f , \tag{3.56}$$

where [recall that $\dim Q(\mathbf{z})=1$] $\lambda(\mathbf{z}^{s-1})$ is a complex-valued function. We shall prove that there exists a unique function $\phi(\mathbf{z}^{s-1})$, analytic and periodic in $\mathcal{J}_a^{s-1}$, real for real $\mathbf{z}^{s-1}$, $\phi(0)\in(-\pi,\pi]$, such that

$$\lambda(z^{s-1})=\exp[i\phi(\mathbf{z}^{s-1})], \quad \phi(\mathbf{z}^{s-1})=\phi(-z^{s-1}) , \tag{3.57}$$

and if (3.45) is fulfilled then $\phi(\mathbf{z}^{s-1})$ is constant:

$$\phi(\mathbf{z}^{s-1})=0,\pi . \tag{3.58}$$

Taking this for granted, it is easy to finish the proof of the theorem. Indeed, as above, if

$$A_s(\mathbf{z})=\exp[-iz_s\phi_s(\mathbf{z}^{s-1})]B(z) , \tag{3.59}$$

one can verify that

$$A_s(\mathbf{z})Q(\mathbf{z}^{s-1},0)=A_s(\mathbf{z}+\mathbf{p})Q(\mathbf{z}^{s-1},0), \quad \mathbf{p}\in\mathbb{Z}^s . \tag{3.60}$$

$$A_s(\mathbf{z})Q(\mathbf{z}^{s-1},0)A_s(\mathbf{z})^{-1}=Q(\mathbf{z}) . \quad (3.61)$$

Moreover, (3.44) and (3.46) for $A_s(\mathbf{z})$ follow from (3.52), (3.53), (3.57), and (3.58). Repeat the construction in one dimension less, starting from $Q(\mathbf{z}^{s-1},0)$. Clearly,

$$A(\mathbf{z})=\prod_{i=0}^{s-1} A_{s-i}(\mathbf{z}^{s-i}) \quad (3.62)$$

is a solution of the Problem C.

We shall prove now (3.57) and (3.58). The invertibility of $T(\mathbf{z}^{s-1})$ implies $\lambda(\mathbf{z}^{s-1})\neq 0$. Let $f\in Q(\mathbf{0},\frac{1}{2})$. There exists a neighborhood X of $\mathbf{0}$ in $\mathbb{C}^{s-1}$ such that $(f,Q(\mathbf{z}^{s-1},\frac{1}{2})f)\neq 0$. Then

$$\lambda(\mathbf{z}^{s-1})=(f,Q(\mathbf{z}^{s-1},\tfrac{1}{2})f)^{-1}(f,Q(\mathbf{z}^{s-1},\tfrac{1}{2})T(\mathbf{z}^{s-1})f)$$

and hence $\lambda(\mathbf{z}^{s-1})$ is analytic in X. By an analytic continuation argument, $\lambda(z^{s-1})$ is analytic in $\mathcal{J}_a^{s-1}$. Hence, the first relation in (3.57) holds true with $\phi(\mathbf{z}^{s-1})$ analytic in $\mathcal{J}_a^{s-1}$. The reality of $\phi(\mathbf{z}^{s-1})$ for $\mathbf{z}^{s-1}\in\mathbb{R}^{s-1}$ follows from the unitarity of $T(\mathbf{z}^{s-1})$. The periodicity of $\lambda(\mathbf{z}^{s-1})$ is obvious. Since $d\lambda/dz_j=i\lambda(d\phi/dz_j)$, $d\phi/dz_j$ are periodic, and hence

$$\phi(\mathbf{z}^{s-1})=\psi(\mathbf{z}^{s-1})+2\pi\sum_{j=1}^{s-1}p_jz_j , \quad (3.63)$$

where $\psi(\mathbf{z}^{s-1})$ is periodic and p_j are integers. We shall show now that (3.53) implies

$$\phi(\mathbf{z}^{s-1})=\phi(-\mathbf{z}^{s-1}) . \quad (3.64)$$

Indeed, from (3.53) and (3.55) it follows that

$$\vartheta T(\mathbf{z}^{s-1})\vartheta=T(-\mathbf{z}^{s-1})^{-1} . \quad (3.65)$$

From (3.38) and (3.43), one has

$$\vartheta Q(\mathbf{z}^{s-1},\tfrac{1}{2})\vartheta=Q(-\mathbf{z}^{s-1},\tfrac{1}{2}) . \quad (3.66)$$

Let now $f\in Q(\mathbf{z}^{s-1},\frac{1}{2})\mathcal{H}$. Using (3.65) and (3.66) and the reality of ϕ one has

$$\vartheta T(\mathbf{z}^{s-1})\vartheta=\exp[-2\pi i\phi(-\mathbf{z}^{s-1})]f$$
$$=\exp[-2\pi i\phi(\mathbf{z}^{s-1})]f ,$$

which proves (3.64). Now (3.64) implies $p_j=0$ in (3.63). Indeed, for example,

$$\phi(-\tfrac{1}{2},0,\ldots,0)=\psi(-\tfrac{1}{2},0,\ldots,0)-p_1/2$$
$$=\psi(\tfrac{1}{2},0,\ldots,0)+p_1/2 ,$$

and the periodicity of ψ implies $p_1=0$. This completes the proof of (3.57). Suppose now (3.45) holds true. Then from (3.54) it follows that

$$IT(\mathbf{z}^{s-1})I=T(-\mathbf{z}^{s-1})^{-1} ,$$

which, together with (3.65), implies

$$I\vartheta T(\mathbf{z}^{s-1})\vartheta I=T(\mathbf{z}^{s-1}) . \quad (3.67)$$

Since $I\vartheta$ is an involution and $[I\vartheta,Q(\mathbf{z})]=0$, if $f\in Q(\mathbf{z})\mathcal{H}$ then $I\vartheta f=\pm f$, which, together with (3.56) and (3.67) implies that $\lambda(\mathbf{z}^{s-1})$ is real. Since λ is of modulus 1 for real $\mathbf{z}^{s-1}$, it follows that $\lambda(\mathbf{z}^{s-1})$ is actually constant: $\lambda(\mathbf{z}^{s-1})=\pm 1$, whereof $\phi(\mathbf{z}^{s-1})$ is either identically zero or equal to π. From this and (3.54) one obtains

$$IA_s(\mathbf{z})IQ(\mathbf{z}^{s-1},0)=\pm\exp(i\pi\beta_sz_s)A_s(-\mathbf{z})Q(\mathbf{z}^{s-1},0) , \quad (3.68)$$

where β_s equals either zero or 1. Combining (3.68) with (3.62), one obtains (3.46).■

Proof of Theorem 3.5. Consider

$$\tilde{\chi}_0(\mathbf{k})=A(\mathbf{k})\chi_0 ,$$

where χ_0 is a normalized vector in $P_0(\mathbf{0})\mathcal{M}$ and $A(\mathbf{k})$ is a solution of Problem C applied to $\tilde{P}_0(\mathbf{k})$. From $\dim P_0(\mathbf{0})=1$ and from (3.30) and (3.31) it follows that $\vartheta\chi_0=\pm\chi_0$, $I\chi_0=\pm\chi_0$. If $\vartheta\chi_0=-\chi_0$ replace χ_0 by $i\chi_0$. In other words, one can chose χ_0 such that

$$\vartheta\chi_0=\chi_0 , \quad I\chi_0=\pm\chi_0 . \quad (3.69)$$

Obviously $\chi_0(\mathbf{k})$ is analytic and periodic in $\mathcal{J}_a^n$. Writing $i\pi\sum_1^n\beta_jk_j=i\mathbf{a}_0\cdot\mathbf{k}$, (3.35) and (3.36) follow from (3.44) and (3.45) and (3.69).■

The proof of Theorems 3.6.ii and 3.6.iii is similar.

Remark. Theorem C.i.a implies the existence of analytic and periodic quasi-Bloch functions in the tight-binding limit where (3.42) for $P_0(\mathbf{k})$ holds true. Moreover, if the crystal has a center of inversion (3.35) and (3.36) are fulfilled with $\mathbf{a}_0=\mathbf{0}$ (see also des Cloizeaux, 1964). Actually, the existence of analytic and periodic quasi-Bloch functions can be proved for complex bands outside the tight-binding limit by the use of a "continuity" argument based on the following.

Proposition 3.1. *Suppose that $Q_i(\mathbf{z})$, $i=1,2$ satisfy (3.37) and (3.38), and that Problem C for $Q_1(\mathbf{z})$ has a solution. Then if*

$$\sup_{z\in\mathcal{J}_a^n}\|Q_1(\mathbf{z})-Q_2(\mathbf{z})\|<1 ,$$

Problem C for $Q_2(\mathbf{z})$ has a solution.

Proof. Apply the Nagy formula (3.47).■

Consider now

$$\hat{P}_0=\int_B^{\oplus}P_0(\mathbf{k})d\mathbf{k} ,$$

i.e.,

$$\hat{P}_0\mathcal{H}=\{f(\mathbf{k})|f(\mathbf{k})=c(\mathbf{k})\chi_0(\mathbf{k}) , \ c(\mathbf{k})\in L^2(B,d\mathbf{k})\} .$$

There are two distinguished based in $\hat{P}_0\mathcal{H}$. The first one (which is actually a basis in generalized sense) is

$$\{\hat{\psi}_{\mathbf{k}_0}(\mathbf{k})\}_{\mathbf{k}_0\in B}=\{\delta(\mathbf{k}-\mathbf{k}_0)\chi_0(\mathbf{k})\}_{\mathbf{k}_0\in B} \ . \tag{3.70}$$

The second one is

$$\{\hat{w}_a(\mathbf{k})\}_{\mathbf{a}\in\Gamma}=\{\exp(i\mathbf{k}\cdot\mathbf{a})\chi_0(\mathbf{k})\}_{\mathbf{a}\in\Gamma} \ . \tag{3.71}$$

The orthonormality of $\hat{w}_{\mathbf{a}}$ comes from

$$(\exp(i\mathbf{k}\cdot\mathbf{a})\chi_0(\mathbf{k}),\exp(i\mathbf{k}\cdot\mathbf{b})\chi_0(\mathbf{k}))=\exp[i\mathbf{k}\cdot(\mathbf{b}-\mathbf{a})]$$

and the completeness from the fact that

$$c(\mathbf{k})\chi_0(\mathbf{k})=\sum_{\mathbf{a}\in\Gamma}c_{\mathbf{a}}\exp(i\mathbf{k}\cdot\mathbf{a})\chi_0(\mathbf{k}) \ ,$$

where $c_{\mathbf{a}}$ are the Fourier coefficients of $c(\mathbf{k})$.

All the results above are written in the "momentum representation." We shall translate some of them in the "x representation." If $\mathbf{x}\in\mathbb{R}^n$ it can be uniquely written as

$$\mathbf{x}=\mathbf{a}_{\mathbf{x}}+r_{\mathbf{x}} \ , \quad \mathbf{a}_{\mathbf{x}}\in\Gamma \ , \quad \mathbf{r}_{\mathbf{x}}=\sum_{j=1}^{n}r_j\mathbf{a}_j \ , \quad -\tfrac{1}{2}<r_j\le\tfrac{1}{2} \ .$$

Obviously [see (3.13)], $\{S^{-1}\hat{\psi}_{\mathbf{k}}\}_{\mathbf{k}\in B}$ is a generalized basis in $P_0L^2(\mathbb{R}^n)$ and $\{S^{-1}\hat{w}_{\mathbf{a}}\}_{\mathbf{a}\in\Gamma}$ is an orthonormal basis in $P_0L^2(\mathbb{R}^n)$.

Theorem 3.7.i.

$$(S^{-1}\hat{\psi}_{\mathbf{k}})(\mathbf{x})\equiv\psi_{0,\mathbf{k}}(\mathbf{x})=(2\pi)^{-n/2}(\mathrm{vol}Q)^{1/2}\exp(i\mathbf{k}\cdot\mathbf{x})u_{\mathbf{k}}(\mathbf{r}_{\mathbf{x}})$$
$$=(2\pi)^{-n/2}(\mathrm{vol}Q)^{1/2}\exp(i\mathbf{a}_{\mathbf{x}}\cdot\mathbf{k})\exp(i\mathbf{r}_{\mathbf{x}}\cdot\mathbf{k})u_{\mathbf{k}}(\mathbf{r}_{\mathbf{x}})\equiv\exp(i\mathbf{a}_{\mathbf{x}}\cdot\mathbf{k})\tilde{u}_{\mathbf{k}}(\mathbf{r}_{\mathbf{x}}) \ , \tag{3.72}$$

where $u_{\mathbf{k}}\in L^2(Q)$, $\|u_{\mathbf{k}}\|=1$. As a family of vectors in $L^2(Q)$, $\tilde{u}_{\mathbf{k}}$ is the restriction to $\mathbb{R}^n$ of a vector-valued function analytic in $\mathcal{J}_a^n$.

ii.

$$(S^{-1}\hat{w}_{\mathbf{a}})(\mathbf{x})\equiv w_{\mathbf{a}}(\mathbf{x})=w(\mathbf{x}-\mathbf{a})=(T_{\mathbf{a}}w)(\mathbf{x}) \ , \tag{3.73}$$

where

$$w(\mathbf{x})\equiv(S^{-1}w_0)(\mathbf{x}) \tag{3.74}$$

has the properties

$$\overline{w(\mathbf{x})}=w(\mathbf{x}) \ , \tag{3.75}$$

$$w(-x)=\pm w(\mathbf{x}-\mathbf{a}_0) \quad \text{for some } \mathbf{a}_0\in\Gamma \tag{3.76}$$

and for $0\le b<a$ and arbitrarily fixed constants α_j

$$\exp(b|\mathbf{x}|)\left[1+\sum_{j=1}^{n}\alpha_j\partial/\partial x_j\right]w(\mathbf{x})\in L^2(\mathbb{R}^n) \ . \tag{3.77}$$

Proof. From (3.13) it follows that for $f\in\mathcal{H}$

$$(S^{-1}f)(\mathbf{x})=(2\pi)^{-n/2}\sum_{\mathbf{g}}\exp(i\mathbf{g}\cdot\mathbf{x})\int_B\exp(i\mathbf{k}\cdot\mathbf{x})f_{\mathbf{g}}(\mathbf{k})d\mathbf{k} \ . \tag{3.78}$$

Consequently, the "subspace" $\mathcal{M}_{\mathbf{k}_0}=\{\delta(\mathbf{k}-\mathbf{k}_0)f\,|\,f\in\mathcal{M}\}$ corresponds to $\mathcal{H}_{\mathbf{k}_0}=\{f(\mathbf{x})|f(\mathbf{x})=\exp(i\mathbf{k}_0\cdot\mathbf{x})u(\mathbf{x})$; $u(\mathbf{x})=u(\mathbf{x}+\mathbf{a})$, $\mathbf{a}\in\Gamma\}$: $S^{-1}\mathcal{M}_{\mathbf{k}_0}=\mathcal{H}_{\mathbf{k}_0}$. In particular,

$$(S^{-1}\hat{\psi}_{\mathbf{k}_0})(\mathbf{x})=(2\pi)^{-n/2}(\mathrm{vol}Q)^{1/2}\exp(i\mathbf{k}_0\cdot\mathbf{x})u_{\mathbf{k}_0}(\mathbf{r}_{\mathbf{x}}) \ , \tag{3.79}$$

where

$$u_{\mathbf{k}_0}(\mathbf{r}_{\mathbf{x}})=(\mathrm{vol}Q)^{-1/2}\sum_{\mathbf{g}\in\hat{\Gamma}}\exp(i\mathbf{g}\cdot\mathbf{r}_{\mathbf{x}})\chi_{0,\mathbf{g}}(\mathbf{k}_0) \ . \tag{3.80}$$

Let $A:L^2(Q)\to\mathcal{M}$ defined by

$$(Au)_{\mathbf{g}}=(\mathrm{vol}Q)^{1/2}\hat{u}_{\mathbf{g}} \ , \tag{3.81}$$

where

$$\hat{\mathbf{u}}_{\mathbf{g}}=(\mathrm{vol}Q)^{-1}\int_Q\exp(-i\mathbf{g}\cdot\mathbf{r})u(\mathbf{r})d\mathbf{r}$$

are the Fourier coefficients of u. Then (3.80) can be rewritten as

$$Au_{\mathbf{k}_0}=\chi_0(\mathbf{k}_0) \ . \tag{3.82}$$

Consider now that the operators R_j in $L^2(Q)$:

$$(R_ju)(\mathbf{r})=2\pi r_ju(\mathbf{r}) \quad (\mathbf{r}=\textstyle\sum r_j\mathbf{a}_j) \ . \tag{3.83}$$

A simple computation shows that [see (3.15) and (3.16)]

$$A^{-1}W_jA=\exp(iA^{-1}C_jA)=\exp(iR_j) \ ,$$
$$j=1,2,\ldots,n \ ,$$

whereof $A^{-1}C_jA=R_j$ and then

$$A^{-1}W(\mathbf{k})A=\exp\left[i\sum_{j=1}^{n}k_jR_j\right] \ . \tag{3.84}$$

Note that the right-hand side of (3.84) is nothing but the operator of multiplication with $\exp(i\mathbf{k}\cdot\mathbf{r})$. From (3.32), (3.82), and (3.84)

$$A^{-1}\tilde{\chi}_0(\mathbf{k})=A^{-1}W(\mathbf{k})AA^{-1}\chi_0(\mathbf{k})=\tilde{u}_{\mathbf{k}} \ . \tag{3.85}$$

From (3.85) and Theorem 3.5 it follows that, as a family of vectors in $L^2(Q)$, $\tilde{u}_{\mathbf{k}}$ is analytic in $\mathcal{J}_a^n$ and the proof of Theorem 3.7.i is finished.

Consider $\hat{w}(\mathbf{p})$, $\mathbf{p}\in\mathbb{R}^n$, given by

$$\hat{w}(\mathbf{k}+\mathbf{g})=\chi_{0,\mathbf{g}}(\mathbf{k}) \ . \tag{3.86}$$

From the definition of $\hat{w}(\mathbf{p})$ and Theorem 3.5, it follows that $\hat{w}(\mathbf{p})$ is the restriction to $\mathbb{R}^n$ of a function analytic in $\mathcal{J}_a^n$. From Theorem 3.2 and the fact that $\chi_0(\mathbf{k})\in\mathcal{D}(H_0(\mathbf{k}))$, it follows that

$$\sup_{|\mathbf{q}|\le b<a}\sum_{\mathbf{g}}\int_B(1+|\mathbf{k}+\mathbf{g}+i\mathbf{q}|^2)|\chi_{0,\mathbf{g}}(\mathbf{k}+i\mathbf{q})|^2d\mathbf{k}<\infty \ ,$$

whereof for arbitrarily fixed constants α_j, $(1+\sum_1^n \alpha_j p_j)\hat{w}(\mathbf{p})$ is analytic in $\mathcal{J}_a^n$ and

$$\sup_{|\mathbf{q}|\le b<a} \int_{\mathbb{R}^n} \left| \left[1+\sum_1^n \alpha_j(p_j+iq_j) \right] \hat{w}(\mathbf{p}+i\mathbf{q}) \right|^2 d\mathbf{p} < \infty \ . \tag{3.87}$$

By definition and (3.78)

$$w(\mathbf{x}) \equiv w_0(\mathbf{x}) = (S^{-1}\hat{w}_0)(\mathbf{x}) = (2\pi)^{-n/2} \sum_{\mathbf{g}} \int_B \exp[i\mathbf{x}\cdot(\mathbf{g}+\mathbf{k})]\chi_{0,\mathbf{g}}(\mathbf{k})d\mathbf{k} = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \exp(i\mathbf{x}\cdot\mathbf{p})\hat{w}(\mathbf{p})d\mathbf{p} \ ,$$

which together with (3.87) proves (3.77), due to the Paley-Wiener theorem (Paley and Wiener, 1934).

Now, by (3.35) and (3.36),

$$\overline{w(\mathbf{x})} = (2\pi)^{-n/2} \sum_{\mathbf{g}} \int_B \exp[-i\mathbf{x}\cdot(\mathbf{g}+\mathbf{k})]\chi_{0,-\mathbf{g}}(-\mathbf{k})d\mathbf{k} = w(\mathbf{x}) \ ,$$

$$w(-\mathbf{x}) = (2\pi)^{-n/2} \sum_{\mathbf{g}} \int_B \exp[-i(\mathbf{x}-\mathbf{a}_0)\cdot(\mathbf{g}+\mathbf{k})]\chi_{0,-\mathbf{g}}(-\mathbf{k})d\mathbf{k} = w(\mathbf{x}-\mathbf{a}_0) \ .$$

Finally

$$w_{\mathbf{a}}(\mathbf{x}) = (S^{-1}\hat{w}_{\mathbf{a}})(\mathbf{x}) = (2\pi)^{-n/2} \sum_{\mathbf{g}} \int_B \exp[i(\mathbf{x}-\mathbf{a})\cdot(\mathbf{g}+\mathbf{k})\chi_{0,\mathbf{g}}(\mathbf{k})d\mathbf{k} = w(\mathbf{x}-\mathbf{a}) = (T_{\mathbf{a}}w)(\mathbf{x}) . \blacksquare$$

Corollary 3.1.i.

$$H_0 w_{\mathbf{a}} = \sum_{\mathbf{b}\in\Gamma} h_0(\mathbf{a}-\mathbf{b})w_{\mathbf{b}} \tag{3.88}$$

with

$$h_0(\mathbf{a}) = (\mathrm{vol}B)^{-1/2} \int_B \exp(-i\mathbf{k}\cdot\mathbf{a})\lambda_0(\mathbf{k})d\mathbf{k} \ . \tag{3.89}$$

ii. $P_0 H_0 P_0$ is unitary equivalent to the following operator in $l^2(\Gamma)$:

$$H_{0,\mathrm{eff}} f(\mathbf{a}) = \sum_{\mathbf{b}\in\Gamma} h_0(\mathbf{b}-\mathbf{a})f(\mathbf{b}) = \sum_{\mathbf{b}\in\Gamma} h_0(\mathbf{a}-\mathbf{b})f(\mathbf{b}) \ . \tag{3.90}$$

Proof. Straightforward verification. The unitary equivalence is given by $Uf(\mathbf{a}) = \langle w_{\mathbf{a}}, f \rangle$. The last equality in (3.90) follows from the fact that both H_0 and w are real.

Suppose now that the crystal has a center of inversion and that $\mathbf{a}_0 \neq \mathbf{0}$. Let us shift the origin in $\mathbb{R}^3$ in the point $-\mathbf{a}_0/2$. This amounts to considering, instead of H_0, the Hamiltonian $T_{\mathbf{a}_0/2} H_0 T_{-\mathbf{a}_0/2}$. If 0 is the operator given by

$$Of(\mathbf{x}) = f(-\mathbf{x}) \ ,$$

then as one can easily see

$$OT_{\mathbf{c}} = T_{-\mathbf{c}} O \ , \tag{3.91}$$

which implies, taking into account that $[H_0, T_{\mathbf{a}_0}] = 0$,

$$[O, T_{\mathbf{a}_0/2} H_0 T_{-\mathbf{a}_0/2}] = O \ ,$$

i.e., $T_{\mathbf{a}_0/2} H_0 T_{-\mathbf{a}_0/2}$ still has a center of inversion. Moreover, the Wannier function of $T_{\mathbf{a}_0/2} H_0 T_{-\mathbf{a}_0/2}$ corresponding to σ_0 is $T_{\mathbf{a}_0/2} w$, and from (3.91) and (3.76)

$$OT_{\mathbf{a}_0/2} w = T_{-\mathbf{a}_0/2} O w = \pm T_{\mathbf{a}_0/2} w \ . \tag{3.92}$$

In other words, by an appropriate choice of the origin one can take $\mathbf{a}_0 = \mathbf{0}$ in (3.76). As a consequence, without restricting the generality, we shall consider in Sec. V that for crystals with a center of inversion one can choose the Wannier function w such that

$$w(\mathbf{x}) = \pm w(-\mathbf{x}) \ . \tag{3.93}$$

IV. THE ELECTRIC-FIELD CASE

A. The deformed-band subspaces

Consider the Hamiltonian

$$-\Delta + V(\mathbf{x}) + F\mathbf{n}\cdot\mathbf{x} = H_0 + FX_0 = H_F \ , \tag{4.1}$$

where $\mathbf{n}$ is the unit vector along the field direction. Actually, the theory below applies to the more general case of nonhomogeneous but still slowly varying fields (see remark below).

The problem at hand is an example of the general theory of asymptotic invariant subspaces as developed by Nenciu (1981).

Definition 4.1. *Let $H_\varepsilon, P_\varepsilon, \varepsilon \ge 0$ be families of self-adjoint and orthogonal projections, respectively, in a Hilbert space $\mathcal{H}$ satisfying the following conditions:*

i. $\lim_{\varepsilon\to 0} \|P_\varepsilon - P_0\| = 0.$ (4.2)

ii. *Let p be a positive integer. There exist $b_p < \infty$, $\varepsilon_p > 0$, and bounded self-adjoint operators B_ε defined for $\varepsilon \in [0, \varepsilon_p]$ such that*

$$\|B_\varepsilon\| \le b_p \varepsilon^p \tag{4.3}$$

and $P_\varepsilon \mathcal{H}$ are invariant subspaces for $H_\varepsilon - \varepsilon B_\varepsilon$. Then $P_\varepsilon \mathcal{H}$ is said to be asymptotically invariant family of subspaces of order p for H_ε.

As expected $P_\varepsilon\mathcal{H}$ are almost invariant under the evolution given by H_ε.

Proposition 4.1. *Suppose H_ε has an asymptotically invariant family of subspaces of order p. Then*

$$\|(1-P_\varepsilon)\exp(-iH_\varepsilon t)P_\varepsilon\| \le b_p \varepsilon^{p+1}|t| \; . \tag{4.4}$$

In particular, if $H_\varepsilon - \varepsilon B_\varepsilon$ has a normalized eigenvector ϕ_ε, then

$$|\langle \phi_\varepsilon, \exp(-iH_\varepsilon t)\phi_\varepsilon\rangle| \ge 1 - b_p \varepsilon^{p+1}|t| \; . \tag{4.5}$$

Proof. The inequalities (4.4) and (4.5) follow from Definition 4.1 and

$$\exp(-iH_\varepsilon t) = \exp[-i(H_\varepsilon - \varepsilon B_\varepsilon)t] - i\varepsilon \int_0^t \exp[-i(H_\varepsilon - \varepsilon B_\varepsilon)(t-s)] \times B_\varepsilon \exp(-iH_\varepsilon s)ds . \blacksquare \tag{4.6}$$

Suppose now that H_ε is of the form $H_0 + \varepsilon X_0$. The problem is to find conditions on the pair H_0, X_0 under which one can prove the existence of asymptotically invariant subspaces for H_ε.

Theorem 4.1. *Suppose that*

i. *$H_\varepsilon = H_0 + \varepsilon X_0$ is essentially self-adjoint on $\mathcal{D}(H_0)\cap\mathcal{D}(X_0)$.*

ii. *$\exp(iX_0 t)(H_0 - i)^{-1}\exp(-iX_0 t)$ is $p+1$ times norm differentiable.*

iii. *There exist $-\infty < \lambda_1 < \lambda_2 < \infty$ such that $\sigma(H_0) = \sigma_0 \cup \sigma_1$, $\sigma_0 \subset [\lambda_1, \lambda_2]$, $\mathrm{dist}(\sigma_0, \sigma_1) = d > 0$.*

Let P_0 be the spectral projection of H_0 corresponding to σ_0. Then $P_q\mathcal{H}$, $q = 1, 2, \ldots, p$, constructed below [see also (2.4)–(2.7)] are asymptotically invariant families of subspaces of order q for H_ε.

Proof. Having in mind the problem at hand, we shall consider the case $p = \infty$. The proof is by construction. Consider $H_0(t) = \exp(i\varepsilon X_0 t)H_0 \exp(-i\varepsilon X_0 t)$. It is not hard to see that its resolvent $R_0(t;z)$ and the spectral projection corresponding to σ_0, $P_0(t)$ are infinitly norm differentiable, and that there exist finite constants $r_{0,m}$, $c_{0,m}$ such that

$$\|(d^m/dt^m)R_0(t;z)\| \le r_{0,m}\varepsilon^m \; , \tag{4.7}$$

$$\|(d^m/dt^m)P_0(t)\| \le c_{0,m}\varepsilon^m \; . \tag{4.8}$$

Indeed, for $z = i$, (4.7) holds by hypothesis. For arbitrary $z \in \rho(H_0)$, one has to use the identity

$$R_0(t;z) = R_0(t;z_0)[1 + (z - z_0)R_0(t;z_0)]^{-1} \; .$$

The inequality (4.8) follows from (4.7) and the Riesz formula for the spectral projection.

Let $K_0(t)$, $A_0(t)$ be as given by the Lemma A1 (see the Appendix) applied to $P_0(t)$ and

$$B_0 = -\varepsilon^{-1}K_0(0) \; . \tag{4.9}$$

Note that, by construction,

$$B_0 = (1 - 2P_0)[X_0, P_0] \; , \tag{4.10}$$

and that

$$\|B_0\| \le c_{0,1} \; .$$

Consider the self-adjoint operator

$$X_1 = X_0 - B_0 \; . \tag{4.11}$$

By the Stone theorem, for all $f \in \mathcal{D}(X_0)$,

$$(id/dt)[\exp(i\varepsilon X_0 t)\exp(-i\varepsilon X_1 t)]f = K_0(t)\exp(i\varepsilon X_0 t)\exp(-i\varepsilon X_1 t)f$$

which together with Lemma A.1 implies

$$A_0(t) = \exp(i\varepsilon X_0 t)\exp(-i\varepsilon X_1 t) \; . \tag{4.12}$$

From (4.12) and Lemma A.1 one has

$$P_0 = \exp(i\varepsilon X_1)P_0 \exp(-i\varepsilon X_1) \; ,$$

which implies that, for $f \in \mathcal{D}(X_0)\cap\mathcal{D}(H_0)$,

$$P_0(H_0 + \varepsilon X_1)f - (H_0 + \varepsilon X_1)P_0 f = 0 \; .$$

Since $H_0 + \varepsilon X_1 = H_\varepsilon - \varepsilon B_0$ is essentially self-adjoint on $\mathcal{D}(X_0)\cap\mathcal{D}(H_0)$, it follows that

$$[P_0, \exp\{-i(H_\varepsilon - \varepsilon B_0)t\}] = 0 \; . \tag{4.13}$$

Consider now $H_1(t)$ given by

$$H_1(t) = A_0(t)^*[H_0(t) - K_0(t)]A_0(t) \; . \tag{4.14}$$

From the identity

$$R_1(t;z) = A_0(t)^* R_0(t;z)[1 - K_0(t)R_0(t;z)]^{-1}A_0(t) \tag{4.15}$$

and from the fact that $R_0(t;z)$ is infinitely norm differentiable, it follows that $R_1(t;z)$ is infinitely norm differentiable. Note that if H_1 is defined by [see (2.3)]

$$H_1 = H_0 + \varepsilon B_0$$

then

$$H_1(t) = \exp(i\varepsilon X_1 t)H_1 \exp(-i\varepsilon X_1 t) \; , \quad H_\varepsilon = H_1 + \varepsilon X_1 \; .$$

For $\varepsilon < \varepsilon_0 \equiv d/2\|B_0\|$ the spectrum of H_1 is still separated, and we can repeat the whole construction. Obviously one can continue this process indefinitely. Namely, for $q = 0, 1, \ldots,$ starting from H_ε written in the form

$$H_\varepsilon = H_q + \varepsilon X_q \; ,$$

where $\sigma(H_q) = \sigma_{0,q} \cup \sigma_{1,q}$, $\mathrm{dist}(\sigma_{0,q}, \sigma_{1,q}) \equiv d_q > 0$ ($\sigma_{0,q}$ coincide with σ_0 in the limit $\varepsilon \to 0$), we define

P_q = the spectral projection of H_q corresponding to $\sigma_{0,q}$,

$$\begin{aligned}
&H_q(t)=\exp(i\varepsilon X_q t)H_q\exp(-i\varepsilon X_q t)\ ,\\
&P_q(t)=\exp(i\varepsilon X_q t)P_q\exp(-i\varepsilon X_q t)\ ,\\
&K_q(t)=i[1-2P_q(t)](d/dt)P_q(t)\ ,\\
&B_q=-\varepsilon^{-1}K_q(0)\ ,\quad H_{q+1}=H_q+\varepsilon B_q\ ,\quad X_{q+1}=X_q-B_q\ .
\end{aligned}\tag{4.16}$$

Obviously

$$H_\varepsilon=H_{q+1}+\varepsilon X_{q+1}\ ,$$

and the whole procedure can be carried further as far as

$$\varepsilon<\varepsilon_q\equiv\frac{d}{2}\left[\sum_{j=1}^{q}\|B_j\|\right]$$

(which assures that the spectrum of H_{q+1} is still separated). Since by construction

$$[P_q,\exp\{-i(H_\varepsilon-\varepsilon B_q)t\}]=0\ ,$$

the only thing we have to do in order to finish the proof of the theorem is to obtain bounds on $\|B_q\|$. The needed bounds are consequences of the following lemma.

Lemma 4.1. *Let C be a contour (of finite length) surrounding σ_0, satisfying* $\operatorname{dist}(C,\sigma_0)=d/2$. *Then there exist constants $r_{q,m}$, $c_{q,m}$, $q=0,1,2,\ldots$, $m=1,2,\ldots$, such that for $\varepsilon<\varepsilon_{q-1}$ (by definition $\varepsilon_{-1}=\infty$) and $z\in C$,*

$$\begin{aligned}
&\|(d^m/dt^m)R_q(t;z)\|\le r_{q,m}\varepsilon^m\ ,\\
&R_q(t;z)\equiv[H_q(t)-z]^{-1}\ ;
\end{aligned}\tag{4.17}$$

$$\|(d^m/dt^m)P_q(t)\|\le c_{q,m}\varepsilon^{m+q}\ .\tag{4.18}$$

Proof. The proof is by induction over n. The case $q=0$ is given by (4.7) and (4.8). Suppose (4.17) and (4.18) are true for $q-1$. Then (4.17) for q follows from an identity similar to (4.15), relating $R_q(t;z)$ and $R_{q-1}(t;z)$ and the induction hypothesis. For (4.18), observe that from

$$P_{q-1}(t)=A_{q-1}(t)P_{q-1}(0)A_{q-1}(t)^*$$

it follows that $P_{q-1}(0)$ is, for all $t\in\mathbb{R}$, the spectral projection of $A_{q-1}(t)^*H_{q-1}(t)A_{q-1}(t)$ corresponding to σ_{q-1}. Then one can write

$$P_q(t)-P_{q-1}(0)=(2\pi i)^{-1}A_{q-1}(t)^*\left\{\int_C[H_{q-1}(t)-K_{q-1}(t)-z]^{-1}K_{q-1}(t)R_{q-1}(t;z)dz\right\}A_{q-1}(t)\tag{4.19}$$

Now, (4.19) and the induction hypothesis implies (4.18) for q.■

From the definition of $K_q(t)$ and (4.18) for $m=1$ it follows that

$$\|B_q\|\le c_{q,1}\varepsilon^q\ ,$$

which finishes the proof of Theorem 4.1.■

Let us apply the above theory to (4.1) with the obvious identifications. According to Theorem X.38 in Reed and Simon (1978), (4.1) is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)\subset\mathcal{D}(H_0)\cap\mathcal{D}(X_0)$, so the hypothesis (i) of Theorem 4.1. is fulfilled. A simple computation $[G(t)=\exp(-iF\mathbf{n}\cdot\mathbf{x}t)]$ gives

$$H_0(t)\equiv G(t)H_0G(t)^*=(\mathbf{P}-F\mathbf{n}t)^2+V(\mathbf{x})\ ,$$

whereof the infinite differentiability of $[H_0(t)-z]^{-1}$ at $t=0$ is obvious. For an arbitrary t, observe that

$$(d^m/dt^m)R_0(t;z)=G(t)[(d^m/dt^m)R_0(t;z)]_{t=0}G(t)^*\ .$$

In particular,

$$[(d/dt)R_0(t;z)]_{t=0}=F(H_0-z)^{-1}\mathbf{P}\cdot\mathbf{n}(H_0-z)^{-1}\ .$$

The connection between the recurrent construction in the proof of Theorem 4.1. and the recurrent construction given by (2.2)–(2.8) is given by the well-known formula

$$i(d/dt)\exp(-iSt)T\exp(iSt)=\exp(-iSt)[S,T]\exp(iSt)\ .$$

From the definition of B_0,

$$\|B_0\|\le\pi^{-1}\left\|\int_C(H_0-z)^{-1}\mathbf{P}\cdot\mathbf{n}(H_0-z)^{-1}dz\right\|\ ,\tag{4.20}$$

where C is a contour enclosing σ_0. Formula (4.20) gives the means to estimate $\|B_0\|$. For details as well as for the estimations of $\|B_1\|$, $\|B_2\|$, we refer to Nenciu (1987).

Remark. Actually, the theory presented above does not require the homogeneity of the electric field. If instead of X_0 given by (4.1) we take

$$(X_0f)(\mathbf{x})=\Phi(\mathbf{x})f(\mathbf{x})\ ,$$

then, for example,

$$\|B_0\|\le(2\pi)^{-1}\left\|\int_C(H_0-z)^{-1}(\mathbf{P}\cdot\operatorname{grad}\Phi+\operatorname{grad}\Phi\cdot\mathbf{P})\times(H_0-z)^{-1}dz\right\|\ ,$$

so what is needed is the boundedness of the derivatives of the field energy. Even more, if $\Phi(\mathbf{x})=\Phi_1(\mathbf{x})+\Phi_2(\mathbf{x})$, where Φ_1 is uniform, locally L^2 and Φ_2 has bounded derivatives, then writing

$$H_F=H_0+F\Phi_1+F\Phi_2=\tilde{H}_0+F\Phi_2$$

one can develop the whole theory for the pair $\tilde{H}_0$, Φ_2.

B. The one-band Hamiltonian

In this subsection V is considered to be periodic. We shall consider the case in which $\mathbf{n}$ is parallel to one of the vectors of the dual basis, say $\mathbf{g}_1$. If $\mathbf{x}=\sum_{j=1}^3x_j\mathbf{a}_j$, then

$$X_0f(\mathbf{x})=(2\pi/|\mathbf{g}_1|)x_1f(\mathbf{x})\ .\tag{4.21}$$

We shall rewrite $\mathcal{H}$ (see Sec. III) as

$$\mathcal{H}=(\mathrm{vol}B)\int\int_{-1/2}^{1/2}\int \mathcal{M}\, dk_1 dk_2 dk_3 = (\mathrm{vol}B)\int\int_{-1/2}^{1/2} dk_2 dk_3 \mathcal{M}^{\#} , \tag{4.22}$$

where

$$\mathcal{M}^{\#}=\int_{-1/2}^{1/2}\mathcal{M}\, dk_1=\{f_{\mathbf{g}}(k_1)\}_{\mathbf{g}\in\hat{\Gamma},k_1\in[-\frac{1}{2},\frac{1}{2}]} . \tag{4.23}$$

We shall use the self-explanatory notation

$$\mathcal{H}=\int_{B_\perp}^{\oplus} M^{\#} dk_\perp , \tag{4.24}$$

$$H_0=\int_{B_\perp}^{\oplus} H^{\#}_{0,k_\perp} d\mathbf{k}_\perp . \tag{4.25}$$

Let $X_0^{\#}$ be the operator in $\mathcal{M}^{\#}$ given by

$$(X_0^{\#} f)_{\mathbf{g}}(k_1)=-i|\mathbf{g}_1|^{-1}(d/dk_1)f_{\mathbf{g}}(k_1) \tag{4.26}$$

with the domain

$$\mathcal{D}(X_0^{\#})=\{f_{\mathbf{g}}(k_1)|(d/dk_1)f_{\mathbf{g}}(k_1)\in\mathcal{M}^{\#} , \quad f_{\mathbf{g}}(\tfrac{1}{2})=f_{\mathbf{g}+\mathbf{g}_1}(-\tfrac{1}{2})\} . \tag{4.27}$$

Lemma 4.2.

$$SX_0S^{-1}=\int_{B_\perp}^{\oplus} X_0^{\#} d\mathbf{k}_\perp .$$

Proof. The Fourier transform $\hat{X}_0$ of X_0 is

$$\hat{X}_0=-i|\mathbf{g}_1|^{-1}\partial/\partial k_1 ,$$

and then taking into account (3.13), on $\mathcal{S}(\mathbb{R}^3)$

$$(SX_0S^{-1}f)_{\mathbf{g}}(\mathbf{k})=-i|\mathbf{g}_1|^{-1}(\partial/\partial k_1)f_{\mathbf{g}}(\mathbf{k})$$

and

$$f_{\mathbf{g}}(\mathbf{g}_1/2+k_2\mathbf{g}_2+k_3\mathbf{g}_3)=f_{\mathbf{g}+\mathbf{g}_1}(-\mathbf{g}_1/2+k_2\mathbf{g}+k_3\mathbf{g}_3) ,$$

which finishes the proof.■

The next remark is that

$$[B_q,T_{\mathbf{a}}]=0 , \quad q=0,1,2,3,\ldots , \tag{4.28}$$

where $T_{\mathbf{a}}$, $\mathbf{a}\in\Gamma$, is the translation operator $T_{\mathbf{a}}f(\mathbf{x})=f(\mathbf{x}-\mathbf{a})$. For $q=0$, (4.28) follows from (4.10), $[T_{\mathbf{a}},P_0]=0$, and $[X_0,T_{\mathbf{a}}]=\mathbf{n}\cdot\mathbf{a}T_{\mathbf{a}}$. By (4.16), $[H_1,T_{\mathbf{a}}]=0$, $[X_1,T_{\mathbf{a}}]=\mathbf{n}\cdot\mathbf{a}T_{\mathbf{a}}$, which gives (4.28) for $q=1$, etc.

Combining (4.25) with (4.26), one obtains the following.

Proposition 4.2.

$$SH_FS^{-1}=\int_{B_\perp}^{\oplus} H^{\#}_{F,\mathbf{k}_\perp} d\mathbf{k}_\perp , \tag{4.29}$$

where

$$H^{\#}_{F,\mathbf{k}_\perp}=H^{\#}_{0,\mathbf{k}_\perp}+FX_0^{\#} . \tag{4.30}$$

In what follows, we shall consider the spectral properties of $H^{\#}_{F,\mathbf{k}_\perp}$ at fixed $\mathbf{k}_\perp$, and for notational convenience we shall omit $\mathbf{k}_\perp$ as well as the index of k_1.

Applying the general theory to the pair $H_0^{\#}$, $X_0^{\#}$, one constructs $P_q^{\#}$, $B_q^{\#}$, $H_q^{\#}$, $X_q^{\#}$ such that

$$H_F^{\#}=H_q^{\#}+FX_{q+1}^{\#}+FB_q^{\#}\equiv H_q^{\#,W}+FB_q^{\#} , \tag{4.31}$$

$$[H_q^{\#,W},P_q^{\#}]=0 , \quad \|B_q^{\#}\|\le F^q b_q \quad \text{for } 0\le F\le F_q . \tag{4.32}$$

Remark. Since the above construction substantiates the ideas in Wannier (1960), we shall call $H_q^{\#,W}$ the Wannier Hamiltonian of order q. Note that, by construction,

$$H^{\#q}_{F,\mathrm{ob}}\equiv P_q^{\#}H_F^{\#}P_q^{\#}=P_q^{\#}H_q^{\#,W}P_q^{\#} .$$

Let $[L^2(-\frac{1}{2},\frac{1}{2})]^m$ be the Hilbert space

$$[L^2(-\tfrac{1}{2},\tfrac{1}{2})]^m = \left\{\{\phi_j(k)\}_{j=1}^m \,\Big|\, \sum_{j=1}^m \int_{-1/2}^{1/2}|\phi_j(k)|^2dk<\infty\right\} ,$$

and $(d/dk)_{\mathrm{per}}$ the usual first-order differential operator in $[L^2(-\frac{1}{2},\frac{1}{2})]^m$ with periodic boundary conditions.

Theorem 4.2. *For every $q=0,1,2,\ldots$, there exists a positive constant $a_q(F)$, $\lim_{F\to 0}a_q(F)=a$ (see Theorem 3.6), an $m\times m$ Hermitian matrix-valued function $Y_F^q(k)$, and a unitary operator, $Z:P_q^{\#}\mathcal{M}^{\#}\to[L^2(-\frac{1}{2},\frac{1}{2})]^m$ such that*

$$H^q_{F,\mathrm{eff}}=ZP_q^{\#}H_F^{\#}P_q^{\#}Z^{-1}=-iF|\mathbf{g}_1|^{-1}(d/dk)_{\mathrm{per}}+Y_F^q(k) , \tag{4.33}$$

and the matrix elements of $Y_F^q(k)$ are restrictions to $[-\frac{1}{2},\frac{1}{2}]$ of analytic functions in the strip $\mathcal{I}_{a_q^1}$, satisfying

$$Y_F^q(k)=Y_F^q(k+1) . \tag{4.34}$$

Moreover, $Y_F^q(k)$ have asymptotic expansions of any order in F. The asymptotic expansions of $Y_F^q(k)$ and $Y_F^{q+1}(k)$ coincide up to terms of order $O(F^{q+1})$. Up to the second order,

$$Y^q_{F;r,s}(k)=\langle\chi_r(k),H_0(k)\chi_s(k)\rangle_{\mathcal{M}} -iF|\mathbf{g}_1|^{-1}\langle\chi_r(k),d\chi_r(k)/dk\rangle_{\mathcal{M}}+\cdots , \tag{4.35}$$

where $\{\chi_r(k)\}$ is the basis in $P_0(k)\mathcal{M}$ given by Theorem 3.6.iii.

Remark. The main points of this theorem are the analyticity and periodicity properties of Y_F^q. At the nonrigorous level, simple bands, and $q=0$, the formula (4.33) is a familiar result (see, e.g., Callaway, 1974). The (4.33) is the main result of this section: it gives the effective one-band Hamiltonian for the electric case.

Proof. The proof consists essentially in writing $H^{\#q}_{\mathrm{ob}}$ in the "Bloch representation." Consider first the case $q=0$. Let $\{\chi_j(k)\}$ be the basis in $P_0(k)\mathcal{M}$ given by Theorem 3.6 and $\tilde{\chi}_j(k)=W(k)\chi_j(k)$. If $\psi\in P_0^\# \mathcal{M}^\#$, then

$$\psi(k)=\sum_{s=1}^{m} c_s(k)\chi_s(k) ,$$

where

$$c_s(k)=\langle \chi_s(k),\psi(k)\rangle_{\mathcal{M}} .$$

Define Z by

$$(Z\psi)_s(k)=c_s(k) . \tag{4.36}$$

The only thing we have to do is to compute $ZP_0^\# H_F^\# P_0^\# Z^{-1}$. Observe first that, because of Theorem 3.6.iii and the definition of $W(k)$,

$$\chi_{j,\mathbf{g}}(1/2)=\chi_{j,\mathbf{g}+\mathbf{g}_1}(-1/2) ,$$

which together with (4.27) and (4.36) implies that $\psi\in\mathcal{D}(X_0^\#)$ if and only if $c_j(k)$ are in the domain of $(d/dk)_{\mathrm{per}}$. A straightforward computation using Lemma 4.2 gives

$$\begin{aligned}(ZP_0^\# H_F^\# P_0^\# Z^{-1}c)_j(k)&=-iF|\mathbf{g}_1|^{-1}dc_j(k)/dk+\sum_{r=1}^{m}\langle \chi_j(k),[H_0(k)-F|\mathbf{g}_1|^{-1}d/dk]\chi_r(k)\rangle_{\mathcal{M}}c_r(k)\\ &=-iF|\mathbf{g}_1|^{-1}dc_j(k)/dk+\sum_{r=1}^{m}\langle \tilde{\chi}_j(k),[\tilde{H}_0(k)+F|\mathbf{g}_1|^{-1}C_1-iF|\mathbf{g}_1|^{-1}d/dk]\tilde{\chi}_r(k)\rangle_{\mathcal{M}}c_r(k) ,\end{aligned} \tag{4.37}$$

which together with Theorem 3.6.iii and Lemma 3.1 proves (4.33) for $q=0$.

Consider now

$$B_0^\# =(1-2P_0^\#)[X_0^\#,P_0^\#] .$$

A computation similar to the above one (Nenciu and Nenciu, 1982) leads to the conclusion that

$$B_0^\# =\int_{-1/2}^{1/2} B_0(k)dk ,$$

and $\tilde{B}_0(k)=W(k)B_0(k)W(k)^{-1}$ is the restriction to $[-\frac{1}{2},\frac{1}{2}]$ of an operator-valued function analytic and periodic in $\mathcal{J}_a^1$. Then

$$H_1^\# =\int_{-1/2}^{1/2}[H_0(k)+FB_0(k)]dk\equiv\int_{-1/2}^{1/2}H_1(k)dk$$

and the whole construction can be repeated starting from $H_1(k)$ instead of $H_0(k)$: by Theorem 3.6.iii one constructs an analytic and periodic basis in $P_1(k)\mathcal{M}$, etc. If, at the qth step, $\{\chi_j^q(k)\}$ is the basis in $P_q(k)\mathcal{M}$ given by Theorem 3.6.iii, then

$$\begin{aligned}Y_{F;r,s}^q(k)=\langle \tilde{\chi}_r^q(k),[\tilde{H}_0(k)+F|\mathbf{g}_1|^{-1}C_1\\ -iF|\mathbf{g}_1|^{-1}d/dk]\tilde{\chi}_s^q(k)\rangle_{\mathcal{M}} .\end{aligned} \tag{4.38}$$

The existence of the asymptotic expansion for $Y_F^q(k)$ follows from the fact that, during the above construction, only the regular perturbation theory is used. Moreover, due to the fact that at the qth step the perturbation is of order $O(F^q)$, the coefficients of the lower powers of F remain unchanged. Since in $H_1(k)=H_0(k)+FB_0(k)$ the perturbation $FB_0(k)$ is off-diagonal, up to terms of order F^2,

$$Y_{F;r,s}^1(k)=\langle \chi_r(k),[H_0(k)-iF|\mathbf{g}_1|^{-1}d/dk]\chi_s(k)\rangle_{\mathcal{M}} ,$$

which gives (4.35).

Remark. Suppose that the crystal has a center of inversion. Then from Theorem 3.5 (according to the discussion at the end of Sec. III, one can take $\mathbf{a}_0=\mathbf{0}$),

$$\overline{\chi_{0,\mathbf{g}}(k)}=\pm\chi_{0,\mathbf{g}}(k) ,$$

and then

$$2\langle \chi_0(k),d\chi_0(k)/dk\rangle_{\mathcal{M}}=d\langle \chi_0(k),\chi_0(k)\rangle/dk=0 ,$$

i.e., for crystals with a center of inversion, the coefficient of the linear term in the asymptotic expansion of Y_F^q vanishes.

The spectral properties of $H_{F,\mathrm{eff}}^q$ are very simple. In order not to obscure the very simplicity of the problem, let us consider first the simple band case (Avron, 1979).

Proposition 4.1. *Suppose* $m=1$. *Then*

$$\sigma(H_{F,\mathrm{eff}}^q)=\{\lambda_{F,r}^q=2\pi F|\mathbf{g}_1|^{-1}r+c_F^q|r=0,\pm1,\pm2,\ldots\} , \tag{4.39}$$

where

$$c_F^q=\int_{-1/2}^{1/2}Y_F^q(k)dk . \tag{4.40}$$

All the eigenvalues are nondegenerate and the corresponding eigenvectors are

$$\psi_{F,r}^q(k)=\exp[-iF^{-1}|\mathbf{g}_1|g_F^q(k)]\exp(2\pi irk) , \tag{4.41}$$

where

$$g_F^q(k)=\int_{-1/2}^{k}[Y_F^q(k)-c_F^q]dk . \tag{4.42}$$

Proof. Observe first that $g_F^q(k)$ is analytic and periodic in $\mathcal{J}_{a_q}^1$. Consider the gauge transformation

$$Gf(k)=\exp[-iF^{-1}|\mathbf{g}_1|g_F^q(k)]f(k) . \tag{4.43}$$

The point is that the domain of $(d/dk)_{\mathrm{per}}$ is invariant under the action of G. A simple computation gives

$$G^* H^q_{F,\mathrm{eff}} G = -iF|\mathbf{g}_1|^{-1}(d/dk)_{\mathrm{per}} + c^q_F \ , \tag{4.44}$$

whereof (4.39) and (4.41) are obvious.■

The general case, $m>1$, is similar, but the gauge transformation cannot be constructed explicitly. Let $N(k)$ be the solution of the differential equation

$$-iF|\mathbf{g}_1|^{-1} dN(k)/dk = -Y^q_F(k)N(k) \ , \quad N(-\tfrac{1}{2})=1 \tag{4.45}$$

and $M=N(\frac{1}{2})$ the monodromy matrix of (4.45). Since $M^*=M^{-1}$, it can be written as

$$M=\exp(iD) \ , \quad D=D^* \ , \quad \|D\| \le \pi \ . \tag{4.46}$$

Consider, instead of (4.43),

$$Gf(k)=N(k)\exp(ikD)f(k) \ . \tag{4.47}$$

By direct computation

$$G^* H^q_{F,\mathrm{eff}} G = -iF|\mathbf{g}_1|^{-1}[(d/dk)_{\mathrm{per}}+D] \ . \tag{4.48}$$

By construction, $G(k)$ is the restriction to $[-\frac{1}{2},\frac{1}{2}]$ of a matrix-valued function analytic and periodic in $\mathcal{J}^1_{a_q}$. Summarizing the above discussion one obtains the following.

Theorem 4.3. *Let* $2\pi d_j$, ψ_j *be the eigenvalues and an orthonormal system of eigenvectors of D, respectively. Then*

$$\sigma(H^q_{F,\mathrm{eff}}) = \{\lambda_{r,j} = 2\pi F|\mathbf{g}_1|^{-1}(r+d_j) \,|\, r=0,\pm 1,\dots, j=1,\dots,m\} \ ,$$

and

$$\psi_{r,j}(k)=\exp(2\pi irk)G(k)\psi_j$$

is an eigenvector of $H^q_{F,\mathrm{eff}}$ *corresponding to* $\lambda_{r,j}$.

All the theory above has been done at some fixed $\mathbf{k}_\perp = \mathbf{k}_{\perp,0}$. Writing again all indices, the eigenvectors are

$$\psi_{r,j}(k_1;\mathbf{k}_\perp)=\delta(\mathbf{k}_\perp-\mathbf{k}_{\perp,0})\psi_{r,j}(k_1) \ . \tag{4.49}$$

A repetition of the argument in the proof of Theorem 3.7. gives the following.

Proposition 4.2.

$$S^{-1}\psi_{r,j}(\mathbf{x})=\exp[2\pi i(k_{0,2}x_2+k_{0,3}x_3)]u_{\mathbf{k}_{\perp,0};r,j}(\mathbf{x}) \ ,$$

where $u_{\mathbf{k}_{\perp,0};r,j}(\mathbf{x})$ *is periodic in* x_2 *and* x_3, *and exponentially localized in* x_1.

Using the Fourier transform one can write the "Wannier representation" of $H^{\#q}_{F,\mathrm{ob}}$. Consider, for notational convenience, the one-dimensional case. If $\mathcal{F}: L^2(\Gamma) \to L^2[-\frac{1}{2},\frac{1}{2}]$ is given by

$$\mathcal{F}f(k)=\sum_{a\in\Gamma}\exp(2\pi ika/a_1)f_a \ , \quad a=na_1, \ n=0,\pm 1,\dots,$$

then a direct computation gives the following.

Proposition 4.3.

$$(\mathcal{F}^{-1}H^q_{F,\mathrm{eff}}\mathcal{F}f)_a=\sum_{b\in\Gamma}Y^q_{F,a-b}f_b+Faf_a \ ,$$

where

$$Y^q_{F,a}=\int_{-1/2}^{1/2}\exp(-2\pi ika/a_1)Y^q_F(k)dk \ .$$

V. THE MAGNETIC-FIELD CASE

A. The stability of the spectrum

Consider the Hamiltonian

$$[P-\mathbf{A}^0(\mathbf{x})-B\,\mathbf{A}^1(\mathbf{x})]^2+V(\mathbf{x}), \quad \mathbf{x}\in\mathbb{R}^3 \ , \tag{5.1}$$

where $A^0_j(\mathbf{x})\in C^1(\mathbb{R}^3)$, $A^1_j(\mathbf{x})\in C^2(\mathbb{R}^3)$ and

$$|\mathrm{curl}\,\mathbf{A}^1(\mathbf{x})|\le 1, \quad |(\partial/\partial x_j)[\mathrm{curl}\,\mathbf{A}^1(\mathbf{x})]_k|\le 1 \ . \tag{5.2}$$

According to the general theory (Reed and Simon, 1975; Theorem X.34), (5.1) is essentially self-adjoint on $\mathcal{C}^\infty_0(\mathbb{R}^3)$, and we shall denote by H_B its self-adjoint closure. Note that in this subsection $H_0=(\mathbf{P}-\mathbf{A}^0)^2+V$. The following result (Nenciu, 1986) gives the stability of the spectrum of H_0.

Theorem 5.1. *Let* $(\alpha,\beta)\in\mathbb{R}$, *If* $(\alpha,\beta)\subset\rho(H_0)$ (= *the resolvent set of* H_0), *then for sufficiently small B there exist*

$$\alpha\le\alpha_B<\beta_B\le\beta \ , \lim_{B\to 0}\alpha_B=\alpha, \quad \lim_{B\to 0}\beta_B=\beta$$

such that

$$(\alpha_B,\beta_B)\subset\rho(H_B) \ .$$

Remark. The result above is of a very general nature; in particular, it covers the situations met in the theory of the quantized Hall effect for periodic as well as for nonperiodic systems. The idea behind the proof is gauge invariance: for an arbitrary domain $D\subset\mathbb{R}^3$ having finite diameter, there exists a gauge transformation G_D such that $G^*_D H_B G_D - H_0$ is small on functions localized in D.

Proof. Let $\lambda\in(\alpha,\beta)$, $\delta>0$, $(\lambda-\delta,\lambda+\delta)\subset(\alpha,\beta)$. We shall prove that there exist $c>0$ independent of λ, δ, and B; $\eta(B)\to 0$ as $B\to 0$, such that for all $\psi\in\mathcal{C}^\infty_0(\mathbb{R}^3)$ and B

sufficiently small,

$$\|(H_B-\lambda)\psi\| \geq c\delta[1-\eta(B)]\|\psi\| \;, \tag{5.3}$$

which implies [H_B is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3)$]

$$(\lambda - c\delta/2, \lambda + c\delta/2) \subset \rho(H_B) \;, \tag{5.4}$$

for sufficiently small B. Since H_B is self-adjoint, (5.4) proves the theorem.

Without restricting the generality (a constant can be absorbed into V), one can take $\lambda=0$. Moreover, it is sufficient to consider only those $\psi \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ for which

$$\|H_B\psi\| \leq \delta\|\psi\| \tag{5.5}$$

[otherwise (5.3) is satisfied with $c=1$ and $\eta(B)=0$]. Let, for $\mathbf{c}=(c_1,c_2,c_3)\in\mathbb{R}^3$ and $L>0$ (in this subsection an orthonormal basis in $\mathbb{R}^3$ is used)

$$C(L,\mathbf{c}) = \{\mathbf{x} \mid |x_i - c_i| \leq L/2\} \;, \tag{5.6}$$

and let $\chi_{L,\mathbf{c}}(\mathbf{x})$ be the characteristic function of $C(L,\mathbf{c})$, i.e.,

$$\chi_{L,\mathbf{c}}(\mathbf{x}) = \begin{cases} 1 & \text{for } \mathbf{x}\in C(L,\mathbf{c}) \;, \\ 0 & \text{otherwise} \;. \end{cases} \tag{5.7}$$

Define $\phi_{L,\mathbf{c}}(\mathbf{x})$ by the following properties:

$$\begin{aligned} &\phi_{L,\mathbf{c}} \in \mathcal{C}_0^\infty(\mathbb{R}^3) \;, \quad 1 \geq \phi_{L,\mathbf{c}}(\mathbf{x}) > 0 \;, \\ &|(\partial/\partial x_i)\phi_{L,\mathbf{c}}(\mathbf{x})| \leq \gamma_l \;, \\ &|(\partial^2/\partial x_i \partial x_j)\phi_{L,\mathbf{c}}(\mathbf{x})| \leq \gamma_L \;, \\ &\lim_{L\to\infty} \gamma_L = 0 \;, \\ &\phi_{L,\mathbf{c}}(\mathbf{x}) = \begin{cases} 1 & \text{for } \mathbf{x}\in C(L,\mathbf{c}) \;, \\ 0 & \text{for } \mathbf{x}\notin C(2L,c) \;. \end{cases} \end{aligned} \tag{5.8}$$

Let now $\psi_0 \in \mathcal{C}_0^\infty(\mathbb{R}^3)$, satisfying (5.5). Obviously, $\|\psi_0\chi_{L,\mathbf{c}}\|$ is a continuous function of c. Let $\mathbf{c}_0$ be a point of maximum for $\|\psi_0\chi_{L,\mathbf{c}}\|$. Consider $\psi_1 = \psi_0(1-\chi_{5L,\mathbf{c}_0})$ and repeat the procedure, taking $\mathbf{c}_1$ to be a point of maximum for $\|\psi_1\chi_{L,\mathbf{c}}\|$, defining $\psi_2=\psi_1(1-\chi_{5L,\mathbf{c}_1})$, etc. At some $k<\infty$, $\psi_k(1-\chi_{5L,\mathbf{c}_k})\equiv 0$ and the procedure stops.

Consider now

$$\tilde{\psi}_j = \psi_0\phi_{L,\mathbf{c}_j} \;, \quad \phi = \sum_{j=0}^{k} \phi_{L,\mathbf{c}_j} \;. \tag{5.9}$$

By construction, $\tilde{\psi}_j$ have disjoint supports, $\operatorname{supp}\tilde{\psi}_j \subset C(2L,\mathbf{c}_j)$; $|\phi(\mathbf{x})| \leq 1$ and

$$125\|\phi\psi_0\| \geq \|\psi_0\| \;. \tag{5.10}$$

Now

$$\begin{aligned} \|H_B\psi_0\| \geq \|\phi H_B\psi_0\| \geq \|H_B\phi\psi_0\| - \|\psi_0(\mathbf{P}^2\phi) \\ -2(\mathbf{P}\phi)\cdot[(\mathbf{P}-\mathbf{A}^0-B\,\mathbf{A}^1)\psi_0]\| \;. \end{aligned} \tag{5.11}$$

The next step is to control the second term in the right-hand side of (5.11). According to the Theorem 2.4 in Avron, Herbst, and Simon (1978), there exists $0<a<1$, $b<\infty$ such that

$$\|V\psi_0\| \leq a\|(\mathbf{P}-\mathbf{A}^0-B\,\mathbf{A}^1)^2\psi_0\| + b\|\psi_0\| \;,$$

from which

$$\|H_B\psi_0\| \geq (1-a)\|(\mathbf{P}-\mathbf{A}^0-B\,\mathbf{A}^1)^2\psi_0\| - b\|\psi_0\| \;. \tag{5.12}$$

On the other hand,

$$\begin{aligned} \|(P_j - A_j^0 - BA_j^1)\psi_0\|^2 &= (\psi_0, (P_j - A_j^0 - BA_j^1)^2\psi_0) \\ &\leq \|\psi_0\|\,\|(\mathbf{P}-\mathbf{A}^0-\mathbf{A}^1)^2\psi_0\| \;. \end{aligned} \tag{5.13}$$

From (5.5), (5.12), and (5.13), it follows that

$$\|(P_j - A_j^0 - BA_j^1)\psi_0\| \leq [(\delta+b)/(1-a)]^{1/2}\|\psi_0\| \;, \tag{5.14}$$

from which, taking into account (5.8),

$$\begin{aligned} &\|\psi_0(\mathbf{P}^2\phi) - 2(\mathbf{P}\phi)\cdot(\mathbf{P}-\mathbf{A}^0-B\,\mathbf{A}^1)\psi_0\| \leq \mu_L\|\psi_0\| \;, \\ &\lim_{L\to\infty} \mu_L = 0 \;, \end{aligned} \tag{5.15}$$

and consequently [see (5.11)]

$$\|H_B\psi_0\| \geq \|H_B\phi\psi_0\| - \mu_L\|\psi_0\| \;. \tag{5.16}$$

Let us estimate now the first term in the right-hand side of (5.16). Consider, for fixed $\mathbf{c}$,

$$\mathbf{A}^1(\mathbf{c};\mathbf{x}) = \int_0^1 s\,\mathbf{n}(\mathbf{c}+s\mathbf{x}-s\mathbf{c}) \wedge (\mathbf{x}-\mathbf{c})\,ds \;, \tag{5.17}$$

where

$$\mathbf{n}(\mathbf{x}) = \operatorname{curl}\mathbf{A}^1(\mathbf{x}) \;. \tag{5.18}$$

$\mathbf{A}^1(\mathbf{c};\mathbf{x})$ is the vector potential of $\mathbf{n}(\mathbf{x})$ in the transversal gauge corresponding to $\mathbf{c}$; that is,

$$\mathbf{A}^1(\mathbf{c};\mathbf{x})\cdot(\mathbf{x}-\mathbf{c}) = 0 \;, \tag{5.19}$$

$$\operatorname{curl}\mathbf{A}^1(\mathbf{c};\mathbf{x}) = \mathbf{n}(\mathbf{x}) \;. \tag{5.20}$$

By direct computation, from (5.2) and (5.17)

$$\max_{\mathbf{x}\in C(2L,\mathbf{c})} |\operatorname{div}\mathbf{A}^1(\mathbf{c};\mathbf{x})| \leq \text{const}\times L \;. \tag{5.21}$$

Since by definition $\mathbf{n}(\mathbf{x})=\operatorname{curl}\mathbf{A}^1(\mathbf{x})$, (5.20) implies that, for $\mathbf{x}\in C(4L,\mathbf{c})$, there exists a twice differentiable function $g(\mathbf{c};\mathbf{x})$ such that (Spain, 1965)

$$\mathbf{A}^1(\mathbf{x}) - \operatorname{grad}g(\mathbf{c};\mathbf{x}) = \mathbf{A}^1(\mathbf{c};\mathbf{x}) \;. \tag{5.22}$$

Consider the gauge transformation

$$(G_\mathbf{c}f)(\mathbf{x}) = \exp[ig(\mathbf{c};\mathbf{x})\phi_{2L,\mathbf{c}}(\mathbf{x})]f(\mathbf{x}) \;. \tag{5.23}$$

If $\operatorname{supp}f \subset C(2L,\mathbf{c})$, one obtains from (5.22) and (5.23)

$$G_\mathbf{c}^*(\mathbf{P}-\mathbf{A}^0-B\,\mathbf{A}^1)G_\mathbf{c}f = [\mathbf{P}-\mathbf{A}^0-B\,\mathbf{A}^1(\mathbf{c};\cdot)]f \;, \tag{5.24}$$

from which

$$\|H_B\tilde{\psi}_j\| = \|G^*_{\mathbf{c}_j} H_B G_{\mathbf{c}_j} G^*_{\mathbf{c}_j}\tilde{\psi}_j\| \geq \|H_0 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| - \|(G^*_{\mathbf{c}_j} H_B G_{\mathbf{c}_j} - H_0) G^*_{\mathbf{c}_j}\tilde{\psi}_j\|$$
$$\geq \|H_0 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| - B\|[(\mathbf{P}-\mathbf{A}^0)\cdot\mathbf{A}^1(\mathbf{c};\cdot) + \mathbf{A}^1(\mathbf{c};\cdot)\cdot(\mathbf{P}-\mathbf{A}^0)]G^*_{\mathbf{c}_j}\tilde{\psi}_j\| - B^2\|[\mathbf{A}^1(\mathbf{c};\cdot)]^2 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| \ . \tag{5.25}$$

Due to (5.20),

$$\|[(\mathbf{P}-\mathbf{A}^0)\cdot\mathbf{A}^1(\mathbf{c};\cdot) + \mathbf{A}^1(\mathbf{c};\cdot)(\mathbf{P}-\mathbf{A}^0)]G^*_{\mathbf{c}_j}\tilde{\psi}_j\| \leq 2B\sum_{k=1}^{3}\|(P_k - A_k^0)G^*_{\mathbf{c}_j}\tilde{\psi}_j\| \max_{C(2L,\mathbf{c}_j)} |A_k^1(\mathbf{c}_j;\mathbf{x})|$$
$$+ \max_{C(2L,\mathbf{c}_j)} |\mathrm{div}\,\mathbf{A}^1(\mathbf{c}_j;\mathbf{x})|\,\|\tilde{\psi}_j\| \ . \tag{5.26}$$

The factors containing $(P_k - A_k^0)$ are controlled by H_0. Indeed, the repetition of the arguments leading to (5.12) and (5.13) gives

$$\|(P_k - A_k^0)G^*_{\mathbf{c}_j}\tilde{\psi}_j\|^2 \leq \|\tilde{\psi}_j\|\,\|(\mathbf{P}-\mathbf{A}^0)^2 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| \leq \|\tilde{\psi}_j\|(\|H_0 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| + b\|\tilde{\psi}_j\|)/(1-a)$$
$$\leq [\|H_0 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| + (b+1)\|\tilde{\psi}_j\|]^2/(1-a) \ , \tag{5.27}$$

and then

$$\|H_B\tilde{\psi}_j\| \geq \|H_0 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| - 6B\max_{C(2L;\mathbf{c}_j)} |\mathbf{A}^1(\mathbf{c}_j;\mathbf{x})|(1-a)^{-1/2}[\|H_0 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| + (b+1)\|\tilde{\psi}_j\|]$$
$$-[B^2\max_{C(2L;\mathbf{c}_j)} |\mathbf{A}^1(\mathbf{c}_j;\mathbf{x})|^2 + B\max_{C(2L,\mathbf{c}_j)} |\mathrm{div}\,\mathbf{A}^1(\mathbf{c}_j;\mathbf{x})|]\|\tilde{\psi}_j\| \ . \tag{5.28}$$

From (5.2) and (5.17),

$$\max\nolimits_{C(2L,\mathbf{c})} |\mathbf{A}^1(\mathbf{c};\mathbf{x})| \leq \mathrm{const}\times L \ . \tag{5.29}$$

Inserting (5.21) and (5.29) in (5.28), one obtains

$$\|H_B\tilde{\psi}_j\| \geq (1-\mathrm{const}BL)\|H_0 G^*_{\mathbf{c}_j}\tilde{\psi}_j\| - \mathrm{const}(BL + B^2L^2) \ . \tag{5.30}$$

Since by assumption $(-\delta,\delta)\subset\rho(H^0)$, for all $f\in\mathcal{C}_0^\infty(\mathbb{R}^3)$, $\|H_0 f\|\geq\delta\|f\|$ and then for all sufficiently small B and $L = B^{-1/2}$, one obtains from (5.30)

$$\|H_B\tilde{\psi}_j\| \geq [\delta(1-\mathrm{const}B^{1/2}) - \mathrm{const}B^{1/2}]\|\tilde{\psi}_j\|$$
$$\geq \delta(1-\mathrm{const}B^{1/2})\|\tilde{\psi}_j\| \ . \tag{5.31}$$

Observing that $\phi\psi_0 = \sum_{j=0}^k \tilde{\psi}_j$ and using the disjointness of the supports of $\tilde{\psi}_j$, one obtains from (5.31)

$$\|H_B\phi\psi_0\| \geq \delta(1-\mathrm{const}B^{1/2})\|\phi\psi_0\| \ ,$$

which, together with (5.10) and (5.16), proves (5.3).■

B. The one-band Hamiltonian

The Hamiltonian considered in this subsection is

$$H_B = (\mathbf{P} - \mathbf{B}\wedge\mathbf{x}/2)^2 + V(\mathbf{x}) \ , \tag{5.32}$$

where V is periodic with respect to Γ. In what follows, B denotes the magnetic-field strength, i.e., $\mathbf{B} = B\mathbf{n}$, $|\mathbf{n}| = 1$. By $T_{\mathbf{a},\mathbf{B}}$, $\mathbf{a}\in\Gamma$ we denote the magnetic translations

$$T_{\mathbf{a},\mathbf{B}} = G_{\mathbf{a},\mathbf{B}} T_{\mathbf{a}} \ , \tag{5.33}$$

where

$$(G_{\mathbf{a},\mathbf{B}} f)(\mathbf{x}) = \exp[-i(\mathbf{B}\wedge\mathbf{x})\cdot\mathbf{a}/2] f(\mathbf{x}) \tag{5.34}$$

are gauge transformations and $T_{\mathbf{a}}$ are the usual translations. In other words,

$$(T_{\mathbf{a},\mathbf{B}} f)(\mathbf{x}) = \exp[-i(\mathbf{B}\wedge\mathbf{x})\cdot\mathbf{a}/2] f(\mathbf{x}-\mathbf{a}) \ . \tag{5.35}$$

By simple computations,

$$[T_{\mathbf{a},\mathbf{B}}, H_{\mathbf{B}}] = 0 \tag{5.36}$$

and

$$T_{\mathbf{a},\mathbf{B}} T_{\mathbf{b},\mathbf{B}} = \exp[i\mathbf{B}\cdot(\mathbf{a}\wedge\mathbf{b})/2] T_{\mathbf{a}+\mathbf{b},\mathbf{B}}$$
$$\equiv \eta_{\mathbf{a},\mathbf{b};\mathbf{B}} T_{\mathbf{a}+\mathbf{b},\mathbf{B}} \ . \tag{5.37}$$

In particular,

$$T_{\mathbf{a},\mathbf{B}} T_{-\mathbf{a},\mathbf{B}} = 1 \ , \tag{5.38}$$

whereof, taking into account that $T_{\mathbf{a},\mathbf{B}}$ are unitary,

$$T^{-1}_{\mathbf{a},\mathbf{B}} = T_{-\mathbf{a},\mathbf{B}} = T^*_{\mathbf{a},\mathbf{B}} \ . \tag{5.39}$$

From (5.37) and (5.38) it follows that $\{T_{\mathbf{a},\mathbf{B}}\}_{\mathbf{a}\in\Gamma}$ form a projective representation of the group Γ of the discrete translations. Note that $T_{\mathbf{a},\mathbf{B}} T_{\mathbf{b},\mathbf{B}} \neq T_{\mathbf{b},\mathbf{B}} T_{\mathbf{a},\mathbf{B}}$.

Let σ_0 be a simple isolated band of H_0. By Theorem 5.1, for sufficiently small B, H_B has an isolated band σ_B coinciding with σ_0 in the limit $B\to 0$. As before, P_B denotes the spectral projection of H_B corresponding to σ_B, and

$$H_{\mathrm{ob},\mathbf{B}} = P_{\mathbf{B}} H_{\mathbf{B}} P_{\mathbf{B}} \ . \tag{5.40}$$

Theorem 5.2. *There exists* $B_0 > 0$ *such that, for* $0 < B < B_0$,

i. *There exist* $w_{\mathbf{B}}(\mathbf{x}), \alpha > 0$ *such that*

$$\exp(\alpha|\mathbf{x}|)w_{\mathbf{B}}(\mathbf{x})\in L^2(\mathbb{R}^3) , \tag{5.41}$$

and

$$\{T_{\mathbf{a},\mathbf{B}}w_{\mathbf{B}}\equiv w_{\mathbf{a},\mathbf{B}}\}_{\mathbf{a}\in\Gamma} \tag{5.42}$$

is an orthonormal basis in $P_{\mathbf{B}}L^2(\mathbb{R}^3)$. *Moreover,*

$$\overline{w_{\mathbf{a},\mathbf{B}}(\mathbf{x})}=w_{\mathbf{a},-\mathbf{B}}(\mathbf{x}) , \tag{5.43}$$

and if the crystal has a center of inversion, then

$$w_{\mathbf{a},\mathbf{B}}(-\mathbf{x})=\pm w_{-\mathbf{a},\mathbf{B}}(\mathbf{x}) . \tag{5.44}$$

ii.

$$H_{\mathrm{ob},\mathbf{B}}w_{\mathbf{a},\mathbf{B}}=H_{\mathbf{B}}w_{\mathbf{a},\mathbf{B}}=\sum_{\mathbf{b}\in\Gamma}\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}h_{\mathbf{B}}(\mathbf{a}-\mathbf{b})w_{\mathbf{b},\mathbf{B}} , \tag{5.45}$$

where

$$h_{\mathbf{B}}(\mathbf{a})=\langle H_{\mathbf{B}}w_{\mathbf{B}},w_{\mathbf{a},\mathbf{B}}\rangle . \tag{5.46}$$

There exists $\beta>0$ *such that*

$$\exp(\beta|\mathbf{a}|)h_{\mathbf{B}}(\mathbf{a})\in l^{\infty}(\Gamma) , \tag{5.47}$$

$$\overline{h_{\mathbf{B}}(\mathbf{a})}=h_{-\mathbf{B}}(\mathbf{a}) , \quad h_{\mathbf{B}}(\mathbf{a})=\overline{h_{\mathbf{B}}(-\mathbf{a})} , \tag{5.48}$$

and if the crystal has a center of inversion,

$$h_{\mathbf{B}}(\mathbf{a})=h_{-\mathbf{B}}(\mathbf{a}) . \tag{5.49}$$

iii. $h_{\mathbf{B}}(\mathbf{a})$ *has an asymptotic expansion in* **B**,

$$h_{\mathbf{B}}(\mathbf{a})=h_0(\mathbf{a})+\mathbf{B}\cdot\mathbf{h}_1(\mathbf{a})+\cdots ,$$

with

$$\mathbf{h}_1(\mathbf{a})=\langle(\mathbf{P}\wedge\mathbf{x}+\mathbf{x}\wedge\mathbf{P})w,w_{\mathbf{a}}\rangle -i\sum_{\mathbf{b}\in\Gamma}\langle w_{\mathbf{b}},(\mathbf{x}\wedge\mathbf{b})w_{\mathbf{a}}\rangle h_0(\mathbf{b}) . \tag{5.50}$$

If the crystal has a center of inversion, then the coefficients of the odd powers of B vanish.

Proof. We start with some technical preliminaries. A function $u(\mathbf{x})$ will be called exponentially localized if $\exp(\alpha|\mathbf{x}|)u(\mathbf{x})\in L^2(\mathbb{R}^3)$ for some $\alpha>0$. Similarly, $g(\mathbf{a})$ will be called exponentially localized if $\exp(\alpha|\mathbf{a}|)g(\mathbf{a})\in l^{\infty}(\Gamma)$. A finite number of "localization lengths" α will appear during the proof; their minimum is strictly positive. A finite number of constants will appear during the proof; for the sake of simplicity we shall denote all of them by the same letter c. In what follows "for sufficiently small B" is a shorthand for "there exists B_0 such that uniformly for $0<B<B_0$." Since the proof is somewhat complex, in order not to obscure the main ideas, some of the technical points are stated as lemmas; their proofs can be skipped at the first reading. The proof follows essentially Nenciu (1989).

The first lemma is of purely technical nature and describes some simple properties of the exponentially localized functions. We shall abbreviate $\sum_{\mathbf{a}\in\Gamma}\cdots$ by $\sum_{\mathbf{a}}$.

Lemma 5.1.i. *If* u,v *are exponentially localized, then, uniformly in B,*

$$f(\mathbf{a})=|\langle u,T_{\mathbf{a},\mathbf{B}}v\rangle| \tag{5.51}$$

is exponentially localized.

ii. *If* $f\in l^2(\Gamma)$ *and* v *is exponentially localized, then, uniformly in B,*

$$\left|\left|\sum_{\mathbf{a}}f(\mathbf{a})T_{\mathbf{a},\mathbf{B}}v\right|\right|\le c\|f\| . \tag{5.52}$$

iii. *Let* w *be the Wannier function corresponding to* σ_0. *Then for sufficiently small B there exists* $\beta>0$ *such that for* $\mathbf{a}\neq0$

$$|\langle w,T_{\mathbf{a},\mathbf{B}}w\rangle|\le cB\exp(-\beta|\mathbf{a}|) . \tag{5.53}$$

If $f\in l^2(\Gamma)$, *then*

$$(1-cB)\|f\|^2\le\left|\left|\sum_{\mathbf{a}}f(\mathbf{a})T_{\mathbf{a},\mathbf{B}}w\right|\right|^2\le(1+cB)\|f\|^2 . \tag{5.54}$$

iv. *If* $u(\mathbf{x})$, $f(\mathbf{a})$ *are exponentially localized, then, uniformly in B,*

$$v(\mathbf{x})=\sum_{\mathbf{a}}f(\mathbf{a})(T_{\mathbf{a},\mathbf{B}}u)(\mathbf{x})$$

is exponentially localized.

v. *If u is exponenetially localized and* $f\in L^2(\mathbb{R}^3)$,

$$\sum_{\mathbf{a}\in\Gamma}|\langle T_{\mathbf{a}}u,f\rangle|^2\le c\|f\|^2 .$$

Proof i. Observe that if $\gamma=\min\{\alpha,\beta\}$, $\alpha,\beta>0$, then

$$\exp(-\alpha|\mathbf{x}|)\exp(-\beta|\mathbf{x}-\mathbf{a}|)\le\exp(-\gamma|\mathbf{a}|) ,$$

and then

$$|f(\mathbf{a})|\le\exp(-\gamma|\mathbf{a}|)\|\exp(\alpha|\cdot|)u\|\,\|\exp(\beta|\cdot|)v\| .$$

ii. Let $g(\mathbf{a})=|\langle v,T_{\mathbf{a},\mathbf{B}}v\rangle$. By the Young inequality

$$\left|\left|\sum_{\mathbf{a}}f(\mathbf{a})T_{\mathbf{a},\mathbf{B}}v\right|\right|\le\sum_{\mathbf{a},\mathbf{b}}|f(\mathbf{a})|\,|f(\mathbf{b})|g(\mathbf{a}-\mathbf{b})\le\|g\|_1\|f\|^2 ,$$

and, by *i.*, $\|g\|_1<\infty$.

iii. Using $|\exp(i\alpha)-1|\le|\alpha|$ for $\alpha\in\mathbb{R}$ and $\langle w,T_{\mathbf{a}}w\rangle=0$ for $\mathbf{a}\neq\mathbf{0}$,

$$|\langle w,T_{\mathbf{a},\mathbf{B}}w\rangle|\le B|\mathbf{a}|\langle|\cdot|w,T_{\mathbf{a}}w\rangle .$$

Due to $\sup_{y>0}y\exp(-\alpha y)=(e\alpha)^{-1}$, $|\mathbf{x}|w$ is exponentially localized (with a localization length of, say, half the localization length of w), and then, by *i.*, $k(\mathbf{a})=\langle|\cdot|w,T_{\mathbf{a}}w\rangle$ is exponentially localized. As above, $|\mathbf{a}|k(\mathbf{a})$ is exponentially localized. Using the fact that, by (5.37) and (5.39), $|\langle T_{\mathbf{a},\mathbf{B}}w,T_{\mathbf{b},\mathbf{B}}w\rangle|=|\langle w,T_{\mathbf{b}-\mathbf{a},\mathbf{B}}w\rangle|$,

$$\left|\left|\sum_{\mathbf{a}}f(\mathbf{a})T_{\mathbf{a},\mathbf{B}}w\right|\right|^2=\sum_{\mathbf{a},\mathbf{b}}\overline{f(\mathbf{a})}f(\mathbf{b})\langle T_{\mathbf{a},\mathbf{B}}w,T_{\mathbf{b},\mathbf{B}}w\rangle \ge\|f\|^2-\sum_{\mathbf{a}\neq\mathbf{b}}|f(\mathbf{a})| \times|f(\mathbf{b})||\langle w,T_{\mathbf{b}-\mathbf{a},\mathbf{B}}w\rangle| .$$

The use of (5.53) and the Young inequality prove the left inequality in (5.54). The proof of the right inequality in (5.54) is similar.

iv. Let α, β be the localization lengths of f and v, respectively. Then, for $\gamma \le \min\{\alpha/2,\beta\}$,

$$\|\exp(\gamma|\cdot|)v\| \le \sum_{\mathbf{b}} \exp(-\alpha|\mathbf{b}|/2)\,|\exp(\alpha|\mathbf{b}|)f(\mathbf{b})|\,\|\exp(\beta|\cdot-\mathbf{b}|)T_{\mathbf{b}}u\| \le c\|\exp(\beta|\cdot|)u\| .$$

v. Let, for $\beta>0$, $s(\mathbf{x})=\exp(\beta|\mathbf{x}|)u(\mathbf{x})$. Then by the Schwartz inequality

$$|\langle T_{\mathbf{a}}u,f\rangle|^2 \le \|s\|^2\langle |f|,\exp(-2\beta|\cdot-\mathbf{a}|)|f|\rangle ,$$

whereof

$$\sum_{\mathbf{a}} |\langle T_{\mathbf{a}}u,f\rangle|^2 \le \|s\|^2\left\langle |f|,\sum_{\mathbf{a}}\exp(-2\beta|\cdot-\mathbf{a}|)|f|\right\rangle \le c\|f\|^2. ■$$

Most of the algebraic structure we shall use is contained in the following simple lemma.

Lemma 5.2. *Let K be an operator such that* $[T_{\mathbf{a},\mathbf{B}},K]=0$. *and* $f\in\mathcal{D}(K)$. *Then*

$$\langle KT_{\mathbf{b},\mathbf{B}}f,T_{\mathbf{a},\mathbf{B}}f\rangle=\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}k^f_{\mathbf{B}}(\mathbf{a}-\mathbf{b}) , \tag{5.55}$$

where

$$k^f_{\mathbf{B}}(\mathbf{a})=\langle Kf,T_{\mathbf{a},\mathbf{B}}f\rangle . \tag{5.56}$$

Proof. Use (5.37) and (5.39).■

Consider the following "twisted" convolutions in $l^p(\Gamma)$:

$$(f\Box g)(\mathbf{a})=\sum_{\mathbf{b}}\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}f(\mathbf{a}-\mathbf{b})g(\mathbf{b}) . \tag{5.57}$$

The convolution $\Box$ has properties similar to the usual ones. In particular, it is associative,

$$(f\Box g)\Box h=f\Box(g\Box h) , \tag{5.58}$$

and the Young inequality holds,

$$\|f\Box g\|_s \le \|f\|_p\|g\|_q , \quad s^{-1}=p^{-1}+q^{-1}-1 . \tag{5.59}$$

Note, however, that it is not commutative, which makes the corresponding algebra a highly nontrivial object.

Let $m(\mathbf{a})$ be exponentially localized and M be the matrix

$$M_{\mathbf{a},\mathbf{b}}=\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}m(\mathbf{a}-\mathbf{b}) . \tag{5.60}$$

Let $\mathcal{M}$ be the set of matrices of the form (5.60). Easy computations show that

$$\|M\|<\|m\|_1 , \tag{5.61}$$

and $M,N\in\mathcal{M}$ implies $MN\in\mathcal{M}$ and

$$(MN)_{\mathbf{a},\mathbf{b}}=\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}(m\Box n)(\mathbf{a}-\mathbf{b}) . \tag{5.62}$$

Consider now the Gramm matrix (Achieser and Glazman, 1977) corresponding to

$$v_{\mathbf{a},\mathbf{B}}=T_{\mathbf{a},\mathbf{B}}w , \tag{5.63}$$

$$G_{\mathbf{a},\mathbf{b}}=\langle v_{\mathbf{b},\mathbf{B}},v_{\mathbf{a},\mathbf{B}}\rangle . \tag{5.64}$$

By Lemma 5.2, $G\in\mathcal{M}$,

$$G_{\mathbf{a},\mathbf{b}}=\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}g_{\mathbf{B}}(\mathbf{a}-\mathbf{b})=\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}\langle w,T_{\mathbf{a}-\mathbf{b},\mathbf{B}}w\rangle . \tag{5.65}$$

Obviously $g_{\mathbf{B}}(\mathbf{0})=1$, and, by Lemma 5.1.iii for $\mathbf{a}\neq\mathbf{0}$ and B sufficiently small,

$$|g_{\mathbf{B}}(\mathbf{a})|\le cB\exp(-\beta|\mathbf{a}|) , \quad \beta>0 . \tag{5.66}$$

Note that G is Hermitian. Let A be defined by

$$G=1-A . \tag{5.67}$$

Obviously, $A\in\mathcal{M}$, $A_{\mathbf{a},\mathbf{b}}=\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}a(\mathbf{a}-\mathbf{b})$, with

$$a(\mathbf{a})=\begin{cases}0 , & \mathbf{a}=\mathbf{0} ,\\ g_{\mathbf{B}}(\mathbf{a}) , & \mathbf{a}\neq\mathbf{0} .\end{cases} \tag{5.68}$$

By (5.66), for sufficiently small B,

$$\|A\|\le cB , \tag{5.69}$$

so that, for sufficiently small B, $\|A\|<1$ and

$$G=1-A>c>0 , \tag{5.70}$$

From (5.70) it follows (Achieser and Glazman, 1977) that $\{v_{\mathbf{a},\mathbf{B}}\}\mathbf{a}\in\Gamma$ is a (nonorthonormal) basis in $Q_{\mathbf{B}}L^2(\mathbb{R}^3)$ (the closed subspace generated by $\{v_{\mathbf{a},\mathbf{B}}\}_{\mathbf{a}\in\Gamma}$). Since $\|A\|<1$, one can define

$$G^{-1/2}=1+\sum_1^\infty\frac{(2k-1)!!}{k!2^k}A^k . \tag{5.71}$$

Due to (5.62), $G^{-1/2}\in\mathcal{M}$,

$$G^{-1/2}_{\mathbf{a},\mathbf{b}}=\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}g^{-1/2}(\mathbf{a}-\mathbf{b}) \tag{5.72}$$

with

$$g^{-1/2}(\mathbf{a})=\delta_{\mathbf{a},0}+\sum_1^\infty\frac{(2k-1)!!}{k!2^k}a^{\Box k}(\mathbf{a}) . \tag{5.73}$$

Lemma 5.3. *For sufficiently small B,*

$$|g^{-1/2}(\mathbf{a})-\delta_{\mathbf{a},0}|\le Bk(\mathbf{a})$$

with $k(\mathbf{a})$ *exponentially localized.*

Proof. By (5.65) and (5.68) (here $*$ means the usual convolution)

$$|g^{-1/2}(\mathbf{a})-\delta_{\mathbf{a},0}|\le\sum_1^\infty\frac{(2k-1)!!}{k!2^k}|a|^{*k}(\mathbf{a}) \le\sum_1^\infty c^kB^k[\exp(-\beta|\cdot|)]^{*k} . \tag{5.74}$$

Let $e(\mathbf{k})$ be the inverse Fourier transform of $\exp(-\beta|\cdot|)$, i.e.,

$$e(\mathbf{k})=\sum_{\mathbf{a}}\exp(i\mathbf{k}\cdot\mathbf{a}-\beta|\mathbf{a}|) . \qquad (5.75)$$

By Paley-Wiener theorem for Fourier series (see, e.g., des Cloizeaux, 1964), $e(\mathbf{k})$ is analytic and periodic in a complex neighborhood of $\mathbb{R}^3$. The inverse Fourier transform of the right-hand side of (5.74) is

$$\sum_{1}^{\infty}c^kB^k[e(\mathbf{k})]^k=cBe(\mathbf{k})[1-ce(\mathbf{k})]^{-1} . \qquad (5.76)$$

Since $|e(\mathbf{k})|\le c<\infty$ in a complex neighborhood of $\mathbb{R}^3$, the right-hand side of (5.76) is, for sufficiently small B, analytic and periodic in a complex neighborhood of $\mathbb{R}^3$. Then, by the Paley-Wiener theorem, the right-hand side of (5.74) is exponentially localized and the proof is finished.■

Consider now

$$\chi_{\mathbf{a,B}}=\sum_{\mathbf{b}}G_{\mathbf{a,b}}^{-1/2}v_{\mathbf{b,B}} . \qquad (5.77)$$

Since $g^{-1/2}\in l^1(\Gamma)$, $\chi_{\mathbf{a,B}}$ are well defined.

Lemma 5.4. *For sufficiently small B,*

i. $\{\chi_{\mathbf{a,B}}\}_{a\in\Gamma}$ *is an orthonormal basis in* $Q_{\mathbf{B}}L^2(\mathbb{R}^3)$.

ii. $\chi_{\mathbf{a,B}}=T_{\mathbf{a,B}}\chi_{\mathbf{B}}, \quad \chi_{\mathbf{B}}\equiv\chi_{\mathbf{0,B}}$. (5.78)

iii. χ_B *is exponentially localized. Moreover,*

$$|\chi_{\mathbf{B}}(\mathbf{x})-w(\mathbf{x})|\le Bu(\mathbf{x})$$

with $u(\mathbf{x})$ *exponentially localized.*

Proof i. $v_{\mathbf{a,B}}=\sum_b G_{\mathbf{a,b}}^{1/2}\chi_{\mathbf{b,B}}$ and $\{v_{\mathbf{a,B}}\}_{a\in\Gamma}$ is a basis in $Q_{\mathbf{B}}L^2(\mathbb{R}^3)$. Now by (5.77) and the fact that $G^{-1/2}$ is Hermitian,

$$\langle\chi_{\mathbf{a,B}},\chi_{\mathbf{b,B}}\rangle=\sum_{\mathbf{c,d}}G_{\mathbf{b,d}}^{-1/2}G_{\mathbf{d,c}}G_{\mathbf{c,a}}^{-1/2}=\delta_{\mathbf{a,b}} .$$

ii. By (5.38) and (5.65)

$$T_{\mathbf{a,B}}\chi_{\mathbf{B}}=\sum_{\mathbf{b}}G_{\mathbf{0,b}}^{-1/2}T_{\mathbf{a,B}}T_{\mathbf{b,B}}w$$

$$=\sum_{\mathbf{b}}\eta_{\mathbf{a,b;B}}g^{-1/2}(-\mathbf{b})T_{\mathbf{a+b,B}}w$$

$$=\sum_{\mathbf{c}}G_{\mathbf{a,c}}^{-1/2}T_{\mathbf{c,B}}w=\chi_{\mathbf{a,B}} .$$

iii. By Lemma 5.3, for some $\beta>0$,

$$|\chi_{\mathbf{B}}(\mathbf{x})-w(\mathbf{x})|=|\sum_{\mathbf{b}\neq0}g^{-1/2}(-\mathbf{b})T_{\mathbf{b,B}}w(\mathbf{x})|$$

$$\le cB\sum_{\mathbf{b}\neq0}\exp(-\beta|\mathbf{b}|)|T_{\mathbf{b}}w(\mathbf{x})|$$

and the application of Lemma 5.1.iv. finishes the proof.■

Let us compute now $Q_{\mathbf{B}}H_{\mathbf{B}}Q_{\mathbf{B}}\chi_{\mathbf{a,B}}$. By (5.36) and Lemma 5.2,

$$Q_{\mathbf{B}}H_{\mathbf{B}}\chi_{\mathbf{a,B}}=\sum_{\mathbf{b}}\langle\chi_{\mathbf{b,B}},H_{\mathbf{B}}\chi_{\mathbf{a,B}}\rangle\chi_{\mathbf{b,B}}$$

$$=\sum_{\mathbf{b}}\eta_{\mathbf{a,b;B}}h_{\mathbf{B}}^{\chi}(\mathbf{a}-\mathbf{b})\chi_{\mathbf{b,B}} , \qquad (5.79)$$

which is nothing but the fundamental formula (5.45) for $Q_{\mathbf{B}}H_{\mathbf{B}}Q_{\mathbf{B}}$.

We turn now to the relation between $Q_{\mathbf{B}}H_{\mathbf{B}}Q_{\mathbf{B}}$ and $P_{\mathbf{B}}H_{\mathbf{B}}P_{\mathbf{B}}$. The next lemma is again of technical nature.

Lemma 5.5.i. *Let ψ be a real differentiable function with*

$$|\mathrm{grad}\psi|\le\gamma . \qquad (5.80)$$

Then, for sufficiently small α and B,

$$\|\exp(\alpha|\cdot|)[Q_{\mathbf{B}},\psi]\exp(-\alpha|\cdot|)\|\le c\gamma . \qquad (5.81)$$

ii. *Let $\chi_{L,0}$ be the characteristic function of* $C(L,\mathbf{0})$ *[see (5.7)]. Then*

$$\|\chi_{L,0}(P_0-Q_{\mathbf{B}})\|\le cBL^4 . \qquad (5.82)$$

Proof. Due to the fact that

$$[Q_{\mathbf{B}},\psi]=Q_{\mathbf{B}}\psi(1-Q_{\mathbf{B}})-(1-Q_{\mathbf{B}})\psi Q_{\mathbf{B}} ,$$

it is sufficient to prove that

$$\|\exp(\alpha|\cdot|)(1-Q_{\mathbf{B}})\psi Q_{\mathbf{B}}\exp(-\alpha|\cdot|)\|\le c\gamma . \qquad (5.83)$$

Let $f\in L^2(\mathbb{R}^2)$, $h=Q_{\mathbf{B}}\exp(-\alpha|\cdot|)f$, $h_{\mathbf{a}}=\langle\chi_{\mathbf{a,B}},h\rangle$. Using the orthogonality of $\chi_{\mathbf{a,B}}$, one obtains

$$(1-Q_B)\psi h=\sum_{\mathbf{a}}h_{\mathbf{a}}\{[\psi-\psi(\mathbf{a})]\chi_{\mathbf{a,B}}-\sum_{\mathbf{b}}\langle\chi_{\mathbf{b,B}},[\psi-\psi(\mathbf{a})]\chi_{\mathbf{a,B}}\rangle\chi_{\mathbf{b,B}}\} .$$

Taking into account (5.80)

$$|(1-Q_{\mathbf{B}})\psi h(\mathbf{x})|\le\gamma\sum_{\mathbf{a}}|h_{\mathbf{a}}|\{|\mathbf{x}-\mathbf{a}|\,|\chi_{\mathbf{a,B}}(\mathbf{x})|+\sum_{\mathbf{b}}\langle|\chi_{\mathbf{b,B}}|\,|\cdot-\mathbf{a}|\,|\chi_{\mathbf{a,B}}|\rangle|\chi_{\mathbf{b,B}}(\mathbf{x})|\} .$$

Since $|\mathbf{x}|\,|\chi_{\mathbf{B}}(\mathbf{x})|$ is exponentially localized, using Lemma 5.1.i and Lemma 5.1.iv, one obtains

$$|\exp(\alpha|\mathbf{x}|)(1-Q_B)\psi h_{\mathbf{a}}(\mathbf{x})|\le\gamma\sum\exp(\alpha|\mathbf{a}|)|h_{\mathbf{a}}|T_{\mathbf{a}}u(\mathbf{x}) .$$

Now $\exp(\alpha|\mathbf{a}|)|h_{\mathbf{a}}|\le\langle|\chi_{\mathbf{a,B}}|\exp(\alpha|\cdot-\mathbf{a}|),|f|\rangle$ and the use of Lemmas 5.1.ii and 5.1.v finishes the proof of (5.83).

ii. Denoting $f_{\mathbf{a}}=\langle w_{\mathbf{a}},f\rangle$, $f_{\mathbf{a,B}}=\langle\chi_{\mathbf{a,B}},f\rangle$,

$$\chi_{L,0}(P_0-Q_{\mathbf{B}})f=\sum_{\mathbf{a}}(f_{\mathbf{a}}-f_{\mathbf{a,B}})\chi_{L,0}w_{\mathbf{a}}+\sum_{\mathbf{a}}f_{\mathbf{a,B}}\chi_{L,0}(w_{\mathbf{a}}-\chi_{\mathbf{a,B}}) . \qquad (5.84)$$

Using Lemma 5.4.iii,

$$|f_{\mathbf{a}}-f_{\mathbf{a},\mathbf{B}}|=|\langle f,T_{\mathbf{a}}w-G_{\mathbf{a},\mathbf{B}}T_{\mathbf{a}}w_{\mathbf{B}}\rangle|\le|\langle f,T_{\mathbf{a}}(w-\chi_{\mathbf{B}}\rangle|+|\langle f,\{1-\exp[-i(\mathbf{B}\wedge\mathbf{x})\cdot(\mathbf{a}-\mathbf{x})/2]\}T_{\mathbf{a}}\chi_{\mathbf{B}}\rangle|$$
$$\le\|f\|(\|w-\chi_{\mathbf{B}}\|+B|\mathbf{a}|\,\|\,|\cdot|\chi_{\mathbf{B}}\|)\le cB(1+|\mathbf{a}|)\|f\| \ . \tag{5.85}$$

On the other hand,

$$\|\chi_{L,0}w_{\mathbf{a}}\|^2\le\sup_{\mathbf{x}\in\mathbb{R}^3}\chi_{L,0}(\mathbf{x})\exp(-2\beta|\mathbf{x}-\mathbf{a}|)\|\exp(\beta|\mathbf{x}|)w\|^2$$
$$\le c\exp\{-2\beta\,\mathrm{dist}[\mathbf{a},C(L,\mathbf{0})]\} \ . \tag{5.86}$$

From (5.85) and (5.86) the first sum in the right-hand side of (5.84) is bounded by $cB\|f\|L^4$. Analogously, using Lemma 5.4.iii,

$$\|\chi_{L,0}(w_{\mathbf{a}}-\chi_{\mathbf{a},\mathbf{B}})\|\le cB(1+|\mathbf{a}|)\exp\{-\beta\,\mathrm{dist}[\mathbf{a},C(L,\mathbf{0})]\} \ ,$$

whereof

$$\sum_{\mathbf{a}}|f_{\mathbf{a},\mathbf{B}}|\|\chi_{L,0}(w_a-\chi_{\mathbf{a},\mathbf{B}})\|\le cB\|f\|L^4 \ ,$$

and the proof of (5.82) is finished.■

The next lemma is the technical core of the proof of Theorem 5.2.

Lemma 5.6.i.

$$\lim_{B\to 0}\mathrm{dist}[\sigma(Q_{\mathbf{B}}H_{\mathbf{B}}Q_{\mathbf{B}}),\sigma_0]=0 \ , \tag{5.87}$$

$$\lim_{B\to 0}\mathrm{dist}[\sigma((1-Q_B)H_B(1-Q_{\mathbf{B}})),\sigma(H_0)\setminus\sigma_0]=0 \ . \tag{5.88}$$

ii. *For sufficiently small B,*

$$\|(1-Q_B)H_{\mathbf{B}}Q_B\|\le cB \ .$$

Proof i. The proofs of (5.87) and (5.88) are similar: mimic the proof of Theorem 5.1. Consider the example (5.88). Let $f\in\mathcal{D}(H_{\mathbf{B}})\cap(1-Q_{\mathbf{B}})L^2(\mathbb{R}^3)$. The whole construction in the proof of Theorem 5.1 can be done for f (the sum over j contains an infinite number of terms, but this does not affect the proof) and one obtains

$$\|H_{\mathbf{B}}f\|\ge\|H_{\mathbf{B}}\phi f\|-\mu_L\|f\|, \quad \lim_{L\to\infty}\mu_L=0 \ .$$

Taking in the case at hand $G_c=G_{\mathbf{c},\mathbf{B}}$ and then

$$G_{\mathbf{c},\mathbf{B}}^{-1}(\mathbf{P}-\mathbf{B}\wedge\mathbf{x}/2)G_{\mathbf{c},\mathbf{B}}=\mathbf{P}-\mathbf{B}\wedge(\mathbf{x}-c)/2 \ ,$$

one obtains [see (5.30)]

$$\|H_{\mathbf{B}}\tilde{f}_j\|\ge(1-cB)\|H_0G^*_{c_j,\mathbf{B}}\tilde{f}_j\|-c(BL+B^2L^2)\|\tilde{f}_j\| \ . \tag{5.89}$$

Since by assumption $(-\delta,\delta)\cap\sigma(H_0)\setminus\sigma_0=\varnothing$,

$$\|H_0G^*_{c_j,\mathbf{B}}\tilde{f}_j\|\ge\|H_0(1-P_0)G^*_{c_j,\mathbf{B}}\tilde{f}_j\|$$
$$\ge\delta\|(1-P_0)G^*_{\mathbf{c}_j,\mathbf{B}}\tilde{\tilde{f}}_j\| \ . \tag{5.90}$$

Now

$$\|(1-P_0)G^*_{\mathbf{c}_j,\mathbf{B}}\tilde{f}_j-G^*_{c_j,\mathbf{B}}(1-Q_{\mathbf{B}})\tilde{f}_j\|$$
$$=\|(P_0-Q_{\mathbf{B}})T_{-\mathbf{c}_j,\mathbf{B}}\tilde{f}_j\|$$

and, since $\mathrm{supp}T_{-\mathbf{c}_j,\mathbf{B}}\tilde{f}_j\subset C(2L,\mathbf{0})$, the application of Lemma 5.5.ii gives

$$\|(1-P_0)G^*_{\mathbf{c}_j,\mathbf{B}}\tilde{f}_j\|\ge\|(1-Q_{\mathbf{B}})\tilde{f}_j\|-cBL^4 \ . \tag{5.91}$$

Observing that $\tilde{f}_j=\phi_jf=\phi_j\chi_{2L,\mathbf{c}_j}f$, from Lemma 5.5.i, (5.8), $(1-Q_{\mathbf{B}})f=f$, and the definition of $\mathbf{c}_j$, it follows that

$$\|(1-Q_{\mathbf{B}})\tilde{f}_j\|\ge(1-8\gamma_L)\|\tilde{f}_j\| \ . \tag{5.92}$$

Taking B sufficiently small and $L=B^{-1/8}$, one obtains from (5.89), (5.90), (5.91), and (5.92)

$$\|H_{\mathbf{B}}\tilde{f}_j\|\ge\delta(1-cB^{1/2})\|\tilde{f}_j\| \ ,$$

and from this point the proof of (5.87) coincides with the proof of Theorem 5.1.

ii. Let $f\in L^2(\mathbb{R}^3)$, $g=Q_{\mathbf{B}}f=\sum_{\mathbf{a}}g_{\mathbf{a}}T_{\mathbf{a},\mathbf{B}}w$. By Lemma 5.1.iii, for sufficiently small B,

$$\sum_{\mathbf{a}}|g_{\mathbf{a}}|^2\le(1-cB)^{-1}\|g\|^2 \ . \tag{5.93}$$

Now

$$H_{\mathbf{B}}g=\sum_{\mathbf{a}}g_{\mathbf{a}}H_{\mathbf{B}}T_{\mathbf{a},\mathbf{B}}w=\sum_{\mathbf{a}}g_{\mathbf{a}}T_{\mathbf{a},\mathbf{B}}(H_0+BH_1)w \ . \tag{5.94}$$

By Thoerem 3.7, H_1w is exponentially localized, and then by Lemma 5.1.ii and (5.93), for sufficiently small B,

$$\|B\sum_{\mathbf{a}}g_{\mathbf{a}}T_{\mathbf{a},\mathbf{B}}H_1w\|\le cB\|g\|\le cB\|f\| \ . \tag{5.95}$$

Further

$$\sum_{\mathbf{a}}g_{\mathbf{a}}T_{\mathbf{a},\mathbf{B}}H_0w=\sum_{\mathbf{a},\mathbf{b}}g_{\mathbf{a}}h_0(-\mathbf{b})T_{\mathbf{a},\mathbf{B}}G_{\mathbf{b},\mathbf{B}}^{-1}T_{\mathbf{b},\mathbf{B}}w$$
$$=\sum_{\mathbf{a},\mathbf{b}}g_{\mathbf{a}}h_0(-\mathbf{b})\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}T_{\mathbf{a}+\mathbf{b},\mathbf{B}}w+\sum_{\mathbf{a},\mathbf{b}}g_{\mathbf{a}}h_0(-\mathbf{b})T_{\mathbf{a},\mathbf{B}}(G_{\mathbf{b},\mathbf{B}}^{-1}-1)T_{\mathbf{b},\mathbf{B}}w \ . \tag{5.96}$$

Since the first term in the right-hand side of (5.96) belongs to $Q_B L^2(\mathbb{R}^3)$, it is sufficient to estimate the second one.

$$\Big|\sum_{\mathbf{b}} h_0(-\mathbf{b})(G^{-1}_{\mathbf{b},\mathbf{B}}-1)T_{\mathbf{b},\mathbf{B}}w(\mathbf{x})\Big| \le B\sum_{\mathbf{b}}|h_0(-\mathbf{b})|\,|\mathbf{b}|\,|T_{\mathbf{b}}w(\mathbf{x})| \le Bu(\mathbf{x}) ,$$

where $u(\mathbf{x})$ is exponentially localized by Lemma 5.1.iv. Then by (5.93) and Lemma 5.1.ii, the second term in the right-hand side of (5.96) is bounded in norm by $cB\|f\|$, and this together with (5.94) and (5.95) finishes the proof.■

Lemma 5.6 allows the use of regular perturbation theory (Kato, 1966) by considering $Q_{\mathbf{B}}H_{\mathbf{B}}Q_{\mathbf{B}}+(1-Q_{\mathbf{B}})H_{\mathbf{B}}(1-Q_{\mathbf{B}})$ as the unperturbed operator and $Q_{\mathbf{B}}H_{\mathbf{B}}(1-Q_{\mathbf{B}})+(1-Q_{\mathbf{B}})H_{\mathbf{B}}Q_{\mathbf{B}}$ as the perturbation. Denoting

$$R_1(z)=Q_{\mathbf{B}}(H_{\mathbf{B}}-z)^{-1}Q_{\mathbf{B}} ,$$

$$R_2(z)=(1-Q_{\mathbf{B}})(H_{\mathbf{B}}-z)^{-1}(1-Q_{\mathbf{B}}) ,$$

$$V_{12}=Q_{\mathbf{B}}H_{\mathbf{B}}(1-Q_{\mathbf{B}}) ,\quad V_{21}=(1-Q_{\mathbf{B}})H_{\mathbf{B}}Q_{\mathbf{B}} ,$$

$$P_{\mathbf{B}}=Q_{\mathbf{B}}+(2\pi i)\int_C[R_2(z)V_{21}R_1(z)+R_1(z)V_{12}R_2(z)]dz+O(B^2) , \tag{5.97}$$

whereof, for sufficiently small B,

$$\|P_{\mathbf{B}}-Q_{\mathbf{B}}\|<cB . \tag{5.98}$$

Lemma 5.7. *There exists $\alpha>0$ such that, for sufficiently small B,*

$$\|\exp(\alpha|\cdot|)(P_{\mathbf{B}}-Q_{\mathbf{B}})\exp(-\alpha|\cdot|)\|<1 .$$

Proof.

$$\exp(\alpha|\cdot|)Q_{\mathbf{B}}\exp(-\alpha|\cdot|)-Q_{\mathbf{B}} =\int_0^\alpha \exp(t|\cdot|)[|\cdot|,Q_{\mathbf{B}}]\exp(-t|\cdot|)dt .$$

The application of Lemma 5.5.i gives for α small enough

$$\|\exp(\alpha|\cdot|)Q_{\mathbf{B}}\exp(-\alpha|\cdot|)-Q_{\mathbf{B}}\|\le c\alpha . \tag{5.99}$$

From (5.98), (5.99), Corollary A.1, and the triangle inequality it follows that

$$\|\exp(\alpha|\cdot|)(P_{\mathbf{B}}-Q_{\mathbf{B}})\exp(-\alpha|\cdot|)\|\le c(\alpha+B) .■$$

Let U_B be the Nagy transformation matrix (Kato, 1966) relating $Q_{\mathbf{B}}$ and $P_{\mathbf{B}}$:

$$U_{\mathbf{B}}=[1-(P_{\mathbf{B}}-Q_{\mathbf{B}})^2]^{-1/2}[P_{\mathbf{B}}Q_{\mathbf{B}}+(1-P_{\mathbf{B}})(1-Q_{\mathbf{B}})] .$$

U is unitary and

$$P_{\mathbf{B}}=U_{\mathbf{B}}Q_{\mathbf{B}}U_{\mathbf{B}}^{-1} . \tag{5.100}$$

Since $[P_{\mathbf{B}},T_{\mathbf{a},\mathbf{B}}]=[Q_{\mathbf{B}},T_{\mathbf{a},\mathbf{B}}]=0$,

$$[U_{\mathbf{B}},T_{\mathbf{a},\mathbf{B}}]=0 . \tag{5.101}$$

From Lemma 5.7, for sufficiently small α,

$$\|\exp(\alpha|\cdot|)U_{\mathbf{B}}\exp(-\alpha|\cdot|)\|\le c . \tag{5.102}$$

Consider now

$$w_{\mathbf{a},\mathbf{B}}=U_B\chi_{\mathbf{a},\mathbf{B}},\quad w_{\mathbf{B}}\equiv w_{0,\mathbf{B}} . \tag{5.103}$$

Due to (5.101), (5.102), and the fact that U is unitary, (5.41) and (5.42) are fulfilled and $\{w_{\mathbf{a},\mathbf{B}}\}_{\mathbf{a}\in\Gamma}$ is an orthonormal basis in $P_{\mathbf{B}}L^2(\mathbb{R}^3)$.

From (5.97) and Lemma 5.6.ii, for sufficiently small B,

$$\|P_{\mathbf{B}}-Q_{\mathbf{B}}\|\le cB<1 . \tag{5.104}$$

From $\|Q_{\mathbf{B}}\chi_{\mathbf{a},\mathbf{B}}\|=1$, $[Q_{\mathbf{B}},T_{\mathbf{a},\mathbf{B}}]=0$, and (5.104), $N^{-1}=\|P_{\mathbf{B}}\chi_{\mathbf{a},\mathbf{B}}\|=\|P_{\mathbf{B}}\chi_{0,\mathbf{B}}\|\ge 1-\|P_{\mathbf{B}}-Q_{\mathbf{B}}\|>0$, and then one can define

$$\mu_{\mathbf{a},\mathbf{B}}=NP_{\mathbf{B}}\chi_{\mathbf{a},\mathbf{B}}=NT_{\mathbf{a},\mathbf{B}}P_{\mathbf{B}}\chi_{0,\mathbf{B}} . \tag{5.105}$$

By construction, $\|\mu_{\mathbf{a},\mathbf{B}}\|=1$. Moreover, from the fact that $\chi_{0,\mathbf{B}}$ is exponentially localized and from Corollary A1 (see Appendix), it follows that $\mu_{\mathbf{a},\mathbf{B}}$ is exponentially localized. Consider

$$F_{\mathbf{a},\mathbf{b}}=\langle\mu_{\mathbf{b},\mathbf{B}},\mu_{\mathbf{a},\mathbf{B}}\rangle=\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}f_{\mathbf{B}}(\mathbf{a}-\mathbf{b}) ,$$

where

$$f_{\mathbf{B}}(\mathbf{a})=\langle\mu_{0,\mathbf{B}},T_{\mathbf{a},\mathbf{B}}\mu_{0,\mathbf{B}}\rangle .$$

Obviously $f_{\mathbf{B}}(\mathbf{0})=1$ and for $\mathbf{a}\neq 0$

$$f_{\mathbf{B}}(\mathbf{a})=N^2\langle(P_{\mathbf{B}}-Q_{\mathbf{B}})\chi_{0,\mathbf{B}},\chi_{\mathbf{a},\mathbf{B}}\rangle . \tag{5.106}$$

Let $\beta>0$ be the localization length of $(P_{\mathbf{B}}-Q_{\mathbf{B}})\chi_{0,\mathbf{B}}$. Then, from (5.104)

$$\|\exp(\beta|\cdot|/2)(P_{\mathbf{B}}-Q_{\mathbf{B}})\chi_{0,\mathbf{B}}\|^2\le\|\exp(\beta|\cdot|)(P_{\mathbf{B}}-Q_{\mathbf{B}})\chi_{0,\mathbf{B}}\| .$$

$$\|(P_{\mathbf{B}}-Q_{\mathbf{B}})\chi_{0,\mathbf{B}}\|\le cB . \tag{5.107}$$

Starting from (5.106) and (5.107) and repeating the analysis for G, one finds that, for $F>0$, $F^{-1/2}$ can be defined, and the analogue of Lemma 5.3 holds true.

Consider

$$w_{\mathbf{a},\mathbf{B}}=\sum_{\mathbf{b}}F^{-1/2}_{\mathbf{a},\mathbf{b}}\mu_{\mathbf{b},\mathbf{B}},\quad w_B\equiv w_{0,\mathbf{B}} . \tag{5.108}$$

Then the repetition of the proof of Lemma 5.4 shows that (5.41) and (5.42) are fulfilled and $\{w_{\mathbf{a},\mathbf{B}}\}_{a\in\Gamma}$ is an orthonormal basis in $P_{\mathbf{B}}L^2(\mathbb{R}^3)$.

Consider now the symmetry properties of $w_{\mathbf{a},\mathbf{B}}$. Let K be the time-reversal operator in $L^2(\mathbb{R}^3)$

$$Kf(\mathbf{x})=\overline{f(\mathbf{x})} . \tag{5.109}$$

A simple computation leads to

$$KH_{\mathbf{B}}K=H_{-\mathbf{B}} , \tag{5.110}$$

$$KT_{\mathbf{a},\mathbf{B}}K=T_{\mathbf{a},-\mathbf{B}} , \tag{5.111}$$

and, from Theorem 3.7,

$$Kw=w . \tag{5.112}$$

One can easily verify that

$$Kv_{\mathbf{a},\mathbf{B}}=v_{\mathbf{a},-\mathbf{B}}\ ,\quad g_{\mathbf{B}}(\mathbf{a})=\overline{g_{-\mathbf{B}}(\mathbf{a})} \tag{5.113}$$

and, due to $\overline{\eta_{\mathbf{a},\mathbf{b};\mathbf{B}}}=\eta_{\mathbf{a},\mathbf{b};-\mathbf{B}}$,

$$K\chi_{\mathbf{a},\mathbf{B}}=\chi_{\mathbf{a},-\mathbf{B}} \tag{5.114}$$

from (5.110) and (5.114), $KP_{\mathbf{B}}K=P_{-\mathbf{B}}$, $KQ_{\mathbf{B}}K=Q_{-\mathbf{B}}$, which implies

$$KU_{\mathbf{B}}K=U_{-\mathbf{B}}\ , \tag{5.115}$$

which together with (5.114) gives (5.43).

Suppose now that the crystal has a center of inversion, i.e., if O is given by

$$Of(\mathbf{x})=f(-\mathbf{x})\ , \tag{5.116}$$

then (see the remark following the proof of Theorem 3.7)

$$OH_{\mathbf{B}}O=H_{\mathbf{B}}\ ,\quad OP_{\mathbf{B}}O=P_{\mathbf{B}}\ , Ow=\pm w\ . \tag{5.117}$$

As above, by straightforward verifications

$$OT_{\mathbf{a},\mathbf{B}}O=T_{-\mathbf{a},\mathbf{B}}\ ,\quad Ov_{\mathbf{a},\mathbf{B}}=v_{-\mathbf{a},\mathbf{B}}\ ,\quad OQ_{\mathbf{B}}O=Q_{\mathbf{B}},$$

$$g_{\mathbf{B}}(\mathbf{a})=g_{\mathbf{B}}(-\mathbf{a})\ ,\quad O\chi_{\mathbf{a},\mathbf{B}}=\pm\chi_{-\mathbf{a},\mathbf{B}}\ ,\quad OU_{\mathbf{B}}O=U_{\mathbf{B}}\ ,$$

which implies (5.44), and the proof of the first part of the theorem is finished.

The relations (5.45) and (5.46) follow at once from (5.36), (5.37), (5.39), and (5.42). Due to Lemma 5.1.i, to prove (5.47) it is sufficient to verify that, for B sufficiently small, $H_{\mathbf{B}}w_{\mathbf{B}}$ is exponentially localized. This follows from

$$H_{\mathbf{B}}w_{\mathbf{B}}=P_{\mathbf{B}}H_{\mathbf{B}}P_{\mathbf{B}}w_{\mathbf{B}}=(2\pi i)^{-1}\int_C z(H_{\mathbf{B}}-z)^{-1}dz\,w_{\mathbf{B}}$$

and Theorem A.1 (see Appendix).

Using (5.43) and (5.105), from (5.46) it follows that

$$\overline{h_{\mathbf{B}}(\mathbf{a})}=\langle KH_{\mathbf{B}}w_{\mathbf{B}},Kw_{\mathbf{a},\mathbf{B}}\rangle=\langle H_{-\mathbf{B}}w_{-\mathbf{B}},w_{\mathbf{a},-\mathbf{B}}\rangle$$
$$=h_{-\mathbf{B}}(\mathbf{a})\ ,$$

i.e., the first equality in (5.48) holds true. Now, from the fact that $H_{\mathbf{B}}$ is self-adjoint and from (5.36) and (5.39),

$$h_{\mathbf{B}}(\mathbf{a})=\langle H_{\mathbf{B}}w_{\mathbf{B}},w_{\mathbf{a},\mathbf{B}}\rangle=\langle w_{-\mathbf{a},\mathbf{B}},H_{\mathbf{B}}w_{\mathbf{B}}\rangle=\overline{h_{\mathbf{B}}(-\mathbf{a})}\ ;$$

i.e., the second equality in (5.48) holds true.

Similarly, if the crystal has a center of inversion, from (5.44)

$$h_B(\mathbf{a})=h_{\mathbf{B}}(-\mathbf{a})\ ,$$

which together with (5.48) gives (5.49).

Consider finally the asymptotic expansion of $h_{\mathbf{B}}(\mathbf{a})$. Clearly, $v_{\mathbf{a},\mathbf{B}}$ has an asymptotic expansion in B. Then $O_{\mathbf{B}}$ has an asymptotic expansion, and by (5.97) $P_{\mathbf{B}}$ has also an asymptotic expansion. Now (5.98) and (5.46) imply the existence of the asymptotic expansion for $h_{\mathbf{B}}(\mathbf{a})$. Note that, due to the fact that the perturbation is off diagonal, up to terms of order B^2 [see (5.79)], $h_{\mathbf{B}}(\mathbf{a})=h_{\mathbf{B}}^{\chi}(\mathbf{a})$, i.e., up to terms of order B^2,

$$h_{\mathbf{B}}(\mathbf{a})=(g_{\mathbf{B}}^{-1/2}\square h_{\mathbf{B}}^{w}\square g_{\mathbf{B}}^{-1/2})(\mathbf{a})\ , \tag{5.118}$$

where

$$h_{\mathbf{B}}^{w}(\mathbf{a})=\langle H_{\mathbf{B}}w,T_{\mathbf{a},\mathbf{B}}w\rangle\ . \tag{5.119}$$

Indeed, note that

$$U_{\mathbf{B}}=P_{\mathbf{B}}Q_{\mathbf{B}}+(1-P_{\mathbf{B}})(1-Q_{\mathbf{B}})+O(B^2)\ . \tag{5.120}$$

On the other hand, since $R_2(z)$ is analytic inside C,

$$P_{\mathbf{B}}H_{\mathbf{B}}P_{\mathbf{B}}=(2\pi i)^{-1}\int_C z(H_B-z)^{-1}dz=Q_{\mathbf{B}}H_{\mathbf{B}}Q_{\mathbf{B}}-\left[(2\pi i)^{-1}\int_C z(R_1V_{12}R_2+R_2V_{21}R_1)dz\right]+O(B^2)\ . \tag{5.121}$$

From (5.120) and (5.121) it follows that

$$Q_{\mathbf{B}}U_{\mathbf{B}}^{*}P_{\mathbf{B}}H_{\mathbf{B}}P_{\mathbf{B}}U_{\mathbf{B}}Q_{\mathbf{B}}=Q_{\mathbf{B}}H_{\mathbf{B}}Q_{\mathbf{B}}+O(B^2)\ . \tag{5.122}$$

Now

$$\langle w_{\mathbf{B}},H_{\mathbf{B}}w_{\mathbf{a},\mathbf{B}}\rangle=\langle\chi_{0,\mathbf{B}},Q_{\mathbf{B}}U_{\mathbf{B}}^{*}P_{\mathbf{B}}H_{\mathbf{B}}P_{\mathbf{B}}U_{\mathbf{B}}Q_{\mathbf{B}}\chi_{\mathbf{a},\mathbf{B}}\rangle\ ,$$

which gives (5.118).

Using (5.118) and (5.119), one obtains (5.50). The fact that the coefficients of the odd powers of B vanish follows from (5.49).■

Corollary 5.1. $P_{\mathbf{B}}H_{\mathbf{B}}P_{\mathbf{B}}:P_{\mathbf{B}}L^2(\mathbb{R}^3)\to P_{\mathbf{B}}L^2(\mathbb{R}^3)$ *is unitary equivalent to the following operator in* $l^2(\Gamma)$:

$$H_{\mathrm{eff},\mathbf{B}}f(\mathbf{a})=\sum_{\mathbf{b}}\eta_{\mathbf{b},\mathbf{a};\mathbf{B}}h_{\mathbf{B}}(\mathbf{b}-\mathbf{a})f(\mathbf{b})\ . \tag{5.123}$$

Proof. Consider the operator $V:P_{\mathbf{B}}L^2(\mathbb{R}^3)\to l^2(\Gamma)$:

$$Vf(\mathbf{a})=\langle w_{\mathbf{a},\mathbf{B}},f\rangle\ .$$

By direct computation, $VP_{\mathbf{B}}H_{\mathbf{B}}P_{\mathbf{B}}V^{-1}=H_{\mathrm{eff},\mathbf{B}}$.■

Consider now the following bounded operator in $L^2(\mathbb{R}^3)$:

$$H_{\mathrm{PO},\mathbf{B}}f(\mathbf{x})=\sum_{\mathbf{c}\in\Gamma}h_{\mathbf{B}}(\mathbf{c})\exp[i(\mathbf{P}-\mathbf{B}\wedge\mathbf{x}/2)\cdot\mathbf{c}]f(\mathbf{x})\ . \tag{5.124}$$

Theorem 5.3. *The spectra of (5.123) and (5.124) coincide as sets.*

Proof. Let, for $\mathbf{r}\in Q$,

$$\Gamma_{\mathbf{r}}=\{\mathbf{a}_{\mathbf{r}}=\mathbf{a}+\mathbf{r}|\mathbf{r}\in Q\ ,\ \mathbf{a}\in\Gamma\}\ .$$

Note that $\mathbb{R}^3=\cup\Gamma_{\mathbf{r}}$, and then $L^2(\mathbb{R}^3)$ can be written as a direct integral of $l^2(\Gamma_{\mathbf{r}})$:

$$L^2(\mathbb{R}^3)=\int_Q^{\oplus} l^2(\Gamma_r)d\mathbf{r}[f_a(\mathbf{r})=f(\mathbf{r}+\mathbf{a})] .$$

In each $l^2(\Gamma_r)$ consider the operator

$$H_{\text{eff},\mathbf{B},\mathbf{r}}f(\mathbf{a}_r) = \sum_{c\in\Gamma}\exp[-i\mathbf{B}\cdot(\mathbf{a}_r\wedge\mathbf{c})/2]h_{\mathbf{B}}(\mathbf{c})f(\mathbf{a}_r+\mathbf{c}) . \quad (5.125)$$

Observe that $\exp(i\mathbf{P}\cdot\mathbf{c})f(\mathbf{x})=f(\mathbf{x}+c)$ and $[P\cdot\mathbf{c},(\mathbf{B}\wedge\mathbf{x})/2]=0$. It follows that $H_{\text{PO},\mathbf{B}}$, as given by (5.116), is nothing but

$$H_{\text{PO},\mathbf{B}}=\int_Q^{\oplus} H_{\text{eff},\mathbf{B},\mathbf{r}}d\mathbf{r} . \quad (5.126)$$

Since the spectra of $H_{\text{eff},\mathbf{B},\mathbf{r}}$ are independent of $\mathbf{r}$ and coincide with the spectrum of $H_{\text{eff},\mathbf{B}}$, the Theorem follows from the fact that by (5.126) the spectrum of $H_{\text{PO},\mathbf{B}}$ equals the union over Q of $H_{\text{eff},\mathbf{B},\mathbf{r}}$.■

Let us remark that, if

$$\lambda_{\mathbf{B}}(\mathbf{k})=\sum_{b\in\Gamma}h_{\mathbf{B}}(\mathbf{b})\exp(i\mathbf{k}\cdot\mathbf{b}) ,$$

then $H_{\text{PO},\mathbf{B}}$ is the Weyl quantization of $\lambda_{\mathbf{B}}(\mathbf{k})$. From the proof of Theorem 5.3 it follows the spectrum of $H_{\text{PO},\mathbf{B}}$ is infinitely degenerate with respect to the spectrum of $H_{\text{eff},\mathbf{B}}$.

Finally, let us prove (2.31). This follows from (5.99) and the following.

Lemma 5.8. *For all $B>0$,*

$$\|Q_{\mathbf{B}}-P_0\|=1 . \quad (5.127)$$

Proof. The argument in the proof of Lemma 5.1.i gives

$$|\langle v_{\mathbf{B},\mathbf{a}},w_{\mathbf{a}+\mathbf{b}}\rangle| \le \text{const}\times\exp(-\alpha|\mathbf{b}|) . \quad (5.128)$$

By the Riemann-Lebesgue lemma (Reed and Simon, 1975), for fixed $\mathbf{b}$

$$\lim_{\mathbf{a}\to\infty}\langle v_{\mathbf{B},\mathbf{a}},w_{\mathbf{a}+\mathbf{b}}\rangle=0 . \quad (5.129)$$

On the other hand,

$$\|Q_{\mathbf{B}}-P_0\|\ge 1-\inf_{\mathbf{a}\in\Gamma}\sum_{\mathbf{b}}|\langle v_{\mathbf{B},\mathbf{a}}w_{\mathbf{a}+\mathbf{b}}\rangle|^2 . \quad (5.130)$$

From (5.128), (5.129), and the Lebesgue-dominated convergence theorem, the second term in the right-hand side of (5.130) vanishes.■

VI. OTHER APPROACHES

A. The Stark-Wannier states

The Stark-Wannier states can be described not only (as in Sec. IV) in terms of spectral concentration, but also by resonances understood as complex poles of the analytic continuation of certain matrix elements of the resolvent to the nonphysical sheet. This point of view, having its roots in the famous Breit-Wigner formula, has been very successful in the atomic case, where a very detailed description of the Stark effect in atoms and molecules exists (see, e.g., the reviews by Hunziker, 1980, and Herbst, 1981).

As for the periodic (one-dimensional) case, one of the first results in this direction was obtained by Herbst and Howland (1981), as follows.

Suppose $V(x)$ is the restriction to $\mathbb{R}$ of a function analytic in $|\text{Im}z|<\alpha_0$ and satisfies a growth estimate. Then the "translated" Hamiltonian

$$H_F(-i\alpha)=-d^2/dx^2+V(x-i\alpha)+F(x-i\alpha) , \quad |\alpha|<\alpha_0$$

has its essential spectrum contained in $\mathbb{R}-i\alpha F=\{\lambda\in\mathbb{C}|\lambda=x-i\alpha F, x\in\mathbb{R}\}$.

The point of this result is that if $H_F(-i\alpha)$ has some discrete spectrum outside $\mathbb{R}-i\alpha F$, then due to $[H_F,T_a]=aFT_a$, this discrete spectrum has the form of Stark-Wannier ladders of complex eigenvalues. The *existence* of the discrete spectrum for $H_F(-i\alpha)$ has been proved by Agler and Froese (1985) for the case when $V(x)$ is a trigonometric polynomial and the field is *sufficiently large.* The last condition is very unpleasant from the physical point of view, and it will be very nice to remove it.

Much more detailed results have been obtained recently by Bentosela and Grecchi (1991) and by Combes and Hislop (1990). Using the ideas recently developed about shape resonances in quantum mechanics—spectral deformations, geometric perturbation theory exponential decay estimates of eigenfunctions (Combes *et al.*, 1987; Heiffer and Sjöstrand, 1986; Hislop and Segal, 1989)—they were able to prove (in the semiclassical limit) the existence of the Stark-Wannier resonances as well as to obtain bounds on the imaginary part of the resonance position, leading to exponential bounds on the width of the resonances for some regimes of the fields (e.g., Combes and Hislop require $F>\text{const}\hbar^{\alpha}$, $0<\alpha<1$). Even more precise results have been obtained by Buslaev and Dmitrieva (1991): by pushing very far the semiclassical method (see Sec. VIc) they were able not only to prove the existence of the resonances but also, under some simplifying assumptions, to give an asymptotic formula for the imaginary part of the resonances.

Alternatively, Avron (1979) has proved for general potentials (i.e., for potentials without analyticity properties) that, for *complex values* of F, H_F has only discrete spectra. This result has been extended recently by Bentosela *et al.* (1988) to a very large class of potentials (including, e.g., δ-like potentials). Moreover, they proved that the Stark-Wannier states are analytic as functions of F in a disc, $|F-iF_0|<F_0$, $F_0>0$, tangent to the real axis at the origin. An asymptotic expansion up to the second order is also given. Unfortunately, again, the physical values of the field lie outside the region for which the results are proved.

Using the Livsic matrix theory (see, e.g., Howland, 1975) and the Fermi golden rule, Avron (1982) proved, for potentials with a finite number of gaps, that the width of the Stark-Wannier resonances is exponentially small. Moreover, he discovered that the widths of the Stark-Wannier resonances have an intrinsically complicated behavior: the width oscillates over different orders of magnitude as the field changes slightly. One can understand these oscillations as a consequence of a resonance phenomenon. Suppose that the zero-field Hamiltonian has many (generically an infinite number) isolated bands. Then at nonzero fields, if the interband coupling is neglected, the spectrum contains the union of the corresponding Stark-Wannier ladders of eigenvalues depending on F [see, e.g., (2.19)]. The interband coupling turns all these eigenvalues into resonances. Consider two resonances with quite different widths $\gamma_1 \gg \gamma_2$, whose positions cross each other as the field changes. While away from crossing, the widths are on different scales; at crossing, via the "interaction" given by the interband coupling, both resonance will have widths of order γ_1. Now if one takes into account that, generically, the number of the Stark-Wannier ladders is infinite so that the "frequency" of the crossing is in some sense dense, one obtains the complicated behavior of the widths as the field changes. Related results and numerical computations are contained in Bentosela, Grecchi, and Zironi (1983). For more details the reader should consult the above-cited paper which contains a nice discussion of the subject. Let us note that the main open problem of the subject is to prove that the width of the Stark-Wannier reosnances is exponentially small for the general case.

The approaches described above are in some sense complementary to the result described in Sec. IV. While, from the conceptual point of view, the resonances viewed as complex poles have the advantage of being clearly defined, the spectral concentration approach developed in Sec. IV seems to be superior from the practical point of view. In particular, it gives explicit algorithms for the computation of the positions of the resonances and of the bounds for their lifetimes, for physical values of the fields. One can hope that a combination of the two approaches will produce in the near future results as precise as the existent ones for the atomic case.

B. The Peierls-Onsager effective Hamiltonian

The Peierls-Onsager effective Hamiltonian is discussed in recent papers by Béllissard (1987b) and Helffer and Sjöstrand (1989a, 1989b). Their effective Hamiltonians are somewhat different from the effective Hamiltonian given in Sec. V.

Béllissard defines the effective Hamiltonian by the Feschbach projection method originating in nuclear physics (Feschbach, 1958).

Let H be a self-adjoint operator in $\mathcal{H}$, P an orthogonal projection in $\mathcal{H}$, $\mathcal{K}=P\mathcal{H}$, $Q=(1-P)$. Suppose that $PHQ+QHP$ is bounded with respect to $PHP+QHQ$. The resummation of the Neumann series for $(H-z)^{-1}$ (with $PHP+QHQ$ as the unperturbed operator), at Imz sufficiently large, gives

$$(H-z)^{-1}=R_2(z)+[1-R_2(z)V_{2I}][H_{\text{eff}}^F(z)-z]^{-1} \times[1-V_{12}R_2(z)] , \tag{6.1}$$

where $R_1(z)=(PHP-z)^{-1}$, $R_2(z)=(QHQ-z)^{-1}$, $V_{12}=PHQ$, $V_{21}=QHP$, and

$$H_{\text{eff}}^F(z)=PHP-V_{12}R_2(z)V_{21}:\mathcal{K}\to\mathcal{K} . \tag{6.2}$$

The formula (6.2) gives at once the Feschbach lemma.

Lemma 6.1. *Let $\lambda\in\mathbb{R}\cap\rho(QHQ)$. Then λ belongs to the spectrum of H if and only if it belongs to the spectrum of $H_{\text{eff}}^F(\lambda)$.*

In this way the spectral problem for H has been replaced by the spectra problem for $H_{\text{eff}}^F(z)$ in the subspace $\mathcal{K}$.

The Grushin (1970) method, used by Helffer and Sjöstrand, is (in this context) related to the Feschbach method. Consider the Hilbert space $\mathcal{H}\oplus\mathcal{K}$ and the following operator in it:

$$\mathcal{P}(z)=\begin{bmatrix} H-z & R_- \\ R_+ & 0 \end{bmatrix} ,$$

where $R_+\mathcal{H}\to\mathcal{K}$ is given by

$$R_+f=Pf$$

and $R_-=R_+^*$

Lemma 6.2. *Suppose*

$$\mathcal{P}^{-1}(z)=\begin{bmatrix} E(z) & E_-(z) \\ E_+(z) & H_{\text{eff}}^G(z)-z \end{bmatrix}$$

exists. Then $(H-z)^{-1}$ exists if and only if $[H_{\text{eff}}^F(z)-z]^{-1}$ exists. Actually,

$$(H-z)^{-1}=E(z)-E_-(z)[H_{\text{eff}}^G(z)-z]^{-1}E_+(z) ,$$

$$[H_{\text{eff}}^G(z)-z]^{-1}=-R_+(H-z)^{-1}R_- .$$

Proof. Direct verification.■

Again, by Lemma 6.2, the spectral problem for H is replaced by the corresponding spectral problem for $H_{\text{eff}}F(z)$ in $\mathcal{K}$.

To apply the above results to the magnetic-field case one takes $\mathcal{K}=\mathcal{N}_{\mathbf{B}}$ (see Sec. II E). One can prove (Helffer and Sjöstrand, 1989a, 1989b) that Lemma 6.2 can be applied. Then, written in the (nonorthogonal) basis $\{v_{\mathbf{B},\mathbf{a}}\}_{\mathbf{a}\in\Gamma}$, $H_{\text{eff}}^{F,G}(z)$ take a form similar to (2.40), with $h_{\mathbf{B}}$ depending on the spectral variable z. Very recently, along these lines, Helffer and Sjöstrand (1989)c) were able to construct an effective Hamiltonian in order to treat the de Haas–van Alphen effect under more general conditions on the zero-field Hamiltonian: the nondegeneracy of $\lambda_0(\mathbf{k})$ is required only a small neighborhood of the Fermi energy.

Let us stress that the spectral problems for $H_{\text{eff}}^{F,G}(z)$ in the subspace $\mathcal{K}$ are nonlinear: the operators themselves depend on the energy. For methods to cope with such nonlinear spectral problems we refer the reader to Helffer and Sjöstrand (1988). On the other hand, as already stated the Grushin method works also in the case of the overlapping bands, which is the most common case in real crystals. A review of the work of Helffer and Sjöstrand is contained in the recent CIME Lectures by Sjöstrand (1989).

Let us mention that the Feschbach scheme has been used in the Born-Oppenheimer approximation problem (Combes *et al.*, 1981). Also in this case it is possible to obtain, via the perturbation theory, a "true" effective Hamiltonian, i.e., an effective Hamiltonian which does not depend on the energy.

C. The semiclassical approach

Another route to the "effective Hamiltonians" is based on semiclassical techniques. This approach relies heavily on the modern theory of pseudodifferential and Fourier integral operators, and a detailed exposition is outside the scope of the present review. At the formal level this approach is beautifully described in a recent review by Buslaev (1988). Rigorous results for the magnetic field case were obtained independently by Guillot, Ralston, and Trubowitz (1988). One can expect more results in the near future.

There are many (essentially equivalent) ways to understand these methods. The main point is that [for the sake of simplicity we shall discuss the magnetic field case, but the scheme in Buslaev (1988) is general] for $B \to 0$ there are two spatial scales in the system: the first one of the order of the linear dimensions, a, of the periodicity cell and the second one of order a/B, on which the vector potential varies appreciably. This makes possible the use of the method of two-scale expansions (homogenization) (see, e.g., Benssousan, Lions, and Papanicolaou, 1978). This amounts to considering, in the first approximation, $\mathbf{x}$ and $B\mathbf{x}$ as independent variables. At a more precise level, instead of the eigenvalue problem

$$[(-i\,\mathrm{grad}_{\mathbf{x}} - B\mathbf{n}\wedge\mathbf{x}/2)^2 + V(\mathbf{x})]u(\mathbf{x}) = Eu(\mathbf{x}) , \qquad (6.3)$$

one has to consider the eigenvalue problem

$$[(-i\,\mathrm{grad}_{\mathbf{x}} - iB\,\mathrm{grad}_{\mathbf{y}} - \mathbf{n}\wedge\mathbf{y}/2)^2 + V(\mathbf{x})]u(\mathbf{x},\mathbf{y};\mathbf{B}) = Eu(\mathbf{x},\mathbf{y};B) . \qquad (6.4)$$

Note that, if in the solution $u(\mathbf{x},\mathbf{y};B)$ of (6.4) we let $\mathbf{y}=B\mathbf{x}$, then it becomes a solution of (6.3). In the variable $\mathbf{x}$, $u(\mathbf{x},\mathbf{y},B)$ is required to be periodic. Now if (6.4) is regarded as an equation for the vector-valued function $\mathbf{y}\to u(\cdot,\mathbf{y};B)$, then (6.4) has exactly the form on which semiclassical methods can be applied; i.e., one looks for local solutions of the form

$$u(\mathbf{x},\mathbf{y};B) = \exp[i\tau(\mathbf{y})/B]\sum_0^\infty (iB)^n u_n(\mathbf{x},\mathbf{y}) , \quad \tau(\mathbf{y}) \in \mathbb{R} .$$

Then, using the method initiated by Keller (Keller, 1958; Keller and Rubinov, 1960), and developed independently by Maslov (Maslov, 1972; Maslov and Fedoryuk, 1976; Duistermaat, 1974) to construct global solutions out of local ones, one obtains approximate eigenvalues and eigenvectors.

The basic steps of the construction involve an associated Hamilton-Jacobi equation and then a classical Hamiltonian system. Now, if $E \in \sigma_0$ and $\sigma_0 = \{\lambda_0(\mathbf{k})\}$ is a simple band, then the *same Hamiltonian* structure appears in the semiclassical approximation for the "effective" Hamiltonian

$$H_{\mathrm{eff}} = \lambda_0(-i\,\mathrm{grad}_{\mathbf{x}} - \mathbf{B}\wedge\mathbf{x}/2) . \qquad (6.5)$$

As a consequence, to the *leading* order in B, the eigenvalues of H_B coincide (in the sense of spectral concentration) with the eigenvalues of the operator given by (6.5). Note that, while the effective Hamiltonian obtained in Sec. V is exact, the Hamiltonian (6.5) is an approximate one and corresponds to the leading-order $h_B(\mathbf{a}) = h_0(\mathbf{a})$ in (5.123). Let us stress, however, that the semiclassical theory is able to give the while asymptotic expansion in powers of B for the eigenvalues and eigenvectors of H_B (see, e.g., the remark following the main theorem in Guillot, Ralston, and Trubowitz, 1988).

While the theory in Sec. V, as well as the related approaches of Béllissard (1987, 1988), Helffer and Sjöstrand (1989a, 1989b), originates in the heuristics put forward by Peierls (1933), Luttinger (1951), and Wannier (1962), the semiclassical theory is closer in spirit to the approach developed by Blount (1962b), Roth (1962) and Zak (1972). The rigorous theory along these lines is far from being complete and new results are expected to appear. For more references we refer the reader to Zak (1972), Buslaev (1988), and Guillot, Ralston, and Trubowitz (1980).

D. The Harper equation

The effective Hamiltonian $H_{\mathrm{eff},\mathbf{B}}$ is a generalization of the famous Harper operator (Harper, 1955). Actually, $H_{\mathrm{eff},\mathbf{B}}$ reduces to the Harper operator in the tight-binding limit.

Consider for simplicity a two-dimensional system with the magnetic field perpendicular to its plane. Moreover, consider Γ to be a square lattice of unit length, so that $\mathbf{a} = \{m,n\}$, $m,n \in \mathbb{Z}$. Then the effective Hamiltonian (2.40) takes the form

$$H_{\mathrm{eff},\mathbf{B}} f(m,n) = \sum_{p,q\in\mathbb{Z}} \exp[-iB(mq-np)/2] h_{\mathbf{B}}(p,q) f(m+p,n+q) .$$

Suppose now that the crystal has a center of inversion, and, moreover, make the tight-binding approximation; this amounts to considering only $h_{\mathbf{B}}(0,0)=E_0$, $h_{\mathbf{B}}(0,1)=h_{\mathbf{B}}(0,-1)=h_1$, $h_{\mathbf{B}}(1,0)=h_{\mathbf{B}}(-1,0)=h_2$ to be different from zero. Then

$$(H_{\text{eff},\mathbf{B}}-E_0)f(m,n)\equiv H_H f(m,n)=h_1[\exp(-iBm/2)f(m,n+1)+\exp(iBm/2)f(m,n-1)] \\ +h_2[\exp(inB/2)f(m+1,n)+\exp(-inB/2)f(m-1,n)]$$

which is just the Harper operator. The most common form of the Harper operator can be obtained by going to the Landau gauge. More precisely, consider the gauge transformation

$$Uf(m,n)=\exp(-iBmn/2)f(m,n) .$$

By direct computation,

$$U^*H_H Uf(m,n)=h_2[f(m+1,n)+f(m-1,n)] \\ +h_1[\exp(-iBm)f(m,n+1) \\ +\exp(iBm)f(m,n-1)] . \quad (6.6)$$

Since $U^*H_H U$ commutes with translations in the second variable, its eigenfunctions have the form

$$f(m,n)=\exp(-ikn)f(m) , \quad k\in[0,2\pi) . \quad (6.7)$$

Introducing (6.7) into (6.6), one obtains that the spectrum Σ_{B,h_1,h_2} of $U^*H_H U$ is the union over $k\in[0,2\pi)$ of the spectra $\Sigma^k_{\mathbf{B},h_1,h_2}$ of the operators

$$H^k_{B,h_1,h_2}f(m,n)=h_2[f(m+1)+f(m-1)] \\ +2h_1\cos(Bm+k)fm . \quad (6.8)$$

Factorizing h_2 and writing $\mu=h_1/h_2$, $B=2\pi\alpha$, one obtains that (up to a scale factor) the spectrum of H_H equals $\Sigma^{\alpha,\mu}=\bigcup_k \Sigma^{\alpha,\mu}_k$, where $\Sigma^{\alpha,\mu}_k$ are the spectra of

$$H^{\alpha,\mu}_k f(m)=f(m+1)+f(m-1) \\ +2\mu\cos(2\pi\alpha m+k)f(m) . \quad (6.9)$$

In spite of its apparent simplicity, the spectrum of $H^{\alpha,\mu}_k$ is a very compacated and beautiful object. This fact has been discovered by Hofstadter (1976) when he produced numerically his famous "buterfly." The main point is that, by Floquet-Bloch theory, if $\alpha=p/q$ is rational, $\Sigma^{\alpha,\mu}$ is the union of q bands. Now when $q\to\infty$, the number of bands increases indefinitely, and the idea of Hofstadter was to show how the repartition of these bands depends on the expansion of α as a continuous fraction (finite in the case where α is rational). This permits one to imagine the spectrum in the irrational case, which is usually assumed to be a Cantor set. In the past two decades the Hofstadter buterfly has been much studied. Basic ideas, partially heuristic, appeared in Azbel (1964), Wannier (1978), Claro and Wannier (1979), Wilkinson (1984, 1986, 1987), and Sokoloff (1985). Mathematical techniques ranging from semiclassical analysis of pseudodifferential operators to C^* algebras have been used to prove rigorously different properties which appear on the Hofstadter buterfly: Béllissard and Simon (1982), Simon (1982), Helffer and Sjöstrand (1988, 1989a, 1989b) van Mouche (1989), and Choi *et al.* (1990). For a nice discussion of the Hofstadter buterfly based both on rigorous results as well as on numerical computations, we refer the reader to Guilement, Helffer, and Treton (1989). Basically, although the fact that $\Sigma^{\alpha,\mu}$ is a Cantor set for irrational α has not been proved in full generality, one can say that the Hofstadter buterfly is well understood. The main problem is to extend the results to $H_{\text{eff},\mathbf{B}}$. Up to now only partial results for some small perturbations of the Harper operator have been obtained (Helffer and Sjöstrand, 1988, 1989a, 1989b, 1989c).

APPENDIX

Consider a continuously differentiable family of orthogonal projections $Q(s)$, $s\in\mathbb{R}$. A transformation function (Kato, 1966; Reed and Simon, 1978) for $Q(s)$ is a family $T(s)$ of unitary operators satisfying

$$Q(s)=T(s)Q(0)T(s)^{-1} , \quad T(0)=1 . \quad (A1)$$

The following construction goes back to Krein and Daletskii and to Kato [see the references in (Krein, 1967) and (Kato, 1966)].

Lemma A.1. *If $K(s)$ is given by*

$$K(s)=i[1-2Q(s)](d/ds)Q(s) \quad (A2)$$

then

i. *$K(s)$ is self-adjoint.*

ii. $Q(s)K(s)Q(s)=0$.

$$(A3)$$

iii. *The (unique) solution of*

$$i(d/ds)A(s)=K(s)A(s) , \quad A(0)=1 \quad (A4)$$

is a transformation function for $Q(s)$, i.e.,

$$Q(s)=A(s)Q(0)A(s)^{-1} . \quad (A5)$$

iv. $Q(s)[(d/ds)A(s)]Q(0)=0.$

$$(A6)$$

v. *If $Q(s)$ is the restriction to $\mathbb{R}$ of a bounded projection-valued function, analytic in a complex neighborhood $\mathcal{W}$ of $\mathbb{R}$, then $A(s)$ is the restriction to $\mathbb{R}$ of a bounded with a bounded inverse operator-valued function analytic in $\mathcal{W}$.*

Proofs. i–iv are direct verifications (Messiah, 1969). For *v*, see Kato (1966), Reed and Simon (1978).■

The property (A6) has a nice geometric interpretation: if $\dim Q(s)=1$, $\psi_0\in Q(0)\mathcal{H}$, and $\psi(s)=A(s)\psi_0$, then

$$\langle \psi(s),(d/ds)\psi(s)\rangle = 0 \ , \tag{A7}$$

i.e., $\psi(s)$ is a parallel transport in $\mathcal{H}$ (Simon, 1983).

In what follows we shall consider the "unperturbed" Hamiltonian in Sec. V.A,

$$H_0 = (\mathbf{P} - \mathbf{A}^0)^2 + V \ . \tag{A8}$$

We shall prove that (see below for the precise meaning) the Green function $G_0(\mathbf{x},\mathbf{y};z)$ corresponding to H_0 vanishes exponentially when $|\mathbf{x}-\mathbf{y}| \to \infty$. The idea of proof is due to Combes and Thomas (see Helffer and Sjöstrand, 1989b for related results).

Theorem A.1. *Let* $z \in \rho(H_0)$. *There exist* $\alpha(z) > 0$, $M < \infty$ *such that, for* $0 \le \alpha \le \alpha(z)$, *and all* $\mathbf{a} \in \mathbb{R}^3$

$$\|\exp(\alpha|\cdot - \mathbf{a}|)(H_0 - z)^{-1}\exp(-\alpha|\cdot - \mathbf{a}|)\| \le M \ . \tag{A9}$$

Moreover,

$$\lim_{\alpha\to 0} \exp(\alpha|\cdot - \mathbf{a}|)(H_0 - z)^{-1}\exp(-\alpha|\cdot - \mathbf{a}|) - (H_0 - z)^{-1}\| = 0 \ . \tag{A10}$$

The meaning of (A9) is that if f is exponentially localized then $(H_0 - z)^{-1} f$ is also exponentially localized.

Proof. Consider

$$g_{\mathbf{a}}(\mathbf{x}) = [(\mathbf{x} - \mathbf{a})^2 + 1]^{1/2} \ . \tag{A11}$$

Since

$$\sup_{\mathbf{a},\mathbf{x} \in \mathbb{R}^3} |g_{\mathbf{a}}(\mathbf{x}) - |\mathbf{x} - \mathbf{a}|| = 1 \ ,$$

it is sufficient to prove the theorem with $|\mathbf{x} - \mathbf{a}|$ replaced by $g_{\mathbf{a}}(\mathbf{x})$.

By direct verification,

$$|\mathrm{grad} g_{\mathbf{a}}(\mathbf{x})| \le 1 \ , \quad |\mathrm{grad}^2 g_{\mathbf{a}}(\mathbf{x})| \le 2 \ . \tag{A12}$$

Consider, for $\alpha > 0$, $f \in \mathcal{D}(H_0)$

$$\begin{aligned} \exp(\alpha g_{\mathbf{a}})(H_0 - z)\exp(-\alpha g_{\mathbf{a}}) f &= [(\mathbf{P} - \mathbf{A}^0 + i\alpha\,\mathrm{grad} g_{\mathbf{a}})^2 + V - z] f \\ &= (H_0 - z + \alpha H_1) f = [1 + \alpha H_1 (H_0 - z)^{-1}](H_0 - z) f \ , \end{aligned} \tag{A13}$$

where

$$H_1 = 2i\,\mathrm{grad} g_{\mathbf{a}} \cdot (\mathbf{P} - \mathbf{A}^0) + i\,\mathrm{grad}^2 g_{\mathbf{a}} - \alpha|\mathrm{grad} g_{\mathbf{a}}|^2 \ . \tag{A14}$$

The main point of the proof is that H_1 is H_0 bounded, i.e.,

$$\|H_1 (H_0 - z)^{-1}\| \le v(z) < \infty \ . \tag{A15}$$

Since V is $(\mathbf{P} - \mathbf{A}^0)^2$ bounded (Avron *et al.*, 1978), it is sufficient to prove that H_1 is $(\mathbf{P} - \mathbf{A}^0)^2$ bounded, and this is obvious from (A14). It follows that, for

$$|\alpha| < v(z)^{-1} \ , \tag{A16}$$

$[1 + \alpha H_1 (H_0 - z)^{-1}]$ is invertible, and then by (A13)

$$\|[\exp(\alpha g_{\mathbf{a}})(H_0 - z)\exp(-\alpha g_{\mathbf{a}})]^{-1}\| \le M < \infty \tag{A17}$$

On the other hand, for $f \in \mathcal{C}_0^\infty(\mathbb{R}^3)$,

$$\exp(\alpha \mathbf{g}_{\mathbf{a}})(H_0 - z)^{-1}\exp(-\alpha g_{\mathbf{a}})\exp(\alpha g_{\mathbf{a}})(H_0 - z)\exp(-\alpha g_a) f = f \ ,$$

which implies

$$[\exp(\alpha g_{\mathbf{a}})(H_0 - z)\exp(-\alpha g_{\mathbf{a}})]^{-1} = \exp(\alpha g_{\mathbf{a}})(H_0 - z)^{-1}\exp(-\alpha g_{\mathbf{a}}) \ ;$$

and the proof of (A9) is finished.

Now

$$\begin{aligned} \|\exp(\alpha g_{\mathbf{a}})(H_0 - z)^{-1}\exp(-\alpha g_{\mathbf{a}}) - (H_0 - z)^{-1}\| &= \|(H_0 - z)^{-1}\| \, \|[1 + \alpha H_1 (H_0 - z)^{-1}]^{-1} - 1\| \\ &\le \alpha v(z)[1 - \alpha v(z)]^{-1} \|(H_0 - z)^{-1}\| \end{aligned}$$

which implies (A10).■

Corollary A.1. *Suppose H_0 has an isolated band σ_0, and let P_0 be the spectral projection of H_0 corresponding to σ_0. There exist $\alpha_0 > 0$, $M < \infty$ such that for $0 \le \alpha \le \alpha_0$, and all $\mathbf{a} \in \mathbb{R}^3$,*

$$\|\exp(\alpha|\cdot-\mathbf{a}|)P_0\exp(-\alpha|\cdot-\mathbf{a}|)\| \le M \ , \tag{A18}$$

$$\lim_{\alpha\to 0}\|\exp(\alpha|\cdot-\mathbf{a}|)P_0\exp(-\alpha|\cdot-\mathbf{a}|)-P_0\| = 0 \ . \tag{A19}$$

Proof. By the Riesz formula,

$$P_0 = (2\pi)^{-1}\int_C (H_0 - z)^{-1} dz \ ,$$

where C is a contour of finite length enclosing σ_0, (A18) and (A19) follow from (A9) and (A10), respectively.■

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