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1982 J. Phys. A: Math. Gen. 15 3313

(http://iopscience.iop.org/0305-4470/15/10/034)

J. Phys. A: Math. Gen. 15 (1982) 3313–3328. Printed in Great Britain

# Dynamics of Bloch electrons in external electric fields: II. The existence of Stark–Wannier ladder resonances

A Nenciu† and G Nenciu‡

Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, SU-141980, Dubna, USSR

Received 25 March 1982

**Abstract.** The problem of the existence of the Stark–Wannier ladder for the Bloch electrons in homogeneous electric fields is considered. If the direction of the electric field coincides with one of the reciprocal lattice vectors, as is well known, the Hamiltonian of the problem can be written as a direct integral of one-dimensional-like Hamiltonians. For these Hamiltonians, the existence of Stark–Wannier ladders of well separated resonances is proved. The wavefunctions corresponding to these resonances are shown to decay exponentially along the field direction.

## 1. Introduction

This is the second in a series of papers dealing, at a rigorous level, with the dynamics of the Bloch electrons in external electric fields. The Hamiltonian of the problem is of the form

$$H^{\varepsilon} = H_0 + \varepsilon X_0 \qquad \varepsilon = eE$$

where $H_0 = -\Delta + V_{\text{per}}$ is the 'unperturbed' periodic Hamiltonian, and $\varepsilon X_0 = eE\boldsymbol{n}x$, $|\boldsymbol{n}| = 1$, is the potential energy of the electric field. In this paper, we shall consider the controversial problem of the existence of the Stark–Wannier (SW) ladder. Originally, it was believed that an SW ladder exists in the following sense: in the Hilbert space of states $\mathscr{H}$, there exists a 'one-band' subspace $\mathscr{K}$ such that $\mathscr{K}$ is invariant under $H^{\varepsilon}$ (i.e. with respect to the decomposition $\mathscr{H} = \mathscr{K} \oplus \mathscr{K}^{\perp}$, $H^{\varepsilon}$ takes a diagonal form) and $H^{\varepsilon}$ restricted to $\mathscr{K}$ has a discrete spectrum of the form $\alpha + \beta\varepsilon n$ where $\alpha$, $\beta$ are constants, $n = 0, \pm 1, \pm 2, \ldots$. In the one-dimensional case (and very probably, also in the three-dimensional case), this possibility is ruled out by the fact that the spectrum of $H^{\varepsilon}$ is absolutely continuous (Avron *et al* 1977). So, if the SW ladder exists, its levels must, in fact, be resonances. This situation can be viewed as follows. The subspace $\mathscr{K}$ (which actually can depend on $\varepsilon$) is not exactly invariant under $H^{\varepsilon}$, but only 'asymptotically' invariant (see Nenciu (1981) for a precise definition) in the sense that the non-diagonal part of $H^{\varepsilon}$ is a bounded operator of order $\varepsilon^{p}$, $p > 0$. In this case, even if the 'one-band' Hamiltonian $P_{\varepsilon} H^{\varepsilon} P_{\varepsilon}$, where $P_{\varepsilon}$ is the orthogonal projection on $\mathscr{K}$, has a discrete spectrum, the 'tunnelling' due to the non-diagonal part of $H^{\varepsilon}$, $P_{\varepsilon} H^{\varepsilon}(1 - P_{\varepsilon}) + \text{HC}$ results in a finite width of the levels. Let $\lambda$, $\psi_{\lambda}$ be an

† Permanent address: IFTM, Central Institute of Physics, PO Box Mg 7 Bucharest, Romania.
‡ IFIN, Central Institute of Physics, PO Box Mg 6 Bucharest, Romania.

eigenvalue and the corresponding eigenfunction of $P_\varepsilon H^\varepsilon P_\varepsilon$. If, following Avron *et al* (1975), we take

$$\gamma^2 \sim ((H^\varepsilon - \lambda)\psi_\lambda, (H^\varepsilon - \lambda)\psi_\lambda) \equiv (\Delta\lambda)^2$$

as a measure of the width, then

$$\gamma^2 \sim (\psi_\lambda, (P_\varepsilon H^\varepsilon(1-P_\varepsilon) + \text{HC})^2 \psi_\lambda).$$

Clearly, in order that the level structure of $P_\varepsilon H^\varepsilon P_\varepsilon$ is not washed by the effect of the non-diagonal part, it is necessary for $\gamma$ to be smaller than the level spacing. All the existing derivations use as $\mathcal{K}$ the subspace corresponding to an isolated band of $H_0$ either simple or composed by mutually non-intersecting branches (Avron *et al* 1977, Avron 1979, Callaway 1974, Hacker and Obermair 1970). The rigorous derivations are for one-dimensional systems, although the results can be extended to the three-dimensional case (see, however, the discussion below) if the localised Wannier functions corresponding to the considered band are supposed to exist (see Kohn (1959), des Cloizeaux (1964) for the problem of the existence of Wannier functions). In all cases considered, the spacing between the SW levels is of order $\varepsilon$, and $\gamma$ is also of the order $\varepsilon$ (Avron *et al* 1975). This fact has led Avron *et al* (1975) (see also Zak 1969, Rabinovitch and Zak 1971, Zak 1972) to the conclusion that the existing derivations of the SW ladder are inconclusive. This controversy generated a lot of approximate and numerical computations (Berezhkovskii and Ovchinnikov 1976, Banavar and Coon 1978, Nagai and Kondo 1980, Bentosela *et al* 1981), all of them indicating the existence of well separated SW resonances. In order to clarify this problem, one needs to prove that:

(i) one can choose $\mathcal{K}$ such that the non-diagonal part is of the order of $\varepsilon^{p+1}$, $p > 0$; and

(ii) the spectrum of $P_\varepsilon H^\varepsilon P_\varepsilon$ has the structure of an SW ladder, with spacing between levels of the order $\varepsilon$.

Problem (i) has been solved in the previous paper (Nenciu and Nenciu 1980, 1981) substantiating an old idea (Kane 1959, Wannier 1960) that one can redefine the bands of $H^\varepsilon$ such that the non-diagonal part of $H^\varepsilon$ is of the order $\varepsilon^{n+1}$, $n$ being a positive integer. More exactly, we constructed recurrently a sequence of periodic operators $H_n(\varepsilon)$, $n = 0, 1, 2, \ldots$, $H_0(\varepsilon) = H_0$, such that the non-diagonal part of $H^\varepsilon$ with respect to the bands of $H_n(\varepsilon)$ is bounded and of the order $\varepsilon^{n+1}$. Moreover, the bands of $H_n(\varepsilon)$ go smoothly to the bands of $H_0$ as $\varepsilon \to 0$. The diagonal part of $H^\varepsilon$ is an orthogonal sum of 'one-band Hamiltonians' $H^{\mathrm{W}}_{i,n}(\varepsilon)$ ($i$ being the band index) which we have called 'effective Wannier Hamiltonians' of order $n$.

In this paper we shall consider problem (ii). In contradistinction to the previous papers on the SW ladder, we shall consider the general, multi-dimensional case. We shall assume that the direction of the homogeneous electric field coincides with one of the reciprocal lattice vectors. Consequently, since the components of the crystal momentum perpendicular to the direction of the electric field are constants of motion, the problem can be reduced to the one-dimensional one, and, in what follows, we shall discuss this reduced problem. At this point we should like to stress that the reduced one-dimensional problem has special features compared with the true one-dimensional problem and these features complicate its study. First, the Hamiltonian is not a differential operator, and therefore one cannot use the powerful theory of ordinary differential equations, in particular, we cannot use the deep results of Kohn (1959). Second, while for the true one-dimensional systems the degeneracy of bands is an accidental phenomenon, for the three-dimensional systems, and then for the corresponding reduced one-dimensional problems, the degeneracy of bands is the generic case, and so we are forced to deal with intersecting bands. We shall prove that $H^{W}_{i,n}(\varepsilon)$ is a direct integral (over the components of the crystal momentum perpendicular to the electric field) of operators, whose spectrum consists of $m$ intertwined ladders, all with the same spacing of the order of $\varepsilon$, $m$ being the degeneracy of the corresponding band. As to the eigenfunctions, we shall prove that they are exponentially localised along the direction of the field. This exponential localisation plays an important role in understanding the Zener and Franz–Keldysh effects.

Two remarks are in order. First, as has been anticipated by Wannier (1969), the theory of the SW ladder, as it is developed here, parallels, to some extent, the theory of the Stark effect in atoms, both of them being particular cases of the same general mathematical theory (Nenciu 1981). Second, as has been stressed by Wannier (1960), the analysis gets into difficulty, if the direction of the field does not coincide with that of the reciprocal lattice vectors. Even if this does not happen, since the spacing between levels is proportional to the inverse of the linear dimension of the Brillouin zone along the field direction, we deal with an SW pattern, varying erratically for infinitely small variations in angle. This fact led Wannier (1960) to question the 'physical reality' of the SW ladder in three dimensions. The discussion of this point is beyond the scope of this paper and will be discussed in a subsequent paper of this series.

Section 2 contains the proofs of some spectral properties of $H_0$. We believe that some results in § 2, especially proposition 2, are interesting in themselves. Section 3 contains the spectral analysis of $H^{W}_{i,n}(\varepsilon)$.

## 2. The construction of quasi-Bloch functions

The 'unperturbed' periodic Hamiltonian is

$$H_0 = -\Delta + V_{\text{per}}. \tag{2.1}$$

As for the periodic potential, we shall assume that it is local and square integrable over the unit cell.

Let $\{\boldsymbol{a}_i\}_{i=1}^{3}$ be a basis in $\mathbb{R}^3$ and $\{\boldsymbol{K}_i\}_{i=1}^{3}$ be the dual basis, i.e.

$$\boldsymbol{a}_i\boldsymbol{K}_j = 2\pi\delta_{ij}.$$

Without loss of generality, we shall take the length of $\boldsymbol{K}_1$ to be $2\pi$. Let $Q$ be the basic period cell for the basis $\{\boldsymbol{a}_i\}$ and $B$ be the basic period cell for $\{\boldsymbol{K}_i\}$ (the Brillouin zone). The fact that $|\boldsymbol{K}_1| = 2\pi$ means that the length of the Brillouin zone along the $\boldsymbol{K}_1$ direction is $2\pi$.

*Theorem 1.* (Reed and Simon 1978). Let $V$ be a real function on $\mathbb{R}^3$ with

$$V(\boldsymbol{x}+\boldsymbol{a}_i) = V(\boldsymbol{x}) \qquad i = 1, 2, 3. \tag{2.2}$$

Let

$$\mathscr{H}' = l^2(\mathbb{Z}^3) = \left\{\{\psi_{m_1,m_2,m_3}\}\Big| \sum_{m_1,m_2,m_3=-\infty}^{+\infty} |\psi_{m_1,m_2,m_3}|^2 < \infty\right\} \tag{2.3}$$

and

$$\mathscr{H} = \int_B^{\oplus} \mathscr{H}' \, \mathrm{d}\boldsymbol{k}. \tag{2.4}$$

Suppose $V \in L^2(Q)$ and $\hat{V}_{\boldsymbol{m}}(\boldsymbol{m} = (m_1, m_2, m_3))$ are the Fourier coefficients of $V$ as a function on $Q$, i.e. for $\boldsymbol{m} \in \boldsymbol{Z}^3$,

$$\hat{V}_{\boldsymbol{m}} = (\mathrm{vol}\, Q)^{-1} \int_Q \exp\left(-\mathrm{i} \sum_{j=1}^{3} m_j \boldsymbol{K}_j \boldsymbol{x}\right) V(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}. \tag{2.5}$$

For $\boldsymbol{k} \in \mathbb{C}^3$, define the operator $H_0(\boldsymbol{k})$ in $\mathscr{H}'$ by

$$(H_0(\boldsymbol{k})\psi)_{\boldsymbol{m}} = \left(\boldsymbol{k} + \sum_{j=1}^{3} m_j \boldsymbol{K}_j\right)^2 \psi_{\boldsymbol{m}} + \sum_{\boldsymbol{n} \in \boldsymbol{Z}^3} \hat{V}_{\boldsymbol{n}} \psi_{\boldsymbol{m}-\boldsymbol{n}} \tag{2.6}$$

with the domain

$$\mathscr{D}(H_0(\boldsymbol{k})) = \mathscr{D}_0 = \left\{ \psi \in \mathscr{H}' \,\middle|\, \sum_{\boldsymbol{m} \in \boldsymbol{Z}^3} |\boldsymbol{m}|^2 |\psi_{\boldsymbol{m}}|^2 < \infty \right\}.$$

Then:

(i) for $\boldsymbol{k} \in \mathbb{R}^3$, $H_0(\boldsymbol{k})$ is self-adjoint,
(ii) $H_0(\boldsymbol{k})$ is an entire analytic family of type A,
(iii) for $\boldsymbol{k} \in \mathbb{C}^3$, $H_0(\boldsymbol{k})$ has a compact resolvent, and
(iv) let $U: L^2(\mathbb{R}^3, \mathrm{d}\boldsymbol{x}) \to \mathscr{H}$ be given by

$$(Uf)_{\boldsymbol{m}}(\boldsymbol{k}) = \hat{f}\left(\boldsymbol{k} + \sum_{j=1}^{3} m_j \boldsymbol{K}_j\right) \qquad \boldsymbol{k} \in B. \tag{2.7}$$

Then $U$ is unitary and

$$U H_0 U^{-1} = \int_B^{\oplus} H_0(\boldsymbol{k}) \, \mathrm{d}\boldsymbol{k}. \tag{2.8}$$

*Proof.* For the proof of this theorem, see Reed and Simon (1978).

In what follows, $k_1$, $k_2$, $k_3$ denote the coordinates of $\boldsymbol{k}$ with respect to the basis $\boldsymbol{K}_i |\boldsymbol{K}_i|^{-1}$. We are interested in the properties of $H_0(\boldsymbol{k})$ as a function of $k_1$ at $\boldsymbol{k}_\perp = (k_2, k_3)$ fixed. In order to emphasise this fact, we shall write

$$H_0(\boldsymbol{k}_1, \boldsymbol{k}_\perp) \equiv H_{0,\boldsymbol{k}_\perp}(k_1)$$

and, moreover, in the cases when no confusion is possible, we shall omit $\boldsymbol{k}_\perp$.

Let $\sigma(k_1)$ be the (discrete) spectrum of $H_0(k_1)$.

*Definition.* A non-void part $\sigma^0(k_1)$ of $\sigma(k_1)$, $k_1 \in [0, 2\pi]$ is said to be an isolated band of $H_0(k_1)$ if there exist continuous functions on $[0, 2\pi]$, $f_1(k_1)$, $f_2(k_1)$ and a positive constant $c > 0$, such that

$$-\infty < f_1(k_1) < f_2(k_1) < \infty \qquad \sigma^0(k_1) \subset [f_1(k_1), f_2(k_1)]$$

$$[f_i(k_1) - c, f_i(k_1) + c] \cap \sigma(k_1) = \varnothing \qquad i = 1, 2 \qquad k_1 \in [0, 2\pi].$$

From the physics textbooks (Kittel 1963) one can learn that, at least for non-degenerate bands, $\sigma^0(k_1)$ is the restriction of a periodic function. The precise statement (which is probably folk-lore, but we do not know a proper reference) is as follows.

Let $J_d$ be the strip $|\mathrm{Im}\, k_1| < d$, $\mathrm{Re}\, k_1 \in \mathbb{R}$.

*Proposition 1.* Let $\sigma^0_{k_\perp}(k_1)$ be an isolated band of $H_{0,k_\perp}(k_1)$. Then:

(i) There exist positive integers $m$, $p$; $p \le m$; functions $\lambda_j(k_1)$, $j = 1, 2, \ldots, p$ analytic in the strip $J_d$ and real for $k_1 \in \mathbb{R}$; positive integers $r_1, \ldots, r_p$ satisfying $\Sigma_{i=1}^{p} r_i = m$, such that

$$\sigma^0_{k_\perp}(k_1) = \{\lambda_i(k_1)\}_{i=1}^{p} \qquad k_1 \in [0, 2\pi]$$

each $\lambda_i(k_1)$ having multiplicity $r_i$.

(ii) The set $\{\lambda_i(k_1)\}_{i=1}^{p}$ is periodic with period $2\pi$, and each $\lambda_i(k_1)$ is periodic with a period at most $2\pi p$.

*Remarks.* (1) Note that the existence of some points for which two or more of the functions $\lambda_i(k_1)$ have the same value (intersection or degeneracy points) is allowed. The number of degeneracy points in $[0, 2\pi]$ is finite due to the analyticity properties.

*Proof.* Let $V: \mathcal{H}' \to \mathcal{H}'$ be the unitary operator given by

$$(V\psi)_{m_1,m_2,m_3} = \psi_{m_1-1,m_2,m_3}. \tag{2.9}$$

Since $V$ is unitary and 1 is not an eigenvalue of $V$, there exists a unique self-adjoint operator $M$, such that $\|M\| \le 1$ and

$$V = \exp(2\pi \mathrm{i} M). \tag{2.10}$$

The bounded operator valued function

$$V(k_1) = \exp(\mathrm{i} k_1 M) \qquad k_1 \in \mathbb{C} \tag{2.11}$$

is obviously an entire function.

Consider the following family of operators

$$K_{0,k_\perp}(k_1) = V(k_1) H_{0,k_\perp}(k_1) V^{-1}(k_1). \tag{2.12}$$

A simple but tedious calculation shows that

$$K_{0,k_\perp}(k_1) = K_{0,k_\perp}(k_1 + 2\pi). \tag{2.13}$$

Since $K_{0,k_\perp}(k_1)$ and $H_{0,k_\perp}(k_1)$ are unitary equivalent, they have the same spectrum and then $\sigma(k_1) \equiv \sigma(H_{0,k_\perp}(k_1))$ as a set, is periodic, i.e.

$$\sigma(k_1) = \sigma(k_1 + 2\pi). \tag{2.14}$$

Defining $\sigma^0(k_1)$ for all $k_1 \in \mathbb{R}$ by periodicity, it follows that $\sigma^0(k_1)$ is isolated for all $k_1 \in \mathbb{R}$ and

$$\mathrm{dist}(\sigma^0(k_1), \sigma(k_1)/\sigma^0(k_1)) \ge c > 0 \qquad \text{all } k_1 \in \mathbb{R}.$$

Now, the existence of $\lambda_i(k_1)$, as well as their analyticity properties, follows from the theory of perturbation for analytic families of type A (Reed and Simon 1978). In particular, the analyticity of $\lambda_i(k_1)$ at the degeneracy points follows from the famous Rellich theorem (Reed and Simon 1978, Kato 1966). The only thing we have to verify is the periodicity properties.

As an isolated part of $\sigma(k_1)$, $\sigma^0(k_1)$ is a periodic set. Since because of the analyticity the number of intersection points in every compact is finite, without loss of generality, we can assume that 0 is not an intersection point. Clearly, if $t_i$ is the smallest integer such that $\lambda_i(2\pi t_i)=\lambda_i(0)$, then the period of $\lambda_i(k_1)$ is $2\pi t_i$. Since for all integers $t$ the set $\sigma^0(2\pi t)$ of possible values of $\lambda_i(2\pi t)$ does not depend on $t$ and contains $p$ points, it follows that $t_i \leqslant p$, and the proof is completed.

*Lemma 1.* Let $\mathscr{H}$ be a separable Hilbert space and $J_d=\{z\in\mathbb{C} \mid |\mathrm{Im}\, z|<d, d>0\}$. Let $\Pi(z)$ be a projection-valued analytic function in $J_d$ satisfying:

(i) $\Pi(z)=\Pi^*(z) \qquad z\in\mathbb{R}$

(ii) $\Pi(z)=\Pi(z+2\pi) \qquad z\in J_d$.

Then, there exists an analytic family $A(z)$ of invertible operators with the properties:

$(a)$ $A(z)\Pi(0)A^{-1}(z)=\Pi(z) \qquad A(0)=1$

$(b)$ $A^*(z)=A^{-1}(z) \qquad z\in\mathbb{R}$

$(c)$ $A(z+2\pi)=A(z) \qquad z\in J_d$.

*Remarks.* (2) Without the periodicity conditions, the above result goes back to Sz-Nagy (1946/47) (see Kato 1966, Reed and Simon 1978). For finite-dimensional Hilbert spaces, related results concerning the periodic case are given in Sibuya (1965) with completely different proofs.

*Proof.* We shall construct $A(z)$ in two steps.

The first step (Reed and Simon 1978). Let $L(z)$, $B(z)$ be given by

$$L(z)=\mathrm{i}(1-2\Pi(z))\frac{\mathrm{d}\Pi(z)}{\mathrm{d}z} \tag{2.15}$$

$$\mathrm{i}\frac{\mathrm{d}B(z)}{\mathrm{d}z}=L(z)B(z) \qquad B(0)=1. \tag{2.16}$$

We refer to Reed and Simon (1978) for the proof of the fact that $B(z)$ is analytic and invertible in $J_d$ and satisfies the conditions $(a)$ and $(b)$ of lemma 1.

The second step. Consider $B(2\pi)$. Since

$$B(z)\Pi(0)B^{-1}(z)=\Pi(z) \tag{2.17}$$

it follows from $\Pi(0)=\Pi(2\pi)$ that

$$B(2\pi)=B_1\oplus B_2 \tag{2.18}$$

where the orthogonal sum is according to the decomposition

$$\mathscr{H}=\Pi(0)\mathscr{H}\oplus(1-\Pi(0))\mathscr{H}. \tag{2.19}$$

Since $B_1$ and $B_2$ are unitary operators, one can take the logarithm, i.e. there exist bounded self-adjoint operators $C_1$, $C_2$ in $\Pi(0)\mathscr{H}$ and $(1-\Pi(0))\mathscr{H}$ respectively, such that $\|C_i\|\leqslant 1$, $i=1, 2$, and

$$B(2\pi)=\exp(2\pi\mathrm{i}C) \qquad C=C_1\oplus C_2. \tag{2.20}$$

Obviously $[C, \Pi(0)]=0$, and consequently,

$$[\Pi(0), \exp(\mathrm{i}zC)]=0. \tag{2.21}$$

We claim now that the family

$$A(z)=B(z)\exp(-\mathrm{i}zC) \tag{2.22}$$

satisfies all the conditions $(a)$–$(c)$ of lemma 1. Combining (2.17) and (2.22) one obtains the property $(a)$ for $A(z)$. Since $B(z)$ is unitary for $z \in \mathbb{R}$ (Reed and Simon 1978) and $C$ is self-adjoint, it follows that $A(z)$ is unitary for $z \in \mathbb{R}$. Since $B(z)$ is analytic and invertible in $J_d$, $A(z)$ has the same properties. Finally, using (2.16), the fact that $\Pi(z)$ and $K(z)$ are periodic and (2.21) for $z = 2\pi$, one can easily verify recurrently that

$$\frac{\mathrm{d}^n}{\mathrm{d}z^n} A(z)\bigg|_{z=0} = \frac{\mathrm{d}^n}{\mathrm{d}z^n} A(z)\bigg|_{z=2\pi}$$

which completes the proof.

We are now prepared to prove the following basic proposition.

*Proposition 2.* Let $\sigma^0(k_1) = \{\lambda_i(k_1)\}_{i=1}^p$, $\Sigma_{i=1}^p r_i = m$ be an isolated band of $H_0(k_1)$, and $P_0(k_1)$ its corresponding spectral projection. Then, there exist a positive constant $d_0 > 0$ and $m$ valued vector functions $\chi_i^0(k_1) \in \mathscr{H}'$, $i = 1, 2, \ldots, m$ analytic in the strip $J_{d_0}$, $\chi_i^0(k_1) = \chi_i^0(k_1 + 2\pi)$ such that $\{V^{-1}(k_1)\chi_i^0(k_1)\}_1^m$ is an orthonormed basis in $P_0(k_1)\mathscr{H}'$.

*Remarks.* (3) Proposition 2 asserts the existence of quasi-Bloch functions $\chi_i^0(k_1)$ (Blount 1962, des Cloizeaux 1964) which are analytic and periodic in $k_1$ at $\boldsymbol{k}_\perp$ fixed. For one-dimensional systems and non-degenerated bands, proposition 2 reduces to some fundamental results by Kohn (1959) and des Cloizeaux (1964). Let us note that via the Paley–Wiener theorem, proposition 2 implies the existence of Wannier functions decreasing exponentially in the $\boldsymbol{a}_1$ direction. We should like to stress that proposition 2 does not imply the exponential decrease of Wannier functions in *all* directions. In order to prove this, one needs the generalisation of proposition 2 asserting the analyticity and periodicity in all variables $k_1$, $k_2$, $k_3$. This is not a trivial problem, because of some topological difficulties. This problem is beyond the scope of this paper (for which the result contained in proposition 2 is sufficient) and will be considered elsewhere.

*Proof.* From the fact that $H_0(k_1)$ is an entire function and the fact that $\sigma^0(k_1)$ is isolated, using the formula

$$P_0(k_1) = \frac{1}{2\pi \mathrm{i}} \int_C \frac{1}{H_0(k_1) - z} \, \mathrm{d}z$$

where $C$ is a contour enclosing $\sigma^0(k_1)$, it follows that there exists $d_0 > 0$ (see e.g. Bentosela 1979) such that $P_0(k_1)$ is analytic in $J_{d_0}$. From (2.12) and (2.13) it follows that

$$\Pi_0(k_1) = V(k_1) P_0(k_1) V^{-1}(k_1)$$

is periodic and then satisfies all the conditions of lemma 1. Let $A(k_1)$ be given by lemma 1 applied to $\Pi_0(k_1)$ and $\{\chi_i^0\}_1^m$ be a basis in $P_0(0)\mathscr{H}'$. Then, from (2.12) and lemma 1 one can easily see that

$$\chi_i^0(k_1) = A(k_1)\chi_i^0 \qquad i = 1, 2, \ldots, m \tag{2.23}$$

have all the required properties.

We shall end this section by writing $X_0$ in a convenient form. Taking (see the introduction) $\boldsymbol{n} = (2\pi)^{-1}\boldsymbol{K}_1$, then

$$(X_0 f)(\boldsymbol{x}) = x_1 f(\boldsymbol{x}) \qquad \boldsymbol{x} = \sum_{i=1}^{3} x_i \boldsymbol{a}_i. \tag{2.24}$$

Consider the Hilbert space $\tilde{\mathscr{H}}$

$$\tilde{\mathscr{H}} = \int_{[0,2\pi]}^{\oplus} \mathscr{H}' \, \mathrm{d}k_1 \tag{2.25}$$

with a self-explanatory notation

$$\mathscr{H} = J \int_{B_\perp}^{\oplus} \tilde{\mathscr{H}} \, \mathrm{d}\boldsymbol{k}_\perp \tag{2.26}$$

$J$ being the Jacobian $J = (|\boldsymbol{K}_1| |\boldsymbol{K}_2| |\boldsymbol{K}_3|)^{-1} \boldsymbol{K}_1 \cdot (\boldsymbol{K}_2 \times \boldsymbol{K}_3)$. We shall denote the elements of $\tilde{\mathscr{H}}$ by $\{\psi_{\boldsymbol{m}}(k_1)\}_{\boldsymbol{m} \in \mathbf{Z}^3; k_1 \in [0,2\pi]}$. Consider the operator $\tilde{X}_0$ given by

$$\{(\tilde{X}_0 \psi)_{\boldsymbol{m}}(k_1)\} = \left\{ \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}k_1} \psi_{\boldsymbol{m}}(k_1) \right\}$$

$$\mathscr{D}(\tilde{X}_0) = \{\{\psi_{\boldsymbol{m}}(k_1)\} | \{\mathrm{d}\psi_{\boldsymbol{m}}(k_1)/\mathrm{d}k_1\} \in \tilde{\mathscr{H}};\ \psi_{m_1,m_2,m_3}(2\pi) = \psi_{m_1+1,m_2,m_3}(0)\}. \tag{2.27}$$

*Proposition 3.* Let $X_0$ be the self-adjoint operator in $L^2(\mathbb{R}^3, \mathrm{d}\boldsymbol{x})$

$$(X_0 f)(\boldsymbol{x}) = x_1 f(\boldsymbol{x}) \qquad \boldsymbol{x} = \sum_{i=1}^{3} x_i \boldsymbol{a}_i$$

on its natural domain. Then

$$U X_0 U^{-1} = \int_{B_\perp}^{\oplus} \tilde{X}_0 \, \mathrm{d}\boldsymbol{k}_\perp. \tag{2.28}$$

The simple proof of this proposition is left to the reader.

The operator $\tilde{X}_0$ is a self-adjoint extension of $\mathrm{i}\,\mathrm{d}/\mathrm{d}k_1$ described by somewhat unusual boundary conditions. The next remark is that $\tilde{X}_0$ is related to a more familiar self-adjoint extension of $\mathrm{i}\,\mathrm{d}/\mathrm{d}k_1$. Let

$$\tilde{V} = \int_{[0,2\pi]}^{\oplus} V(k_1) \, \mathrm{d}k_1 \qquad \tilde{M} = \int_{[0,2\pi]}^{\oplus} M \, \mathrm{d}k_1 \tag{2.29}$$

(remember that $V(k_1) = \exp(\mathrm{i}k_1 M)$) and $\mathrm{i}(\mathrm{d}/\mathrm{d}k_1)_{\mathrm{per}}$, the self-adjoint operator, is given by

$$\left\{ \left( \mathrm{i} \left( \frac{\mathrm{d}}{\mathrm{d}k_1} \right)_{\mathrm{per}} \psi \right)_{\boldsymbol{m}} (k_1) \right\} = \left\{ \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}k_1} \psi_{\boldsymbol{m}}(k_1) \right\}$$

$$\mathscr{D}\left( \mathrm{i} \left( \frac{\mathrm{d}}{\mathrm{d}k_1} \right)_{\mathrm{per}} \right) = \left\{ \{\psi_{\boldsymbol{m}}(k_1)\} \middle| \left\{ \frac{\mathrm{d}}{\mathrm{d}k_1} \psi_{\boldsymbol{m}}(k_1) \right\} \in \mathscr{H}';\ \psi_{\boldsymbol{m}}(0) = \psi_{\boldsymbol{m}}(2\pi) \right\}. \tag{2.30}$$

*Proposition 4.*

$$\tilde{V} \tilde{X}_0 \tilde{V}^{-1} = \mathrm{i}(\mathrm{d}/\mathrm{d}k_1)_{\mathrm{per}} + \tilde{M}. \tag{2.31}$$

*Proof.* This is an immediate consequence of the differentiability of $V(k_1)$ and of the fact that

$$(V(2\pi)\psi)_{m_1,m_2,m_3} = \psi_{m_1-1,m_2,m_3}.$$

## 3. The spectral properties of the effective Wannier Hamiltonian of arbitrary order

Having the description of $H_0$ and $X_0$, we return now to $H^\varepsilon = H_0 + \varepsilon X_0$. It is known that $H^\varepsilon$ is self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(X_0)$ (Reed and Simon 1975). Denoting

$$\tilde{H}_{0,k_\perp} = \int_{[0,2\pi]}^{\oplus} H_{0,k_\perp}(k_1)\,\mathrm{d}k_1 \tag{3.1}$$

from theorem 1 and proposition 3 it follows that

$$UH^\varepsilon U^{-1} = \int_{B_\perp}^{\oplus} H^\varepsilon(k_\perp)\,\mathrm{d}k_\perp \tag{3.2}$$

where

$$\tilde{H}^\varepsilon(k_\perp) = \tilde{H}_{0,k_\perp} + \varepsilon\tilde{X}_0. \tag{3.3}$$

In what follows, we shall discuss the spectral properties of $\tilde{H}^\varepsilon(k_\perp)$. For notational convenience, we shall omit the variable $k_\perp$. The zeroth-order theory developed in Nenciu and Nenciu (1981) applied to $\tilde{H}^\varepsilon$ gives the following. Let $\sigma^0(k_1)$ be an isolated band of $\tilde{H}_0$, $P_0(k_1)$ be the spectral projection of $H_0(k_1)$ corresponding to $\sigma^0(k_1)$ and

$$\tilde{P}_0 = \int_{[0,2\pi]}^{\oplus} P_0(k_1)\,\mathrm{d}k_1. \tag{3.4}$$

Define (for the rigorous justification, see Nenciu and Nenciu (1981))

$$\tilde{B}_0 = [\![ \mathrm{i}(1-2\tilde{P}_0)[\tilde{X}_0, \tilde{P}_0] ]\!] \tag{3.5}$$

where $[\![\ldots]\!]$ means the extension by continuity. $\tilde{B}_0$ is a bounded self-adjoint periodic operator, i.e.

$$\tilde{B}_0 = \int_{[0,2\pi]}^{\oplus} B_0(k_1)\,\mathrm{d}k_1 \tag{3.6}$$

and $\|\tilde{B}_0\| \leqslant$ constant.

Define

$$\tilde{X}_1 = \tilde{X}_0 + \tilde{B}_0. \tag{3.7}$$

Note that by construction

$$\tilde{H}^\varepsilon = \tilde{H}_0 + \varepsilon\tilde{X}_0 = \tilde{H}_0 + \varepsilon\tilde{X}_1 - \varepsilon\tilde{B}_0 \equiv \tilde{H}_1 + \varepsilon\tilde{X}_1 \qquad [\tilde{H}_0 + \varepsilon\tilde{X}_1, \tilde{P}_0] = 0. \tag{3.8}$$

For $\varepsilon$ sufficiently small, $\tilde{H}_1$ has an isolated band $\sigma^1(k_1)$, which in the limit $\varepsilon \to 0$ coincides with $\sigma^0(k_1)$. Repeating the above construction, starting from $\tilde{H}^\varepsilon = \tilde{H}_1 + \varepsilon\tilde{X}_1$ one can define $\tilde{P}_1, \tilde{B}_1, \tilde{H}_2, \tilde{X}_2$, and in general, recurrently, $\tilde{P}_n, \tilde{B}_n, \tilde{H}_{n+1}, \tilde{X}_{n+1}$, such that

$$\tilde{H}^\varepsilon = \tilde{H}_n + \varepsilon\tilde{X}_{n+1} - \varepsilon\tilde{B}_n \equiv \tilde{H}_n^{\mathrm{W}} - \varepsilon\tilde{B}_n \qquad [\tilde{H}_n^{\mathrm{W}}, \tilde{P}_n] = 0. \tag{3.9}$$

We have called $\tilde{H}_n^{\mathrm{W}}$ the effective Wannier Hamiltonian of order $n$ (see Kane (1959), Wannier (1960) for heuristic discussions). The main result in Nenciu and Nenciu (1981) is that

$$\|\tilde{B}_n\| \leq b_n \varepsilon^n. \tag{3.10}$$

It follows that up to terms of the order $\varepsilon^{n+1}$

$$\tilde{H}^\varepsilon \simeq \tilde{P}_n \tilde{H}^\varepsilon \tilde{P}_n \oplus (1-\tilde{P}_n)\tilde{H}^\varepsilon(1-\tilde{P}_n). \tag{3.11}$$

Note also that since $\tilde{P}_n \tilde{B}_n \tilde{P}_n = 0$

$$\tilde{P}_n \tilde{H}^\varepsilon \tilde{P}_n = \tilde{P}_n \tilde{H}_n^{\mathrm{W}} \tilde{P}_n.$$

The main aim of this paper is to study the spectral properties of $\tilde{P}_n \tilde{H}_n^{\mathrm{W}} \tilde{P}_n$. The reason is the following. Suppose that $\tilde{P}_n \tilde{H}_n^{\mathrm{W}} \tilde{P}_n$ has an eigenvalue $\lambda$ with the corresponding eigenvector $\psi_\lambda$. It follows from what has been said above that $\lambda$, $\psi_\lambda$ are the quasi-eigenvalue and quasi-eigenvector, respectively, of the order $(n+1)$ for $\tilde{H}^\varepsilon$, in the sense that

$$\|\tilde{H}^\varepsilon \psi_\lambda - \lambda \psi_\lambda\| \leq b_n \varepsilon^{n+1}. \tag{3.12}$$

Let $(L^2([0, 2\pi]))^m$ be the Hilbert space

$$(L^2([0,2\pi]))^m = \left\{ \{\varphi_i(k)\}_{i=1}^m, k \in [0, 2\pi] \,\middle|\, \sum_{i=1}^m \int_0^{2\pi} |\varphi_i(k)|^2 \, \mathrm{d}k < \infty \right\},$$

$Y_n(k)$ be an $m \times m$ Hermitian matrix valued function on $[0, 2\pi]$ and $\mathrm{i}(\mathrm{d}/\mathrm{d}k)_{\mathrm{per}}$ the usual first-order differential operator in $(L^2([0, 2\pi]))^m$ with periodic boundary conditions.

*Theorem 2.* There exist a positive constant $d_n > 0$, an integer $m$, and a unitary operator

$$W : \tilde{P}_n \mathscr{H} \to (L^2([0, 2\pi]))^m$$

such that

$$W\tilde{P}_n \tilde{H}_n^{\mathrm{W}} \tilde{P}_n W^{-1} = \mathrm{i}\varepsilon(\mathrm{d}/\mathrm{d}k)_{\mathrm{per}} + Y_n(k; \varepsilon) \tag{3.13}$$

where the matrix elements of $Y_n(k; \varepsilon)$ are restriction to $k \in [0, 2\pi]$ of analytic functions in the strip $J_{d_n}$, satisfying

$$Y_{n,lp}(k; \varepsilon) = Y_{n,lp}(k+2\pi; \varepsilon). \tag{3.14}$$

*Remarks.* (4) The main point of this theorem is the analyticity and periodicity properties of $Y_n(k; \varepsilon)$. At the non-rigorous level, the result in the case of non-degenerated bands is familiar (see e.g. Callaway 1974). At the rigorous level, for one-dimensional systems and non-degenerated bands, see Avron (1979), Avron *et al* (1977). In the three-dimensional case, and intersecting bands, even the fact that $Y_n(k; \varepsilon)$ is bounded at the degeneracy points seems not to be known.

*Proof.* We shall start with the proof for $n = 0$.

Let $\{V^{-1}(k)\chi_i^0(k)\}_1^m$ be the basis in $P_0(k)\mathscr{H}'$ given by proposition 2. If $\psi \in \tilde{P}_0 \mathscr{H}$ then

$$\{\psi_p(k)\} = \left\{ \sum_{l=1}^m C_l(k)(V^{-1}(k)\chi_l^0(k))_p \right\} \tag{3.15}$$

where

$$c_l(k) = (V^{-1}(k)\chi_l^0(k), \psi(k))_{\mathcal{H}'}$$
$$= \sum_{p\in\mathbf{Z}^3} (\overline{V^{-1}(k)\chi_l^0(k)})_p \psi_p(k). \tag{3.16}$$

We shall define

$$W : \tilde{P}_0\mathcal{H} \to (L^2([0, 2\pi]))^m$$

by

$$\{(W\psi)_l(k)\} = \{c_l(k)\}. \tag{3.17}$$

Obviously, $W$ is unitary, and the only thing we have to do is to compute

$$W\tilde{P}_0\tilde{H}_0^W\tilde{P}_0W^{-1} = W\tilde{P}_0(\tilde{H}_0 + \varepsilon\tilde{X}_0)\tilde{P}_0W^{-1}.$$

A simple calculation shows that

$$(W\tilde{P}_0\tilde{H}_0\tilde{P}_0W^{-1}c)_i(k) = \sum_{j=1}^{m} (\chi_i^0(k), V(k)H_0(k)V^{-1}(k)\chi_j^0(k))_{\mathcal{H}'}c_j(k). \tag{3.18}$$

Now $(\chi_i^0(k), V(k)H_0(k)V^{-1}(k)\chi_j^0(k))_{\mathcal{H}'}$ is the restriction to $k \in [0, 2\pi]$ of the function

$$(\chi_i^0(k), V(k)H_0(k)V^{-1}(k)\chi_j^0(k))_{\mathcal{H}'} = \sum_{p\in\mathbf{Z}^3} \overline{\chi_{i,p}^0(\bar{k})}(V(k)H_0(k)V^{-1}(k)\chi_j^0(k))_p$$

which is analytic in $J_{d_0}$ and by (2.12), (2.13) and proposition 2, it is periodic with the period $2\pi$.

Using proposition 4 and the fact that $\chi_i^0(k)$ are differentiable, one can see that the domain of $W\tilde{P}_0\tilde{X}_0\tilde{P}_0W^{-1}$ is

$$\{\{c_l(k)\}_1^m | \{\mathrm{d}c_l(k)/\mathrm{d}k\}_1^m \in (L^2([0, 2\pi]))^m;\ c_l(0) = c_l(2\pi)\}$$

and

$$(W\tilde{P}_0\tilde{X}_0\tilde{P}_0W^{-1}c)_j = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}k}c_j(k) + \sum_{l=1}^{m}\left[(\chi_j^0(k), M\chi_l^0(k))_{\mathcal{H}'} + \mathrm{i}\left(\chi_j^0(k), \frac{\mathrm{d}}{\mathrm{d}k}\chi_l^0(k)\right)_{\mathcal{H}'}\right]c_l(k). \tag{3.19}$$

Note that the hermiticity of the matrix with elements $\mathrm{i}(\chi_j^0(k), \mathrm{d}\chi_l^0(k)/\mathrm{d}k)$ follows from the fact that $(\chi_j^0(k), \chi_l^0(k)) = \delta_{jl}$ and then $(\mathrm{d}/\mathrm{d}k)(\chi_j^0(k), \chi_l^0(k)) = 0$. Again, the functions appearing in the right-hand side of (3.19) are the restriction of $(\chi_j^0(\bar{k}), M\chi_l^0(k))_{\mathcal{H}'}$ and $(\chi_j^0(\bar{k}), \mathrm{d}\chi_l^0(k)/\mathrm{d}k)_{\mathcal{H}'}$, analytic in $J_{d_0}$. Then (3.18) and (3.19) proves theorem 2, with

$$Y_{0,lp}(k;\varepsilon) = (\chi_l^0(k), V(k)H_0(k)V^{-1}(k)\chi_p^0(k))_{\mathcal{H}'}$$
$$+ \varepsilon[(\chi_l^0(k), M\chi_p^0(k))_{\mathcal{H}'} + \mathrm{i}(\chi_l^0(k), \mathrm{d}\chi_p^0(k)/\mathrm{d}k)_{\mathcal{H}'}]. \tag{3.20}$$

Consider now $\tilde{B}_0$. Using the fact that

$$(\tilde{V}\tilde{P}_0\tilde{V}^{-1}\psi)_p(k) = \sum_{j=1}^{m} (\chi_j^0(k), \psi(k))_{\mathcal{H}'}\chi_{jp}^0(k)$$

and proposition 4, a straightforward calculation gives for $\psi \in \mathscr{D}(\tilde{V}\tilde{X}_0\tilde{V}^{-1})$

$$
\begin{aligned}
(\tilde{V}[\tilde{X}_0, \tilde{P}_0]\tilde{V}^{-1}\psi)_p(k) = \sum_{j=1}^{m} [&(\chi_j^0(k), \psi(k))_{\mathscr{H}'}(M\chi_j^0)_p(k) \\
&+ (\mathrm{i}\, \mathrm{d}\chi_j^0(k)/\mathrm{d}k - (M\chi_j^0)(k), \psi(k))_{\mathscr{H}'}\chi_{j,p}^0(k) \\
&+ \mathrm{i}(\chi_j^0(k), \psi(k))_{\mathscr{H}'}\, \mathrm{d}\chi_{j,p}^0(k)/\mathrm{d}k]
\end{aligned}
\tag{3.21}
$$

whence it follows that $V(k)B_0(k)V^{-1}(k)$ is the restriction to $[0, 2\pi]$ of a bounded operator valued function, analytic, and periodic in $J_{d_0}$. Then

$$
\tilde{H}_1 = \tilde{H}_0 - \varepsilon\tilde{B}_0 = \int_{[0,2\pi]}^{\oplus} [H_0(k) - \varepsilon B_0(k)]\, \mathrm{d}k \equiv \int_{[0,2\pi]}^{\oplus} H_1(k)\, \mathrm{d}k
$$

and

$$
K_1(k) = V(k)H_1(k)V^{-1}(k)
$$

is analytic and periodic in $J_{d_0}$.

Then, starting from $\tilde{H}_1$, instead of $\tilde{H}_0$, the whole theory developed for $\tilde{H}_0$ goes through. The formula obtained for $Y_1$ is (3.20) where $H_0(k)$ has been replaced by $H_1(k)$ and $\chi_j^0(k)$ by the corresponding basis in $V(k)P_1(k)V^{-1}(k)$, namely $\chi_j^1(k)$. The procedure can be repeated indefinitely and the proof of theorem 2 is finished.

Using the arguments in Avron *et al* (1977), one can prove that the spectrum of $\mathrm{i}\varepsilon(\mathrm{d}/\mathrm{d}k)_{\mathrm{per}} + Y_n(k;\varepsilon)$ consists of $m$ intertwined ladders, all with the same spacing $\varepsilon$. In fact, the use of the theory of differential equations with periodic coefficients (see e.g. Cronin 1980) allows a rather detailed description of the eigenvalues and eigenvectors of $\mathrm{i}\varepsilon(\mathrm{d}/\mathrm{d}k)_{\mathrm{per}} + Y_n(k;\varepsilon)$.

Let $N(k;\varepsilon)$ be the unitary $m \times m$ matrix given by the equation

$$
\mathrm{i}\varepsilon\, \mathrm{d}N(k;\varepsilon)/\mathrm{d}k = -Y(k;\varepsilon)N(k;\varepsilon) \qquad N(0;\varepsilon) = 1 \tag{3.22}
$$

and

$$
\exp(2\pi\mathrm{i}\theta_q), \qquad \theta_q \in [0, 1]; \qquad \psi_q \qquad q = 1, 2, \ldots, m
$$

be the eigenvalues and corresponding set of orthonormal eigenvectors, respectively, of the unitary matrix $N(2\pi;\varepsilon)$.

*Theorem 3.* The spectrum of $\mathrm{i}\varepsilon(\mathrm{d}/\mathrm{d}k)_{\mathrm{per}} + Y(k;\varepsilon)$ in $(L^2([0, 2\pi]))^m$, where $Y(k;\varepsilon)$ has the properties stated in theorem 2, is discrete. Its eigenvalues are given by

$$
\lambda_{s,q} = \varepsilon(s + \theta_q) \qquad s = 0, \pm 1, \pm 2, \ldots \qquad q = 1, 2, \ldots, m. \tag{3.23}
$$

A complete set of eigenvectors is given by

$$
\psi_{s,q}(k) = K_{s,q}^{-1/2} \exp(\mathrm{i}\varepsilon^{-1}\lambda_{s,q}k)N(k;\varepsilon)\psi_q \tag{3.24}
$$

where $K_{s,q}$ is the normalisation factor.

*Remarks.* (5) Concerning the spectrum, theorem 3 generalises the results in Avron (1979) and Avron *et al* (1977) to the case of three-dimensional systems, intersecting bands and the $n$th-order one-band approximation. But the main point of this theorem is that the components of $\psi_{s,q}(k)$ are restrictions to $k \in [0, 2\pi]$ of functions analytic and periodic in a strip $J_d$.

*Proof.* Since $\mathrm{i}(\mathrm{d}/\mathrm{d}k)_{\mathrm{per}}$ has a compact resolvent and $Y(k;\varepsilon)$ is bounded, it follows that $\mathrm{i}\varepsilon(\mathrm{d}/\mathrm{d}k)_{\mathrm{per}}+Y(k;\varepsilon)$ has a compact resolvent, and then its spectrum is discrete. The eigenvalue problem for $\mathrm{i}\varepsilon(\mathrm{d}/\mathrm{d}k)_{\mathrm{per}}+Y(k;\varepsilon)$ is equivalent to the problem of finding the values $\lambda$, for which the evolution equation with periodic coefficients

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}k}y(k)=-\frac{1}{\varepsilon}[Y(k;\varepsilon)-\lambda]y(k) \tag{3.25}$$

admits periodic solutions. The number of independent periodic solutions of (3.25) equals the multiplicity of the eigenvalue $\lambda$. Let $N(k;\varepsilon;\lambda)$ be the fundamental matrix of (3.25), i.e.

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}k}N(k;\varepsilon;\lambda)=-\frac{1}{\varepsilon}[Y(k;\varepsilon)-\lambda]N(k;\varepsilon;\lambda) \qquad N(0;\varepsilon;\lambda)=1. \tag{3.26}$$

The fundamental result in the theory of differential equations with periodic coefficients (Cronin 1980) says that the number of independent periodic solutions of (3.25) equals the multiplicity $r$ of the eigenvalue 1 of $N(2\pi;\varepsilon;\lambda)$, and if $\psi_{q_1},\ldots,\psi_{q_r}$ is a basis in the corresponding subspace ($N(2\pi;\varepsilon;\lambda)$ is here understood as a unitary operator in $\mathbb{C}^m$), then a system of $r$ independent periodic solutions of (3.25) is given by

$$\psi_{qi}(k)=N(k;\varepsilon;\lambda)\psi_{qi}. \tag{3.27}$$

Taking into account that

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}k}N(k;\varepsilon;\lambda)=-\frac{1}{\varepsilon}[Y(k;\varepsilon)-\lambda]N(k;\varepsilon;\lambda) \qquad N(0;\varepsilon;\lambda)=1 \tag{3.28}$$

the verification of theorem 3 is immediate.

Translated in the '$\boldsymbol{x}$ representation', the analyticity and periodicity properties of $\psi_{s,q}(k)$ give the exponential decay along $\boldsymbol{a}_1$. As is well known, the direct integral decomposition of $L^2(\mathbb{R}^3,\mathrm{d}\boldsymbol{x})$ in the '$\boldsymbol{x}$ representation' is

$$L^2(\mathbb{R}^3,\mathrm{d}\boldsymbol{x})=\int_B^{\oplus}\mathcal{H}(\boldsymbol{k})\,\mathrm{d}\boldsymbol{k}$$

where

$$\mathcal{H}(\boldsymbol{k})=\left\{\psi_{\boldsymbol{k}}(\boldsymbol{x})=\exp(\mathrm{i}\boldsymbol{k}\boldsymbol{x}')u_{\boldsymbol{k}}(\boldsymbol{x});\ u_{\boldsymbol{k}}(\boldsymbol{x})\ \text{periodic}\,|\,\|\psi_{\boldsymbol{k}}(\boldsymbol{x})\|^2=\int_Q|u_{\boldsymbol{k}}(\boldsymbol{x})|^2\,\mathrm{d}\boldsymbol{x}\right\}.$$

It is not hard to verify that

$$\begin{aligned}\tilde{\mathcal{H}}(\boldsymbol{k}_\perp)&=\int_{[0,2\pi]}^{\oplus}\mathcal{H}(k_1,\boldsymbol{k}_\perp)\,\mathrm{d}k_1\\&=\Big\{\psi_{\boldsymbol{k}_\perp}(\boldsymbol{x})=\exp[2\pi\mathrm{i}(|\boldsymbol{K}_2|^{-1}k_2x_2+|\boldsymbol{K}_3|^{-1}k_3x_3)]\tilde{u}_{\boldsymbol{k}_\perp}(\boldsymbol{x});\ \tilde{u}_{\boldsymbol{k}_\perp}(\boldsymbol{x})\ \text{periodic}\\&\qquad\text{in } x_2 \text{ and } x_3\,|\,\|\psi_{\boldsymbol{k}_\perp}(\boldsymbol{x})\|^2=(\mathrm{vol}\,Q)^{-1}\int_{Q_\perp}\mathrm{d}x_2\,\mathrm{d}x_3\int_{-\infty}^{+\infty}\mathrm{d}x_1|\tilde{u}_{\boldsymbol{k}_\perp}(\boldsymbol{x})|^2\Big\}.\end{aligned}$$

*Theorem 4.* For all $a<d_0$

$$\exp(a|x_1|)(U^{-1}W^{-1}\psi^0_{s,q})_{\boldsymbol{k}_\perp}(\boldsymbol{x})\in\tilde{\mathcal{H}}(\boldsymbol{k}_\perp).$$

*Proof.* Using the definition (2.7) of $U$ and (3.17) of $W$, we have

$$(U^{-1}W^{-1}\psi^0_{s,q})_{k_\perp}(\boldsymbol{x}) = \exp[2\pi i(|\boldsymbol{K}_2|^{-1}k_2x_2+|\boldsymbol{K}_3|^{-1}k_3x_3)](2\pi)^{-1}\sum_{m_2,m_3}\exp[2\pi i(m_2x_2+m_3x_3)] \times(2\pi)^{-1/2}\int_{-\infty}^{+\infty}dp_1\,\exp(ip_1x_1)h_{m_2,m_3}(p_1)$$

where

$$h_{m_2,m_3}(p_1)=h_{m_2,m_3}(k_1+2\pi m_1)=\sum_{l=1}^{m}\psi^0_{s,q;l}(k_1)(V^{-1}(k_1)\chi^0_l(k_1))_{m_1,m_2,m_3}.$$

From the periodicity of $\chi^0_l(k_1)$ and $\psi^0_{s,q;l}(k_1)$ and the definition of $V(k_1)$, it follows that $h_{m_2,m_3}(p_1)$ is analytic in the strip $J_{d_0}$ and

$$\sum_{m_2,m_3}\int_{-\infty+ia}^{+\infty+ia}|h_{m_2,m_3}(p_1)|^2\,dp_1<\infty \qquad |a|<d_0$$

which via the Paley–Wiener theorem applied to the vectorial function $h_{m_2,m_3}(p_1)$ implies that if

$$c_{m_2,m_3}(x_1)=(2\pi)^{-1/2}\int_{-\infty}^{+\infty}dp_1\,\exp(ip_1x_1)h_{m_2,m_3}(p_1)$$

then

$$\sum_{m_2,m_3}\int_{-\infty}^{+\infty}\exp(2a|x_1|)|c_{m_2,m_3}(x_1)|^2\,dx_1<\infty$$

which, together with the Plancherel theorem, completes the proof.

*Remarks.* (6) The result in theorem 4 extends to arbitrary $n$ (replacing, of course, $d_0$ by $d_n$).

(7) In general, $\boldsymbol{a}_1$ and $\boldsymbol{K}_1$ are not parallel, and moreover, for a given $\boldsymbol{K}_1$ there is a freedom in the choice of $\boldsymbol{a}_1$. However, since $\boldsymbol{a}_1\boldsymbol{K}_1=2\pi$ they are not orthogonal, and then exponential decay along $\boldsymbol{a}_1$ is equivalent to the exponential decay along $\boldsymbol{K}_1$.

(8) Although for all $n=0,1,\ldots$ the spectrum of $\tilde{P}_n\tilde{H}^\varepsilon\tilde{P}_n$ consists of $m$ intertwined SW ladders of eigenvalues, all of them having the same spacing between eigenvalues, it is not allowed to take the limit $n\to\infty$, because the iterative construction of $\tilde{P}_n$ seems not to be convergent as $n\to\infty$, but only asymptotic.

In fact, although a direct proof of the divergence of the iterative construction of $\tilde{P}_n$ as $n\to\infty$ does not exist, there exists an indirect one (at least, for the one-dimensional case): if the iterative construction of $\tilde{P}_n$ converges (in norm) as $n\to\infty$, then our results imply, for sufficiently small $\varepsilon$, the existence of a SW ladder of eigenvalues for $H^\varepsilon$, and this contradicts the fact that the spectrum of $H^\varepsilon$ is absolutely continuous. Our results imply that as $\varepsilon\to 0$, the width of SW resonances decreases faster than any power of $\varepsilon$. This fits the heuristic arguments of Zener (1943), as well as recent numerical calculations of Bentosela *et al* (1981), giving an exponential decrease of the width of the SW resonances.

(9) Our next remark concerns the existence of closed bands (Wannier and Fredkin 1962, Wannier 1962). In spite of the strong criticism of Zak (1968) and the recognition by Wannier (1969) that the problem might be more complicated, it seems that there

exists a widespread opinion (Callaway 1974) that, without relying on power expansions in the field strength, one can prove rigorously that Bloch bands closed in time exist. We shall point out below that, due to a tacitly assumed hypothesis which turns out to be wrong, the existence of *bona fide* Bloch bands (i.e. indexed by a discrete index) closed in time does not follow from the Wannier and Fredkin arguments. Although in a different form, our argument is the same as the argument of Zak (1968). For simplicity, we shall consider the one-dimensional case and assume that the periodic potential $V(x) = V(x+a)$ is twice differentiable. The basic idea of Wannier and Fredkin is to consider the operator

$$\Phi = \exp(-i2\pi(\varepsilon a)^{-1}H^{\varepsilon}).$$

It is easy to see that $\Phi$ commutes with the translation operator $((T_a f)(x) = f(x+a))$, so that $\Phi$ can be written as a direct integral over the Brillouin zone

$$\Phi = \int_B^{\oplus} \Phi(k)\,\mathrm{d}k.$$

Wannier and Fredkin (see also Wannier 1962, 1969) tacitly assumed that the spectrum of $\Phi(k)$ is *discrete*, whence the existence of the closed bands as well as of the SW ladder follows. Unfortunately, the fact that the spectrum of $H^{\varepsilon}$ is absolutely continuous (Avron *et al* 1977) implies that the spectrum of $\Phi(k)$ is continuous (i.e. $\Phi(k)$ has no eigenvalues) for all $k \in B$. Indeed, suppose $\Phi(k_0)$ has the eigenvalue $\lambda_0$, for some $k_0 \in B$. Then, an argument of Wannier (1969) shows that $\lambda_0$ is an (infinitely degenerated) eigenvalue of $\Phi$. On the other hand, the fact that the spectrum of $H^{\varepsilon}$ is absolutely continuous implies, via the spectral theory, that $\Phi$ has only a continuous spectrum.

(10) Finally, let us mention some other mathematical approaches. For a complex field ($\mathrm{Im}\,\varepsilon \neq 0$) Avron (1979) proved the existence of SW ladder eigenvalues. For real $\varepsilon$ and periodic potentials with some analytic properties Herbst and Howland (1981) proved that certain matrix elements of $(H^{\varepsilon} - z)^{-1}$ have meromorphic continuation from $\mathrm{Im}\, z > 0$ to $\mathrm{Im}\, z < 0$. One can hope that this continuation has ladder poles in order to describe the SW resonances. However, besides the restriction to one-dimensional systems, one expects the proofs to be rather complicated.

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