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Dynamics of Bloch electrons in external electric fields: I. Bounds for interband transitions and effective Wannier Hamiltonians

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Abstract. Upper bounds on the interband transitions for Bloch electrons in homogeneous electric fields are obtained. The bounds are powerful enough to imply the existence of 'oscillating Bloch electrons' in weak electric fields. The existence of the effective Wannier Hamiltonians of arbitrary order is also proved.

1. Introduction

This is the first in a series of papers dealing with the dynamics of Bloch electrons in external electric fields. Since the first paper by Bloch (1928), a large body of literature has been accumulated about this subject. In spite of this, mainly due to some subtle mathematical phenomena which appear, few rigorous results are known and matters like the existence of oscillating Bloch electrons, effective Wannier Hamiltonians, Stark–Wannier ladder, etc are still controversial. The aim of this series of papers is to obtain rigorous results about the dynamics of Bloch electrons in external electric fields and to settle some of the existing debates.

The main aim of the present paper is to prove a result announced already (Nenciu and Nenciu 1980). In the second section, the problem is described and the main results are stated. The third section contains the first-order theory. The recent result due to Bentosella (1979) is shown to be a particular case of our first-order theory. The fourth section contains the general theory and the proof of the main results. In the last section, we shall indicate some straightforward generalisations. As already announced (Nenciu and Nenciu 1980), the proof follows essentially the proof of the adiabatic theorem (Nenciu 1980) with some simplifications, due to the time independence of the starting Hamiltonian.

2. Description of the problem and the main results

The Hamiltonian we shall consider in this paper is of the form

$$H^{\varepsilon} = H_0 + \varepsilon X_0 \qquad (2.1)$$

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where ($\hbar = 1$)

$$H_0 = -(1/2m)\Delta + V(\boldsymbol{x}) \equiv T + V, \qquad \boldsymbol{x} \in \mathbb{R}^3, \tag{2.2}$$

$$(X_0 f)(\boldsymbol{x}) = \boldsymbol{n} \cdot \boldsymbol{x} f(\boldsymbol{x}), \qquad f \in L^2(\mathbb{R}^3), \tag{2.3}$$

where $\boldsymbol{n}$ is the unit vector along an arbitrary fixed direction. The Hamiltonian (2.1) describes the dynamics of an electron of mass m in the potential $V(\boldsymbol{x})$ and under the influence of the electric field $\boldsymbol{E} = (\varepsilon/e)\boldsymbol{n}$. About V we shall suppose that

$$\lim_{a\to\infty} \left\| V \frac{1}{T+a} \right\| = 0, \tag{2.4}$$

i.e. V is T bounded, with relative bound zero. The condition (2.4) is a rather weak one; it is sufficient that $V(\boldsymbol{x})$ be uniformly locally L^2 (Reed and Simon 1975, theorem XIII 96). In particular, if $V(\boldsymbol{x})$ is periodic, i.e. for some basis $\{\boldsymbol{a}_i\}_{i=1,2,3} \in \mathbb{R}^3$, $V(\boldsymbol{x}+\boldsymbol{a}) = V(\boldsymbol{x})$, it is sufficient for $V(\boldsymbol{x})$ to be square integrable over the unit cell. The condition (2.4) implies via the Kato–Rellich theorem (Kato 1966, theorem 4.3 ch V) that H_0 is self-adjoint on $\mathscr{D}(T)$. It is known (Reed and Simon 1975, theorem X38) that H^ε is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

Let σ_0 be the spectrum of H_0. We shall suppose that there exist $\lambda_1, \lambda_2 \in \mathbb{R}$, such that

$$\begin{aligned} &\sigma_0 = \sigma_0^0 \cup \sigma_0^1, && \sigma_0^0 \neq \varnothing, \\ &\sigma_0^0 \subset [\lambda_1, \lambda_2], && \sigma_0^1 \subset \mathbb{R}\backslash[\lambda_1, \lambda_2], \\ &\operatorname{dist}(\sigma_0^0, \sigma_0^1) = d > 0. \end{aligned} \tag{2.5}$$

Let us stress that we shall not make any assumption about the nature of σ_0^0, so our results apply for periodic systems, as well as for disordered ones (as far as a forbidden gap exists (Nenciu and Nenciu 1981)).

Let P_0 be the spectral projection of H_0 corresponding to σ_0^0 and

$$r_0(\varepsilon; t) = \|(1-P_0)\exp(-\mathrm{i}H^\varepsilon t)P_0\|. \tag{2.6}$$

Obviously $1 - r_0^2(\varepsilon; t)$ is a lower bound for the probability of finding at time t the electron in a state corresponding to σ_0^0, if at $t = 0$ the electron is with probability one in a state corresponding to σ_0^0. The main problem we shall be concerned with is to obtain upper bounds on $r_0(\varepsilon; t)$. The main result obtained in § 3 is that (see theorems 3.1 and 3.2)

$$r_0(\varepsilon; t) \leqslant \varepsilon(C_1 + C_2 t) \tag{2.7}$$

for some constants $0 < C_1, C_2 < \infty$. In the periodic case, in order to establish the existence of oscillating Bloch electrons in weak fields (Kittel 1963, Zak 1972, Nenciu and Nenciu 1980), one needs to show that $r_0(\varepsilon; t) \ll 1$ for t of order $T = 1/\varepsilon|\boldsymbol{a}|$, where $|\boldsymbol{a}|$ is the linear dimension of the unit cell. Clearly, the bound (2.7) is not sufficient. In fact, $\varepsilon C_2 T$ is less than one only for sufficiently large forbidden gaps. On the other hand, physical arguments suggest that

$$\lim_{\varepsilon\to 0} r_0(\varepsilon; T) = 0 \tag{2.8}$$

irrespective of the smallness of the forbidden gap. Bounds on $r_0(\varepsilon; T)$ powerful enough to imply (2.8) are obtained in § 4. More exactly, it is proved that for a given integer n, there exist $0<\varepsilon_n, b_n, C_k^n<\infty$, $k=1,2,\ldots,n+1$ such that for $0<\varepsilon<\varepsilon_n$

$$r_0(\varepsilon;t)\leqslant\sum_{k=1}^{n+1}C_k^n\varepsilon^k+b_n\varepsilon^{n+1}t. \tag{2.9}$$

Moreover, during the proof of (2.9) the following construction emerges. We shall construct a sequence of bounded operators B_n, $n=0,1,2,\ldots$, with the following properties.

(i) B_n is well defined for $\varepsilon<\varepsilon_n$ and

$$\|B_n\|\leqslant b_n\varepsilon^n. \tag{2.10}$$

(ii) Let $H_n(\varepsilon)$ be defined for $\varepsilon<\varepsilon_n$ by

$$H_n(\varepsilon)=H_0-\varepsilon\sum_{k=0}^{n-1}B_k, \qquad n=1,2,\ldots. \tag{2.11}$$

Then $\varepsilon\Sigma_{k=0}^{n-1}\|B_k\|<d/2$, so that $H_n(\varepsilon)$ still has a gap in its spectrum. Let P_n be the spectral projection of $H_n(\varepsilon)$ corresponding to the part of its spectrum which coincides with σ_0^0 in the limit $\varepsilon\to0$. Then

$$\|(1-P_n)\exp(-\mathrm{i}H^\varepsilon t)P_n\|\leqslant b_n\varepsilon^{n+1}t. \tag{2.12}$$

(iii) If $H_n^{\mathrm{W}}(\varepsilon)$ is defined by

$$H_n^{\mathrm{W}}(\varepsilon)=H^\varepsilon+\varepsilon B_n \tag{2.13}$$

or

$$H_n^{\mathrm{W}}(\varepsilon)=H_n(\varepsilon)+\varepsilon X_{n+1} \tag{2.14}$$

where

$$X_n=X_0+\sum_{k=0}^{n-1}B_k \tag{2.15}$$

then

$$[H_n^{\mathrm{W}}(\varepsilon),P_n]=0. \tag{2.16}$$

(iv) Suppose that $V(\boldsymbol{x})$ is periodic and $T(\boldsymbol{a}_i)$, $i=1,2,3$, are the unitary operators representing the translations with the basis vectors of the lattice. Then

$$[B_n,T(\boldsymbol{a}_i)]=0 \tag{2.17}$$

and consequently

$$[H_n(\varepsilon),T(\boldsymbol{a}_i)]=0, \tag{2.18}$$

$$[X_n,T(\boldsymbol{a}_i)]=[X_0,T(\boldsymbol{a}_i)]=\boldsymbol{n}\cdot\boldsymbol{a}_i. \tag{2.19}$$

We have called $H_n^{\mathrm{W}}(\varepsilon)$ effective Wannier Hamiltonians of order n, since the approximative Hamiltonians of the above sort were discussed for the first time by Wannier (1960) (see also Wannier 1962, Zak 1976).

3. The first-order theory

We shall start with a few observations.

(1) Consider the family of self-adjoint operators

$$H_0(t)=U_0^*(t)H_0U_0(t), \qquad U_0(t)=\exp(-\mathrm{i}\varepsilon X_0 t),$$
$$\mathscr{D}[H_0(t)]=U_0(t)\mathscr{D}(H_0). \tag{3.1}$$

Since $U_0(t)\mathscr{D}(H_0)=\mathscr{D}(H_0)$ we have $\mathscr{D}[H_0(t)]=\mathscr{D}(H_0)$. Moreover, as can be easily seen

$$H_0(t)=(\boldsymbol{p}-\varepsilon\boldsymbol{n}t)^2/2m+V(\boldsymbol{x}), \qquad \boldsymbol{p}=-\mathrm{i}\nabla. \tag{3.2}$$

(2) For $z\in\rho[H_0(t)]=\rho(H_0)$ let

$$R_0(t;z)=1/(H_0(t)-z). \tag{3.3}$$

Then, $R_0(t;z)$ is norm differentiable as a function of t and

$$\frac{\mathrm{d}}{\mathrm{d}t}R_0(t;z)=\varepsilon U_0^*(t)\frac{1}{H_0-z}\frac{\boldsymbol{p}\cdot\boldsymbol{n}}{m}\frac{1}{H_0-z}U_0(t). \tag{3.4}$$

To see this, note first that the operator

$$\frac{1}{H_0-z}\frac{\boldsymbol{p}\cdot\boldsymbol{n}}{m}\frac{1}{H_0-z}$$

is bounded and

$$\lim_{t\to0}\left\|\frac{1}{t}[R_0(t;z)-R_0(0;z)]-\varepsilon\frac{1}{H_0-z}\frac{\boldsymbol{p}\cdot\boldsymbol{n}}{m}\frac{1}{H_0-z}\right\|=0. \tag{3.5}$$

The general case follows from (3.5), remarking that

$$\frac{\mathrm{d}}{\mathrm{d}t}R_0(t;z)=U_0^*(t)\left(\frac{\mathrm{d}}{\mathrm{d}t}R_0(t;z)\right)_{t=0}U_0(t). \tag{3.6}$$

(3) By definition, $H_0(t)$ and H_0 have the same spectrum. We shall denote by

$$P_0(t)=U_0^*(t)P_0U_0(t) \tag{3.7}$$

the spectral projection of $H_0(t)$ corresponding to σ_0^0. $P_0(t)$ is norm differentiable and the norm of the derivative does not depend on t. In fact

$$\frac{\mathrm{d}}{\mathrm{d}t}P_0(t)=\varepsilon U_0^*(t)\left(\frac{1}{2\pi\mathrm{i}}\int_C\frac{1}{H_0-z}\frac{\boldsymbol{p}\cdot\boldsymbol{n}}{m}\frac{1}{H_0-z}\,\mathrm{d}z\right)U_0(t) \tag{3.8}$$

where C is a contour surrounding σ_0^0. The formula (3.8) follows from (3.4) and the usual formula relating the spectral projectors and the resolvent of a self-adjoint operator.

(4) The following construction, which is crucial for our theory, goes back to Kato (1950) (see also Kato 1966, ch II, 4.2, Messiah 1966, ch XVII).

Lemma 3.1. Let $P(t)$, $t\in\mathbb{R}$ be a family of orthogonal projections, having continuous norm derivative with respect to t.

(i) If $K(t)$ is defined by

$$K(t)=\mathrm{i}(1-2P(t))\,\mathrm{d}P(t)/\mathrm{d}t \tag{3.9}$$

then $K(t)$ is a family of bounded self-adjoint operators and

$$[P(t), K(t)] = -\mathrm{i}\, \mathrm{d}P(t)/\mathrm{d}t. \tag{3.10}$$

(ii) The equation

$$\mathrm{i}\, \mathrm{d}A(t)/\mathrm{d}t = K(t)A(t), \qquad A(0) = 1, \tag{3.11}$$

has a unique solution satisfying $A^{-1}(t) = A^*(t)$ and

$$A(t)P(0) = P(t)A(t). \tag{3.12}$$

(5) Let $K_0(t)$, $A_0(t)$ be given by the construction in lemma 3.1, applied to $P_0(t)$, and

$$B_0 = (1/\varepsilon)K_0(0). \tag{3.13}$$

Consider now the self-adjoint operator

$$X_1 = X_0 + B_0, \qquad \mathscr{D}(X_1) = \mathscr{D}(X_0). \tag{3.14}$$

By direct calculation (which is allowed by Stone's theorem)

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}[\exp(\mathrm{i}\varepsilon X_0 t)\exp(-\mathrm{i}\varepsilon X_1 t)]f = K_0(t)\exp(\mathrm{i}\varepsilon X_0 t)\exp(-\mathrm{i}\varepsilon X_1 t)f, \qquad f \in \mathscr{D}(X_0), \tag{3.15}$$

which implies

$$A_0(t) = \exp(\mathrm{i}\varepsilon X_0 t)\exp(-\mathrm{i}\varepsilon X_1 t). \tag{3.16}$$

From (3.7), (3.12) and (3.16) it follows that

$$[P_0, \exp(-\mathrm{i}\varepsilon X_1 t)] = 0, \qquad \text{for all } t \in \mathbb{R} \tag{3.17}$$

which implies that if $f \in \mathscr{D}(X_1)$, then $P_0 f \in \mathscr{D}(X_1)$ and

$$X_1 P_0 f - P_0 X_1 f = 0. \tag{3.18}$$

We are now ready to prove the main result of this section.

Theorem 3.1.

$$r_0(\varepsilon; t) = \|(1 - P_0)\exp(-\mathrm{i}H^\varepsilon t)P_0\| < \varepsilon\|B_0\|t. \tag{3.19}$$

Proof. From (3.18) and the fact that H^ε is essentially self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(X_0)$, it follows that

$$[\exp[-\mathrm{i}(H_0 + \varepsilon X_1)t], P_0] = 0 \tag{3.20}$$

which together with the Schrödinger equation written in the form

$$\exp[\mathrm{i}(H_0 + \varepsilon X_1)t]\exp(-\mathrm{i}H^\varepsilon t) = 1 + \varepsilon\int_0^t \exp[\mathrm{i}(H_0 + \varepsilon X_1)u]B_0\exp(-\mathrm{i}H^\varepsilon u)\,\mathrm{d}u \tag{3.21}$$

implies (3.19).

One can easily obtain extensions of the above result. Let $b(\boldsymbol{x})$ be a bounded function and B be the operator of multiplication with $b(\boldsymbol{x})$. Suppose that $\varepsilon\|B\| < d/2$. Let P_B be the spectral projection of $H_0 - \varepsilon B$ corresponding to the spectrum included in

$\{\lambda \mid \operatorname{dist}(\lambda, \sigma_0^0) < \varepsilon\|B\|\}$ and

$$P_B(t) = \exp[\mathrm{i}\varepsilon(X_0+B)t]P_B \exp[-\mathrm{i}\varepsilon(X_0+B)t]. \tag{3.22}$$

Since X_0 commutes with B

$$P_B(t) = \exp(\mathrm{i}\varepsilon Bt)\exp(\mathrm{i}\varepsilon X_0 t)P_B \exp(-\mathrm{i}\varepsilon X_0 t)\exp(-\mathrm{i}\varepsilon Bt) \tag{3.23}$$

and, exactly as above,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}&\exp(\mathrm{i}\varepsilon X_0 t)P_B \exp(-\mathrm{i}\varepsilon X_0 t)\\ &= \varepsilon \exp(\mathrm{i}\varepsilon X_0 t)\left(\frac{1}{2\pi\mathrm{i}}\int_C \frac{1}{H_0-\varepsilon B-z}\frac{\boldsymbol{p}\cdot\boldsymbol{n}}{m}\frac{1}{H_0-\varepsilon B-z}\,\mathrm{d}z\right)\\ &\quad\times\exp(-\mathrm{i}\varepsilon X_0 t)\end{aligned} \tag{3.24}$$

and it follows that $P_B(t)$ is norm differentiable. From this point, all the theory developed above applies and the result is the following.

Theorem 3.2.

$$r_B(\varepsilon\,;t) \equiv \|(1-P_B)\exp(-\mathrm{i}H^\varepsilon t)P_B\| \leqslant \left\|\left(\frac{\mathrm{d}}{\mathrm{d}t}P_B(t)\right)_{t=0}\right\| t. \tag{3.25}$$

Remarks

3.1. Supposing that we know that on a dense set $X_0P_0 - P_0X_0$ is well defined and bounded, it is easy to see that its extension by continuity, denoted by $[X_0, P_0]$, equals $(\mathrm{i}/\varepsilon)[\mathrm{d}P_0(t)/\mathrm{d}t]_{t=0}$. We can reformulate the result in theorem 3.1 as

$$r_0(\varepsilon\,;t) \leqslant \varepsilon\|[P_0, X_0]\|t. \tag{3.26}$$

Of course the same comment applies to theorem 3.2. Moreover, in this case the theory in the first part of this section becomes unnecessary since we can define X_1 and B_0 by

$$\begin{aligned}X_1 &= P_0X_0P_0 + (1-P_0)X_0(1-P_0),\\ B_0 &= (1-P_0)X_0P_0 + P_0X_0(1-P_0) = (1-2P_0)[P_0, X_0].\end{aligned} \tag{3.27}$$

3.2. We shall outline the proof of the fact that the bound obtained recently by Bentosella (1979) is a particular case of (3.26). Consider the case when P_0 corresponds to a non-degenerate isolated band of a periodic system. Bentosella took as $b(\boldsymbol{x})$ the periodic function which equals $-\boldsymbol{n}\cdot\boldsymbol{x}$ in the first cell. For ε sufficiently small, P_B corresponds to a non-degenerate isolated band of $H_0 - \varepsilon B$. Let $w_m^1(\boldsymbol{x}) = w^1(\boldsymbol{x} - \boldsymbol{R}_m)$ be the Wannier functions of this band (which are supposed to be sufficiently localised, such that all are in the domain of X_0).

Let

$$f \in P_B L^2(\mathbb{R}^3), \qquad \|f\| = 1, \qquad f(\boldsymbol{x}) = \sum_m C_m w_m^1(\boldsymbol{x}), \qquad \sum_m |\boldsymbol{R}_m|^2|C_m|^2 < \infty. \tag{3.28}$$

Let

$$g(\boldsymbol{x}) = \sum_m \boldsymbol{n}\cdot\boldsymbol{R}_m C_m w_m^1(\boldsymbol{x}). \tag{3.29}$$

Obviously $\|g\|<\infty$ and $(1-P_B)g=0$. Then

$$\begin{aligned}\|[P_B,(X_0+B)]f\| &= \|(1-P_B)(X_0+B)P_Bf\| \\ &= \|(1-P_B)[g-(X_0+B)f]\| \\ &\leqslant \left\|\sum_m C_m(\boldsymbol{n}\cdot(\boldsymbol{x}-\boldsymbol{R}_m)+b(\boldsymbol{x}))w^1(\boldsymbol{x}-Rm)\right\| \\ &\leqslant \mathcal{M}\left(\sum_m |C_m|^2\right)^{1/2}\leqslant \mathcal{M}\end{aligned} \tag{3.30}$$

where $\mathcal{M}$ is the same as in Bentosella's paper.

4. The general theory

We shall start by remarking that (3.2), (3.7), (3.9) and (3.11) imply the following.

Lemma 4.1. $R_0(t;z)$, $P_0(t)$, $K_0(t)$ and $A_0(t)$ are indefinitely norm differentiable functions of $t\in\mathbb{R}$.

Let us consider now $H_1(t)$ given by

$$\begin{aligned}&H_1(t)=A_0^*(t)[H_0(t)-K_0(t)]A_0(t)=\exp(\mathrm{i}\varepsilon X_1t)(H_0-\varepsilon B_0)\exp(-\mathrm{i}\varepsilon X_1t),\\ &\mathscr{D}[H_1(t)]=A_0(t)\mathscr{D}[H_0(t)].\end{aligned} \tag{4.1}$$

Obviously, $\sigma[H_1(t)]=\sigma_1$ is independent of t and for $\varepsilon<\varepsilon_1=d/2\|B_0\|$ is a union of two disjoint sets

$$\sigma_1=\sigma_1^0\cup\sigma_1^1,\qquad \sigma_1^0\subset\{\lambda\mid \operatorname{dist}(\lambda,\sigma_0^0)<\varepsilon\|B_0\|\}. \tag{4.2}$$

Following the construction of the previous section, we can define $P_1(t)$ as the spectral projection of $H_1(t)$, corresponding to σ_1^0 and $K_1(t)$, $A_1(t)$, B_1 by formulae similar to (3.9), (3.11) and (3.13).

Lemma 4.2. $R_1(t;z)$, $P_1(t)$, $K_1(t)$ and $A_1(t)$ are indefinitely norm differentiable functions of $t\in\mathbb{R}$.

Proof. It is sufficient to consider $R_1(t;z)$ for $\operatorname{dist}(z,\sigma_0^0)>\varepsilon\|B_0\|$. Writing

$$R_1(t;z)=A_0^*(t)R_0(t;z)[1-K_0(t)R_0(t;z)]^{-1}A_0(t), \tag{4.3}$$

the indefinite norm differentiability of $R_1(t;z)$ follows from lemma 4.1.

One can continue this process indefinitely. At the nth step, the value of ε for which the procedure can be carried out is

$$\varepsilon<\varepsilon_n=d\left(2\sum_{j=0}^{n-1}\|B_j\|\right)^{-1}. \tag{4.4}$$

The recurrence relations are

$$X_{n+1}=X_n+B_n, \tag{4.5}$$

$$H_{n+1}=H_n-\varepsilon B_n, \tag{4.6}$$

$$H_{n+1}(t)=A_n^*(t)[H_n(t)-K_n(t)]A_n(t)=\exp(\mathrm{i}\varepsilon X_{n+1}t)H_{n+1}\exp(-\mathrm{i}\varepsilon X_{n+1}t), \tag{4.7}$$

and the repetition of the theory in the previous section leads to the following theorem.

Theorem 4.1. For $\varepsilon<\varepsilon_n$, $n=0, 1, 2, \ldots,$

$$r_n(t)=\|(1-P_n)\exp(-\mathrm{i}H^\varepsilon t)P_n\|\leqslant\varepsilon\|B_n\|t, \tag{4.8}$$

$$[P_n, \exp[-\mathrm{i}(H_n+\varepsilon X_{n+1})t]]=0. \tag{4.9}$$

Theorem 4.2. For $\varepsilon<\varepsilon_n$, $n=0, 1, 2, \ldots,$ there exists $b_n<\infty$ such that

$$\|B_n\|\leqslant\varepsilon^n b_n. \tag{4.10}$$

The main body of the proof is contained in the following lemma.

Lemma 4.3. Let C be a contour enclosing σ_0^0 and satisfying $\mathrm{dist}(C, \sigma_0^0)\geqslant d/2$. Then there exist constants $a_{n,m}$, $b_{n,m}$, $n=0, 1, \ldots, m=1, 2, \ldots,$ such that for $\varepsilon\leqslant\varepsilon_n$

$$\|\mathrm{d}^m R_n(t; z)/\mathrm{d}t^m\|\leqslant\varepsilon^m a_{n,m}, \tag{4.11}$$

$$\|\mathrm{d}^m P_n(t)/\mathrm{d}t^m\|\leqslant\varepsilon^{n+m} b_{n,m}. \tag{4.12}$$

The proof is by induction over n.

$n=0$:

$$\|\mathrm{d}^m R_0(t;z)/\mathrm{d}t^m\|=\|(\mathrm{d}^m R_0(t; z)/\mathrm{d}t^m)_{t=0}\|\leqslant\varepsilon^m a_{0,m} \tag{4.13}$$

follows from

$$\frac{\mathrm{d}}{\mathrm{d}t}R_0(t; z)=\varepsilon R_0(t; z)\frac{\boldsymbol{p}\cdot\boldsymbol{n}-\varepsilon t}{m}R_0(t; z). \tag{4.14}$$

Now (4.12) for $n=0$ follows from (4.13) and

$$\left\|\left(\frac{\mathrm{d}^m}{\mathrm{d}t^m}P_0(t)\right)_{t=0}\right\|\leqslant\frac{1}{2\pi}\int_C\left\|\left(\frac{\mathrm{d}^m}{\mathrm{d}t^m}R_0(t; z)\right)_{t=0}\right\||\mathrm{d}z|. \tag{4.15}$$

Supposing (4.11) and (4.12) are true for $n-1$, (4.11) for n follows from the formula

$$R_n(t; z)=A_{n-1}^*(t)R_{n-1}(t)[1-K_{n-1}(t)R_{n-1}(t)]^{-1}A_{n-1}(t). \tag{4.16}$$

Finally (4.12) for n follows from the formula

$$P_n(t)-P_{n-1}(0)=\frac{1}{2\pi\mathrm{i}}A_{n-1}^*(t)\left(\int_C\frac{1}{H_{n-1}(t)-K_{n-1}(t)-z}K_{n-1}(t)R_{n-1}(t; z)\,\mathrm{d}z\right)A_{n-1}(t). \tag{4.17}$$

Formula (4.17) follows from the fact that

$$A_{n-1}(t)P_{n-1}(0)=P_{n-1}(t)A_{n-1}(t) \tag{4.18}$$

which is true by construction, implying that $P_{n-1}(0)$ is the spectral projection of $A_{n-1}^*(t)H_{n-1}(t)A_{n-1}(t)$ corresponding to σ_{n-1}^0 for all $t\in\mathbb{R}$. This finishes the proof of lemma 4.3.

Now (4.10) is implied by (4.12) for $m=1$ and the definition of B_n and the proof of theorem 4.2 is finished.

Finally, suppose that $V(\boldsymbol{x})$ is periodic and let $T(\boldsymbol{a}_i)$ be the translation operators. Either using

$$T(\boldsymbol{a}_i)X_0 - X_0 T(\boldsymbol{a}_i) = \boldsymbol{n}\cdot\boldsymbol{a}_i \tag{4.19}$$

or directly from (3.2), it follows that

$$[H_0(t), T(\boldsymbol{a}_i)] = 0, \qquad t\in\mathbb{R}. \tag{4.20}$$

Then by construction it follows that

$$[B_k, T(\boldsymbol{a}_i)] = 0, \qquad k = 0, 1, 2, \ldots, \tag{4.21}$$

and then

$$[H_m, T(\boldsymbol{a}_i)] = 0, \qquad m = 0, 1, 2, \ldots. \tag{4.22}$$

$$[X_m, T(\boldsymbol{a}_i)] = -\boldsymbol{n}\cdot\boldsymbol{a}_i. \tag{4.23}$$

Remarks

4.1. Leaving the full discussion for a future publication, we shall comment a little on the controversial existence of the Stark–Wannier ladder. For simplicity, we shall consider the one-dimensional case. Moreover, we shall take P_0 corresponding to a single non-degenerate band. Then, P_n will correspond to a non-degenerate band of H_n. The nth-order effective Wannier Hamiltonian H_n can be written as an orthogonal sum

$$H_n^{\mathrm{W}}(\varepsilon) = P_n H_n^{\mathrm{W}}(\varepsilon) P_n \oplus (1-P_n) H_n^{\mathrm{W}}(\varepsilon)(1-P_n). \tag{4.24}$$

Now, $P_n H_n^{\mathrm{W}}(\varepsilon) P_n$ has a pure non-degenerate point spectrum (Avron *et al* 1977, Avron 1979)

$$P_n H_n^{\mathrm{W}}(\varepsilon) P_n \psi_p^{(n)} = (\varepsilon a p + \delta)\psi_p^{(n)}, \qquad p = 0, \pm 1, \pm 2, \ldots, \tag{4.25}$$

where δ is a certain constant and a is the lattice constant. Due to (4.10), $\psi_p^{(n)}$ is a pseudoeigenvalue of order n of the full Hamiltonian in the sense that (Reed and Simon 1975, ch XII 5)

$$\|H^{\varepsilon}\psi_p^{(n)} - (\varepsilon a p + \delta)\psi_p^{(n)}\| \leqslant b_n \varepsilon^{n+1}, \tag{4.26}$$

indicating a spectral concentration of order n. Moreover, since the one-dimensional projector associated with $\psi_p^{(n)}$ commutes with $H_n^{\mathrm{W}}(\varepsilon)$, it follows that

$$|(\psi_p^{(n)}, \exp(-\mathrm{i}H^{\varepsilon}t)\psi_p^{n})|^2 \geqslant 1 - b_n^2 \varepsilon^{2(n+1)} t^2, \tag{4.27}$$

indicating a rather long lifetime of the pseudo-eigenstate $\psi_p^{(n)}$. Let us stress that while the spectral concentration in the sense of (4.26) is of the order ε^n, the spacing between pseudo-eigenvalues is of the order of ε. In this sense, one can say that at low electric fields, a Stark–Wannier ladder of well separated resonances exists (see also Avron (1979) for related results).

4.2. Our last remark is about the existence of an effective Hamiltonian having no interband transitions. If the constants b_n appearing in (4.10) satisfy

$$|b_n| \leqslant C^n, \qquad C < \infty \tag{4.28}$$

then H_n and X_n converge to well defined operators H_∞, X_∞ for sufficiently small ε, $H_\infty + \varepsilon X_\infty = H^\varepsilon$ and $[P_\infty, H^\varepsilon] = 0$. Unfortunately, it seems that (4.28) is not true and the above scheme does not work, so if H_n converges in some sense to an operator H_∞, this is at best in some asymptotical sense (see also Wannier and Van Dyke (1968) for a discussion of this point).

5. Generalisation and remarks

The first remark is that in order to obtain bounds of the form (2.9), the homogeneity of the electric field is not really needed. The whole theory works if (2.3) is generalised to

$$(X_0 f)(\boldsymbol{x}) = \Phi(\boldsymbol{x}) f(\boldsymbol{x}), \tag{5.1}$$

the only condition being that $\Phi(\boldsymbol{x})$ be differentiable and its derivatives be bounded on $\mathbb{R}^3$. Of course, in this case the translation invariance of H_n, $n = 1, 2, \ldots$, is lost. Moreover, bounds on the interband transition probabilities can be obtained also in the case when the electric field is not constant in time.

Another generalisation is that in the case of a homogeneous electric field and perdiodic potential, the whole theory works if a forbidden gap exists in the following sense. Let $\sigma_0(\boldsymbol{k}) = \{\lambda_0^i(\boldsymbol{k})\}_{i=0}^{\infty}$ be the (discrete) spectrum of H_0, at a fixed value of crystal momentum. If $\sigma_0^0 = \{\lambda \,|\, \lambda = \lambda_0^0(\boldsymbol{k}), \boldsymbol{k} \in B, \lambda_0^0(\boldsymbol{k}) \text{ is continuous}\}$, then the condition (2.5) can be replaced by

$$\inf_{\boldsymbol{k} \in B} \operatorname{dist}(\lambda_0^0(\boldsymbol{k}), \{\sigma_0(\boldsymbol{k}) \backslash \lambda_0^0(\boldsymbol{k})\}) \geq d > 0 \tag{5.2}$$

where B is the first Brillouin zone. In other words, the condition is that a forbidden gap exists at each value of the crystal momentum.

Our last remark concerns the numerical values of the constants appearing in (2.12), (3.25), etc. For the typical values $d = 6 \times 10^{-19}$J, $a = 5 \times 10^{-10}$ m, Bentosella claims (Bentosella 1979) that for his choice of B

$$r_{\mathrm{Ben}}(\varepsilon; T) \leq 4 \times 10^{-2} \tag{5.3}$$

without any assumption on V, as far as $E \leq 10^7$ V m^{-1}. However, we were not able to follow his arguments leading to the above estimates (and we suspect one of them to be incorrect).

Our (rough) estimations lead, under the assumption that $V(\boldsymbol{x})$ is bounded and

$$\operatorname*{ess\,sup}_{\boldsymbol{x} \in \mathbb{R}^3} V(\boldsymbol{x}) - \operatorname*{ess\,inf}_{\boldsymbol{x} \in \mathbb{R}^3} V(\boldsymbol{x}) \lesssim 6 \times 10^{-17} \text{ J} \tag{5.4}$$

give the weaker results

$$r_0(\varepsilon; T) \leq 5 \times 10 \tag{5.5}$$

and

$$r_1(\varepsilon; T) \leq 8 \times 10^{-7} E \qquad \text{for } E \lesssim 10^8 \text{ V m}^{-1}. \tag{5.6}$$

A detailed study of the numerical values of the constants appearing in the theory will be published.

References

Avron J E 1979 *J. Phys. A: Math. Gen.* **12** 2393–8
Avron J E, Zak J, Grossmann A and Gunther L 1977 *J. Math. Phys.* **18** 918–21
Bentosella F 1979 *Commun. Math. Phys.* **68** 173–82
Bloch F 1928 *Z. Phys.* **52** 555
Kato T 1950 *J. Phys. Soc. Japan* **5** 435–9
—— 1966 *Perturbation Theory for Linear Operators* (Berlin: Springer)
Kittel Ch 1963 *Quantum Theory of Solids* (New York: Wiley)
Messiah A 1960 *Mecanique Quantique* Tome II (Paris: Dunod)
Nenciu A and Nenciu G 1980 *Phys. Lett.* **78**A 101–2
Nenciu A and Nenciu Gh 1981 *J. Phys. A: Math Gen.* **14** L109–12
Nenciu Gh 1980 *J. Phys. A: Math. Gen.* **13** L15–8
Reed M and Simon B 1975 *Methods of Modern Mathematical Physics* vol II (New York: Academic)
Wannier G H 1960 *Phys. Rev.* **117** 432–9
—— 1962 *Rev. Mod. Phys.* **34** 645–55
Wannier G H and Van Dyke J P 1968 *J. Math. Phys.* **9** 899–904
Zak J 1973 *Solid State Phys.* **27** 1–62
—— 1976 *Commun. Phys.* **1** 73–9