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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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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[1], 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[2]. 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[3] 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 generalizations. As already announced[2] the proof follows essentially the proof of the adiabatic theorem[4] 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

$$H^{\epsilon} = H_0 + \epsilon X_0 , \tag{2.1}$$

where $(\hbar = 1)$,

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

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

where $\vec{n}$ 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 $V(\vec{x})$ and under the influence of the electric field $\vec{E} = \frac{\epsilon}{e}\vec{n}$. About V we shall suppose that

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

i.e., V is T bounded, with relative bound zero. The condition (2.4) is a rather weak one; it is sufficient that $V(\vec{x})$ be uniformly locally L^2 (ref. /5/, Th.XIII 96). In particular, if $V(\vec{x})$ is periodic, i.e., for some basis $\{\vec{a}_i\}_{i=1,2,3} \in \boldsymbol{R}^3$, $V(\vec{x}+\vec{a}) = V(\vec{x})$, it is sufficient to be square integrable over the unit cell. The condition (2.4) implies via the Kato-Rellich theorem (ref. /6/, Th.4.3. Chapter V) that H_0 is self-adjoint on $D(T)$. It is known (ref. /5/, Th.X 38) that H^ϵ is essentially self-adjoint on $C_0^\infty(\boldsymbol{R}^3)$.

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

$$\sigma_0 = \sigma_0^0 \cup \sigma_1^1, \quad \sigma_0 \neq \phi,$$

$$\sigma_0^0 \subset [\lambda_1, \lambda_2], \quad \sigma_0^1 \subset \boldsymbol{R} \setminus [\lambda_1, \lambda_2], \tag{2.5}$$

$$\mathrm{dist}(\sigma_0^0, \sigma_0^1) = d > 0 .$$

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[7]).

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

$$\gamma_0(\epsilon, t) = \| (1 - P_0) \exp(-iH^\epsilon t) P_0 \| . \tag{2.6}$$

Obviously $1 - \gamma_0^2(\epsilon, t)$ is a lower bound for the probability to find at the 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 $\gamma_0(\epsilon, t)$. The main result obtained in section 3 is that (see Ths.3.1. and 3.2.)

$$\gamma_0(\epsilon, t) \le \epsilon(C_1 + C_2 t) \tag{2.7}$$

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 [8,9], one needs to show that $\gamma_0(\epsilon,t) \ll 1$ for t of order $T=\frac{1}{\epsilon|\vec{a}|}$, where $|\vec{a}|$ is the linear dimension of the unit cell. Clearly, the bound (2.7) is not sufficient. In fact, $\epsilon C_2 T$ is less than one only for sufficiently large forbidden gaps. On the other hand, physical arguments suggest that

$$\lim_{\epsilon\to 0}\gamma_0(\epsilon,T)=0, \tag{2.8}$$

irrespective of the smallness of the forbidden gap. Bounds on $\gamma_0(\epsilon,t)$, powerful enough to imply (2.8), are obtained in section 4. More exactly, it is proved that for a given integer n, there exist $0<\epsilon_n, b_n, C_k^n<\infty$, $k=1,2,\ldots,n$ such that for $0<\epsilon<\epsilon_n$

$$\gamma_0(\epsilon,t)\le \sum_{k=1}^{n} C_k^n\epsilon^k + b_n\epsilon^{n+1}t. \tag{2.9}$$

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

i. B_n is well defined for $\epsilon<\epsilon_n$ and

$$\|B_n\|\le b_n\epsilon^n \tag{2.10}$$

ii. Let $H_n(\epsilon)$ be defined for $\epsilon<\epsilon_n$ by

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

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

$$\|(1-P_n)\exp(-iH^\epsilon t)P_n\|\le b_n\epsilon^{n+1}t. \tag{2.12}$$

iii. If $H_n^w(\epsilon)$ is defined by

$$H_n^W(\epsilon)=H^\epsilon+\epsilon B_n, \tag{2.13}$$

or, otherwise,

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

where

$$X_n = X_0 + \sum_{k=0}^{n-1} B_k \ , \qquad (2.15)$$

then

$$[H_n^W(\epsilon), P_n] = 0. \qquad (2.16)$$

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

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

and, consequently,

$$[H_n(\epsilon), T(\vec{a}_i)] = 0, \qquad (2.18)$$

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

We have called $H_n^W(\epsilon)$ effective Wannier Hamiltonians of order n, since the approximative Hamiltonians of the above sort have been discussed for the first time by Wannier /10/ (see also refs. /11,12/).

3. THE FIRST ORDER THEORY

We shall start with a few observations.

1. Consider the family of self-adjoint operators

$$H_0(t) = U_0^*(t)\, H_0\, U_0(t)\ ; \quad U_0(t) = \exp(-i\epsilon X_0 t),$$

$$D(H_0(t)) = U_0^*(t)\, D(H_0). \qquad (3.1)$$

Since $U_0^*(t)\,D(H_0) = D(H_0)$, we have $D(H_0(t)) = D(H_0)$. Moreover, as it can be easily seen

$$H_0(t) = \frac{1}{2m}(\vec{p} - \epsilon\vec{n}t)^2 + V(\vec{x})\ ; \quad \vec{p} = -i\nabla\ . \qquad (3.2)$$

2. Let for $z \in \rho(H_0(t)) = \rho(H_0)$

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

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

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

To see this, note first that the operator $\frac{1}{H_0 - z} \frac{\vec{p}\cdot\vec{n}}{m} \frac{1}{H_0 - z}$ is bounded and

$$\lim_{t\to 0} \|\frac{1}{t}(R_0(t;z) - R_0(0;z)) - \epsilon \frac{1}{H_0 - z} \frac{\vec{p}\cdot\vec{n}}{m} \frac{1}{H_0 - z}\| = 0. \tag{3.5}$$

The general case follows from (3.5), remarking that

$$\frac{d}{dt} R_0(t;z) = U_0^*(t) [\frac{d}{dt} R_0(t;z)]_{t=0} U_0(t). \tag{3.6}$$

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

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

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,

$$\frac{d}{dt} P_0(t) = \epsilon U_0^*(t) [\frac{1}{2\pi i} \int_C \frac{1}{H_0 - z} \frac{\vec{p}\cdot\vec{n}}{m} \frac{1}{H_0 - z} dz] U_0(t), \tag{3.8}$$

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

4. The following construction, which is crucial for our theory, goes back to Kato[13] (see also refs.[6], Chapter II, § 4.2, and ref.[14], Chapter 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

$$K(t) = i(1 - 2P(t)) \frac{d}{dt} P(t) \tag{3.9}$$

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

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

ii. The equation

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

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

$$B_0 = \frac{1}{\epsilon}K_0(0). \tag{3.13}$$

Consider now the self-adjoint operator

$$X_1 = X_0 + B_0; \quad D(X_1) = D(X_0). \tag{3.14}$$

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

$$i\frac{d}{dt}(e^{i\epsilon X_0 t}\, e^{-i\epsilon X_1 t})f = K_0(t)\, e^{i\epsilon X_0 t}\, e^{-i\epsilon X_1 t} f; \tag{3.15}$$

$$f \in D(X_0),$$

which implies

$$A_0(t) = e^{i\epsilon X_0 t}\, e^{-i\epsilon X_1 t}. \tag{3.16}$$

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

$$[P_0, e^{-i\epsilon X_1 t}] = 0, \qquad \text{all } t \in \boldsymbol{R}, \tag{3.17}$$

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

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

We are now ready to prove the main results of this section:

Theorem 3.1.

$$\gamma_0(\epsilon;t) \equiv \|(1-P_0)e^{-iH^{\epsilon}t}\, P_0\| < \epsilon\, \|B_0\|\, t. \tag{3.19}$$

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

$$[e^{-i(H_0+\epsilon X_1)t}, P_0] = 0, \tag{3.20}$$

which together with the Schrödinger equation written in the following form

$$e^{i(H_0+\epsilon X_1)t} \quad e^{-iH^\epsilon t} = 1 + \epsilon \int_0^t e^{i(H_0+\epsilon X_1)u} B_0 e^{-iH^\epsilon u} du \tag{3.21}$$

implies (3.19).

One can easily obtain extentions of the above result. Let $b(\vec{x})$ be a bounded function and B be the operator of multiplication with $b(\vec{x})$. Suppose that $\epsilon \|B\| < d/2$. Let P_B be the spectral projection of $H_0 - \epsilon B$ corresponding to the spectrum included in $\{\lambda | \text{dist.}(\lambda, \sigma_0^0) < \epsilon \|B\|\}$ and

$$P_B(t) = e^{i\epsilon(X_0+B)t} P_B e^{-i\epsilon(X_0+B)t}. \tag{3.22}$$

Since X_0 commutes with B

$$P_B(t) = e^{i\epsilon X_0 t} e^{i\epsilon Bt} P_B e^{-i\epsilon X_0 t} e^{-i\epsilon Bt}, \tag{3.23}$$

and, exactly as above,

$$\frac{d}{dt} e^{i\epsilon X_0 t} P_B e^{-i\epsilon X_0 t} = \epsilon e^{i\epsilon X_0 t} [\frac{1}{2\pi i} \int_C \frac{1}{H_0 - \epsilon B - z} \frac{\vec{p}\vec{n}}{m} \cdot \frac{1}{H_0 - \epsilon B - z} dz] e^{-i\epsilon X_0 t}, \tag{3.24}$$

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

Theorem 3.2.

$$\gamma_B(\epsilon, t) = \|(1-P_B) e^{-iH^\epsilon t} P_B\| \leq \|[\frac{d}{dt} P_B(t)]_{t=0}\| t. \tag{3.25}$$

Remarks.

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

$$\gamma_0(\epsilon, t) \leq \epsilon \|[P_0, X_0]\| t. \tag{3.26}$$

Of course, the same comment applies to Th.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

$$X_1 = P_0 X_0 P_0 + (1-P_0) X_0 (1-P_0)$$

$$B_0 = (1-P_0) X_0 P_0 + P_0 X_0 (1-P_0) = (1-2P_0)[P_0, X_0] . \tag{3.27}$$

3.2. We shall outline the proof of the fact that the bound obtained recently by Bentosella [3] is a particular case of (3.26). Consider the case when P_0 corresponds to a nondegenerated isolated band of a periodic system. Bentosella tooks as $b(\vec{x})$ the periodic function which equals $-\vec{n}\vec{x}$ in the first cell. For ϵ sufficiently small, P_B corresponds to a nondegenerated isolated band of $H_0 - \epsilon B$. Let $\omega'_m(\vec{x}) = \omega'(\vec{x} - \vec{R}_m)$ 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

$$f \in P_B L^2(\boldsymbol{R}^3), \qquad \|f\| = 1, \quad f(\vec{x}) = \sum_m C_m \omega'_m(\vec{x}),$$

$$\sum_m |\vec{R}_m|^2 |C_m|^2 < \infty . \tag{3.28}$$

Let

$$g(\vec{x}) = \sum_m \vec{n}\cdot\vec{R}_m C_m \omega'_m(\vec{x}) . \tag{3.29}$$

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

$$\|[P_B, (X_0 + B)] f\| = \|(1-P_B)(X_0 + B) P_B f\| =$$

$$= \|(1-P_B)(g - (X_0 + B) f)\| \leq \tag{3.30}$$

$$\leq \|\sum_m C_m (\vec{n}(\vec{x} - \vec{R}_m) + b(\vec{x}))\,\omega'(\vec{x} - \vec{R}_m)\| \leq \mathfrak{M} \sqrt{\sum_m |C_m|^2} = \mathfrak{M},$$

where $\mathfrak{M}$ 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:

Lemma 4.1.
$R_0(t;z)$, $P_0(t)$, $K_0(t)$, $A_0(t)$ are indefinitely norm differentiable functions of $t \in \mathbf{R}$.
Let us consider now $H_1(t)$ given by

$$H_1(t) = A_0^*(t)[H_0(t) - K_0(t)]A_0(t) = e^{i\epsilon X_1 t}(H_0 - \epsilon B_0)e^{-i\epsilon X_1 t}, \tag{4.1}$$

$$D(H_1(t)) = A_0^*(t)\, D(H_0(t)).$$

Obviously, $\sigma(H_1(t)) = \sigma_1$ is independent of t and for $\epsilon < \epsilon_1 = \dfrac{d}{2\|B_0\|}$ is a union of two disjoint sets

$$\sigma_1 = \sigma_1^0 \cup \sigma_1^1 , \tag{4.2}$$

$$\sigma_1^0 \subset \{\lambda \mid \mathrm{dist}(\lambda, \sigma_0^0) < \epsilon \|B_0\|\} .$$

Following the construction from 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.
$R_1(t;\ z)$, $P_1(t)$, $K_1(t)$, $A_1(t)$ are indefinitely norm differentiable functions of $t \in \mathbf{R}$.
Proof: It is sufficient to consider $R_1(t;z)$ for $\mathrm{dist}(z, \sigma_0^0) > \epsilon \|B_0\|$.
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 n-th step, the value of ϵ for which the procedure can be carried out is

$$\epsilon < \epsilon_n = \frac{d}{2\sum_{j=0}^{n-1} \|B_j\|} . \tag{4.4}$$

The recurrence relations are

$$X_{n+1} = X_n + B_n , \qquad (4.5)$$

$$H_{n+1} = H_n - \epsilon B_n , \qquad (4.6)$$

$$H_{n+1}(t) = A_n^*(t)\,[H_n(t) - K_n(t)\,]\,A_n(t) = e^{i\epsilon X_n t}\, H_{n+1}\, e^{-i\epsilon X_n t}, \qquad (4.7)$$

and the repetition of the theory in the previous section leads to

Theorem 4.1.
For $\epsilon < \epsilon_n$, $n = 0,1,\ldots$

$$\gamma_n(t) = \|(1-P_n)\, e^{-iH' t} P_n\| < \epsilon \|B_n\| t , \qquad (4.8)$$

$$[P_n . e^{-i(H_n + \epsilon X_{n+1})t}] = 0 . \qquad (4.9)$$

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

$$\|B_n\| \leq \epsilon^n b_n . \qquad (4.10)$$

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 $\mathrm{dist}(C,\sigma_0^0) \geq \frac{d}{2}$. Then, there exist constants $a_{n,m}$, $b_{n,m}$, $n = 0,1,\ldots$, $m = 1,2,\ldots$ such that for $\epsilon \leq \epsilon_n$

$$\left\| \frac{d^m}{dt^m} R_n(t;z) \right\| \leq \epsilon^m a_{n,m} , \qquad (4.11)$$

$$\left\| \frac{d^m}{dt^m} P_n(t) \right\| \leq \epsilon^{n+m} b_{n,m} . \qquad (4.12)$$

The proof is by induction over n .

$n = 0$.

$$\left\| \frac{d^m}{dt^m} R_0(t;z) \right\| = \left\| \left[\frac{d^m}{dt^m} R_0(t;z) \right]_{t=0} \right\| \leq \qquad (4.13)$$

$$\leq \epsilon^m a_{0,m}$$

follows from

$$\frac{d}{dt} R_0(t;z) = \epsilon R_0(t;z) \frac{\vec{p}\vec{n} - \epsilon t}{m} R_0(t;z) . \tag{4.14}$$

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

$$\| [\frac{d^m}{dt^m} P_0(t)]_{t=0} \| \leq \frac{1}{2\pi} \int_C \| [\frac{d^m}{dt^m} R_0(t;z)]_{t=0} \| \; |dz| . \tag{4.15}$$

Supposing (4.11), (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 following formula

$$P_n(t) - P_{n-1}(0) =$$

$$= \frac{1}{2\pi i} A^*_{n-1}(t) [\int_C \frac{1}{H_{n-1}(t) - K_{n-1}(t) - z} K_{n-1}(t) R_{n-1}(t;z) \, dz] A_{n-1}(t) . \tag{4.17}$$

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^0_{n-1} for all $t \in \boldsymbol{R}$. 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 Th.4.2. is finished.

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

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

or directly from (3.2), it follows that

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

Then, by construction it follows that

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

and then

$$[H_m, T(\vec{a}_i)] = 0, \quad [X_m, T(a_i)] = -\vec{n}\vec{a}_i, \quad m = 0,1,2,\ldots \tag{4.22}$$

Finally (2.9) follows from (2.10), (2.11), (2.12) and

$$\gamma_0(\epsilon, t) \leq 2\|P_n - P_0\| + \gamma_n(\epsilon, t). \tag{4.23}$$

Remarks.

4.1. Leaving the full discussion for a future publication, we shall comment a little bit on the controversal 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 nondegenerated band. Then, P_n will correspond to a nondegenerate band of H_n. The n-th order effective Wannier Hamiltonian H_n can be written as an orthogonal sum

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

Now, $P_n H_m^W(\epsilon) P_n$ has a pure nondegenerated point spectrum [15,16].

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

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 total Hamiltonian in the sense that (ref. [5], Chapter XII.5)

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

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

$$|(\psi_p^{(n)}, e^{-iH^\epsilon t}\psi_p^{(n)})|^2 \geq 1 - b_n^2 \epsilon^{2(n+1)} t^2 \tag{4.27}$$

indicating a rather long lifetime of the pseudoeigenstate $\psi_p^{(n)}$. Let us stress that while the spectral concentration in the sense of (4.26) is of the order ϵ^n, the spacing between pseudoeigenvalues 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 ref. [16] 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

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

then H_n and X_n converge to well defined operators H_∞, X_∞ for sufficiently small ϵ, $H_\infty+\epsilon X_\infty = H^\epsilon$ and $[P_\infty, H^\epsilon]=0$. 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 ref./17/ for a discussion about this point).

5. GENERALIZATION 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 generalized to

$$(X_0 f)(\vec{x}) = \phi(\vec{x}) f(\vec{x}), \tag{5.1}$$

the only condition being that $\phi(\vec{x})$ be differentiable and its derivatives be bounded on $\mathbf{R}^3$. 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 generalization is that in the case of homogeneous electric field and periodic potential, the whole theory works if a forbidden gap exists in the following sense. Let $\sigma_0(\vec{k}) = \{\lambda_0^i(\vec{k})\}_{i=0}^{\infty}$ be the (discrete) spectrum of H_0, at a fixed value of crystal momentum. If $\sigma_0^0 = \{\lambda \mid \lambda = \lambda_0^0(\vec{k}), \vec{k}\in B, \lambda_0^0(\vec{k})$ continuous $\}$, then the condition (2.5) can be replaced by

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

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 $d = 6\cdot 10^{-19}$ J, $a = 5\cdot 10^{-10}$ m, Bentosella claims /3/ that for his choice of B

$$\gamma_{Ben.}(\epsilon;T) \leq 4\cdot 10^{-2} \tag{5.3}$$

without any assumption on V, as far as $E \lesssim 10^7$ V/m. 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 $V(\vec{x})$ is bounded and

$$\operatorname*{ess\,sup}_{\vec{x}\in \mathbf{R}^3} V(\vec{x}) - \operatorname*{ess\,inf}_{\vec{x}\in \mathbf{R}^3} V(\vec{x}) \lesssim 6\cdot 10^{-17}\ \mathrm{J}, \qquad (5.4)$$

to the weaker results

$$\gamma_0(\epsilon;T) \leq 5\cdot 10 \qquad (5.5)$$

and

$$\gamma_1(\epsilon;T) \leq 8\cdot 10^{-7}\, E, \qquad \text{for} \quad E \lesssim 10^8 \frac{V}{m}. \qquad (5.6)$$

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

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