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DYNAMICS OF BLOCH ELECTRONS IN TIME DEPENDENT ELECTRIC FIELDS

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Abstract. Upper bouns on interband transitions, leading to the existence of oscillating Bloch electrons are proved, for the case of periodic potential and (or) the electric field slowly varying in time.
Key words: *Bloch electrons, electric fields, electron-phonon interaction*.

1. INTRODUCTION

The problem of the dynamics of Bloch electrons in a constant external electric field has begun with the papers of Wannier [1, 2] and continued for some decades. The existence of Stark-Wannier resonances and of oscillating Bloch electrons has been rigorously proved in the papers [3-6] and confirmed experimentally [7]. We shall start with a brief review of the main results in the literature.

The theory describing this problem is based on one-electron approximation without electron-phonon interaction. For simplicity, we shall present the actual situation for one dimensional case, but the results were obtained for any dimensions [3,4].

The hamiltonian of the perturbed system is

$$H^{\varepsilon} = H_0 + \varepsilon X_0; \qquad \varepsilon = -eE \tag{1.1}$$

where ($\hbar = 1$; E is the electric field):

$$\begin{gathered} H_0 = -\frac{1}{2m}\frac{d^2}{dx^2} + V(x) \\ (X_0 f)(x) = xf(x) \\ V(x+a) = V(x) \end{gathered} \tag{1.2}$$

a being the lattice constant.

About the spectrum of H_0, $\sigma(H_0) = \sigma_0$, it is supposed that there exists an isolated band σ_0^0 separated by the rest of the spectrum:

$$\sigma_0 = \sigma_0^0 \cup \sigma_0^1; \qquad \sigma_0^0 \neq \emptyset$$

$$dist\left(\sigma_0^0, \sigma_0^1\right) = d > 0$$

This means that, as far as a forbidden gap exists in the spectrum of H_0, the results apply.

Wannier [1,2] believed that on can redefine the bands of H_0 such that the one-band hamiltonian

$$P_\varepsilon H^\varepsilon P_\varepsilon$$

where P_ε is the orthogonal projection on the Hilbert space of states corresponding to a deformed band, has a discrete spectrum, while the nondiagonal part of H^ε, which is a measure of the transition probability, vanishes:

$$P_\varepsilon H^\varepsilon (1 - P_\varepsilon) + h.c. = 0$$

Zak [8] argued that closed bands (with no interband transitions) cannot exist. The existence of closed bands would imply the existence of eigenvalues (with square integrable eigenfunctions) for H^ε, but the rigorous result of Avron et al. [9] proved that the spectrum of H^ε is absolutely continous.

Nenciu and Nenciu [3,4] proved that one can redefine recurrently the bands of H_0 so that although the subspace corresponding to an isolated band is not exactly invariant under the evolution given by H^ε, the interband transitions are small, in the sense that the nondiagonal part of H^ε is a bounded operator of order ε^{n+1}, $n > 0$. The diagonal part of H^ε

$$P_n H^\varepsilon P_n$$

where P_n is the orthogonal projection corresponding to the deformed band, has a *discrete spectrum (the Stark-Wannier ladder)* of the form

$$\alpha + \varepsilon\, a\, n\,.$$

where α is a constant and a the lattice constant. This means that in times of the order of period of the oscillatory motion of an electron in an isolated band, $T = \frac{2\pi}{\varepsilon a}$, the transitions are of the order ε^n, $n > 0$ and the one-band spectrum of H^ε consists of equally spaced resonances.

The invention of semiconductor supperlattice has allowed the experimental observation of Stark-Wannier ladder in the optical spectra [10], of Bloch oscillations [11] and the harmonic spatial motion of the electron [12]

The problem we are dealing with in this paper concerns the dynamics of Bloch electrons in a slowly varying in time electric field and some of the results discussed above are generalizated to this case.

Now, the hamiltonian of the system is

$$H^{\varepsilon,\omega}(t) = H_0 + \varepsilon\, X_0 F(\omega\, t) \tag{1.4}$$

with $F(u)$ and all its derivatives $F^{(n)}(u)$ bounded. The case $F = const.$ is the one discussed above.

Heuristically, for small ω one expects by an adiabatic argument, that the interband transitions are still small, so one can hope the same type of results. Indeed, in what follows we shall develop for the hamiltonian (1.4) a similar theory as for the time independent case [3].

The content of the paper is as follows: Section 2 is devoted to first order theory and the result is that in spite of the unboundness of the perturbation given by the time dependent external electric field, the interband transitions are of the order εt, irrespective of the value of ω. Since this estimation is not good enough, in Section 3 the second order theory is developed and the interband transitions are proved to be of order $\left(\varepsilon^2 + \varepsilon\omega\right)t$, a result which covers most physical situations. The Section 4 contains conclusions, in particular possible extentions are outlined.

2. THE FIRST ORDER THEORY

If $U^{\varepsilon}(t)$ is the solution of Schrödinger equation

$$i\frac{d}{dt}U^{\varepsilon}(t) = H^{\varepsilon}U^{\varepsilon}(t); \quad U^{\varepsilon}(0) = 1$$

and P_0 is the spectral projection of H_0 corresponding to the isolated band σ_0^0, we want to show that the interband transitions are bounded by:

$$\gamma_0(\varepsilon, t) = \left\|(1 - P_0)U^{\varepsilon}(t)P_0\right\| \le \varepsilon\, b_0 \int_0^t \left|F(\omega u)\right| du \tag{2.1}$$

b_0 being a constant. Obviously, if at $t = 0$ the probability to find the electron in a state corresponding σ_0^0 is one, $1 - \gamma_0^2(t)$ is a lower bound for the probability to find the electron at time $t \neq 0$ in a state corresponding to σ_0^0. The inequality (2.1) means that, if $F(u)$ is bounded, the transitions are of the order of ε.

First we shall prove that

$$\left\|(1 - P_0)U^{\varepsilon}P_0\right\| = \left\|\left(1 - \tilde{P}_0(t)\right)W^0(t)\tilde{P}_0(0)\right\| \tag{2.2}$$

where $W^0(t)$ is

$$W^0(t) = U_0^*(t)U^{\varepsilon}(t) \tag{2.3}$$

$U_0(t)$ being the unitary operator

$$U_0(t) = e^{-i\varepsilon x\int_0^t F(\omega u)du} \qquad (2.4)$$

From (2.3), by direct computation, one obtains that the equation satisfied by $W^0(t)$ is

$$i\frac{d}{dt}W^0(t) = \tilde{H}_0(t)W^0(t) \qquad (2.5)$$

where

$$\tilde{H}_0(t) = U_0^*(t)H_0U_0(t) \qquad (2.6)$$

Then (2.2) results immediately:

$$\begin{aligned}&\left\|(1-P_0)U^{\varepsilon}(t)P_0\right\| = \\ &\left\|U_0(t)U_0^*(t)U^{\varepsilon}(t)P_0 - U_0(t)U_0^*(t)P_0U_0(t)U_0^*(t)U^{\varepsilon}(t)P_0\right\| = \qquad (2.7)\\ &\left\|\left(1-\tilde{P}_0(t)\right)W^0(t)\tilde{P}_0(0)\right\|\end{aligned}$$

where: $\tilde{P}_0(t) = U_0^*(t)P_0U_0(t)$; $\tilde{P}_0(0) = P_0$.

To obtain bounds for interband transitions, we shall prove that one can find a new operator $\Omega^0(t)$ with the properties:

$$\left(1-\tilde{P}_o(t)\right)\Omega^0(t)\tilde{P}^0(0) = 0 \qquad (2.8)$$

and

$$\Omega^0(t) - W^0(t) \sim O(\varepsilon) \qquad (2.9)$$

Indeed, if we take $\Omega^0(t)$ as given by the equation:

$$i\frac{d}{dt}\Omega^0(t) = \left(\tilde{H}_0(t) + \tilde{K}_0(t)\right)\Omega^0(t); \quad \Omega^0(0) = 1 \qquad (2.10)$$

where:

$$\tilde{K}_0(t) = i\left[1-2\tilde{P}_0(t)\right]\frac{d\tilde{P}_0(t)}{dt} \qquad (2.11)$$

$\Omega^0(t)$ fulfils (2.8) due to the following generalization of the Kato-Krein lemma [13].

<u>*Lemma:*</u>

Let $P(t)$, $t \in \Re$ be a family of orthogonal projections, having continuous norm derivatives with respect to t and $A(t)$ a family of self-adjoint operators.

If $K_A(t)$ is given by

$$K_A(t)=A(t)+(1-2P(t))\left(i\frac{d}{dt}P(t)-[A(t),P(t)]\right) \tag{2.12}$$

then

$$K_A(t)=K_A^*(t)$$

and the equation

$$i\frac{dY(t)}{dt}=K_A(t)Y(t); \quad Y(0)=1 \tag{2.13}$$

has a unique solution satisfying

$$P(t)=Y(t)P(0)Y^*(t) \tag{2.14}$$

In order to obtain (2.8), we take $Y(t)=\Omega^0(t); P(t)=P_0(t); A(t)=\tilde{H}_0(t)$, with $[\tilde{H}_0(t),\tilde{P}_0(t)]=0$.

Having $\Omega^0(t)$ given by the equation (2.10) and due to (2.8), the interband transitions are bounded by:

$$\gamma_0(t)\le\left\|(1-2\tilde{P}_0(t))\left(W^0(t)-\Omega^0(t)\right)\tilde{P}_0(0)\right\|+\left\|(1-2\tilde{P}_0(t))\Omega^0(t)\tilde{P}_0(0)\right\|\le$$

$$\le\left\|W^0(t)-\Omega^0(t)\right\|\le\int_0^t\left\|\tilde{K}_0(u)\right\|du=\int_0^t\left\|\frac{d\tilde{P}_0(u)}{dt}\right\|du \tag{2.15}$$

To evaluate $\left\|\frac{d\tilde{P}_0(t)}{dt}\right\|$ we use the Riesz formula relating the spectral projection and the resolvent of a self-adjoint operator:

$$\tilde{P}_0(t)=\frac{1}{2\pi i}\int_{(\Gamma)}\tilde{R}_0(t,z)dz \tag{2.16}$$

where (Γ) is a contour surrounding σ_0^0 and

$$\tilde{R}_0(t,z)=U_0^*(t)\frac{1}{H_0-z}U_0(t) \tag{2.17}$$

By a direct computation, one obtains:

$$\frac{d\tilde{P}_0(t)}{dt}=\varepsilon F(\omega t)U_0^*(t)\frac{1}{2\pi i}\int_{(\Gamma)}\frac{1}{H_0-z}\frac{p}{m}\frac{1}{H_0-z}dz\,U_0(t) \tag{2.18}$$

where $p=-i\frac{d}{dx}$.

The operator $\frac{1}{H_0 - z}\frac{p}{m}\frac{1}{H_0 - z}$ is bounded and

$$\left\|\frac{1}{H_0 - z}\frac{p}{m}\frac{1}{H_0 - z}\right\| \le \left\|\frac{1}{H_0 - z}\right\|\left\|\frac{p}{m}\frac{1}{H_0 - z}\right\| \le const. \tag{2.19}$$

For the proof of this relation, see [14].

Having all the above results, one obtains the bound for the first order transitions:

$$\gamma_0(t) \le \varepsilon\, b_0 \int_0^t |F(\omega u)| du \sim \varepsilon; \quad b_0 = const. \tag{2.20}$$

Now, we remark that such a bound announced in Equation (2.1)is not sufficient since, in times of the order of the period of oscillation of Bloch electrons, $T = \frac{2\pi}{\varepsilon a}$,

$$\gamma_0(T) \le const.$$

while the physical arguments suggest that

$$\lim_{\varepsilon \to 0} \gamma_0(T) = 0$$

irrespective of the smallness of the forbidden gap and more powerful estimations are needed.

3. THE SECOND ORDER THEORY

To obtain a better estimation for the interband transitions, we shall follow the same way as in the first order theory: more exactly, we will find a bound for

$$\gamma_1(t) = \left\|(1 - P_1(t))U^{\varepsilon}(t)P_1(0)\right\|, \tag{3.1}$$

where we have to choose $P_1(t)$.

Let us consider the following operator:

$$\tilde{H}_0(t) - \tilde{K}_0(t) \tag{3.2}$$

where: $\tilde{H}_0(t) = U_0^*(t) H_0 U_0(t);$

$$\tilde{K}_0(t) = i\left(1 - 2\tilde{P}_0(t)\right)\frac{d\tilde{P}_0(t)}{dt}$$

and $\tilde{P}_0(t)$ is given by (2.7).

A straightforward computation gives for the operator given by (3.2) the following:

$$\tilde{H}_0(t) - \tilde{K}_0(t) = U_0^*(t)\{H_0 - \varepsilon F(\omega t)B\}U_0(t) \tag{3.3}$$

where

$$B = (1 - 2P_0)\frac{1}{2\pi}\int_{(\Gamma)} \frac{1}{H_0 - z}\frac{p}{m}\frac{1}{H_0 - z}dz \tag{3.4}$$

Obviously, this operator and the unitary operator representing the translations with the basis vector of lattice a, T_a, commute

$$[B, T_a] = 0$$

and consequently, if we denote

$$H_1(t) = H_0 - \varepsilon F(\omega t)B$$

it results that

$$[H_1(t), \mathrm{T_a}] = 0 \tag{3.5}$$

which means that $H_1(t)$ still has a gap in its spectrum and there exists an isolated band σ_1^0 in the spectrum $\sigma(H_1(t))$ if

$$\varepsilon |F(\omega t)| < \frac{d}{2\|B\|}$$

We propose for $P_1(t)$ the operator:

$$P_1(t) = \frac{1}{2\pi i}\int_{(\Gamma)} \frac{1}{H_1(t) - z}dz \tag{3.6}$$

(the spectral projection of $H_1(t)$ corresponding to σ_1^0) and we shall prove that

$$\gamma_1(t) \le \int_0^t \left\| \frac{d\tilde{P}_1(u)}{du} \right\| du \tag{3.7}$$

where $\tilde{P}_1(t)$ is the operator:

$$\tilde{P}_1(t) = A_0^*(t)U_0^*(t)P_1(t)U_0(t)A_0(t) \tag{3.8}$$

The operator $A_0(t)$ is the solution of the equation:

$$i\frac{dA_0(t)}{dt} = \tilde{K}_0(t)A_0(t) \tag{3.9}$$

where $\tilde{K}_0(t)$ is:

$$\tilde{K}_0(t) = i(1 - 2\tilde{P}_0(t))\frac{d\tilde{P}_0(t)}{dt}$$

Following the same steps as in the first order theory, $\gamma_1(t)$ given by (3.1)

:

$$\gamma_1(t) = \left\| \left(1 - \tilde{P}_1(t)\right) W^1(t) \tilde{P}_1(0) \right\| \tag{3.10}$$

where $W^1(t)$ is:

$$W^1(t) = U_1^*(t) U^\varepsilon(t) \tag{3.11}$$

$U_1(t)$ being the unitary operator:

$$U_1(t) = U_0(t) A_0(t) \tag{3.12}$$

To obtain bounds for (3.10), we will find an operator $\Omega^1(t)$ satisfying:

$$\left\| \left(1 - \tilde{P}_1(t)\right) \Omega^1(t) \tilde{P}_1(0) \right\| = 0 \tag{3.13}$$

and

$$\Omega^1(t) - W^1(t) \sim O\left(\varepsilon^2, \varepsilon\omega\right) \tag{3.14}$$

The operator $\Omega^1(t)$ is the solution of equation (2.13), where

$$A(t) = \tilde{H}_1(t)$$

and:

$$\tilde{H}_1(t) = A_0^*(t)\left(\tilde{H}_0(t) - K_0(t)\right) A_0(t) \tag{3.15}$$

The operator $\tilde{P}_1(t)$ given by (3.8) is then the spectral projection of $\tilde{H}_1(t)$:

$$\tilde{P}_1(t) = \frac{1}{2\pi i} \int_{(\Gamma)} \frac{1}{\tilde{H}_1(t) - z} dz \tag{3.16}$$

so that

$$\left[\tilde{P}_1(t), \tilde{H}_1(t)\right] = 0 \tag{3.17}$$

It results that

$$\gamma_1(t) \le \left\| W^1(t) - \Omega^1(t) \right\| \le \int_0^t \left\| \frac{d\tilde{P}_1(u)}{du} \right\| du \tag{3.18}$$

To compute the derivative $\frac{d\tilde{P}_1(t)}{dt} = \frac{d}{dt}\left(\tilde{P}_1(t) - \tilde{P}_0(0)\right)$ we use (3.8) and (2.14):

$$\tilde{P}_1(t)-\tilde{P}_0(0)=A_0^*(t)U_0^*(t)\frac{1}{2\pi i}\int_{(\Gamma)}\frac{1}{H_1(t)-z}dzU_0(t)A_0(t)-$$

$$-A_0^*(t)U_0^*(t)P_0U_0(t)A_0(t)=$$

$$=A_0^*(t)\frac{1}{2\pi i}\int_{(\Gamma)}\left(\frac{1}{U_0^*(t)H_1(t)U_0(t)-z}-\frac{1}{\tilde{H}_0(t)-z}\right)dzA_0(t)$$

But

$$U_0^*(t)H_1(t)U_0(t)=\tilde{H}_0(t)-\tilde{K}_0(t)$$

and then

$$\tilde{P}_1(t)-\tilde{P}_0(0)=A_0^*(t)\frac{1}{2\pi i}\int_{(\Gamma)}\frac{1}{\tilde{H}_0(t)-\tilde{K}_0(t)-z}\tilde{K}_0(t)\frac{1}{\tilde{H}_0(t)-z}dzA_0(t)$$

so,

$$\frac{d}{dt}\tilde{P}_1(t)=\frac{d}{dt}\left(\tilde{P}_1(t)-\tilde{P}_0(0)\right)=$$

$$=iA_0^*(t)\tilde{K}_0(t)\frac{1}{2\pi i}\int_{(\Gamma)}\frac{1}{\tilde{H}_0(t)-\tilde{K}_0(t)-z}\tilde{K}_0(t)\frac{1}{\tilde{H}_0(t)-z}dzA_0(t)-$$

$$-iA_0^*(t)\frac{1}{2\pi i}\int_{(\Gamma)}\frac{1}{\tilde{H}_0(t)-\tilde{K}_0(t)-z}\tilde{K}_0(t)\frac{1}{\tilde{H}_0(t)-z}dz\tilde{K}_0(t)A_0(t)+ \qquad (3.19)$$

$$+A_0^*(t)\frac{1}{2\pi i}\frac{d}{dt}\left(\int_{(\Gamma)}\frac{1}{\tilde{H}_0(t)-\tilde{K}_0(t)-z}\tilde{K}_0(t)\frac{1}{\tilde{H}_0(t)-z}dz\right)A_0(t)$$

The norm of the first two terms are of the order:

$$\left\|\tilde{K}_0(t)\right\|^2=\left\|\frac{d\tilde{P}_0(t)}{dt}\right\|^2$$

so, we are left to compute the norm of

$$\frac{d}{dt}\left(\frac{1}{\tilde{H}_0(t)-\tilde{K}_0(t)-z}\tilde{K}_0(t)\frac{1}{\tilde{H}_0(t)-z}\right)=$$

$$\frac{d}{dt}\left\{\frac{1}{\tilde{H}_0(t)-z}\frac{1}{1-\tilde{K}_0(t)\left(\tilde{H}_0(t)-z\right)^{-1}}\tilde{K}_0(t)\frac{1}{\tilde{H}_0(t)-z}\right\} \qquad (3.20)$$

The norm of (3.20) contains terms proportional to $\left\|\frac{d\tilde{R}_0(t)}{dt}\right\|\left\|\tilde{K}_0(t)\right\|\cdot$, $\left\|\frac{d\tilde{K}_0(t)}{dt}\right\|\left\|\tilde{K}_o(t)\right\|$, $\left\|\frac{d\tilde{K}_0(t)}{dt}\right\|$.

From the definition of $\tilde{R}_0(t)=U_0^*(t)\frac{1}{H_0-z}U_0(t)$ one obtains:

$$\frac{d\tilde{R}_0(t)}{dt}=\varepsilon F(\omega t)U_0^*(t)\frac{1}{H_0-z}\frac{p}{m}\frac{1}{H_0-z}U_0(t)$$

so that

$$\left\|\frac{d\tilde{R}_0(t)}{dt}\right\|\sim O(\varepsilon) \qquad (3.21)$$

From (2.11), (2.18) and (2.19) it results that

$$\left\|\tilde{K}_0(t)\right\|=\left\|\frac{d\tilde{P}_0(t)}{dt}\right\|\sim O(\varepsilon) \qquad (3.22)$$

Further,

$$\frac{d\tilde{K}_0(t)}{dt}=-2i\left(\frac{d\tilde{P}_0(t)}{dt}\right)^2+i\left(1-2\tilde{P}_0(t)\right)\frac{d^2\tilde{P}_0(t)}{dt^2} \qquad (3.23)$$

and we have to evaluate $\left\|\frac{d^2\tilde{P}_0(t)}{dt^2}\right\|$.

Having $\frac{d\tilde{P}_0(t)}{dt}$ given by (2.18), by a direct computation one obtains:

$$\frac{d^2\tilde{P}_0(t)}{dt^2}=\varepsilon\omega F'(\omega t)U_0^*(t)MU_0(t)+i\varepsilon^2F(\omega t)U_0^*(t)[x,M]U_0(t) \qquad (3.24)$$

where

$$M=\frac{1}{2\pi i}\int_{(\Gamma)}\frac{1}{H_0-z}\frac{p}{m}\frac{1}{H_0-z}dz$$

But

$$\left[x,\frac{1}{H_0-z}\frac{p}{m}\frac{1}{H_0-z}\right]=\left[x,\frac{1}{H_0-z}\right]\frac{p}{m}\frac{1}{H_0-z}+$$
$$+\frac{1}{H_0-z}\left[x,\frac{p}{m}\right]\frac{1}{H_0-z}+\frac{1}{H_0-z}\frac{p}{m}\left[x,\frac{1}{H_0-z}\right]$$

so $[x, M]$ is bounded and finally, from (3.21), (3.22) and (3.24) one obtains for (3.18) the follwing:

$$\gamma_1(\varepsilon,\omega,t) \le \varepsilon^2 C_1 \int_0^t |F(\omega u)| du + \varepsilon\omega C_2 \int_0^t |F'(\omega u)| du \tag{3.25}$$

with C_1 and C_2 constants. This is a better bound for the transition rate since, for times of order $T = \frac{2\pi}{\varepsilon a}$,

$$\gamma_1(\varepsilon,\omega,T) \xrightarrow[\varepsilon\to 0]{} 0$$

a condition not fulfilled by the result in Section 2.

4. CONCLUSIONS

The main result of this note is the proof of the existence of "deformed" bands in the case of small slowly varying in time external electric fields. The interband transitions for these deformed bands were proved to be bounded by (see (3.19)):

$$\gamma_1(\varepsilon,\omega,t) \le \left(const.\varepsilon^2 + const.\varepsilon\omega \right) \tag{4.1}$$

This result implies that in physical situations, one can neglect the interband transitions and study the dynamics for each isolated band separately. In this case, the analysis is much more complicated since the deformed one-band hamiltonian depends on time. It turns out that for a fixed t, the spectrum is still of Stark-Wannier ladder type, the distance between levels being $\varepsilon\, aF(\omega t)$.

In the limit of small ω, the in-band dynamics can be analysed by adiabatic type methods.

Although in most physical situations the result (4.1) is sufficient, if there are problems in which a more precise result is needed, one can generalize the recurrent construction in [3] to the present setting and prove the existence of deformed bands for any $n = 1,2,3,\ldots$, for which the interband transitions are at most of the order

$$\gamma_n(\varepsilon,\omega,t) \sim O\left(\varepsilon^n + \varepsilon^{n-1}\omega + \ldots\ldots\varepsilon\omega^{n-1} \right) \tag{4.2}$$

(one has to remark that the limit $n \to \infty$ has no meaning, as the constants involved blow up very rapidly).

The details concerning the in-band dynamics as well as the proof of (4.2) will be given elsewhere.

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