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DYNAMICS OF BLOCH ELECTRONS IN EXTERNAL ELECTRIC FIELDS.

The Existence of Ladder Resonances

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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

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

where $H_0 = -\Delta + V_{per.}$ is the "unperturbed" periodic Hamiltonian, and $\epsilon X_0 = eE\vec{n}\vec{x}$, $|\vec{n}| = 1$, is the potential energy of the electric field. In this paper, we shall consider the controversial problem of the existence of the Stark-Wannier (S-W) ladder. Originally, it was believed that an S-W ladder exists in the following sense: in the Hilbert space of states $\mathcal{H}$, there exists a "one-band" subspace $\mathcal{K}$ such that $\mathcal{K}$ is invariant under H^{ϵ} (i.e., with respect to the decomposition $\mathcal{H} = \mathcal{K} \oplus \mathcal{K}^{\perp}$, H^{ϵ} takes a diagonal form) and H^{ϵ} restricted to $\mathcal{K}$ has a discrete spectrum of the form $\alpha + \beta\epsilon n$, α, β -constants, $n = 0, \pm 1, \pm 2, \ldots$ In the one-dimensional case (and very probable, in the three-dimensional case also) this possibility is ruled out by the fact that the spectrum of H^{ϵ} is absolutely continuous (see ref. [1]). So, if the S-W ladder exists, its levels must be in fact resonances. This situation can be viewed as follows. The subspace $\mathcal{K}$ (which actually can depend on ϵ) is not exactly invariant under H^{ϵ}, but only "asymptotically" invariant (see ref. [2] for a precise definition) in the sense that the non-diagonal part of H^{ϵ} is a bounded operator of order ϵ^{p}, $p > 0$. In this case, even if the "one band" Hamiltonian $P_{\epsilon} H^{\epsilon} P_{\epsilon}$, where P_{ϵ} is the orthogonal projection on $\mathcal{K}$, has discrete spectrum, the "tunneling" due to the nondiagonal part of H^{ϵ}, $P_{\epsilon} H^{\epsilon} (1-P_{\epsilon}) + \mathrm{h.c.}$ results in a finite width of the levels. Let λ, ψ_{λ} be an eigenvalue and the corresponding eigenfunction of $P_{\epsilon} H^{\epsilon} P_{\epsilon}$. If, following Avron et al. [3], we shall take

$$\gamma^2 \sim ((H^{\epsilon} - \lambda)\psi_{\lambda} , (H^{\epsilon} - \lambda)\psi_{\lambda}) \equiv (\Delta\lambda)^2$$

as a measure of the width, then

$$\gamma^2 \sim (\psi_{\lambda} , (P_{\epsilon} H^{\epsilon} (1-P_{\epsilon}) + \mathrm{h.c.})^2 \psi_{\lambda}) .$$

Clearly, in order that the level structure of $P_\epsilon H^\epsilon P_\epsilon$ be not washed by the effect of the nondiagonal part it is necessary for γ to be smaller than the level spacing. All the existing derivations use as K the subspace corresponding to an isolated band of H_0 either simple or composed by mutually nonintersecting branches /1, 4-6/. The rigorous derivations are for one-dimensional systems, although the results can be carried to the three-dimensional case (see, however, the discussion below) if the localized Wannier functions corresponding to the considered band are supposed to exist (see refs./7,8/) for the problem of the existence of Wannier functions). In all cases considered the spacing between the S-W levels is of order ϵ, and γ is also of the order ϵ /3/.

This fact has led Avron et al./3/ (see also refs./9-11/) to the conclusion that the existing derivations of the S-W ladder are inconclusive. This controversy generated a lot of approximate and numerical computations /12-14/ all of them indicating the existence of well separated S-W resonances. In order to clarify this problem, one needs to prove that:

a. One can choose K such that the nondiagonal part is $\sim\epsilon^p$, $p > 1$.

b. The spectrum of $P_\epsilon H^\epsilon P_\epsilon$ has the structure of an S-W ladder, with spacing between levels of the order ϵ.

The problem a. has been solved in the previous paper /15/ substantiating an old idea /16,17/ that one can redefine the bands of H^ϵ such that the nondiagonal part of H^ϵ is of the order ϵ^{n+1}, n being a positive integer. More exactly, we constructed recurrently a sequence of periodic operators $H_n(\epsilon)$ $n = 0,1,2,\dots$, $H_0(\epsilon) = H_0$, such that the nondiagonal part of H^ϵ with respect to the bands of $H_n(\epsilon)$ is bounded and of the order ϵ^{n+1}. Moreover, the bands of $H_n(\epsilon)$ go smoothly to the bands of H_0 as $\epsilon \to 0$. The diagonal part of H^ϵ is an orthogonal sum of "one band Hamiltonians" $H^W_{i,n}(\epsilon)$ (i being the band index) which we have called "effective Wannier Hamiltonians" of order n.

In this paper we shall consider the problem b. In contradistinction to the previous papers on the S-W ladder, we shall consider the general, multidimensional case. We shall assume that the direction of the homogeneous electric field coincides with one of the reciprocical lattive vectors. Consequenly, 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 a one-dimensional one and, in what follows, we shall discuss this reduced problem. At this point we would like to stress that the reduced one-dimensional problem has special features as 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/7/. 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 $H^W_{i,n}(\epsilon)$ is a direct integral (over the components of the crystal momentum perpendicular to the electric field) of operators, whose spectrum consists of m interwined ladders, all with the same spacing $\sim\epsilon$, m being the degeneracy of the corresponding band. As to the eigenfunctions, we shall prove that they are exponentially localized along the direction of the field. This exponential localization plays an important role in understanding the Zener and Franz-Keldysh effects.

Two remarks are in order. First, as has been anticipated by Wannier/18/, the theory of the S-W 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 /2/. Second, as it has been stressed by Wannier/17/, the analysis gets into difficulty, if the direction of the field does not coincide with that of the reciprocical 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 S-W pattern, varying erratically for infinitely small variation in angle. This fact led Wannier/17/ to question the "physical reality" of the S-W 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.

During the proofs, we shall heavily use the results obtained in/19/ (from now, quoted as I) about some analyticity and periodicity properties of the Bloch functions. Moreover, we shall use all the notations in I without further explanations.

2. THE SPECTRAL PROPERTIES OF THE EFFECTIVE WANNIER HAMILTONIAN OF ARBITRARY ORDER

Starting from the description of H_0 and X_0 in I we consider now $H^\epsilon = H_0 + \epsilon X_0$. It is known that H^ϵ is self-adjoint on $D(H_0) \cap D(X_0)$ (see ref./20/).

Denoting

$$\tilde{H}_{0,\vec{k}_\perp} = \int_{[0,2\pi]}^{\oplus} H_{0,\vec{k}_\perp}(k_1)\, dk_1 , \tag{1}$$

from Theorem 1I* and Proposition 3 it follows that

$$U H^\epsilon U^{-1} = \int_{B_\perp}^{\oplus} \tilde{H}^\epsilon(\vec{k}_\perp)\, d\vec{k}_\perp , \tag{2}$$

where

$$\tilde{H}^\epsilon(\vec{k}_\perp) = \tilde{H}_{0,\vec{k}_\perp} + \epsilon \tilde{X}_0 . \tag{3}$$

In what follows, we shall discuss the spectral properties of $\tilde{H}^\epsilon(k_\perp)$. For notational convenience, we shall omit the variable $\vec{k}_\perp$. The first order theory developed in ref./15/ applied to $\tilde{H}^\epsilon$ gives the following. Let $\sigma^\circ(k_1)$ be an isolated band of $\tilde{H}_0$, $P_0(k_1)$ be the spectral projection of $H_0(k_1)$ corresponding to $\sigma^\circ(k_1)$ and

$$\tilde{P}_0 = \int_{[0,2\pi]}^{\oplus} P_0(k_1)\, dk_1 . \tag{4}$$

Define (for the rigorous justification see ref./15/)

$$\tilde{B}_0 = [\, i(1-2\tilde{P}_0)[\tilde{X}_0, \tilde{P}_0]\,] , \tag{5}$$

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

$$\tilde{B}_0 = \int_{[0,2\pi]}^{\oplus} B_0(k_1)\, dk_1 \tag{6}$$

and $\|\tilde{B}_0\| \le$ const.

Define

$$\tilde{X}_1 = \tilde{X}_0 + \tilde{B}_0 . \tag{7}$$

Note that by construction

$$\tilde{H}^\epsilon = \tilde{H}_0 + \epsilon \tilde{X}_0 = \tilde{H}_0 + \epsilon \tilde{X}_1 - \epsilon \tilde{B}_0 \equiv \tilde{H}_1 + \epsilon \tilde{X}_1 , \qquad [\tilde{H}_0 + \epsilon \tilde{X}_1, \tilde{P}_0] = 0 . \tag{8}$$

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*I indicates the corresponding formula in I. For example theorem 1I and (I.2.12) means Theorem 1 and formula (2.12), respectively, in ref./19/.

For ϵ sufficiently small, $\tilde{H}_1$ has an isolated band $\sigma^1(k_1)$, which in the limit $\epsilon \to 0$ coincides with $\sigma^\circ(k_1)$. Repeating the above construction, starting from $\tilde{H}^\epsilon = \tilde{H}_1 + \epsilon \tilde{X}_1$, 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

$$\tilde{H}^\epsilon = \tilde{H}_n + \epsilon \tilde{X}_{n+1} - \epsilon \tilde{B}_n \equiv \tilde{H}_n^W - \epsilon \tilde{B}_n , \qquad [\tilde{H}_n^W, \tilde{P}_n] = 0 . \tag{9}$$

We have called $\tilde{H}_n^W$ the effective Wannier Hamiltonian of order n (see refs./16,17/ for heuristic discussions). The main result in ref./15/ is that

$$\|\tilde{B}_n\| \le b_n \epsilon^n . \tag{10}$$

It follows that up to terms of the order ϵ^{n+1}

$$\tilde{H}^\epsilon \simeq \tilde{P}_n \tilde{H}^\epsilon \tilde{P}_n \oplus (1-\tilde{P}_n)\tilde{H}^\epsilon(1-\tilde{P}_n) . \tag{11}$$

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

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

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

$$\|\tilde{H}^\epsilon \psi_\lambda - \lambda\psi_\lambda\| \le b_n \epsilon^{n+1} . \tag{12}$$

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

$$(L^2([0,2\pi]))^m = \{\, \{\phi_i(k)\}_{i=1}^m, k\in[0,2\pi] \mid \sum_{i=1}^m \int_0^{2\pi} |\phi_i(k)|^2 dk < \infty \,\} ,$$

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

Theorem 1. There exist: a positive constant $d_n > 0$, an integer m, and a unitary operator

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

such that

$$W\tilde{P}_n \tilde{H}_n^W \tilde{P}_n W^{-1} = i\epsilon\left(\frac{d}{dk}\right)_{per.} + X_n(k;\epsilon) \qquad (13)$$

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

$$X_{n,\ell p}(k;\epsilon) = X_{n,\ell p}(k+2\pi;\epsilon). \qquad (14)$$

Remarks 1. The main point of this Theorem is the analyticity and periodicity properties of $X_n(k;\epsilon)$. At the nonrigorous level, the result in the case of nondegenerated bands is familiar, (see, e.g., ref.[5]). At the rigorous level, for one-dimensional systems and nondegenerated bands, see refs.[1,4]. In the three-dimensional case, and intersecting bands, even the fact that $X_n(k;\epsilon)$ is bounded at the degeneracy points seems not to be known.

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

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

$$\{\psi_{\vec{p}}(k)\} = \left\{\sum_{\ell=1}^m c_\ell(k)\,(V^{-1}(k)\chi_\ell^\circ(k))_{\vec{p}}\right\}, \qquad (15)$$

where

$$c_\ell(k) = (V^{-1}(k)\chi_\ell^\circ(k),\psi(k))_{\mathcal{H}'} = \sum_{\vec{p}\in \mathbf{Z}^3}\overline{(V^{-1}(k)\chi_\ell^\circ(k))_{\vec{p}}}\,\psi_{\vec{p}}(k). \qquad (16)$$

We shall define

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

by

$$\{(W\psi)_\ell(k)\} = \{c_\ell(k)\}. \qquad (17)$$

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

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

A simple calculation shows that

$$(W\tilde{P}_0\tilde{H}_0\tilde{P}_0W^{-1}c)_i(k) = \sum_{j=1}^m(\chi_i^\circ(k),\ V(k)H_0(k)V^{-1}(k)\chi_j^\circ(k))_{\mathcal{H}'}c_j(k). \qquad (18)$$

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

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

which is analytic in J_{d_0} and by (I.2.12), (I.2.13) and Proposition 2I it is periodic with the period 2π.

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

$$\left\{\{c_\ell(k)\}_1^m \,\middle|\, \left\{\frac{d}{dk}c_\ell(k)\right\}_1^m\in(L^2([0,2\pi]))^m;\ c_\ell(0)=c_\ell(2\pi)\right\},$$

and

$$(W\tilde{P}_0\tilde{X}_0\tilde{P}_0W^{-1}c)_j(k) = i\frac{d}{dk}c_j(k) + \sum_{\ell=1}^m\left[(\chi_j^\circ(k), M\chi_\ell^\circ(k))_{\mathcal{H}'} + i\left(\chi_j^\circ(k),\frac{d}{dk}\chi_\ell^\circ(k)\right)_{\mathcal{H}'}\right]c_\ell(k). \qquad (19)$$

Note that the hermiticity of the matrix with elements $i(\chi_j^\circ(k), \frac{d}{dk}\chi_\ell^\circ(k))$ follows from the fact that $(\chi_j^\circ(k),\chi_\ell^\circ(k))=\delta_{j\ell}$ and then $\frac{d}{dk}(\chi_j^\circ(k),\chi_\ell^\circ(k))=0$. Again, the functions appearing in the r.h.s. of (19) are the restriction of $(\chi_j^\circ(\bar{k}), M\chi_\ell^\circ(k))_{\mathcal{H}'}$ and $(\chi_j^\circ(\bar{k}),\frac{d}{dk}\chi_\ell^\circ(k))_{\mathcal{H}'}$, analytic in J_{d_0}. Then (18) and (19) proves Theorem 1 with

$$X_{0,\ell p}(k;\epsilon) = (\chi_\ell^\circ(k), V(k)H_0(k)V^{-1}(k)\chi_p^\circ(k))_{\mathcal{H}'} + \epsilon\left[(\chi_\ell^\circ(k), M\chi_p^\circ(k))_{\mathcal{H}'} + i\left(\chi_\ell^\circ(k),\frac{d}{dk}\chi_p^{\circ}(k)\right)_{\mathcal{H}'}\right]. \qquad (20)$$

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

$$(\tilde{V}\tilde{P}_0\tilde{V}^{-1}\psi)_{\vec{p}}(k) = \sum_{j=1}^m(\chi_j^\circ(k),\psi(k))_{\mathcal{H}'}\chi^\circ_{j\vec{p}}(k),$$

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

$$(\tilde{V}[\tilde{X}_0,\tilde{P}_0]\tilde{V}^{-1}\psi)_{\vec{p}}(k) = \sum_{j=1}^m[(\chi_j^\circ(k),\psi(k))_{\mathcal{H}'}(M\chi_j^\circ)_{\vec{p}}(k) + (i\frac{d}{dk}\chi_j^\circ(k) -$$

$$(M\chi_j^\circ)(k),\ \psi(k))_{\mathcal{H}}\,\chi^\circ_{j,\vec p}(k) + i(\chi_j^\circ(k),\psi(k))_{\mathcal{H}}\frac{d}{dk}\chi^\circ_{j,\vec p}(k)], \tag{21}$$

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

$$\tilde H_1 = \tilde H_0 - \epsilon \tilde B_0 = \int^{\oplus}_{[0,2\pi]} [H_0(k) - \epsilon B_0(k)]\,dk = \int^{\oplus}_{[0,2\pi]} H_1(k)\,dk,$$

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 obtained formula for X_1 is (20) where $H_0(k)$ has been replaced by $H_1(k)$ and $\chi_j^\circ(k)$ 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 1 is finished.

Using the arguments in [1] one can prove that the spectrum of $i\epsilon\,(\frac{d}{dk})_{per.} + X_n(k;\epsilon)$ consists of m interwined ladders, all with the same spacing ϵ. In fact, the use of the theory of differential equations with periodic coefficients (see, e.g., ref. [21]) allows a rather detailed description of the eigenvalues and eigenvectors of $i\epsilon\,(\frac{d}{dk})_{per.} + X_n(k;\epsilon)$.

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

$$\begin{aligned} i\epsilon \frac{d}{dk} N(k;\epsilon) &= -X(k;\epsilon)\,N(k;\epsilon);\\ N(0;\epsilon) &= 1, \end{aligned} \tag{22}$$

and

$$\exp(2\pi i\theta_q),\quad \theta_q \in [0,1];\quad \psi_q,\quad q = 1,\dots,m$$

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

<u>Theorem 2</u>. The spectrum of $i\epsilon\,(\frac{d}{dk})_{per.} + X(k;\epsilon)$ in $(L^2([0,2\pi]))^m$, where $X(k;\epsilon)$ has the properties stated in Theorem 1, is discrete. Its eigenvalues are given by

$$\begin{aligned} \lambda_{s,q} = \epsilon\,(s+\theta_q);\quad & s = 0, \pm1, \pm2, \dots,\\ & q = 1,2,\dots,m. \end{aligned} \tag{23}$$

A complete set of eigenvectors is given by

$$\psi_{s,q}(k) = K^{-1/2}_{s,q}\,.\exp(i\epsilon^{-1}\lambda_{s,q}\cdot k)\,N(k;\epsilon)\,\psi_q, \tag{24}$$

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

<u>Remarks 2</u>. Concerning the spectrum, Theorem 2 generalizes the results in refs. [1,4] to the case of three-dimensional systems, intersecting bands and n-th order one-band approximation. But the main point of this Theorem is that the components of $\psi_{s,q}(k)$ are restriction to $k\in[0,2\pi]$ of functions analytic and periodic in a strip J_d.

<u>Proof.</u> Since $i(\frac{d}{dk})_{per.}$ has compact resolvent and $X(k;\epsilon)$ is bounded, it follows that $i\epsilon(\frac{d}{dk})_{per.} + X(k;\epsilon)$ has compact resolvent, and then its spectrum is discrete. The eigenvalue problem for $i\epsilon(\frac{d}{dk})_{per.} + X(k;\epsilon)$ is equivalent to the problem of finding the values λ, for which the evolution equation with periodic coefficients

$$i\frac{d}{dk} J(k) = -\frac{1}{\epsilon}[X(k;\epsilon) - \lambda]\,J(k) \tag{25}$$

admits periodic solutions. The number of independent periodic solutions of (25) equals the multiplicity of the eigenvalue λ. Let $N(k;\epsilon;\lambda)$ be the fundamental matrix of (25), i.e.,

$$\begin{aligned} i\frac{d}{dk} N(k;\epsilon;\lambda) &= -\frac{1}{\epsilon}[X(k;\epsilon) - \lambda]\,N(k;\epsilon;\lambda),\\ N(0;\epsilon;\lambda) &= 1. \end{aligned} \tag{26}$$

The fundamental result in the theory of differential equations with periodic coefficients ([21] says that the number of independent periodic solutions of (25) equals the multiplicity r of the eigenvalue 1 of $N(2\pi;\epsilon;\lambda)$, and if $\psi_{q_1},\dots,\psi_{q_r}$ is a basis in the corresponding subspace ($N(2\pi;\epsilon;\lambda)$ is here understood as a unitary operator in $\mathbf{C}^m$), then a system of r independent periodic solutions of (25) is given by

$$\psi_{q_i}(k) = N(k;\epsilon;\lambda)\,\psi_{q_i}. \tag{27}$$

Taking into account that

$$\begin{aligned} i\frac{d}{dk} N(k;\epsilon;\lambda) &= -\frac{1}{\epsilon}[X(k;\epsilon) - \lambda]\,N(k;\epsilon;\lambda),\\ N(0;\epsilon;\lambda) &= 1, \end{aligned} \tag{28}$$

the verification of Theorem 2 is immediate.

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

$$L^2(\mathbf{R}^3, d\vec{x}) = \int_B^{\oplus} \mathcal{K}(\vec{k})\, d\vec{k} ,$$

where

$$\mathcal{K}(\vec{k}) = \{ \psi_{\vec{k}}(\vec{x}) = \exp(i\vec{k}\vec{x})\, u_{\vec{k}}(\vec{x}); \quad u_{\vec{k}}(\vec{x}) - \text{periodic} \,|$$

$$\|\psi_{\vec{k}}(\vec{x})\| = \int_Q |u_{\vec{k}}(\vec{x})| \, d\vec{x} \} .$$

It is not hard to verify that

$$\tilde{\mathcal{K}}(\vec{k}_\perp) \equiv \int_{[0,2\pi]}^{\oplus} \mathcal{K}(k_1, \vec{k}_\perp)\, dk_1 =$$

$$= \{ \psi_{\vec{k}_\perp}(\vec{x}) = \exp\{2\pi i[|\vec{K}_2|^{-1} k_2 x_2 + |\vec{K}_3|^{-1} k_3 x_3]\}\, \tilde{u}_{\vec{k}_\perp}(\vec{x});\ \tilde{u}_{\vec{k}_\perp}(\vec{x}) \text{ periodic in}$$

$$x_2 \text{ and } x_3 \mid \|\psi_{\vec{k}_\perp}(\vec{x})\|^2 = (\mathrm{vol}\, Q_\cap)^{-1} \int_{Q_\perp} dx_2 dx_3 \int_{-\infty}^{+\infty} dx_1 |\tilde{u}_{\vec{k}_\perp}(\vec{x})|^2 \} .$$

<u>Theorem 3</u>. For all $a < d_0$,

$$\exp(a|x_1|)\,(U^{-1} W^{-1} \psi^\circ_{sq})_{\vec{k}_\perp}(\vec{x}) \in \tilde{\mathcal{K}}(\vec{k}_\perp).$$

<u>Proof.</u> Using the definitions (I.2.7) of U and (17) of W, we have

$$(U^{-1} W^{-1} \psi^\circ_{sq})_{\vec{k}_\perp}(\vec{x}) =$$

$$= \exp[2\pi i(|\vec{K}_2|^{-1} k_2 x_2 + |\vec{K}_3|^{-1} k_3 x_3)]\,(2\pi)^{-1} \sum_{m_2 m_3} \exp[2\pi i(m_2 x_2 + m_3 x_3)] \times$$

$$\times (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} dp_1 \exp(ip_1 x_1)\, h_{m_2,m_3}(p_1),$$

where

$$h_{m_2,m_3}(p_1) = h_{m_2,m_3}(k_1 + m_1 2\pi) = \sum_{\ell=1}^{m} \psi^\circ_{sq;\ell}(k_1)\,(V^{-1}(k_1)\chi^\circ_\ell(k_1))_{m_1 m_2 m_3}.$$

From the periodicity of $\chi^\circ_\ell(k_1)$ and $\psi^\circ_{sq;\ell}(k_1)$ 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

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

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

$$c_{m_2,m_3}(x_1) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{+\infty} dp_1 \exp(ip_1 x_1)\, h_{m_2,m_3}(p_1),$$

then

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

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

<u>Remarks 3</u>. The result in Theorem 3 extends to arbitrary n (replacing, of course, d_0 by d_n).

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

5\. Although for all $n = 0,1,\ldots$ the spectrum of $\tilde{P}_n H^\epsilon \tilde{P}_n$ consists of m interwined S-W 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 ϵ, the existence of a S-W ladder of eigenvalues for H^ϵ, and this contradicts the fact that the spectrum of H^ϵ is absolutely continuous. Our results imply that as $\epsilon \to 0$, the width of S-W resonances decreases faster than any power of ϵ. This fits the heuristic arguments of Zener /22/, as well as recent numerical calculations of Bentosela et al. /23/, giving an exponential decrease of the width of the S-W resonances.

6\. Our next remark concerns the existence of closed bands /24,25/. In spite of the strong criticism of Zak /26/ and the recognition by Wannier /18/ that the problem might be more complicated, it seems that there exists a widerspread opinion /5/ 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 with the argument of Zak[26]. 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

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

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

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

Wannier and Fredkin (see also refs. [18,25]) tacitly assumed that the spectrum of $\Phi(k)$ is discrete, wherefrom the existence of the closed bands as well as of the S-W ladder follows. Unfortunately, the fact that the spectrum of H^{ϵ} is absolutely continuous[1] 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 λ_0, for some $k_0 \in B$. Then, an argument of Wannier[18] shows that λ_0 is an (infinitely degenerated) eigenvalue of Φ. On the other hand, the fact that the spectrum of H^{ϵ} is absolutely continuous, implies, via the spectral theorem, that Φ has only continuous spectrum.

10. Finally, let us mention some other mathematical approaches. For a complex field ($\mathrm{Im}\,\epsilon \neq 0$) Avron[4] proves the existence of S-W ladder eigenvalues. For real ϵ and periodic potentials with some analytic properties Herbst and Howland[27] proved that certain matrix elements of $(H^{\epsilon} - z)^{-1}$ 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 S-W resonances. However, besides the restriction to one-dimensional systems, one expects the proofs to be rather complicated.

REFERENCES

1. Avron J.E. et al. J.Math.Phys., 1977, 18, p.918.
2. Nenciu G. Comm.Math.Phys., 1981, 82, p.121.
3. Avron J.E., Günther L., Zak J. Solid State Comm., 1975, 16, p.189.
4. Avron J.E. J.Phys.A: Math.Gen., 1979, 12, p.2393.
5. Callaway J. Quantum Theory of the Solid State. N.Y.-London, Academic Press, 1974.
6. Hacker K., Obermain G. Z.Phys., 1970, 234, p.1.
7. Kohn W. Phys.Rev., 1959, 115, p.809.
8. Des Cloizeaux J. Phys.Rev., 1964, 135, p.A698.
9. Zak J. Phys.Rev., 1969, 181, p.1366.
10. Rabinovitch A., Zak J. Phys.Rev., 1971, B4, p.2358.
11. Zak J. Solid State Physics, 1972, 27, p.1.
12. Berezhkovskii A.M., Ovchinnikov A.A. Sov.Phys.Solid State, 1976, 18, p.1908.
13. Banavar J.R., Coon D.D. Phys.Rev., 1978, B17, p.3744.
14. Nagai S., Kondo J. J.Phys.Soc.Jap., 1980, 49, p.1255.
15. Nenciu A., Nenciu G. J.Phys.A: Math.Gen., 1981, 14, p.2817.
16. Kane E.O. J.Phys.Chem.Solids, 1959, 12, p.191.
17. Wannier G.H. Phys.Rev., 1960, 117, p.432.
18. Wannier G.H. Phys.Rev., 1969, 181, p.1364.
19. Nenciu A., Nenciu G. E17-82-207, JINR, Dubna, 1982.
20. Reed M., Simon B. Methods of Modern Mathematical Physics. Academic Press, N.Y., 1975, vol.II.
21. Cronin J. Differntial Equations. N.Y., Basel: Marcel Dekker, 1980.
22. Zener C. Proc.Roy.Soc. (London), 1943, A145, p.523.
23. Bentosela F., Grecchi V., Zironi F. Preprint CPT-81, Marseille, 1981, p.1337.
24. Wannier G.H., Fredkin D.R. Phys.Rev., 1962, 125, p.1910.
25. Wannier G.H. Rev.Mod.Phys., 1962, 34, p.645.
26. Zak J. Phys.Rev.Lett., 1968, 20, p.1477.
27. Herbst I.W., Howland J.S. Comm.Math.Phys., 1981, 80, p.23.

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Ненчу А., Ненчу Г. E17-82-208
Динамика блоховских электронов во внешнем электрическом поле.
Существование лестничных резонансов

Изучается проблема существования лестничных резонансов при наличии внешнего электрического поля для общего трехмерного кристалла и вырожденных зон. Гамильтониан проблемы описывается в виде прямого интеграла квазиодномерных гамильтонианов. Для квазиодномерного гамильтониана доказывается существование лестничных резонансов, отделенных друг от друга. Волновые функции, соответствующие этим резонансам, убывают экспоненциально в направлении электрического поля. Доказательство основано на аналитичности и периодичности квазиблоховских функций.

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Nenciu A., Nenciu G. E17-82-208
Dynamics of Bloch Electrons in External Electric Fields.
The Existence of Ladder Resonances

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 it 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 wave functions corresponding to these resonances, are shown to decay exponentially along the field direction.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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