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Analyticity and asymptotics for the Stark–Wannier states†

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Abstract. It is proved that the Stark-Wannier states, as functions of the electric field, are analytic in a disc tangential to the real axis at the origin, with asymptotic expansion to the second order which coincides with the Wannier approximation up to the first order.

1. Introduction

We consider the motion of an electron in a one-dimensional crystal, under the action of an external uniform electric field of strength F.

For this problem Wannier (1960, 1969) obtained, by means of the approximation of the decoupled bands, bound states distributed along ladders and linear in F.

This suggests that the actual problem admits metastable states related to resonances (called Stark-Wannier states) as has been proved in some particular cases (Agler and Froese 1985) for large values of F. In the case of sufficiently singular potentials, such as the Krönig-Penny ones with distributions of the δ type, it is believed that one can have actual bound states (see Bentosela *et al* 1985, Berezhkovskii and Ovchinnikov 1976, Ferrari *et al* 1985).

Avron (1979) has proved that for complex values of the field there exist ladders of eigenvalues which will also be called Stark-Wannier states. The numerical analysis of the states (Ferrari *et al* 1985) has suggested that they are analytic in F in a region of the complex plane. Such states, as functions of F, should exhibit couples of branch points of the Bender-Wu type due to crossings (Bender and Wu 1969, Ferrari *et al* 1985) which accumulate asymptotically at the origin in real directions. The numerical analysis agrees with the conjecture that resonances exist for small $F>0$ and are the limits of these states as $\Im F \to 0$. Because of such crossings, avoided crossings arise for the resonances, and they have been studied by Avron (1982), Bentosela *et al* (1982a, b) and Ferrari *et al* (1985).

In this paper we prove that the Stark-Wannier states are analytic in a disc tangent to the real axis at the origin and are radially asymptotic up to the second order with an expansion which extends the Wannier approximation.

Moreover we extend the existence result at complex field by Avron (1979) to potentials infinitesimally small with respect to the kinetic energy in the sense of the forms, thus including the distribution potentials of the type of the Dirac delta.

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The results are obtained using the crystal momentum representation (CMR), perturbation theory, operator techniques and the method of the asymptotic expansion for a saddle point. The expansion to the second order obtained here can be used as an improvement on the Wannier approximation for the resonances.

In § 2 we prove the existence and the analyticity of the Stark–Wannier states for F in a disc tangent to the real axis at the origin. In § 3 we prove the asymptotism of a power series expansion truncated to the second order, which coincides with the Wannier approximation up to the first order.

2. Analyticity of eigenvalues

Hypothesis 2.1. Let V be a real tempered distribution, invariant under translation by 2π. Let the corresponding symmetric quadratic form $\gamma(\phi,\psi)=V(\bar{\phi}\psi)$, with $\phi,\psi\in C_0^\infty(\mathbf{R})$, satisfy the following condition:

$$\forall a>0, \exists b\in R\colon \gamma(\phi,\phi)\leqslant a\left\langle\phi, -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi\right\rangle+b\langle\phi,\phi\rangle \qquad \forall\phi\in C_0^\infty(\mathbf{R}). \tag{2.1}$$

Under the above hypothesis there exists a unique self-adjoint operator, denoted by $H_\mathrm{B}=-\mathrm{d}^2/\mathrm{d}x^2+V$ obtained by the KLMN theorem (Reed and Simon 1975, p 167) such that

$$\langle\phi, H_\mathrm{B}\psi\rangle=\left\langle\phi, -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi\right\rangle+\gamma(\phi,\psi) \qquad \forall\phi,\psi\in C_0^\infty(\mathbf{R}).$$

Moreover H_B and $p^2=-\mathrm{d}^2/\mathrm{d}x^2$ have the same form-domain. H_B will also be called the Bloch operator. From (2.1) it follows that H_B is bounded from below. Without loss of generality from now on we shall suppose that H_B is positive. Periodic potentials $V\in L^2_{\mathrm{loc}}(\mathbf{R})$ are contained in the above class of hypothesis 2.1 since, as multiplication operators, they are infinitesimally small with respect to $-\mathrm{d}^2/\mathrm{d}x^2$ (see Reed and Simon 1978). Another example is given by the Krönig–Penny model, with $V=\Sigma_{j\in\mathbf{Z}}\,\delta_{2j\pi}$, where $\delta_{2j\pi}(\phi)=\phi(2j\pi)$, $\forall\phi\in C_0^\infty(\mathbf{R})$ (Reed and Simon 1975, p 168).

Lemma 2.2. Let V satisfy hypothesis 2.1. For $F\in\mathbf{C}$, $\Im F\neq 0$, let

$$H_\mathrm{F}\phi=H_\mathrm{B}\phi+Fx\phi \qquad \forall\phi\in C_0^\infty(\mathbf{R}).$$

Then there exist $a(F)>0$ and $b(F)>0$ such that

$$\|H_\mathrm{F}\phi\|^2+a(F)\|\phi\|^2\geqslant b(F)(\|H_\mathrm{B}\phi\|^2+\|x\phi\|^2) \qquad \forall\phi\in C_0^\infty(\mathbf{R}). \tag{2.2}$$

Proof. For sake of simplicity let $F=i$. If $\phi\in C_0^\infty(\mathbf{R})$, a core for both H_B and V as quadratic forms, we have:

$$\langle H_i\phi, H_i\phi\rangle=\langle H_\mathrm{B}\phi, H_\mathrm{B}\phi\rangle+\langle x\phi, x\phi\rangle+\langle \mathrm{i}x\phi, H_\mathrm{B}\phi\rangle+\langle H_\mathrm{B}\phi, \mathrm{i}x\phi\rangle.$$

Now x is self-adjoint and ϕ, $x\phi$ are in the form-domain $Q(H_\mathrm{B})$ of H_B. Thus:

$$\begin{aligned}\langle \mathrm{i}x\phi, H_\mathrm{B}\phi\rangle+\langle H_\mathrm{B}\phi, \mathrm{i}x\phi\rangle&=\mathrm{i}\langle\phi,[p^2,x]\phi\rangle+\gamma(\phi,\mathrm{i}x\phi)+\gamma(\mathrm{i}x\phi,\phi)\\&=\langle\phi,2p\phi\rangle+2\Re\,\gamma(\phi,\mathrm{i}x\phi)\\&=\langle\phi,2p\phi\rangle\end{aligned}$$

since $\gamma(\phi,\mathrm{i}x\phi)=\mathrm{i}\gamma(\phi,x\phi)$ is purely imaginary. Here $p=-\mathrm{i}(\mathrm{d}/\mathrm{d}x)$.

To obtain (2.2) we notice that, by hypothesis 2.1, as quadratic forms on $C_0^\infty(\mathbf{R})\times C_0^\infty(\mathbf{R})$ we have:

$$2p\leq\alpha^{-1}p^2+\alpha\leq H_\mathrm{B}+b_1\leq\tfrac{1}{2}H_\mathrm{B}^2+b_2$$

for some α, b_1, $b_2>0$.

Lemma 2.3. Let $F\in\mathbf{C}$ be fixed with $\Im F\neq 0$. Then H_F defines a closed operator on the domain $\mathbf{D}(H_\mathrm{F})=\mathbf{D}(H_\mathrm{B})\cap\mathbf{D}(x)$, with compact resolvent satisfying

$$\|[H_\mathrm{F}-z]^{-1}\|\leq\frac{1}{\mathrm{dist}(z,\Theta_\mathrm{F})}\tag{2.3}$$

where $\Theta_\mathrm{F}=\{z\in\mathbf{C}\colon \Re z\geq\cot(\theta)\Im z\}$ is the numerical range of H_F and $\theta=\arg(F)$.

Proof. Since H_B is positive, $H_\mathrm{B}+Fx$ has numerical range in the above half-plane Θ_F. In order to show that H_F has compact resolvent, we decompose it in the sum $(1-\eta)p^2+Fx+B_\eta$, where $1>\eta>0$, and $B_\eta=\eta p^2+V$.

By hypothesis 2.1 B_η is well defined and its domain contains $\mathbf{D}(p^2)\cap\mathbf{D}(x)$. By the closed graph theorem it is relatively bounded with respect to $(1-\eta)p^2+Fx$, and choosing η sufficiently small, the relative bound is much less than 1. Therefore by the usual resolvent formula, since $(1-\eta)p^2+Fx$ has compact resolvent (Herbst 1979) H_F has compact resolvent too.

Finally (2.3) follows immediately since H_F is accretive (up to a phase factor).

Remark. By the unitary translation $(T_{2\pi}\phi)(x)=\phi(x+2\pi)$ we have $T_{2\pi}H_\mathrm{F}T_{2\pi}^{-1}=H_\mathrm{F}+2\pi F$. Thus, if $\sigma(H_\mathrm{F})$ is not empty, it consists of ladders of the form $\{E_0+2j\pi F\}_{j\in\mathbf{Z}}$.

Let P_n denote the (orthogonal) projection onto the subspace $\mathscr{H}_n$, such that the spectrum of the restriction of H_B to $\mathscr{H}_n$ is just the nth band $[\alpha_n,\beta_n]$. Then we set $P_n'=1-P_n$ and

$$\begin{aligned}H_{\mathrm{F},1}&=P_1H_\mathrm{F}P_1\\ H'_{\mathrm{F},1}&=P_1'H_\mathrm{F}P_1'\\ W_1&=P_1xP_1'+P_1'xP_1\end{aligned}\tag{2.4}$$

whence $H_\mathrm{F}=H_{\mathrm{F},1}+H'_{\mathrm{F},1}+FW_1$.

$H_{\mathrm{F},1}$ is the Stark-Wannier operator relative to the band $[\alpha_1,\beta_1]$, with a spectrum given by the ladder of simple eigenvalues $\{\lambda_1+2\pi Fj\}_{j\in\mathbf{Z}}$, where λ_n, $n=1,2,\ldots$, is the mean value of the band function $E_n(k)$ (described below). Its numerical range is contained in the strip

$$\{z\in\mathbf{C}\colon \alpha_1\leq\Re z-\Im z\cot\theta\leq\beta_1\}.$$

$H'_{\mathrm{F},1}$ has compact resolvent and numerical range in the half-plane

$$\{z\in\mathbf{C}\colon \alpha_2\leq\Re z-\Im z\cot\theta\}.$$

Lemma 2.4. The operator W_1 defined in (2.4) is bounded.

Proof. We have $W_1=[P_1,x]P_1'+P_1'[x,P_1]$. Now, from the proof of lemma 2.2 it follows that $\forall\alpha>0$, $\forall\varphi\in C_0^\infty(\mathbf{R})$

$$|\langle\varphi,[H_\mathrm{B},x]\varphi\rangle|\leq\frac{1}{\alpha}\langle\varphi,H_\mathrm{B}\varphi\rangle+\alpha\langle\varphi,\varphi\rangle.\tag{2.5}$$

Thus (2.5) holds $\forall\varphi \in Q(H_{\mathrm{B}})$, the form domain of H_{B}. Choosing $\psi \in \mathrm{Range}(H_{\mathrm{B}}-z)$, with $z \notin \sigma(H_{\mathrm{B}})$ ($z \in \mathbf{R}$ for simplicity), let $\varphi = (H_{\mathrm{B}}-z)^{-1}\psi$. Then (2.3) implies:

$$\begin{aligned}
&|\langle (H_{\mathrm{B}}-z)^{-1}\psi, [H_{\mathrm{B}}, x](H_{\mathrm{B}}-z)^{-1}\psi\rangle| \\
&\qquad \leqslant \frac{1}{\alpha}\langle H_{\mathrm{B}}(H_{\mathrm{B}}-z)^{-1}\psi, (H_{\mathrm{B}}-z)^{-1}\psi\rangle + \alpha\|(H_{\mathrm{B}}-z)^{-1}\psi\|^2 \\
&\qquad \leqslant |\langle \psi, (H_{\mathrm{B}}-z)^{-1}\psi\rangle| + \left(\alpha + \frac{|z|}{\alpha}\right)\|(H_{\mathrm{B}}-z)^{-1}\psi\|^2 \\
&\qquad \leqslant c\|\psi\|^2.
\end{aligned}$$

Hence

$$[x, P_1] = -(2\pi \mathrm{i})^{-1} \oint_{\Gamma_1} (H_{\mathrm{B}}-z)^{-1}[H_{\mathrm{B}}, x](H_{\mathrm{B}}-z)^{-1}\, \mathrm{d}z$$

is bounded on $\mathrm{Range}(H_{\mathrm{B}}-z)$, which is dense. Therefore W_1 is bounded too.

In the following L_1 will denote the norm of W_1. Notice that the proof of lemma 2.4 can be given in a much simpler way within the crystal momentum representation (see § 3).

Theorem 2.5. Let V satisfy hypotheses 2.1 and 3.2. Consider the nth isolated band of the corresponding Bloch operator H_{B}, with isolation distance $2\delta_n$. Then there exists $\varepsilon_n > 0$ such that for $F \in B_{\varepsilon_n}(\mathrm{i}\varepsilon_n) \equiv \{z \in \mathbf{C}: |z - \mathrm{i}\varepsilon_n| < \varepsilon_n\}$ the operator H_{F} has exactly one ladder of eigenvalues lying within the strip

$$S_n = \{z \in \mathbf{C}: \alpha_n - \delta_n + \Im z \cot\theta < \Re z < \beta_n + \delta_n + \Im z \cot\theta\}. \tag{2.6}$$

Such eigenvalues, as functions of F, are analytic in $B_{\varepsilon_n}(\mathrm{i}\varepsilon_n)$.

Proof. For simplicity, let $n=1$ and $2\delta_1 = \alpha_2 - \beta_1 = 2\delta$. Let $H_{\mathrm{F}}(\beta) = H_{\mathrm{F}} - (1-\beta)FW_1$. Consider the lines $\alpha_1 - \delta + \Im z \cot\theta = \Re z$ and $\beta_1 + \delta + \Im z \cot\theta = \Re z$.

We want to show that they are contained in the resolvent set of $H_{\mathrm{F}}(\beta)$ uniformly in $\beta \in [0, 1]$, for all $F \in B_{\varepsilon_n}(\mathrm{i}\varepsilon_n)$.

This implies that the first Stark-Wannier ladder does not go out of the strip S_1 and no other ladder enters the strip when β varies in $[0, 1]$.

Let us now consider $H_{\mathrm{F}}(\beta)$ for fixed F: it represents an analytic family of type A on the whole complex plane with $H_{\mathrm{F}}(1) = H_{\mathrm{F}}$ and $H_{\mathrm{F}}(0) = H_{\mathrm{F},1} + H'_{\mathrm{F},1}$. Indeed

$$H_{\mathrm{F}}(\beta) = H_{\mathrm{F},1} + H'_{\mathrm{F},1} + \beta F W_1 \tag{2.7}$$

by (2.4) and the definition of $H_{\mathrm{F}}(\beta)$. Now we want to estimate the resolvent as follows:

$$\begin{aligned}
\|(H_{\mathrm{F}}(\beta)-z)^{-1}\| &= \|(H_{\mathrm{F}}(0)-z)^{-1}(1 + F\beta W_1(H_{\mathrm{F}}(0)-z)^{-1})\| \\
&\leqslant \frac{2(\delta\sin\theta)^{-1}}{1 - 2L_1|F|(\delta\sin\theta)^{-1}}
\end{aligned} \tag{2.8}$$

for all F such that

$$L_1|F|2(\delta\sin\theta)^{-1} < 1 \tag{2.9}$$

uniformly for z in the above quoted lines. In order to prove (2.8) we use the decomposition

$$\|(H_F(0)-z)^{-1}\| \leq \|(H_{F,1}-z)^{-1}\| + \|(H'_{F,1}-z)^{-1}\| \leq \frac{2}{\delta \sin\theta} \tag{2.10}$$

if z belongs to one of the two lines considered above. In fact the distance of z from the numerical range of $H_{F,1}(H'_{F,1})$ is not less than $\delta \sin\theta$.

Now notice that inequality (2.9) defines the ball $B_{\varepsilon_1}(\mathrm{i}\varepsilon_1)$ for $\varepsilon_1 = (\delta/4L_1)$ (a simple application of the sine theorem to the right triangle constructed by the vectors F and $2\mathrm{i}\varepsilon_1$ in the complex plane).

The eigenvalues of $H_F(\beta)$ (an analytic family of type A) are continuous in β (counting multiplicity).

On the other hand, notice that not only $H_F(1)$, but also $H_F(\beta)$, $\beta \in [0, 1]$, has invariant discrete spectrum with respect to translation by $2\pi F$, since W_1 commutes with a translation by 2π.

Thus we can consider the spectrum on a cylinder defined by $\mathbf{C}/2\pi F$; then in the region $S_1/2\pi F$ we find just one eigenvalue for $\beta = 0$. Now from the norm-continuity (in β) of the resolvents and from the bound (2.8) on the boundary of $S_1/2\pi F$ there is still a unique isolated eigenvalue for any $\beta \in [0, 1]$. Therefore there exists a unique eigenvalue $E_1(F)$ near the eigenvalue λ_1 of $H_{F,1}$, for any F in the disc $B_{\varepsilon_1}(\mathrm{i}\varepsilon_1)$.

Since H_F is an analytic family of type A, the eigenvalue $E_1(F)$ is analytic as long as it is isolated, and the theorem is proved.

3. Asymptotics

From the above obtained analyticity of the eigenvalues in a disc we can now prove the existence of an asymptotic perturbation expansion up to the second order for the eigenvalues. Such an expansion coincides, up to the first order, with the Wannier approximation under the following further assumption.

Hypothesis 3.1. We assume that V satisfies the parity condition

$$V\varphi = V\psi \qquad \text{if} \qquad \psi(x) = \varphi(-x) \qquad \forall \varphi \in C_0^\infty(\mathbf{R}) \qquad \forall x \in \mathbf{R}. \tag{3.1}$$

We note that the perturbation expansion cannot be simply obtained by the Rayleigh-Schrödinger method, since there is no unperturbed eigenvalue. Hence the problem compels us to choose the Wannier approximation, i.e. the decoupled band approximation as an unperturbed model.

To this end we have to introduce the crystal momentum representation (CMR) (Bentosela 1979, Blount 1962), which we now briefly recall.

We consider the unitary transformation $U: L^2(\mathbf{R}) \to \mathscr{H}$ defined by $(U\psi)(k, K) = \varphi(k, K) = \hat{\psi}(k+K)$, where $\hat{\psi}$ denotes the Fourier transform of ψ. The sequence $\{\varphi(k, K)\}_{K \in \mathbf{Z}}$ belongs to $\mathscr{H}'(k) = l^2$, for almost all $k \in B$, where B is the torus $\mathbf{R}/1$ called the Brillouin zone, and $\mathscr{H} = \int_B^\oplus \mathscr{H}'(k)\,\mathrm{d}k$.

Then we obtain

$$UH_B U^{-1} = \int_B^\oplus H(k)\,\mathrm{d}k \tag{3.2}$$

where

$$(H(k)a)(K) = (T(k)a)(K) + (\tilde{V}a)(K)$$
$$= (k+K)^2 a(K) + \sum_{j\in\mathbf{Z}} V_j a(K-j) \tag{3.3}$$

for any $a(K)$ of the form $a(K) = \varphi(k, K) = (U\psi)(k, K)$ for some $\psi \in \mathbf{D}(H_B)$. Here V_j denotes the jth Fourier coefficient of V: $V_j \in \mathbf{R}$ by hypothesis 3.1.

Notice that $\mathscr{H}(k)$ is an analytic family of type A in k. $\tilde{V}$ is infinitesimally small in the form sense with respect to $T(k)$, $k \in B$, exactly as V is with respect to $-\mathrm{d}^2/\mathrm{d}x^2$ (hypothesis 2.1). As a consequence, $H(k)$ has compact resolvent as $T(k)$ (see theorem XIII.68 of Reed and Simon (1978)) and it is bounded from below. We shall suppose it is positive for any $k \in B$.

Then for any k there exists a sequence of eigenvalues $0 \leqslant E_1(k) \leqslant E_2(k) \leqslant \ldots \leqslant E_n(k) \leqslant \ldots$ with orthonormal eigenvectors $\{\omega_1^{(k)}(K)\}_{K\in\mathbf{Z}}, \ldots, \{\omega_n^{(k)}(K)\}_{K\in\mathbf{Z}}, \ldots$.

Hypothesis 3.2. We assume that the eigenvalues $E_n(k)$ of $T(k) + \tilde{V}$ are simple.

This means that all the gaps (β_n, α_{n+1}) are non-empty (about such a hypothesis see theorem XIII.91 of Reed and Simon (1978)). Such eigenvalues, as function of k, are called band functions and they are analytic, even and periodic with period one and they are strictly monotone in $[0, \frac{1}{2}]$. In particular in the open interval $(0, \frac{1}{2})$ the derivatives of $E_n(k)$ are positive for n odd and negative for n even (Reed and Simon 1978). We have $\alpha_n = \min_k E_n(k)$, $\beta_n = \max_k E_n(k)$.

We now define

$$\lambda_n = \langle E_n \rangle = \int_B E_n(k)\,\mathrm{d}k. \tag{3.4}$$

Since $V_K = V_{-K} \in \mathbf{R}\ \forall K \in \mathbf{Z}$, the set of real-valued functions is left invariant by $H(k)$. Thus we can restrict ourselves to considering only real-valued eigenfunctions $\omega_n^{(k)}$ of the real eigenvalues $E_n(k)$, without loss of generality, with the property that $\omega_n^{(k)}(K) = \omega_n^{(-k)}(-K)$.

Moreover, since $H(k)$ is analytic of type A, we may assume that each $\omega_n^{(k)}$ is a vector-valued analytic function. In particular there exists $\partial\omega_n^{(k)}/\partial k \in l^2$.

Now it easily follows that

$$\left\langle \omega_n^{(k)}, \frac{\partial \omega_m^{(k)}}{\partial k} \right\rangle_{l^2} = -\left\langle \omega_m^{(k)}, \frac{\partial \omega_n^{(k)}}{\partial k} \right\rangle_{l^2} \qquad \forall n, m \in \mathbf{N}\ \forall k$$

by normalisation. In particular

$$\left\langle \omega_n^{(k)}, \frac{\partial \omega_n^{(k)}}{\partial k} \right\rangle = 0.$$

A sequence $b \in l^2$ can be written

$$b(K) = \sum_{m=1}^{\infty} a_m(k)\omega_m^{(k)}(K) \tag{3.5}$$

where

$$a_m(k) = \sum_{K\in\mathbf{Z}} \omega_m^{(k)}(K) b(K).$$

A unitary transform $\tilde{U}: L^2(\mathbf{R}) \to \oplus_{m=1}^{\infty} \mathscr{H}_m$, where $\mathscr{H}_m = L^2(B) \forall m$, is defined by

$$(\tilde{U}\psi)_m(k) = \sum_{j\in\mathbf{Z}} \omega_m^{(k)}(j)(U\psi)(k,j) = \langle \omega_m^{(k)}, (U\psi)(k,\cdot)\rangle_{l^2}. \tag{3.6}$$

Notice that $\tilde{U}$ is unitary since $\tilde{U}^{-1}$ is defined on $\oplus_{m=1}^{\infty}\mathscr{H}_m$ by (3.5) with $b(K) = (U\psi)(k, K)$, and $\int_{-\infty}^{+\infty}|\psi(x)|^2\,\mathrm{d}x = \Sigma_{m=1}^{\infty}\int_B |a_m(k)|^2\,\mathrm{d}k$ if $a_m = (\tilde{U}\psi)_m$.

Let us consider the unitary transformation of H_{F} given by

$$\tilde{H}_{\mathrm{F}} = \tilde{U}H_{\mathrm{F}}\tilde{U}^{-1} = \tilde{H}_{\mathrm{B}} + F\tilde{U}x\tilde{U}^{-1}. \tag{3.7}$$

Formally, we have

$$\tilde{H}_{\mathrm{F}} = \tilde{H}_{\mathrm{B}} + FX + \mathrm{i}FD \tag{3.8}$$

on the elements $a = (a_m)_m$ of $\oplus_{m=1}^{\infty}\mathscr{H}_m$ such that $a_m \in C^1(B)\,\forall m$, and only a finite number of a_m is not identically zero, where

$$(\tilde{H}_{\mathrm{B}}a)_m(k) = E_m(k)a_m(k) \tag{3.9a}$$

$$(Xa)_m(k) = \sum_{n=1}^{\infty} X_{m,n}a_n(k) \tag{3.9b}$$

$$(Da)_m(k) = \frac{\partial a_m(k)}{\partial k} \tag{3.9c}$$

with

$$X_{m,n}(k) = \mathrm{i}\left\langle \omega_m^{(k)}, \frac{\partial\omega_n^{(k)}}{\partial k}\right\rangle_{l^2} = -X_{n,m}(k) = -X_{m,n}(-k). \tag{3.10}$$

Let us consider $\tilde{H}_{\mathrm{F}}$ and the corresponding Stark-Wannier approximation $\tilde{H}_{\mathrm{B}} + \mathrm{i}FD$, which corresponds to neglecting the FX term connecting different bands.

The operator $\tilde{H}_{\mathrm{B}} + \mathrm{i}FD$ acts in the space $\oplus_{m=1}^{\infty}\mathscr{H}_m$ the following way:

$$\tilde{H}_{\mathrm{B}} + \mathrm{i}FD = \tilde{U}\left(\sum_{m=1}^{\infty} P_m H_F P_m\right)\tilde{U}^{-1}. \tag{3.11}$$

The eigenvalue problem for (3.11)

$$\tilde{H}_{\mathrm{B}}a + \mathrm{i}FDa = \lambda a \tag{3.12}$$

where $a = \{a_m\}_{m\in\mathbf{N}}$, can be separated:

$$E_n(k)a_n(k) + \mathrm{i}F\frac{\partial a_n(k)}{\partial k} = \lambda a_n(k) \qquad \forall n \in \mathbf{N}.$$

The solutions are of the form

$$a_n(k) = c_n \exp\left((\mathrm{i}F)^{-1}\int_{-1/2}^{k} (\lambda - E_n(\tau))\,\mathrm{d}\tau\right) \tag{3.13}$$

with the condition that $a_n(k)$ be a function defined on the torus B: $a_n(-\frac{1}{2}) = a_n(\frac{1}{2})$, i.e.

$$\lambda = \lambda_{n,j} = \int_{-1/2}^{1/2} E_n(k)\,\mathrm{d}k + 2\pi jF \qquad \forall j \in \mathbf{Z}. \tag{3.14}$$

The eigenvectors are given by

$$(\psi^{n,j}(k))_m = \delta_m^n \exp\left((\mathrm{i}F)^{-1}\int_{-1/2}^{k}(\lambda_{n,j} - E_n(\tau))\,\mathrm{d}\tau\right). \tag{3.15}$$

We split the interband operator X into two terms:

$$X = \tilde{U}W_1\tilde{U}^{-1} + (X - \tilde{U}W_1\tilde{U}^{-1}).$$

$\tilde{W}_1 = \tilde{U}W_1\tilde{U}^{-1}$ contains the interband terms between the first band and the others. $X' = X - \tilde{W}_1$ contains the interband terms between all the bands except the first one. With this notation $\tilde{H}_F$ can be written as:

$$\tilde{H}_F = \tilde{H}_B + iFD + FX' + F\tilde{W}_1.$$

We set

$$H(F,\eta) = \tilde{H}_B + iFD + FX' + \eta\tilde{W}_1. \tag{3.16}$$

We now consider $\eta\tilde{W}_1$ as a perturbation of $\tilde{H}_B + iFD + FX'$, the spectrum of which contains the set $\{\lambda_{1,j}\}$. The eigenvalues of $H(F,\eta)$ are given by

$$E(F,\eta) = \sum_{n=0}^{\infty} c_n(F)\eta^n$$

a convergent expansion with convergence radius $\varepsilon_1 > 0$ independent of $F(\varepsilon_1 = \delta/(4\|W_1\|)$, where 2δ is the isolation distance of the first band as in § 2). Such a series is calculated by the usual perturbation formalism: setting $R_\eta = (H(F,\eta)-z)^{-1}$, for fixed $F \in B_{\varepsilon_1}(i\varepsilon_1)$ such that $0 < \theta_1 \leqslant \arg(F) = \theta \leqslant \theta_2 < \pi$ for $|F|$ sufficiently small, the expansion is given by $\lambda_{1,0} + \eta(\Sigma_{n=0}^{\infty} a_n(F)\eta^n)(\Sigma_{n=0}^{\infty} b_n(F)\eta^n)^{-1}$, according to the usual formulae:

$$a_n(F) = (2\pi i)^{-1} \oint_{|\lambda_{1,0}-z|=|F|\pi} \langle\varphi, (-\tilde{W}_1R_0)^{n+1}\psi\rangle\, dz \tag{3.17a}$$

$$b_n(F) = -(2\pi i)^{-1} \oint_{|\lambda_{1,0}-z|=|F|\pi} \langle\varphi, R_0(-\tilde{W}_1R_0)^n\psi\rangle\, dz. \tag{3.17b}$$

Here the scalar products are in the space $\oplus_{m=1}^{\infty}\mathcal{H}_m$, while ψ is given by (3.15) for $n=1, j=0$, up to a constant factor the following way:

$$\begin{aligned}(\psi(k))_m &= \delta_1^m \exp(-ig(k)/F)\\ &= \delta_1^m \exp\left(-i/F\int_{-\bar{k}}^{k} (\lambda_1 - E_1(\tau))\, d\tau\right)\end{aligned} \tag{3.18}$$

where $\bar{k}$ is the positive value such that $E_1(\bar{k}) = \lambda_1$. Notice that $g(k) > 0, \forall k \neq -\bar{k}$, and $g'(-\bar{k}) = 0$ since $E_1(k)$ is an even function; also $\|\psi\| \leqslant 1$. Finally

$$(\varphi(k))_m = \delta_1^m \qquad \forall k \in B. \tag{3.19}$$

Consider (3.17a) for n even. We have

$$\begin{aligned}a_{2r}(F) &= -(2\pi i)^{-1} \oint_{|\lambda_{1,0}-z|=|F|\pi} \langle\varphi, \tilde{W}_1R_0(\tilde{W}_1R_0\tilde{W}_1R_0)^r\psi\rangle\, dz\\ &= -(2\pi i)^{-1} \oint_{|\lambda_{1,0}-z|=|F|\pi} \langle\varphi, P_1\tilde{W}_1P_1'R_0P_1'\\ &\qquad \times (P_1\tilde{W}_1P_1'R_0P_1'\tilde{W}_1P_1R_0P_1)^r\psi\rangle\, dz\end{aligned} \tag{3.20}$$

because R_0 commutes with both P_1 and P_1', while $P_1\tilde{W}_1P_1 = P_1'\tilde{W}_1P_1' = 0$ $(P_1 + P_1' = 1)$. It follows that $a_{2r}(F) = 0$, $\forall r \in N$, since in the above product a factor $P_1'P_1 = 0$ appears.

In full analogy it turns out that $b_{2r+1}(F)=0$. For the remaining non-zero terms the following estimates hold:

$$|a_{2r+1}(F)|\leq c^r|F|^{-r}$$
$$|b_{2r}(F)|\leq c^r|F|^{-r}. \tag{3.21}$$

In fact $P_1R_0P_1=P_1(E_1+\mathrm{i}FD-z)^{-1}$, where $(E_1a)_m(k)=\delta_1^m E_1(k)a_1(k)$. Moreover the numerical range of $P_1'H_{\mathrm{B}}P_1'$ has distance from λ_1 greater than $2\delta\sin\theta$ (at least for $|F|$ small), so that $P_1'R_0P_1'$ is bounded by $(2\delta\sin\theta)^{-1}$. Furthermore $\|P_1R_0P_1\|\leq 2|F|^{-1}$, since $P_1R_0P_1$ admits a spectral representation in terms of the projections $P_{1,j}$ relative to the ladder $\{\lambda_{1,j}\}_{j\in\mathbf{Z}}=\{\lambda_1+2\pi Fj\}_{j\in\mathbf{Z}}$, with $\Sigma_{j\in\mathbf{Z}}P_{1,j}=P_1$.

The estimates (3.21) follow, since both the vector ψ and the operator $\tilde{W}_1$ are uniformly bounded, and the length of the path is given by $2\pi^2|F|$.

Let us consider now the asymptotic calculus of $a_1(F)$:

$$a_1(F)=(2\pi\mathrm{i})^{-1}\oint_{|\lambda_1-z|=|F|\pi}\langle\varphi,\ \tilde{W}_1P_1'R_0P_1'\tilde{W}_1R_0\psi\rangle\,\mathrm{d}z \tag{3.22}$$

where $R_0\psi=(\lambda_1-z)^{-1}\psi$.

By the residue theorem

$$\begin{aligned}a_1(F)&=-\langle\varphi,\ \tilde{W}_1P_1(H(F,0)-\lambda_1)^{-1}P_1'\tilde{W}_1\psi\rangle\\&=-\langle P_1'(H(F,0)-\lambda_1)^{-1}P_1'\tilde{W}_1\varphi,\ \tilde{W}_1\psi\rangle.\end{aligned} \tag{3.23}$$

Now,

$$|a_1(F)+\langle P_1'(H(0,0)-\lambda_1)^{-1}P_1'\tilde{W}_1\varphi,\ \tilde{W}_1\psi\rangle|=\mathrm{O}(F) \tag{3.24}$$

since $\|(H(F,0)-H(0,0))u\|=\mathrm{O}(F)$ for fixed $u\in\mathbf{D}(H(F,0))$, whence the strong resolvent convergence, with rate of convergence $\mathrm{O}(F)$ on the vector $\tilde{W}_1\varphi$.

We note that

$$\begin{aligned}&\langle P_1'(H(0,0)-\lambda_1)^{-1}P_1'\tilde{W}_1\varphi,\ \tilde{W}_1\psi\rangle\\&\quad=\int_B\sum_{m\neq1}(\tilde{W}_1(k))_{1,m}(E_m(k)-\lambda_1)^{-1}(\tilde{W}_1(k))_{m,1}\exp[-\mathrm{i}g(k)/F]\,\mathrm{d}k.\end{aligned} \tag{3.25}$$

Since $-\bar{k}$ is the only point of minimum of $g(k)$ we can evaluate the asymptotics of (3.25) by the saddle point method (Olver 1974, p 127). It turns out that (3.25) has the following behaviour:

$$F^{1/2}\left(\frac{2\pi}{\mathrm{i}g''(-\bar{k})}\right)^{1/2}\sum_{m\neq1}(\tilde{W}_1(-\bar{k}))_{1,m}(E_m(-\bar{k})-\lambda_1)^{-1}(\tilde{W}_1(-\bar{k}))_{m,1}+\mathrm{O}(F^{3/2}). \tag{3.26}$$

By combining (3.24) and (3.26) we obtain

$$a_1(F)=-F^{1/2}\left(\frac{2\pi}{\mathrm{i}g''(-\bar{k})}\right)^{1/2}\sum_{m\neq1}|(\tilde{W}_1(-\bar{k}))_{1,m}|^2(E_m(-\bar{k})-\lambda_1)^{-1}+\mathrm{O}(F). \tag{3.27}$$

Similarly,

$$b_0(F)=\int_B\exp(-\mathrm{i}g(k)/F)\,\mathrm{d}k=F^{1/2}\left(\frac{2\pi}{\mathrm{i}g''(-\bar{k})}\right)^{1/2}+\mathrm{O}(F^{3/2}). \tag{3.28}$$

Notice that the estimates and the asymptotic behaviours given above are uniform in any angular sector of the form $|\arg(F)-\pi/2|\leq\theta_0<\pi/2$.

In the case $F = \eta$, in any such angular sector we have

$$E(F, F) = \lambda_1 + F^2[a_1(F)(b_0(F))^{-1} + \mathrm{O}(F^{1/2})]$$
$$= \lambda_1 - F^2 \sum_{m \neq 1} |(\tilde{W}_1(-\bar{k}))_{1,m}|^2 (E_m(-\bar{k}) - \lambda_1)^{-1} + \mathrm{O}(F^{5/2}). \quad (3.29)$$

Notice that the coefficient of F^2 is negative, according to the numerical calculation performed in Ferrari *et al* (1985, p 5826). Moreover $(\tilde{W}_1(k))_{n,m}$ is an odd function of k as is $X_{n,m}(k) \forall n, m$ and, since $E_m(k)$ is even for any m, $-\bar{k}$ can be replaced by $\bar{k}$ in (3.29). The above results can be summarised as follows.

Theorem 3.4. The Stark-Wannier eigenvalues $E_{n,j}(F)$, $n \in \mathbf{N}, j \in \mathbf{Z}$ of $H_F = -\mathrm{d}^2/\mathrm{d}x^2 + V + Fx$ are analytic in some disc $B_{\varepsilon_n}(\mathrm{i}\varepsilon_n)$, $\varepsilon_n > 0$ and they admit asymptotic expansion in powers of F, up to the second order, whose linear part coincides with the Wannier expression

$$E_{n,j}(F) = \lambda_n + 2\pi F j - F^2 \sum_{m \neq n} |(\tilde{W}_n(\bar{k}_n))_{n,m}|^2 (E_m(\bar{k}_n) - \lambda_{n,j})^{-1} + \mathrm{O}(F^{5/2}) \quad (3.30)$$

where $\bar{k}_n > 0$ is defined by $E_n(\bar{k}_n) = \lambda_n$. Here $\tilde{W}_n = \tilde{U} W_n \tilde{U}^{-1}$, $W_n = P_n x P'_n + P'_n x P_n$ and P_n is the projection defined in § 2. For all n and j (3.30) holds uniformly in any sector $|\arg(F) - \pi/2| \leq \theta_0 < \pi/2$.

Remark. This result gives a precise meaning to the Stark-Wannier approximation in terms of the asymptotic behaviour (3.30) in complex directions.

We can construct a formal perturbation theory in F of the band functions by a diagonalising unitary multiplication operator of class $C^1(B)$ formally defined by a series.

More precisely one looks for $S(F, k) = \exp[\mathrm{i}FA(F, k)]$ and $\varepsilon(F, k)$, where $A(F, k) = \sum_{n=0}^{\infty} F^n A_n(k)$, $A_n(k)$ is a symmetric matrix, and $(\varepsilon(F, k))_{j,m} = \delta_{j,m} \sum_{n=0}^{\infty} e_{j,n}(k) F^n$ such that

$$\tilde{H}_F = \tilde{H}_B + FX + \mathrm{i}FD$$
$$= S(F, k)[\varepsilon(F, k) + \mathrm{i}FD]S^{-1}(F, k)$$
$$= S(F, k)\varepsilon(F, k)S^{-1}(F, k) + \mathrm{i}FS(F, k)\frac{\partial S^{-1}(F, k)}{\partial k} + \mathrm{i}FD. \quad (3.31)$$

Equality (3.31) is meant to hold to all orders in F (compare with Avron (1982, p 42)); for a wider discussion of the band perturbation see Nenciu and Nenciu (1981, 1982).

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