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LETTER TO THE EDITOR

Wannier ladders and perturbation theory

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Abstract. Following Avron we consider the Stark effect for Bloch electrons in the case of a finite number of gaps. We prove that the ladders of resonances are given by the Wannier decoupled-band approximation and the perturbation theory. The Fermi golden rule yields the width behaviour of Buslaev and Dmitrieva.

Despite the fact that Wannier ladder states seem to play an important role in the understanding of electrical conductivity in crystals [1], experimental observations and theoretical proofs of existence took a long time to appear. Some numerical methods have given the first evidence of the existence of such states as resonances [2]. For the experimental observations it was essential to introduce the superlattices, that is materials which essentially exhibit one-dimensional properties [3,4]. On the theoretical side resonances are defined as eigenvalues of a non-self-adjoint operator [5] and only in the last few years has rigorous proof of the existence of resonances been given. They are based on semiclassical methods, i.e. the existence of resonances is given as the electric field strength goes to zero together with $\hbar$ [6,7] or for large electric field strength [8] or the existence of resonances in crystals and disordered systems is given for large atomic distance [9].

In this paper, making the assumption of a finite number of bands [10,11] we are able to define the resonances by means of a relatively compact perturbation operator with respect to the Wannier decoupled-band (DB) approximation in the Crystal momentum representation (CMR) and we prove the existence of ladders of resonances for arbitrarily small electric field strength; indeed, we have no semiclassical restriction in our method.

The proof of existence we give justifies the Wannier decoupled-band approximation as the basis of a solvable perturbation calculation and some partial results on the behaviour of the resonances suggested for such models. In particular, we prove that the second-order perturbation theory gives the second-order Nenciu [12–14] asymptotic power series and an exponentially small width (Fermi golden rule) [10] in agreement with the Buslaev–Dmitrieva adiabatic approximation [11,15].

Let us notice that, recently, an important connection has been stressed between the Stark–Wannier problem and the quantum-chaos one [16].

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Let us consider a one-dimensional Bloch Hamiltonian with a finite number of gaps; that is, for instance, the periodic Lamé potential of period 2π

$$H_{\mathrm{B}} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + m(m+1)\left(\frac{tK}{\pi}\right)^2 \mathrm{Sn}^2(Kx/\pi, t) \tag{1}$$

where $0 < t < 1$ and $m = 1, 2 \ldots$. Here $Sn(x,t)$ is the Jacobian elliptic function of period $4K(t)$, the potential in (1) is real analytic in the strip $|\mathrm{Im}\, z| \leqslant 2\alpha_0$ where $\alpha_0 \leqslant \pi^2/4K$. The spectrum of H_{B} is given by $m+1$ bands, i.e. only the first m gaps are open [17]. In the following we shall assume $m = 1$ for the sake of simplicity. In the CMR the corresponding operator to the Stark–Wannier Hamiltonian $H_F = H_B + Fx$ takes the form $H_F = H_F^{\mathrm{DB}} + FW$ and acts on $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, where $\mathcal{H}_1 = L^2(\mathcal{B}, \mathrm{d}k)$, $\mathcal{B}$ is the Brillouin zone, that is the torus $\mathbf{R}/1$ with representatives on $(0, +1]$, and $\mathcal{H}_2 = L^2(\mathbf{R}, \mathrm{d}p)$. Here

$$H_F^{DB} = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix} \qquad \text{and} \qquad W = \begin{pmatrix} 0 & X_{1,2} \\ X_{2,1} & X_{2,2} \end{pmatrix} \quad X_{2,1} = X_{1,2}{}^{*} \tag{2}$$

H_F^{DB} is called the Wannier decoupled-band (DB) approximation, $H_1 = \mathrm{i}F\partial_k + \mathcal{E}_1(k)$, $H_2 = \mathrm{i}F\partial_p + \mathcal{E}_2(p)$, $\mathcal{E}_1(k)$ and $\mathcal{E}_2(p)$ are the band functions, $X_{2,1}$ and $X_{1,2}$ are the interband terms between bands and $X_{2,2}$ is the intraband term on the second band (the intraband term on the first one vanishes identically).

In order to obtain the resonances as eigenvalues of a non-self-adjoint operator we use the analytic translation $x \to x - \mathrm{i}\alpha$ (we take $\alpha \leqslant \alpha_0$). The CMR of the distorted operator, which we shall call H_F^{α} or simply H_F, has DB approximation such that $H_1^{\alpha} \equiv H_1$ and $H_2^{\alpha} = H_2 - \mathrm{i}F\alpha$. Hence, the essential spectrum of the DB approximation is $\Sigma_{\mathrm{ess}}(H_F^{\mathrm{DB}}) = -\mathrm{i}F\alpha + \mathbf{R}$ and the discrete spectrum coincides with the Wannier ladder $\{E_{1,j},\ j \in \mathbf{Z}\}$, where $E_{1,j} = \langle\mathcal{E}_1\rangle + 2\pi jF$ and $\langle\mathcal{E}_1\rangle$ denotes the mean value of the first band function.

Let us consider the usual Rayleigh–Schrödinger perturbation theory, where H_F^{DB} is the unperturbed operator and W is a perturbation: $H_F(f) = H_F^{\mathrm{DB}} + fW$, $f \in \mathbf{C}$ is an auxiliary parameter which plays the role of the perturbative one in the perturbation theory (for $f = F$ we have, of course, $H_F(F) = H_F$). As we shall show, the interband term W is bounded and, in particular, relatively compact with respect to the DB approximation; hence, we have the stability of the essential spectrum:

$$\Sigma_{\mathrm{ess}}(H_F) = \Sigma_{\mathrm{ess}}(H_F^{\mathrm{DB}}) = -\mathrm{i}F\alpha + \mathbf{R}\,. \tag{3}$$

Therefore $\Sigma(H_F) - \Sigma_{\mathrm{ess}}(H_F) = \Sigma_{\mathrm{d}}(H_F)$ defines the resonances in the strip $-F\alpha < \mathrm{Im}\, z < 0$, as it is known in the usual x-representation [5].

Indeed, we have the following result.

Proposition. There exists $F_0 > 0$ such that for each fixed F, $0 < F < F_0$ the Stark–Wannier Hamiltonian has one ladder of resonances $E_{1,j}(F)$, $j \in \mathbf{Z}$ which is close, up to a term of order F^2, to the Wannier ladder of eigenvalues and given by $E_{1,j}(F) = E_{1,j}(F, F)$ where $E_{1,j}(f, F) = \sum_{n=0}^{\infty} f^n c_n(F)$ is analytic in f for $|f| \leqslant F$ and it is expressed by the Rayleigh–Schrödinger perturbation formula

$$E_{1,j}(f,F) = E_1 + 2\pi jF - f^2 \frac{\oint_{\Gamma} \langle \psi_1, X_{1,2}[H_2 + fX_{2,2} - E]^{-1} X_{2,1} R_1(f)\psi_1\rangle_{\mathcal{H}_1} \mathrm{d}E}{\oint_{\Gamma} \langle \psi_1, R_1(f)\psi_1\rangle_{\mathcal{H}_1} \mathrm{d}E} \tag{4}$$

where $R_1(f)$ is the projection of the resolvent of $H_F(f)$ on $\mathcal{H}_1$, $E_1 = E_{1,0}$, and Γ is the clockwise contour $|E - E_1| = dF^2$, for suitable $d > 0$.

Remark. Let us stress that the above convergent perturbation series $\sum_n^\infty F^n c_n(F) = E_{1,j}(F)$ has F-dependent coefficients. The asymptotic power series expansion $E_{1,j}(F) \sim \sum_n F^n d_n$ is considered elsewhere [12–14].

We give now a sketch of the proof of the proposition [18]. First of all we need to explicitly consider the interband and intraband operators; they act on $(a_1, a_2) \in \mathcal{H}$ as

$$(X_{2,1}a_1)(p) := X_{2,1}(p)a_1(p) \qquad a_1(p) = a_1(k) \qquad \forall p = k + L \qquad \forall L \in \mathbf{Z}$$
$$X_{2,1}(p) = \mathrm{i}\sum_{J\in\mathbf{Z}} w_1^{(p)}(J) \cdot \partial_p w_2^{(p)}(J) \tag{5a}$$

$$(X_{2,2}a_2)(p) := \sum_{L\in\mathbf{Z}} X_{2,2}^L(p)a_2(p+L)$$
$$X_{2,2}^L(p) = \mathrm{i}\sum_{J\in\mathbf{Z}} w_2^{(p+L)}(J-L)\partial_p w_2^{(p)}(J) \tag{5b}$$

$$(X_{1,2}a_2)(k) := \sum_{L\in\mathbf{Z}} X_{1,2}(k+L)a_2(k+L) \qquad X_{1,2}(p) = \overline{X}_{2,1}(p)\,. \tag{5c}$$

Here $w_1^{(k)}(J)$ and $w_2^{(p)}(J)$ are the Fourier coefficients of the periodic functions $u_{1,2}$ (since the Lamé potential is even, they are real analytic), where $\varphi_1(x,k) = \mathrm{e}^{\mathrm{i}kx}u_1(x,k)$ and $\varphi_2(x,p) = \mathrm{e}^{\mathrm{i}px}u_2(x,p)$ are the Bloch functions. Let us stress that $\varphi_2(x,p)$ are orthonormal functions on $L^2([-\pi,\pi], \mathrm{d}x/2\pi)$, so we have $X_{2,2}^0(p) \equiv 0$.

The important point is that the Bloch functions are regular in the quasi-momentum complex plane with the exception of the branch points $z_1^\pm = k_1 \pm \mathrm{i}h_1$, $k_1 = \frac{1}{2}$ and $h_1 > 0$, and in the strip of width $4\alpha_0$ around the x-real axis. Indeed, analyticity of the Bloch function in the quasi-momentum complex plane plays an important role in proving the boundedness of $X_{2,2}$.

Now, by taking the potential as a perturbation, we have that the periodic Bloch function $u_1(x,k)$ is bounded and $u_2(x,p) = 1 + \mathrm{O}(p^{-1})$, uniformly as p goes to infinity, for x and p in the strips $|\mathrm{Im}\, x| \leqslant 2\alpha_0$ and $|\mathrm{Im}\, p| \leqslant h_1/2$ [19]. Hence, from the exponentially decaying behaviour of the Fourier coefficients of $u_{1,2}$, the following estimates hold:

$$|X_{2,2}^L(p)| \leqslant C\exp[-|L|\alpha_0]/(1+p^2) \qquad \text{and} \qquad |X_{2,1}(p)| \leqslant C\exp[-|p|\alpha_0] \tag{6}$$

and, in particular, W is norm-bounded and, as one can verify, relatively compact (Hilbert-Schmidt) with respect to H_F^{DB}.

In order to prove the proposition we should control $R_1(f)$ as a uniformly bounded operator for $E \in \Gamma$ and $|f| \leqslant F$. We consider the expression

$$R_1(f) = R_1(0)\,[1 - A(f)]^{-1} \qquad \text{where} \qquad A(f) = X_{1,2}\,[1 + Q(f)]^{-1}\,T(f)\,. \tag{7}$$

Here, $Q(f) = fR_2(0)X_{2,2}$, $T(f) = f^2R_2(0)X_{2,1}R_1(0)$ and $R_i(0)$, $i = 1, 2$, are the projection of the resolvent of H_F^{DB} on $\mathcal{H}_i$, that is $R_i(0) = [H_i - E]^{-1}$. We are able to prove that $Q^2(f)$ has norm less than 1 for any $|f| \leqslant F$ and $E \in \Gamma$, for F small enough; so that $A(f)$ is a bounded operator. Analogously, we have a norm bound less than 1 for $A(f)$, so that the uniform boundedness of $R_1(f)$ follows and the Rayleigh–Schrödinger series is convergent for $f = F$. These estimates are based on the explicit expression of $R_i(0)$ as an integral operator and on (6). For instance, the operator $T(f)$ is norm bounded by C/d, where C is a positive constant; therefore the norm of $A(f)$ will be less than 1 for a suitable d. In fact, by fixing $f = F$ for simplicity, we obtain for any $v \in \mathcal{H}_1$

$$(Tv)(p) = \frac{1}{(\mathrm{e}^{\rho}-1)}\psi_2(p)U(p)\int_B \psi_1^{-1}(\tau)v(\tau)\mathrm{d}\tau - \psi_2(p)U(p)\int_0^p \psi_1^{-1}(\tau)v(\tau)\mathrm{d}\tau$$
$$- \psi_2(p)\int_p^{+\infty} U(\tau)\psi_1^{-1}(\tau)v(\tau)\mathrm{d}\tau \tag{8}$$

where $\psi_{1,2}$ are the solutions of $[H_{1,2} - E]\psi_{1,2} = 0$ and $\rho = \mathrm{i}(E - E_1)/F$. The above announced estimate on T holds since the integral

$$U(p) = \int_p^{+\infty} X_{2,1}(\tau)\psi_2^{-1}(\tau)\psi_1(\tau)\mathrm{d}\tau \tag{9}$$

is absolutely convergent and, by the stationary-phase method, it is bounded by $FC\{\exp[-\alpha_0|p|] + \chi_{(-\infty,0]}(p)\}$, where χ_I is the characteristic function on the set I. The norm estimate on Q^2 follows in the same way since $\|Q^2\| = \mathrm{O}(\sqrt{F})$ by the stationary-phase method. The sketch of the proof of the proposition is therefore completed.

Let us state some qualitative results which have been previously discussed and which now, following the convergence of the perturbation series, assume a definitive status. From (4) one can easily obtain the second-order perturbation term for $E_{1,j}(F)$:

$$E_{1,j}^2(F) = E_1 + 2\pi jF - \mathrm{i}F\int_{\mathbb{R}}\psi_2(p)\psi_1(p)^{-1}X_{1,2}(p)\int_p^{+\infty}\psi_1(q)\psi_2(q)^{-1}X_{2,1}(q)\mathrm{d}q\mathrm{d}p\,. \tag{10}$$

Integrating by parts the integral of the right-hand side of (10), we have

$$E_{1,j}^2(F) = E_1 + 2\pi jF - F^2\int_{\mathbb{R}}\frac{X_{1,2}(p)X_{2,1}(p)}{\mathcal{E}_2(p) - \mathcal{E}_1(p)}\mathrm{d}p + \mathrm{O}(F^3)\,. \tag{11}$$

Hence, the second order of the regular perturbation theory gives exactly the second order of the asymptotic expansion [12–14] adapted to the case of a finite number of gaps.

Finally, following Avron [10], we compute rigorously, by the saddle point method, the imaginary part behaviour. In fact, the second-order approximation (Fermi golden rule) gives

$$\operatorname{Im} E_{1,j}^2(F) = -F/2\left|\int_{\mathbb{R}} X_{1,2}(p)\exp\left[\mathrm{i}/F\int_{1/2}^{p}(\mathcal{E}_2(\tau) - \mathcal{E}_1(\tau))\,\mathrm{d}\tau\right]\mathrm{d}p\right|^2 \tag{12}$$

where the saddle point z_1 coincides with a polar singularity of $X_{1,2}(p)$ as well as with a branch point of square root type of the band functions. More precisely, let $w_1^{(p)}$ and $w_2^{(p)}$ be $\ell^2(\mathbf{Z})$ analytic vectors on a connected domain Ω of the Riemann four-sheeted surface of $(p-z_1^+)^{1/4}$ containing the interval $[0,1]$, where they are real orthonormal [20]. Thus we have the bilinear scalar product $\langle w_i, w_j \rangle_{\ell^2} \equiv \delta_i^j$ on all Ω. The z_1^+ singularity connects w_1 with w_2 in the sense that, surrounding z_1^+ clockwise once, we have $w_1 \to w_2$ and $w_2 \to -w_1$. So, we can write, in $z = (p - z_1)$, $w_1^{(p)} = z^{-1/4}(a + bz^{1/2})$ and $w_2^{(p)} = \mathrm{i}z^{-1/4}(a - bz^{1/2})$, where a and b are $\ell^2(\mathbf{Z})$ analytic vectors such that $\langle a, a\rangle \equiv \langle b, b\rangle \equiv 0$ and $\langle a, b\rangle \equiv \frac{1}{2}$. Hence,

$$X_{1,2}(p) = \mathrm{i}\langle w_1^{(p)}, \partial_p w_2^{(p)}\rangle = 1/(4z) + \left(\langle a, \partial_p b\rangle - \langle \partial_p a, b\rangle\right) \tag{13}$$

so that $X_{1,2}(p)$ has isolated polar singularities at $p = z_1^{\pm}$ with residue $\pm\frac{1}{4}$. The stationary-phase evaluation is determined by the minimal angle between two steepest descent directions: $4\pi/3$ and the pole residue. So, one has that

$$\mathrm{Im}\, E_{1,j}^2(F) = -FC\left[1 + \mathrm{O}(F^{2/3})\right]\exp[-2\rho_Z(F)] \tag{14}$$

where $C = \pi^2/18$ and $\rho_Z(F)$ is the Zener length of the effective barrier created by the tilted gap:

$$\rho_Z(F) = \int_{\mathrm{barrier}} |\mathrm{Im}\, p[E_F(x)]|\,\mathrm{d}x = \frac{1}{F}\int_{\mathrm{gap}} |\mathrm{Im}\, p(E)|\,\mathrm{d}E = -\frac{\mathrm{i}}{2F}\oint_{\gamma} \mathcal{E}(p)\,\mathrm{d}p\,. \tag{15}$$

$E_F(x) = E_1 - Fx$, γ is a clockwise regular contour around the cut and $p(\cdot) = \mathcal{E}^{-1}(\cdot)$, $\mathcal{E}(p)$ is the energy function defined by $\mathcal{E}(0) = \mathcal{E}_1(0)$ on the Riemann sheet [11, 20] with a cut linking directly z_1^+ and z_1^-. Let us stress that the asymptotic behaviour (14) of the imaginary part of the resonances agrees with the one given by Buslaev and Dmitrieva by a completely different adiabatic approximation. More precisely, in the one-gap case the Buslaev–Dmitrieva approximation gives for the numerical coefficient of the imaginary part the value $\frac{1}{2}$ that should be compared with our one, that is $\pi^2/18$. The above discrepancy on the numerical coefficient is not unexpected since our perturbation method (Fermi golden rule) does not guarantee the exact asymptotic behaviour up to the numerical coefficient. A similar phenomenon has been already observed in a semiclassical problem [21, p 325]: exactly an extra factor $\pi^2/9$ also appears in the first-order Bremmer approximation for a reflection coefficient.

For the case $m > 1$, the existence of m ladders of resonances follows from the degenerate perturbation theory and one can also prove the existence of (avoided) crossing points. In such a problem one expects an accumulation of crossing points and oscillations of the width [10].

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