# The Lifetime of Wannier Ladder States\*

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I study the width of the Wannier ladder states, i.e, Bloch electrons in external homogeneous field. For periodic potentials with a finite number of gaps, a formula for the width is obtained showing that the width vanishes exponentially fast with the field in accordance with Zener tunneling. The case of infinitely many gaps is studied qualitatively, and it is argued that although the width decreases exponentially "on the average," the detailed bahavior is very complicated. In particular the width oscillates over different orders of magnitude as the field changes slightly. The oscillations are a consequence of a resonance phenomenon.

### 1. THE PROBLEM

The Wannier ladder (also referred to as "Stark ladder" or "Wannier-Stark ladder") [26, 27] is a ladder of resonances for the one dimensional Bloch electron in a homogeneous electric<sup>1</sup> field f:<sup>2</sup>

$$H_{f} = p^{2} + V(x) - fx, \qquad V(x + 2\pi) = V(x), \qquad f > 0,$$
  
$$p \equiv -i \frac{d}{dx}.$$
 (1.1)

The field gives the particle a uniform velocity over the Brillouin zone:  $\dot{k} = f$ . Since k + 1 is identified with k by Bragg reflection (the Brillouin zone is a torus) the motion appears periodic and suggests bound states.<sup>3</sup> A simple tunneling argument says, however, that  $H_f$  supports no bound states, so the above argument indicates at best resonances for (1.1). The behavior of  $H_f$  under the shift  $x \to x + 2\pi$  then says that these form ladders parallel to the real energy axis, and the distance between the rungs in any one ladder is  $2\pi f$ .

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<sup>1</sup> Another possible interpretation of the Hamiltonian is for neutrons in crystals under a gravitational field. A discussion of gravitational interference effects for neutrons is given in Ref. [28] and references therein.

<sup>2</sup> The units are  $2m = \hbar = a/2\pi = 1$ , *a* the lattice spacing. The unit of charge is  $e^2 = \pi \hbar^2/ma$  and the unit of force  $\pi h^2/ma^3$ .

<sup>3</sup> It is instructive to contrast (1.1) with H = p + V(x) - fx. *H* is unitarily equivalent to *p* (see footnote (5)) and has no resonances although it has the same symmetry properties as (1.1). The catch is that p + V(x) has no gaps in the spectrum and does not Bragg scatter.

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The question of existence of the Wannier ladder of resonances has attracted some attention [3, 7, 14, 20, 21, 30, 31]. Although from a rigorous point of view this is still an open problem, considerable progress has been made, and the stand I shall take here, which is suggested by the current status of the problem, is that the ladders exist although a proof is still lacking.<sup>4</sup>

The problem I address is calculating the lifetime of the Wannier ladder. Relatively few works have dealt directly with this question. The work of Berezhkovski and Ovchinikov [8] is the one closest to the one given here, but does not discuss the complicated  $f \rightarrow 0$  structure. I also feel that the treatment given here is simpler and more transparent. Finally, I do not replace the homogeneous field potential by a staircase which [8] does. In [3] the width is calculated for a soluble model. There is an error in this work which is corrected here in an appendix. More importantly, however, the soluble model involves a nonlocal periodic potential with sharp momentum cutoffs, and as a consequence the tunneling mechanisms may, in principle, be irrelevant to Hamiltonians with local periodic potentials. In [7] rigorous estimates are given for  $e^{-itH}\psi$  for times of orders of many periods of oscillations which suggest that the width is at most linear in f for small fields. Somewhat stronger results are described in [20]. One question, which [7, 20] leave open, is whether the width is exponentially small, as is the case in other tunneling phenomena [6, 13, 22]. There is numerical evidence [12] that for a Kronig–Penney model with step potential, mimicking the homogeneous field, which levels off out of the "crystal," the Wannier ladder has indeed exponentially small width.

It may be worthwhile to explain the physics behind the mathematical difficulty of calculating the width. The potential V(x) - fx is shown in Fig. 1.1. A localized state has to tunnel through a distance of order of 1/f to get to the region where, had it been a classical particle, it could sail through to infinity. The classical action associated with such tunneling is of order of 1/f suggesting a width  $\Gamma \sim e^{-D/f}$ . The difficulty with this argument is that it disregards the fact that at each and every bump of the



FIG. 1.1. Periodic plus a weak linear potential.

<sup>4</sup> From the work of Herbst and Howland [14] it follows that if V(x) is, e.g., a trigonometric polynomial, certain matrix elements of the resolvent of  $H_f$  are meromorphic functions of the energy. The poles are the Wannier ladder. No Wannier ladder means that the function is entire which seems unlikely. Existence is of course weaker than observable as the above result of Herbst-Howland does not preclude the possibility that the resonances are extremely broad.

periodic potential the particle both reflects and transmits. Going through many bumps is a complicated interference phenomenon. For example, it is easy to arrange for n bumps to transmit better than a single bump. Moreover, since a quantum particle reflects from a bump even if classically it does not, the number of relevant bumps may exceed O(1/f).

Another aspect of the difficulty is that in the limit of  $f \rightarrow 0$  the localized Wannier state disappears. For f = 0 there are only nonnormalizable Bloch waves. The following toy model illustrates what happens in a simpler setting. Figure 1.2a describes an attractive one dimensional "atom" in an electric field. Figure 1.2b describes a repulsive one dimensional atom in an electric field. In Fig. 1.2a there is a bound state for f = 0 which turns into a resonance for f > 0. The width of the resonance is  $\Gamma \sim f^{2/3}e^{-D/f}$  because the classical action for tunneling is proportional to 1/f. In Fig. 1.2b there is a resonance for  $f \neq 0$  which becomes an extended state as  $f \rightarrow 0$ . The action for tunneling through the barrier is essentially a constant and  $\Gamma \sim f^{2/3}$ . The lifetime is a *power* of the field. Is the lifetime of the Wannier ladder more like Fig. 1.2a or like Fig. 1.2b?

There is, of course, a tremendous literature in semiconductor hysics, starting with Zener [32] on tunneling between bands. I shall not attempt to reference this extensive body of knowledge, let alone review it. The reader may consult the review of Duke [11] and the extensive bibliography it gives. Zener tunneling is related to the Wannier ladder width via, e.g., the "tilted band" picture (Fig. 1.3). (The reader who is uncomfortable with this picture would do best to skip the next paragraph. No use of tilted bands is made again in this paper.)



FIG. 1.2a. Tunneling of a bound state in an electric field.



FIG. 1.2b. Tunneling of a resonance state for a repulsive potential in an electric field.



FIG. 1.3. The tilted band picture for the Zener tunneling of electrons between bands.

The Wannier ladder states are localized in an interval of order  $\Delta \varepsilon / f$ ,  $\Delta \varepsilon$  the band width, and acquire their width by tunneling through an interval of order  $\varepsilon_g / f$  with  $\varepsilon_g$ the gap size. For short times this describes the leaking from the original band. However, for two bands the electron will eventually leak to the original band: The lifetime is infinite. To correct for this, infinitely many bands have to be considered which make the analysis much harder. Nevertheless, already at this stage one can see how a sensitivity to f may come about: There will, in general, be a very high band with a Wannier state in resonance with the first band so something special happens. Which band it is depends on the field f in a sensitive way. In any case, as far as the literature on Zener tunneling goes, there is only little direct contact with the Wannier ladder problem.

In Section 2, I shall describe which kind of periodic potentials lead to a tractable Hamiltonian. As I shall explain, the natural candidates such as the Kronig-Penney or the Mathieu potential  $(\cos(x))$  lead to an intractable Hamiltonian. In Section 3, I analyse the simplest class of such models, and obtain a formula for the width of the Wannier states, which essentially vindicates the intuition based on Zener tunneling. In Section 4, a qualitative analysis extends the treatment of Section 3 to more complicated models and  $\cos x$  in particular. The conclusion is that  $f \rightarrow 0$  behavior is extremely complicated in an intrinsic way. In particular, it depends on certain "rationality" conditions on the field f, and varies over many scales as f changes slightly. Section 4 is the main part of this work. Section 5 is the conclusions and a summary. In an appendix, I give details on an explicitly soluble model with nonlocal periodic potential, and correct some errors in [3]. This model has certain perculiar features, but does support the main point of this work, namely, the intricacy of the  $f \rightarrow 0$  limit, and the large oscillations of the Wannier states lifetime.

## 2. Choosing V

The purpose of this section is to motivate the choice of periodic potentials V such that the analysis of H is simple. As I shall argue  $V(x) = \cos(x)$  or the Kronig-Penney model lead to intractable Hamiltonians.

The simple choices are periodic potentials with a finite number of gaps [18]. This shall now be explained.

It is natural to work in a representation that diagonalizes the Bloch Hamiltonian

 $H_0$  and uses the Bloch waves  $|n, k\rangle$  as a basis. This is known as te crystal momentum or Adams representation and its formalism has been described in a basic review article by Blount [9]. Borrowing from [9] the formula for the position operator, x, in this representation one finds that  $H_f$  takes the form

$$H_f = -if d_k + \varepsilon_n(k) - f X_{mn}(k),$$
  
$$-\frac{1}{2} \leqslant k < \frac{1}{2}.$$
 (2.1)

 $\left|-\frac{1}{2},\frac{1}{2}\right|$  is the Brillouin zone.  $\varepsilon_n(k)$  are the band functions, and in (2.1) a choice of gauge is made so that the intraband interaction of x,  $X_{nn}(k)$ , vanishes identically (the gauge freedom is related to  $|nk\rangle \rightarrow e^{i\varphi(k)} |nk\rangle$  with  $\varphi(k)$  periodic of period one).<sup>5</sup>

Setting  $X_{mn}(k) = 0$  in (2.1) gives (real) Wannier ladders as eigenvalues:

$$E_{j,n} = 2\pi j f + \langle \varepsilon_n \rangle, \qquad j = 0, \pm 1, ...,$$
  
$$\langle \varepsilon_n \rangle = \int_{-1/2}^{1/2} \varepsilon_n(k) \, dk, \qquad \langle \varepsilon_n \rangle \to n^2 \text{ as } n \to \infty.$$
  
(2.2)

Depending on whether f is rational or not, the (approximate) eigenvalues in (2.2) will not (will) be dense one the energy axis. The difficulty is that there is no method to compute how such eigenvalues move into the complex when the  $X_{mn}$  interaction is switched on (a small divisor problem [19]).<sup>6</sup> The available method, Fermi Golden Rule, applies to eigenvalues embedded in a *continuous* spectrum [25]. We shall now choose periodic potentials V(x), such that this is the case.

Finite gap potentials are V(x) such that the Bloch Hamiltonian

$$H_B = p^2 + V(x) \tag{2.3}$$

has only a finite number of gaps in the spectrum. An example is Lamés potential

$$V(x) = m(m+1)(tK/2\pi)^2 sn^2(Kx)$$
(2.4)

with  $K \equiv \int_0^{\pi/2} d\varphi (1 - t^2 \sin^2 \varphi)^{-1/2}$ . If *m* is a positive integer, the number of gaps is *m* [18]. Finite gaps potentials are exceptional. "Most" periodic potentials, like  $\cos(x)$  and the Kronig-Penney have all their gaps open [18, 24]. As we shall see, an

<sup>5</sup> This is imprecise. A gauge may be chosen so that  $X_{nn}(k)$  is k-independent. However, because  $\int X_{nn}(k) dk \pmod{2\pi}$  is gauge invariant, it is not always possible to make the constant vanish by gauge transformation. This subtlety is of no consequence for the sequel. I am indebted to J. Zak for this remark. See also Ref. [33].

<sup>6</sup> This is not precise. There are methods of accelerated convergence, associated with Kolmogorov, Arnold and Moser, that handle small divisors. A beautiful application of these techniques to quantum mechanics has been made by E. Dinaburg and Y. Sinai in *Funckcional. Anal. i Priložen.* 9 (1975), 8, for the almost periodic Schrodinger. However, there is, as yet, no application that I am aware of for a resonance equation. If a KAM approach to the Wannier ladder problem was to be made, there is little doubt that diophantine properties of the field would play an important role (*f* has to be badly approximated by rationals). This provides yet another indication of the curious dependence on *f*. *m*-gap potential in the  $X_{mn} = 0$  approximation will lead to *m*-Wannier ladders embedded in a continuous spectrum—as desired.

For an isolated band,  $\varepsilon_n(k)$  and the Bloch waves are periodic in k with period 1. For this reason, Eq. (2.1) has been solved with periodic boundary conditions in k with period 1 to give Eq. (2.2). When two bands,  $\varepsilon_{n-1}(k)$  and  $\varepsilon_n(k)$ , are not separated by a gap (but are still separated from  $\varepsilon_{n-2}(k)$  and  $\varepsilon_{n+1}(k)$ ), it is convenient to combine them to a single band  $E_n(k)$  over a doubled Brillouin zone  $-1 \le k < 1$ . (For the isolated bands, say,  $\varepsilon_{n+2}(k)$ , keep the old Brillouin zone  $-\frac{1}{2} \le k < \frac{1}{2}$ .)  $E_n(k)$  and the associated Bloch waves have period 2 and so do the relvant boundary conditions in Eq. (2.1). In this manner, one finds different Brillouin zones for different bands. In particular, for an *m*-gap potential, where the first *m*-gaps are open and all other gaps are closed, there are *m* Brillouin zones  $-\frac{1}{2} \le k < \frac{1}{2}$  and one infinite Brillouin zone  $-\infty < k < +\infty$ :

$$H_f = -if d_k + \varepsilon_n(k) - f X_{nl}, \ 1 \le l, \ n \le m+1.$$
(2.5)

 $\varepsilon_n(k+1) = \varepsilon_n(k)$  for n = 1,..., m but  $\varepsilon_{m+1}(k) \sim k^2$  as  $k \to \infty$ . The wave function  $\Psi = (\psi_1(k),...,\psi_m(k),\psi_{m+1}(k))$  satisfies  $\psi_n(k+1) = \psi_n(k)$  for all  $1 \le n \le m$  and the norm is

$$\langle \Psi | \Psi \rangle \equiv \sum_{n=1}^{m} \int_{-1/2}^{1/2} |\psi_1(k)|^2 dk + \int_{-\infty}^{\infty} |\psi_{m+1}(k)|^2 dk.$$
 (2.6)

 $X_{nl}$  operates as follows:

$$(X_{nl}\psi_{l})_{n}(k) = X_{nl}(k)\psi_{l}(k), \qquad n, l \neq m+1,$$

$$(X_{n,m+1}\psi_{m+1})_{n}(k) = \sum_{j=-\infty}^{+\infty} X_{n,m+1}(k+j)\psi_{m+1}(k+j),$$

$$(X_{m+1,n}\psi_{n})_{m+1}(k) = X_{m+1,n}(k)\psi_{n}(k),$$

$$X_{nl}(k) = X_{ln}^{*}(k).$$
(2.7)

In addition

$$X_{nl}(k+1) = X_{nl}(k), \qquad 1 \le n, \ l \le m,$$
  
$$X_{n,m+1}(k) \to 0, \qquad |k| \to \infty.$$
(2.8)

The second assertion in (2.8) follows from the observation

$$[x, H_{B}] = -2ip,$$

$$X_{n,m+1}(k) = +2i\langle n, k | p | m+1, k \rangle / [\varepsilon_{n}(k) - \varepsilon_{m+1}(k)].$$
(2.9)

Now, the Bloch wave of the *n*th band  $|n, k\rangle$  is concentrated, in *p*-space, around  $p \sim \pm n$  and decays exponentially fast away from these points. Similarly, for large k the  $|m+1, k\rangle$  Bloch wave is concentrated in p space about  $p \sim \pm (k + m + 1)$  and decays exponentially away from these points. It follows that the matrix element in Eq. (2.9) is an overlap of exponentially small tails and so decays exponentially fast as  $|k| \rightarrow \infty$ . Note also that the denominator increases like  $k^2$ . The fast decay of  $X_{n,m+1}$  for large k will play an important role in Section 3.

Now, the approximation  $X_{nl}(k) = 0$  gives *m*-Wannier ladders embedded in a *continuous spectrum* which arises from  $-if d_k + \varepsilon_{m+1}(k)$ ,  $-\infty < k < \infty$ . The width can therefore be calculated, in principle at least, by the Fermi Golden Rule. This we do in the next section. In the simplest case<sup>7</sup> m = 1 calculating the width, to leading order in *f*, reduces to an integral.

#### 3. ONE WANNIER LADDER

We need a slight generalization of the Fermi Golden Rule. In its simplest setting the Fermi Golden Rule describes how one eigenvalue, embedded in the continuous spectrum, dissolves into a resonance. The situation at hand is complicated by the following two features. First, there are infinitely many such eigenvalues and the imaginary part results from a parallel shift of a whole ladder. Second, the distance between eigenvalues becomes small as the perturbation becomes small. More precisely, both the level spacing and the coupling to the continuum are proportional to the external field f. It turns out that there is a setting for the Fermi Golden Rule that can accommodate these features. It is associated with what is known as Livsic matrix and is described in detail in [16]. In Eq. (3.1) to (3.4) below a brief recapitulation of this scheme is given.

A comment on background might be useful. Resonances, even in the simplest settings, such as typical textbook examples, are often not understood on a rigorous level and some gained this status only recently [6]. One difficulty is what a resonance actually means. One natural definition—a state which eventually decays exponentially—turns out to be empty in most cases (whenever H is bounded below) and even if not, is often extremely hard to verify in concrete examples [34]. The route adopted here is via complex poles of the analytic continuation of certain matrix elements of the resolvent to the nonphysical sheet. Of course the physical content of such a definition is not a priori clear and it also suffers from the ambiguity of which matrix elements are to be chosen for the purpose of continuation. The virtues are that it is an excellent working tool and indeed most of the recent progress (even calculational!) relies on it. For a review the reader should consult Volume 4 of the Reed–Simon series and the special issue of the *International Journal of Quantum Chemistry*, Volume XIV, 1978. Here resonances are defined as the analytic continuation of the

<sup>&</sup>lt;sup>7</sup> It is known that if m = 0, and the periodic potential has no gaps, then V(x) = const; see Ref. [18]. Clearly, there is no Wannier ladder in this case.

resolvent restricted to a fixed band subspace. In the one-gap case, write  $H_f$  as a 2 × 2 matrix of operators:

$$H = \begin{pmatrix} H_1 & -fX_{1c} \\ -fX_{c1} & H_c \end{pmatrix}, \tag{3.1}$$

 $H_1 = -if d_k + \varepsilon(k), \ -\frac{1}{2} \leq k < \frac{1}{2} \qquad \text{and} \qquad H_c = -if d_p + \mathscr{E}(p), \ -\infty < p < \infty.$ 

In the standard Fermi Golden Rule situation,  $H_1$  in (3.1) is a number and not an operator with discrete spectrum. The analysis is, however, similar:

$$R(E) \equiv (H - E)^{-1} \equiv \begin{pmatrix} R_1(E) & S \\ S^+ & R_c(E) \end{pmatrix}.$$
 (3.2)

We shall look at poles of analytic continuations of  $R_1(E)$ . Since [16]

$$R_{1}(E) = [H_{1} - E - (fX_{1c})(H_{c} - E)^{-1}(fX_{c1})]^{-1},$$
(3.3)

poles of  $R_1(E)$  are "eigenvalues" of

$$h(E) \equiv H_1 - K(E),$$
  

$$K(E) \equiv (fX_{1c})(H_c - E)^{-1}(fX_{c1}),$$
(3.4)

i.e.,  $[h(E) - E] \psi(k) = 0$ ,  $\psi(k + 1) = \psi(k)$ . One verifies<sup>8</sup>

$$(H_{c} - E)^{-1}(p, p') = +\frac{i}{f} e_{E}^{-1}(p) e_{E}(p') \theta(p - p'),$$
  
Im  $E > 0,$  (3.5)  
$$e_{E}(p) \equiv \exp{-\frac{i}{f}} \left( Ep - \int_{0}^{p} \mathscr{E}(t) dt \right)$$

h(E) has no eigenvalues in the upper half plane.<sup>9</sup>

The analytic continuation of h(E) to the lower half plane requires only the analytic continuation of K(E). Formally, the analytic continuation is achieved by taking (3.5) for the kernel of  $(H_c - E)^{-1}$  in K(E) even though it does not have the meaning of the resolvent of  $H_c$  in the lower half plane. K(E) has kernel

$$K(E)(k, k') = if \sum_{mn} X_{1c}(k+m) e_E^{-1}(k+m) e_E(k'+n) \times X_{c1}(k'+n) \theta(k+m-k'-n).$$
(3.6)

<sup>8</sup> Note that  $-if d_p + \mathscr{E}(p)$ ,  $\mathscr{E}(p)$  real, is unitarily equivalent to  $-if d_p$  through  $U = \exp(i/f) \int \mathscr{E}(p) dp$ , the latter is diagonalized by Fourier transform. This is one way to derive (3.5).

<sup>9</sup> This is a consequence of the selfadjointness of  $H_{f}$ .

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For Im E > 0 all the terms with large k + m decay exponentially and the convergence of the sum in (3.6) follows "by inspection." In continuing to Im E < 0 the  $e_E^{-1}$  term in (3.6) grows exponentially. Therefore, the sum in Eq. (3.6) converges only if  $X_{1c}$  and  $X_{c1}$  decay (at least) exponentially. This, however, was established in the previous section. With an exponential falloff for  $X_{1c}$  one establishes that K(E) continues to Im  $\ge -cf$  with some c > 0. If, however,  $X_{1c}$  decay faster than exponential Im E will continue to, say Im E > -c independent of f.

Note that h(E) has the nice feature that the original problem of embedded eigenvalues, (3.1), has been converted to one of isolated eigenvalues perturbed by the nonselfadjoint operator K(E). The nonselfadjointness of K(E) is responsible for the possibility of complex eigenvalues. Moreover, one can now resort to the standard, time independent perturbation theory. For K(E) = 0 h(E) has the real eigenvalues given in Eq. (2.2).

First order perturbation theory gives the Fermi Golden Rule

Since the second term in (3.7) is manifestly real

Im 
$$E = -\frac{f}{2} \left| \int_{-\infty}^{\infty} dq \, g_0(q) \right|^2 < 0.$$
 (3.8)

It is now clear from (3.8) and the equation for  $g_0(q)$  that  $\Gamma \equiv -2$  Im E vanishes exponentially fast as f tends to zero. To actually calculate  $\Gamma$  to leading orders in fonce  $\mathscr{E}(q) - \varepsilon(q)$  and  $X_{1c}(q)$  are given, one may use the method of stationary phase. Since in this work no attempt is made to establish the detailed properties of the bands of one-gap potentials, I stop short of such a calculation. The following remark, however, may be useful. As is well known, the method of stationary phase is sensitive to the behavior near the stationary point which, in the present case, is the one of band crossing:  $\mathscr{E}(t_0) = \varepsilon(t_0)$ . For many periodic potentials and  $\cos(x)$  in particular, the bands are branches of one, multisheeted analytic function and band crossings occur at square-root branch points [17]. For this reason it appears reasonable to assume  $\mathscr{E}(p) - \varepsilon(p) = ((1/4)\varepsilon_g^2 + (\varepsilon_g/2\mu) p^2)^{1/2}$ . This is in fact the dispersion originally taken by Zener. However, I want to emphasize that there is no reason why this should be true for a one-gap potential. These are very special, and the general arguments given in [17] do not apply. For all we know, the band crossing may even be a point of analyticity:

$$\mathscr{E}(p) - \varepsilon(p) \sim \varepsilon_{p} + p^{2}/2\mu, \qquad \mu > 0.$$

In this particular case, one finds

$$\Gamma \sim cf^{5/3} |Ai[\varepsilon_g(2\mu/f^2)^{1/3}]|^2 \sim cf^2 \exp{-\frac{2}{3}\varepsilon_g^{3/2}\sqrt{2\mu/f}}.$$
(3.9)

Of course, it is also possible, in principle at least, that the behavior near crossing is neither of the above. For this reason, Eq. (3.9) should be taken as an illustration only. In Ref. [10] there is an extensive discussion of various tunneling formulas obtained by making different assumptions on the dispersion. They would all lead to  $\Gamma \sim Af^{\alpha} \exp(-D/f)$  with different constants A,  $\alpha$ , and D depending on the model. For our purposes, the explicit form of these various constants is of secondary importance.

### 4. WANNIER LADDER INTERACTIONS

In the previous section periodic potentials with a single gap in the band spectrum were shown to give one Wannier ladder whose width is exponentially small with f. This section deals with m such ladders. The new feature that arises for  $m \ge 2$  is the interaction of ladders. As f changes the ladders slide past each other so that on intervals (1/f, 1/f + const) there is at least one near crossing point. The tendency to avoid crossing leads to a complicated  $f \to 0$  behavior.

The m-gaps periodic potentials give m-Wannier ladders. Mimicking the analysis in Section 3 gives the eigenvalue equation

$$[h(E) - E] \psi(k) = 0, \qquad \psi(k+1) = \psi(k),$$
 (4.1)

where  $\psi(k) = (\psi_1(k), ..., \psi_m(k))$  and h(E) in the  $m \times m$  matrix

$$[h(E)]_{jl} = \delta_{jl} [-if d_k + \varepsilon_j(k)] - f X_{jl}(k) - f X_{jc}(H_c - E)^{-1} f X_{cl}, \qquad j, l \in 1, ..., m.$$
(4.2)

Viewing the last term in (4.2) as higher order suggests considering first

$$h_0(E) = -if d_k + \Lambda(k),$$
  

$$[\Lambda(k)]_{jl} \equiv \delta_{jl} \varepsilon_j(k) - f X_{jl}(k).$$
(4.3)

In analysing (4.3) it is useful to describe the ladder interaction in a canonical way. Let U(k) be the unitary transformation that diagonalizes  $\Lambda(k)$ .  $h_0$  takes the form

$$h_0 = -if d_k + \Lambda_D(k, f) - f X_I(k, f),$$
(4.4)



FIG. 4.1. Interacting (dashed line) and noninteracting (solid lines) ladders in the finite band approximation.

where  $\Lambda_D(k, f)$  is a diagonal matrix and  $X_I \equiv iU^{-1}(k) d_k U(k)$  is hermitian. Multiplying U(k) by a diagonal matrix one can always arrange for  $X_I$  to vanish on the diagonal.<sup>5</sup>

 $X_i(k)$  vanishes identically if  $[\Lambda(k), \Lambda(k')] = 0$ . In this case  $h_0$  can be readily diagonalized and gives intersecting curves, as in Fig. 4.1. The asymptotic slopes of the curves, as  $f \to 0$ , is given by  $\langle \varepsilon_j \rangle$ .  $X_i = 0$  is therefore a situation where suitably "rotated" ladders do not interact at all. From this point of view  $X_i$  is the "true" interladder interaction. Of course  $X_i \neq 0$  is atypical. With  $X_i \neq 0$  the eigenvalues tend to avoid crossings,<sup>10</sup> and the qualitative spectrum is shown in the figure in dashed lines. It follows that each individual eigenvalue has an oscillatory component in 1/f. For one eigenvalue, and m = 2, the picture is schematically as in Fig. 4.2.

For *m*-Wannier ladders, the behavior becomes increasingly more complicated. Figure 4.3 describes schematically m = 3. A somewhat unusual feature of this problem is that ladders coming from arbitrarily high energy bands can not be neglected even though the coupling to such bands is weak, because as long as the coupling is not exactly zero, it will affect the behavior near crossing. This peculiar sensitivity is, of course, due to resonance.

It seems more or less clear that the change in qualitative properties due to ladder interactions for  $h_0$  have analogs in h(E). For fixed f, h(E) has resonances with width  $\Gamma_j \rightarrow \infty$  [14]. Typically, levels coming from higher bands tend to have short lifetimes. But, near crossings there is mixing of levels which leads to mixing of the lifetimes.

To calculate the lifetime an estimate for the wave function is needed. Let  $|\psi\rangle$  be a normalized eigenvector of h(E) with eigenvalue E. Clearly

$$\operatorname{Im} E = \langle \psi \mid \operatorname{Im} h(E) \mid \psi \rangle$$
  
=  $-\operatorname{Im} \langle \psi \mid f X_{ic} (H_c - E)^{-1} f X_{cl} \mid \psi \rangle.$  (4.5)

Taking eigenvalues of  $h_0$  as approximations to the exact eigenvectors gives an estimate for the lifetime.

<sup>&</sup>lt;sup>10</sup> A precise statement due to Wigner and von-Neumann [29] is that for  $n \times n$  selfadjoint matrices, those with two-fold degeneracy have codimension 3. The corresponding result in the nonselfadjoint case which is more relevant here is that the codimension is 2 [5].



FIG. 4.2. The dependence on the electric field f of an interacting ladder energy in a two band approximation.



FIG. 4.3. The dependence on the electric field f of an interacting ladder energy in a three band approximation.

When  $X_I = 0$  the eigenfunctions of (4.4) are

$$\exp -\left(\frac{i}{f}\int_{0}^{k}\left[\Lambda_{j}(k,f)-\langle\Lambda_{j}(k,f)\rangle-2\pi fn\right]dk\right).$$
(4.6)

 $\Lambda_j(k, f) \to \varepsilon_j(k)$  as  $f \to 0$  and *n* is an integer. This situation is similar to the one encountered in Section 3, because of the absence of ladder interaction. One finds that each ladder has an exponentially small width, i.e.,  $\Gamma_j \sim e^{-D_j/f}$ . Since  $D_j \neq D_k$  for  $j \neq k$  the lifetimes are of different orders of magnitudes in the sense that  $\Gamma_j/\Gamma_k$  diverges to infinity (or zero) as  $f \to 0$ .

What happens when  $X_I \neq 0$ ?  $X_I$  leads to mixing of the eigenfunctions and consequently to mixing of the lifetimes.

For the sake of orientation consider what happens when complex eigenvalues of a  $2 \times 2$  matrix couple near crossings:

$$M(t) = \begin{pmatrix} t + i\varepsilon & X \\ \overline{X} & i\varepsilon^n \end{pmatrix}.$$
 (4.7)

t is a real variable playing in (4.7) the role of (1/f). t = 0 is the point of near crossing.  $\varepsilon$  is small and plays the role of the width.<sup>11</sup> The two widths  $\varepsilon$  and  $\varepsilon^n$ , n > 1, are of different orders of magnitude as expected of the noninteracting lifetimes in the original problem. The interlevel coupling is hermitian, as  $X_t$  is. The eigenvalues are

$$\frac{1}{2}(t+i\varepsilon+i\varepsilon^{n})\pm\frac{1}{2}[(t+i\varepsilon-i\varepsilon^{n})^{2}+4|X|^{2}]^{1/2}.$$
(4.8)

Suppose now that X becomes small with  $\varepsilon$ . For t of order unity Eq. (4.8) gives imaginary parts of order  $\varepsilon$  and of order  $|X|^2 \varepsilon^{12}$  ( $\varepsilon^n$  if  $|X|^2 \ll \varepsilon^{n-1}$ ). In the terminology used above, the two lifetimes are on different scales. Near crossing,  $|t| < (|X|, \varepsilon)$ , both imaginary parts in Eq. (4.8) are of order  $\varepsilon$  if  $2|X| > \varepsilon$  (and of order  $\varepsilon$  and  $|X|^2/\varepsilon$  if  $2|X| < \varepsilon$ ). The time scale for the decay of the more stable eigenvalue  $(1/\varepsilon)^n$  or  $(|X|^2\varepsilon)^{-1}$  shortens to  $\varepsilon^{-1}$  (or to  $\varepsilon/|X|^2$ ). Note that if  $\varepsilon > 2|X|$  the imaginary parts of (4.8) do not cross at t = 0 and the real parts do while if  $\varepsilon < 2|X|$  it is the other way round. The situation is summarized in Fig. 4.4.

One way to translate these results to the problem at hand is to estimate the mixings of the wave functions (4.6) due to  $X_I$ , and plug in Eq. (3.5) to obtain the lifetime. However, since I am after qualitative results only it is possible to take a short cut. Identify  $\varepsilon$  and  $\varepsilon^n$  with the  $\Gamma_j$  of the two ladders and X with the Zener coupling between the two ladders. Indeed, the overlap between two crossing Wannier states due to the coupling  $X_I$  is

$$\int_{-1/2}^{1/2} X_{I_{jl}}(k') \, dk' \exp \frac{i}{f} \int_{0}^{k'} \left[ \Lambda_{j}(k) - \Lambda_{l}(k) - \langle \Lambda_{j} \rangle + \langle \Lambda_{l} \rangle - 2\pi n_{j} f + 2\pi n_{l} f \right] dk, \quad (4.9)$$

defining X in Eq. (4.7). Since the two levels are near crossing

$$\langle A_i \rangle + 2\pi n_i f \sim \langle A_i \rangle + 2\pi n_i f$$
 (4.10)

and the phase in (4.9) is proportional to the (band gap)/f.  $X^2$  is related to the Zener tunneling between the j and l bands. (Compare Eq. (3.8).)

What does this imply for two Wannier ladders? There are two cases:

(a)  $\Gamma_2 \ll |X|$  when Zener tunneling between the two bands is fast while leaking to infinity of the second ladder is slow. ( $\Gamma_2 > \Gamma_1$  is assumed.)

(b)  $|X| \ll \Gamma_2$ . (This is the normal situation.)

In case (a) the behavior of the imaginary part of the energy is shown schematically in Fig. 4.5. Thus a Wannier ladder that started with a narrow width, say,<sup>12</sup>  $|X|^2 \Gamma_2$ , will, upon crossing with the second ladder, acquire its width  $\Gamma_2$ . In the complex energy plane the ladder performs a "Virginia reel." Since there is crossing at every

<sup>&</sup>lt;sup>11</sup> Of course  $\varepsilon$  is a function of t in the original problem, but here it is convenient to regard them as independent variables.

<sup>&</sup>lt;sup>12</sup> This has the natural interpretation of the width being the product of probabilities of tunneling to the second band and then to the continuum.



FIG. 4.4. Interlevel interaction near "crossing." When the coupling is strong relative to the imaginary parts (the two upper figures), the levels avoid crossing in the real part but the lifetimes cross. When the coupling is weak relative to the imaginary parts, it is the lifetimes that avoid crossing while the real parts cross.



FIG. 4.5. The behavior of the lifetime for two interacting ladders as functions of the field f in the case that the two bands are strongly coupled to each other but weakly coupled to the rest of the spectrum. Note that the overall exponential decrease of the lifetime with f has been factored out.



FIG. 4.6. The same as in Fig. 4.5 except that now the two bands are weakly coupled to each other and one of them is strongly coupled to the continuum.

interval (1/f, 1/f + O(1)) the lifetime will fluctuate between  $\Gamma_1$  and  $\Gamma_2$ . Although both  $\Gamma_1$  and  $\Gamma_2$  are small the fluctuations are large in the sense that  $\Gamma_1/\Gamma_2 \to 0$ .

In (b) the picture is different, and is shown schematically in Fig. 4.6. The ladder has width of order, say,<sup>12</sup>  $|X|^2 \Gamma_2$ , away from crossings. But, in a small interval of size proportional to |X| (related to the Zener tunneling) around the crossing point the width increases and is of order  $|X|^2/\Gamma_2$ . ( $\Gamma_2 \ll 1$  is assumed.) This differs from the one in (a) in that as f becomes smaller the size of the intervals where the width is large shrinks fast to zero. However, in both cases near the crossing the width changes by many orders of magnitudes (a factor of  $(\Gamma_2)^2$  in (b) and a factor of  $|X|^2$  in (a)).

This picture can now be generalized to *m*-ladders. As long as levels cross in pairs and there are no simultaneous crossings of three or more, the behavior near the crossing point is as if there are only the two relevant levels. The behavior of the width, for one level, is shown schematically in Fig. 4.7.

Thus a Wannier level that started with a long lifetime will, upon crossing with a "wider" level k, acquire a shorter lifetime. The larger the number of gaps or ladders, the larger the available k's, and the more frequent the crossing.

Since  $\Gamma_m \to \infty$  as *m* does, while the coupling to high bands decreases with *m*, the interactions between the ladders effectively stop for  $m \ge m_0$  with  $\Gamma_{m_0}$  of order one, say. However,  $m_0$  increases as *f* becomes small, which implies that in the  $f \to 0$  limit there are essentially infinitely many interacting ladders. The spikes in Fig. 4.7 will presumably be everywhere dense although the total measure under them may be quite small.



FIG. 4.7. The schematic behavior of a Wannier state lifetime as a function of the field f when the field is small. After an overall exponential behavior is factored out one finds a complicated behavior ranging over many scales.

This suggests that for a typical periodic potential, such as the Mathieu  $V(x) = \cos x$ , where there are infinitely many gaps, a Wannier ladder state has width that is sensitive to f. The width is a complicated function of f in an essential way: It has Cantor-like behavior,

Finally, I point out that the absense of scale, typical to "Cantor-like" behavior, is not uncommon in solid state physics. Other examples are Bloch electrons in magnetic fields |15| and almost periodic potentials [1, 2].

## 5. CONCLUSIONS AND SUMMARY

Qualitative arguments suggest that the lifetime of the Wannier ladder may have an intrinsically complicated behavior for small fields: The widths change dramatically as f changes slightly. This results from resonances between low and high bands. The analysis has, at its present stage, limited quantitative power.

As is well known, the Wannier ladder has been a tantalizing experimental problem [30]. The common attitude is that this is due to technical reasons having to do with the difficulty in realizing the idealization embodied in the one electron Hamiltonian (e.g., collision with phonons, impurities, many body effects, etc., may not be neglected). It has been suggested by some, and J. Zak in particular, that the problem may be one of principle, namely, that even the idealization in Eq. (1.1) may not have sufficiently long-lived resonances [31].<sup>13</sup> For example, if the lifetime decreases linearly (or slower) with f the resolution of an individual level may be poor.

The present work was partly motivated by a talk given by Eva Andrei at Caltech, in which she described a new experimental approach based in part on the following observation: In superlattices [23], the ratio of band gaps to band widths can be made large compared to typical values in semiconductors. This should give the Wannier ladder states a longer lifetime. A second virtue is that the Brillouin zone in superlattices is very small, so with moderate fields one has the possibility that the electron may wrap around the Brillouin zone for many times before it scatters. Finally, the period potential is produced via an optical grating which causes the relevant Schrodinger equations to separate and gives a one dimensional problem.

This spurred me to investigate afresh whether the width of the ladder in one dimension is given, as the folklore says, by a Zener type formula and so is exponentially small or whether it may be so wide for Zak's criticism to apply. I should emphasize, however, that there does not appear to be a convincing argument, [3, 4, 7, 20] notwithstanding, for the width to be linear with the field.

For special periodic potentials which I discussed in Section 3, the behavior of the width is calculated and found to be essentially as predicted by the Zener argument, i.e., exponentially small. However, for typical periodic potentials, say,  $\cos x$ , due to interactions of ladders coming from high energy band the width oscillates wildly as

<sup>&</sup>lt;sup>13</sup> More accurately, Zak pointed out that existing derivations of the Wannier ladders were inadequate.

function of the field. The  $f \rightarrow 0$  behavior is so bizarre that each individual level essentially covers presumably an exponentially narrow strip through wild oscillations.

It should be stressed that only the one dimensional problem has been treated here. In quantum mechanics, spectral properties are sensitive to dimensionality so it is not obvious how, if at all, the one dimensional results transfer to three. Of course, the experiments with grating, sketched above, are one dimensional, but for most solid state applications this is not the case. One additional complication in higher dimensions is that the semiclassical orbit  $\vec{k}(t) = \vec{ft} + \vec{k_0}$  may or may not cover the Brillouin zone ergodically according to the rationality of the direction  $\vec{f}$ .

As is well known, a Bloch electron in homogeneous magnetic field exhibits sensitive dependence on B having to do with rationality of the flux through a unit cell [10, 15, 31]. Here a vaguely related phenomenon takes place in one dimension and homogeneous electric field. The lifetime of the Wannier states is sensitive to the field.

On the day this paper was sent to the printer, I received a letter from V. Grecchi which describes the results of numerical computations which seem to agree with the picture proposed in Section 4. Grecchi, together with E. Zironi, considered the following model: A finite one dimensional Kronig-Penny crystal (with attractive delta functions) and a step-like electric field applied to the crystal only: Namely, for a crystal of length L the potential is zero to the left of the crystal and is fL to its right.

In this model it is straightforward to calculate the transfer matrix for each unit cell. The transfer matrix for the whole crystal is then calculated numerically to yield the reflection coefficient. The resonances are defined as complex poles in the analytic continuation of the relection coefficient to complex energies. By considering a finite crystal and defining resonances this way Greechi and Zironi achieve in fact a more realistic model than the one presented here (an infinite crystal and resonances as certain poles of the resolvent). It is therefore reassuring that both models seem to agree on the essential features.

As f changes slightly  $(\Delta f/f \sim 1/15)$ , Grecchi and Zironi find changes in three orders of magnitude in  $\Gamma$ . The plot of  $-f \ln \Gamma(f)$  as a function of f reveals a bump and a step in the particular range of parameters they communicated to me. The step is presumably a consequence of a do-si-do of a narrow and a wide resonance (i.e., an exchange of widths) while the bump forms when the two resonances advance and retire as in a minuet.

## APPENDIX: A SOLUBLE MODEL

Here I shall describe a soluble model for the Wannier ladder with a nonlocal periodic potential V. The model was described first in [3] and is close in spirit to the finite gap potentials. Because of the nonlocal nature of V the situation here is different from that treated in the paper. The reason for the inclusion is to correct certain errors in [3].



FIGURE A.1

1

Let

$$H_0 = p^2 / 2m - fx, (A.1)$$

$$H = H_0 + vV, \tag{A.2}$$

where in momentum space V has kernel

$$V(p, p') = \delta(p - p' - 1)\chi_{01}(p') + \delta(p - p' + 1)\chi_{-1,0}(p').$$
(A.3)

One verifies that  $V = V^+$  and commutes with translation  $x \to x + 2\pi$ . The corresponding Bloch Hamiltonian has one gap in its spectrum, and the band spectrum is shown schematically in Fig. A.1. The anomalous second band is a consequence of nonlocality. The resolvent for  $H_0$  has kernel

$$R_{0}(E) = (H_{0} - E)^{-1}(p, p') = +\frac{i}{f} e_{E}^{-1}(p) e_{E}(p') \theta(p - p'), \qquad (A.4)$$
$$\operatorname{Im}(E/f) > 0,$$
$$e_{F}(p) = \exp{-\frac{i}{f}} (Ep - p^{3}/6m).$$

Notice that under the complex translation  $x \rightarrow x + a$ 

$$H_a \equiv T_a H T_a^{-1} = H_0 - fa + v \{ e^{-ia} T_{-1} \chi_{01} + e^{ia} T_1 \chi_{-10} \},$$
(A.5)

where  $T_K$  is the translation  $p \rightarrow p + K$ . Equation (A.5) is relevant in that we shall look for resonances in the translation analytic sense, i.e., eigenvalues of  $H_a$  for complex *a* but independent of *a* [14] for, say, Im a > 0 (for real *a*,  $H_a$  has no eigenvalues, of course). Schrodinger's equation for the eigenvalues of  $H_a$  is

$$\psi_a(p) = v R_0^{(a)}(E) \ V^{(a)} \psi_a(p), \tag{A.6}$$

$$\psi_q(p) = 0, \qquad p < -1,$$
 (A.6i)

$$\varphi_a(p) = \beta \int_{-1}^{p} \left[ K_t^{-1}(p') e^{-ia} \right] \varphi_a(p'+1) dp', \quad -1$$

$$\varphi_a(p) = \varphi_a(0) + \beta \int_0^p \left[ Q_I^{-1}(p') e^{ia} \right] \varphi_a(p'-1) \, dp', \qquad 0$$

$$\varphi_a(p) = \varphi_a(1), \qquad 1 < p, \tag{A.6iv}$$

where

$$\varphi(p) \equiv e_E(p) \psi(p),$$

$$K_E(p) \equiv e_E^{-1}(p) e_E(p+1),$$

$$Q_E(p) \equiv e_E^{-1}(p) e_E(p-1),$$

$$t = E + af,$$

$$\beta = -iv/f.$$
(A.7)

If we choose Im a > -Im(E/f),  $\psi(p) \to 0$  as  $p \to \infty$  exponentially. Except for this boundary condition that dictates a minimal choice of Im *a*, the equations are *a*-independent since the square brackets in (A.6ii, iii) are. This is the notion of translation analytic resonance. Differentiating (A.6ii) and substituting (A.6iii) and then differentiating again results in

$$\varphi''(p) + \left(\frac{d\ln K_E(p)}{dp}\right)\varphi'(p) - \beta^2\varphi(p) = 0, \quad -1 (A.8)$$

This is the harmonic oscillator is disguise since

$$\varphi(p) \equiv [K_E(-1)/K_E(p)]^{1/2} Y(s)$$
(A.9)

gives

$$2mvs \equiv p + \frac{1}{2},$$
  
$$\hbar^2 \ddot{Y}(s) + [1 - s^2 + i\hbar] Y(s) = 0, \qquad \hbar \equiv f/2mv^2.$$
(A.10)

The limit  $f \to 0$  is therefore the semiclassical limit  $\hbar \to 0$ .

The boundary condition, at p = -1, for Eq. (A.10) is incorporated in the integral equation (A.6ii), which is a Dirichlet boundary condition. This gives

$$Y(s) = Y_o(D/2) Y_e(s) + Y_e(D/2) Y_o(s),$$
  

$$D \equiv 1/2mv.$$
(A.11)

 $Y_{o,e}$  are the odd, even solutions of (A.10). Now that Eq. (A.11) and (A.9) give  $\varphi(p)$  on  $-1 , we use Eq. (A.6ii) to get <math>\varphi(p)$  on the interval 0 by differentiating

$$\beta \varphi(p+1) = K_E(p) \, \varphi'(p), \qquad -1$$

This can be rewritten as

$$\varphi'(p) = \beta Q_E(p+1) \varphi(p+1), \quad -1 (A.12')$$

Equation (A.12') gives the second boundary condition to make the differential equation (A.10) a decent eigenvalue problem, by substituting p = -1. This relates  $\varphi'(-1)$  and  $\varphi(0)$ . Since  $\varphi(0) = 2Y_o(D/2) Y_e(D/2)$ , Eq. (A.12') at p = -1 reads

$$\exp\frac{i}{f}\left(E-\frac{1}{6M}\right) = \frac{i\hbar}{2} \frac{d\ln(Y_o/Y_e)}{ds} \bigg|_{s-D/2}.$$
 (A.13)

Equation (A.13) is an explicit equation for the resonance energies E. Clearly, if E solves (A.13) so does  $E + 2\pi f$ , giving the requisite ladder.

To calculate E in the limit  $f \rightarrow 0$  we can, by (A.10), use WKB to evaluate the rhs of (A.13). This gives

$$\exp\frac{i}{f}\left(E - \frac{1}{6M}\right) \sim \frac{i(1+D/2+i\hbar)^{1/2}}{\sin(2/\hbar)\int_0^{D/2} (1+t^2-i\hbar)^{1/2} dt}.$$
 (A.14)

So for  $\Gamma = -2 \operatorname{Im} E$  we find

We find

$$tgh^{-2}(\theta) \geqslant R \geqslant 1$$
 (A.16)

so  $\Gamma \ge 0$  as it should. Moreover, since  $\hbar$  is proportional to f the width oscillates between 0 and cf with period 1/f (Fig. A.2). This behavior is reminiscent of (although simpler than) the behavior discussed in Sections 4 and 5 for local potentials.



FIGURE A.2

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