Metastable Bloch oscillators

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Abstract. We give in a rigorous way the time behavior of the metastable Bloch oscillators for weak electric field. The validity of the Fermi Golden Rule, with the change of the numerical pre-factor suggested by Kane and Blount, is definitely proved. Moreover, we give a new version of the acceleration theorem and the localization of Bloch oscillators in the adiabatic limit.

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Our aim is to give a better description and understanding of the dynamics of an electron in an one-dimensional crystal moving under the effect of an homogeneous external field, usually called Bloch oscillators (BO) [1] or Wannier-Stark (WS) problem [2]. The WS Hamiltonian is

$$H = \frac{p^2}{2m} + V(x) + eFx, \quad V(x) = V(x+d)$$

where $V(x)$ is the periodic crystal potential with period d, e is the electron charge and F is the strength of the electric field. If a single band packet is initially localized about a given value k_0 of the crystal momentum (quasi-momentum) variable then oscillations of the electron wavefunction (hereafter called Bloch oscillators) with period $T_B = 2\pi\hbar/|eF|d$ are expected because of the acceleration theorem [3] and the periodicity of the band function. Actually, BO are observable in superlattices [4], but not in bulk materials [5].

On the other side, at each period we make experience of a tunneling effect and the state gradually goes into the other bands. Therefore, the BO behavior depends on the value of the probability of transmission [6]. The transmission across a barrier created by a "tilted gap" goes back to Zener [7] and it was identified with the transition between close levels in adiabatic problems.

Some time later, Wannier discussed the existence of metastable states (hereafter SW states) or resonances on a sound basis [8]. Recently, it was proved the existence of ladders of resonances by means of the regular perturbation series starting from the Wannier approximation and it was computed their lifetime by means of the Fermi Golden Rule (FGR), that is at the second perturbation order approximation [9]. At this order a $(\pi/3)^2$ numerical pre-factor appeared. In contrast, the estimate given by Buslaev and Dmitrieva [10], by means of an adiabatic approximation in the x-space, shows the absence of this factor. Therefore the validity of the FGR was put in doubt, and, for what concerns the probability of transmission, Kane and Blount [11] proposed the elimination of the same numerical pre-factor.

We discuss now the first point of this letter: the exact computation of WS resonances and the validity of the FGR for weak electric field. To this end we consider here a simplified model with two bands, one finite and the other infinite [12], and where the contributions due to phonons, interactions, impurities, etc., are neglected. We assume also, for the sake of definiteness, $\hbar^2 = 2m$, $f = eF > 0$, $d = 2\pi$ and the crystal potential symmetric (i.e. $V(-x) = V(x)$). The crystal momentum representation of the WS Hamiltonian operator has the form

$$H_f = H_f^{DB} + f\tilde{X}$$

and it acts on $L^2(\mathcal{B}, dk) \oplus L^2(R, dp)$ where $\mathcal{B} = [0, 1)$ is the Brillouin zone; k denotes the crystal momentum variable in the finite band and p denotes the crystal momentum variable in the infinite band (sometimes are both denoted by p for the sake of simplicity). $H_f^{DB} = \mathrm{diag}(H_1, H_2)$ is the decoupled band approximation, $H_1 = if\frac{d}{dk} + \mathcal{E}_1(k)$, $H_2 = if\frac{d}{dp} + \mathcal{E}_2(p)$ and $\tilde{X}$ is the coupling term. We stress that the first band function $\mathcal{E}_1(k)$ is a periodic function with period 1 while the second band function $\mathcal{E}_2(p)$ has the asymptotic behavior $\mathcal{E}_2(p) = (p-1/2)^2(1+O(p^{-1}))$ as p goes to infinity; moreover they are real-analytic functions with branch points of square root type at $k_c = 1/2 + ir_c$ and $\bar{k}_c$, $r_c > 0$: $\Lambda(k_c) = \Lambda(\bar{k}_c) = 0$ where $\Lambda(p) = \mathcal{E}_2(p) - \mathcal{E}_1(p)$ [13].

The discrete spectrum of the decoupled band approximation H_f^{DB} consists of one ladder of simple real eigenvalues $e_j(f) = \langle \mathcal{E}_1 \rangle + 2\pi j f$, $j = 0, \pm 1, \pm 2, \ldots$, where $\langle \mathcal{E}_1 \rangle$ is the mean value of the first band function, with associated eigenvectors $\phi_j = (\omega_j, 0)$, where

$$\omega_j(k) = \exp\left[i2\pi jk + (i/f)\int_0^k [\mathcal{E}_1(\nu) - \langle \mathcal{E}_1 \rangle] d\nu \right].$$

When we restore the coupling term $\tilde{X}$ then the ladder of real eigenvalues $e_j(f)$ becomes a ladder of resonances $E_j(f) = E_0(f) + 2\pi jf$, $\Im E_0(f) < 0$, associated to WS states.

In order to exactly compute these resonances we introduce now a technical hypothesis [14] regarding the anti-Stokes line such that $\Im\left[\int_{\bar{k}_c}^p \Lambda(\nu)d\nu\right] = 0$ and starting at the Kohn singularity $\bar{k}_c$ with asymptotic direction $\pi/6$. The hypothesis says that the anti-Stokes line has no other points with the same imaginary part of $\bar{k}_c$. Under this hypothesis the FGR is true and we give now an idea of the proof leaving to a forthcoming paper the detailed proof [15]. Let $E_j(f)$ be a resonance and let $\Phi_j^\lambda = (\Omega_j, \Gamma_j^\lambda)$ be the associated wave function:

$$[H_f^\lambda - E_j(f)]\Phi_j^\lambda = 0 \tag{1}$$

where $\|\Gamma_j^\lambda\|_{L^2(R)} = O(f)$ as f goes to zero. Resonances are defined here as complex discrete eigenvalues, in the strip $f\Im\lambda < \Im z < 0$, of the non-symmetric operator $H_f^\lambda = \mathcal{U}_\lambda H_f \mathcal{U}_\lambda^{-1}$ where $\mathcal{U}_\lambda$ is an one-parameter family of analytic distortions [16]. For the sake of simplicity we drop λ if not necessary. By means of the Adams-Wannier method [17] we obtain

$$\Omega_j(k) = \omega_j(k)\exp[ig_n(k,f)] + O(f^n)$$

for any positive integer n where $g_n(k,f)$ is a real-valued function. Therefore $\langle \Omega_j, \Omega_{j'} \rangle_{L^2(\mathcal{B})} = \delta_j^{j'} + O(f^\infty)$. By multiplying (1) by the vector $(\Omega_j, 0)$ and by using the first resolvent formula, then we obtain the following expression for the imaginary part of the resonance:

$$\Im E_j(f) = -(|I(f)|^2/2) f e^{-2\rho_Z} (1 + O(f))$$

as f goes to zero where

$$\rho_Z = -(i/f) \int_{\Re \bar{k}_c}^{\bar{k}_c} \Lambda(p) dp. \tag{2}$$

By means of the convergent perturbation series, by introducing the "semi-classical action" variable $s(p) = (1/f) \int_{\bar{k}_c}^{p} \Lambda(\nu) d\nu$ and by making the above assumption on the anti-Stokes line then we have $I(f) = \sum_{n=0}^{\infty} I_n(f)$ where this series is uniformly convergent for f small enough and where [18]

$$I_n(f) = 2(i\pi/6)^{2n+1}/(2n+1)! + O(f^{2/3}).$$

Hence, it follows that $I(f) = i + o(1)$ as f goes to zero. Therefore we have shown, under a technical condition surely true in a class of double band models, the validity of the FGR for the WS problem where we replace the numerical pre-factor $|I_0| = \pi/3$ with 1. The transition from $\pi/3$ to 1 goes as the sinus series. There is evidence that the correct result is also given by Adams-Wannier iteration scheme by means of the Abel sum of the series

$$1 = \pi/3 + \pi/3 \sum_{n=1}^{\infty} (1/6)_n (-1/6)_n \beta^n/(n!)^2,$$

where $\beta = 1 - 0$ and $(\alpha)_n = \alpha(\alpha+1)...(\alpha+n-1)$.

Let us stress that (2) could also be written as

$$\rho_Z = \int_{\text{barrier}} |\Im p(E(x))| dx,$$

where $E(x) = E_1^t - fx$ and E_1^t is the top of the first band; hence, it represents the Agmon length of the Zener barrier. Moreover, going back to the true units and using a recent result [19] it follows that ρ_Z can be directly written in terms of the periodic potential $V(x)$, and so the imaginary part of the resonance is given by:

$$\Im E_j(f) = -(d/4\pi) f e^{-2\rho_Z} (1 + o(1))$$

as f goes to zero, where

$$\rho_Z = \frac{m\pi}{8|eF|\hbar^2}\int_0^d [V(x) - \langle V\rangle]^2 dx \tag{3}$$

and $\langle V\rangle$ is the mean value of the crystal potential. Now, since [20]

$$P = 2|\Im E_j|/\hbar = pT_B^{-1},$$

where T_B^{-1} is the frequency of the periodic motion in the band and P is the probability of transmission of a single WS state per unit time, then the leading term of the probability of transmission p per period is given by [21]

$$p = e^{-2\rho_Z}. \tag{4}$$

We discuss now the second point of this letter: the time behavior of BO and the single band version of the acceleration theorem [22]. Let $\psi^t(k)$ be a state initially in the first band, i.e. $\psi^0(k) = (a^0(k), 0)$. Let c_j be the Fourier coefficients of the series $a^0(k) = \sum_{j\in Z} c_j\Omega_j(k) + O(f^\infty)$, i.e. $c_j = \langle e^{idjk}, a^0/\Omega_0\rangle_{L^2(\mathcal{B})}$. The projection on the first band of the state has the following time behavior

$$a^t(k) = |c|^2\Omega_0^t(k)\left[\left(a^0/\Omega_0\right)(k - ft/\hbar) + O(f^\infty)\right] \tag{5}$$

for any $d_1/f < t < d_2/|\Im E_0(f)|$, for some $d_1, d_2 > 0$ independent of f, where $c = 1 + O(f^2)$ and $\Omega_0^t(k) = e^{-iE_0t/\hbar}\Omega_0(k)$. So we have BO, with period T_B and tunneling probability (4), for at least two $c_j \neq 0$ and the single band version of the acceleration theorem for localized $a^0(k)$. In this case we have a connection between T_B, the probability of transmission p and the SW states lifetime (coinciding with the BO lifetime). Notice that the interval of validity of (5) contains a number of periods T_B of the order $e^{d_3/f}$ for some $d_3 > 0$. In order to prove (5) we consider the time evolution of the state $\psi^t(k)$. By an analytic complex distortion $\mathcal{U}_\lambda$ with $\Im\lambda < 0$ then we have [23]

$$\begin{aligned}\psi^t &= \sum_{j\in Z}\frac{1}{2\pi i}\oint_{\gamma_j}\mathcal{U}_\lambda^{-1}P_j\mathcal{U}_\lambda\psi^0\frac{e^{-iEt/\hbar}dE}{E_j(f) - E} + \\ &\quad + \frac{1}{2\pi i}\oint_{\tilde\gamma}\mathcal{U}_\lambda^{-1}[H_f^\lambda - E]^{-1}\mathcal{U}_\lambda\psi^0 e^{-iEt/\hbar}dE\end{aligned}$$

where γ_j is a closed circle surrounding the resonance $E_j(f)$, $\tilde\gamma$ is a closed path surrounding the line $f\lambda + R$ and P_j is the eigenprojection on the eigenspace spanned by Φ_j^λ. Therefore, the time behavior of the state ψ^t is described by means of a superimposition of the WS resonant states up to an error of the order $O(e^{t\Im\lambda f/\hbar})$ which can be neglected for $t > d_1/f$. The eigenprojection P_j can be computed by means of the vector $c(\Omega_j, 0)$, where $c \equiv c(\lambda)$ is a normalization constant independent of j, obtaining so the time behavior (5).

Since f is small, it is relevant to consider the adiabatic behavior of the BO, obtained for large t such that $\tau = ft/\hbar$ is fixed, when $a^0(k)$ is a continuous and f—independent function. The adiabatic behavior, obtained by a distributional limit, is given by

$$a^t(k) \sim a_f^\tau(k) = e^{i\pi/4}\omega_0(k)\sqrt{\pi f/|\mathcal{E}_1'(k)|} \times$$
$$\times (a^0/\omega_0)(k-\tau)\left[\delta(k-\tau/2) + i\delta(k-\tau/2-\pi/d)\right]$$

for small f when $d\tau/2\pi$ is not integer (otherwise $a_f^\tau(k) = a^0(k)$), greater than $dd_1/2\pi\hbar$ and less than d_4/f for some $d_4 > 0$ (δ denotes the Dirac delta). It directly follows from (5) because of the limit $\Omega_0^t(k) \to \omega_0(k)$ and the stationary phase effect. Therefore, we have a natural localization at two points in the crystal momentum space. These two points move with the same velocity, given by half of the one of the acceleration theorem, and the distance between them is half of the width of the Brillouin zone. In particular, at each period T_B one of these points reaches the point of minimal distance between the two bands and so the connection between T_B, p and $|\Im E_0(f)|$ has the same meaning.

Let us close with a brief discussion of BO for a model with two (or more) finite bands [24]. Ad discussed in a previous paper [25], for certain classes of potentials we have beating effect before the decay of the state when the two ladders of resonances cross. At such values of the electric field we have quasi periodic damped oscillations and the state is spread over the two bands. In the other cases we have the same picture of the single ladder model for any value of the electric field.

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Bibliography

1. Bloch F, Z. Phys. **52** (1928) 555; see also Bentosela F, Commun. Math. Phys. **68** (1979) 173.

2. It has been object of an increasing interest in the last years since the introduction of superlattices; see, for instance, Di Carlo A, Pötz W and Vogl P, Phys. Rev. B **50** (1994) 8358 and the references therein. Recently, attention has been also directed to WS problems with strongly singular potentials given by a sequence of Dirac δ', see Avron J, Exner P and Last Y, Phys. Rev. Lett. **72** (1994) 896.

3. Acceleration theorem says that $\hbar\langle\dot{k}(t)\rangle = eF$, see for instance §6.1.1 in Callaway J *Quantum theory of the solid state* (Academic Press, New-York, 1974).

4. Waschke C, Roskos H G, Schwedler R, Leo K, Kurz H, Köhler K, Phys. Rev. Lett. **70** (1993) 3318.

5. The accepted reason consists in the phonon scattering effect; see, for instance, the paper by Rossi F *Bloch oscillations and Wannier-Stark localization in semiconductor superlattice* to appear on *Theory of transport properties of semiconductor nanostructures* edited by Schöll E (1996).

6. A first computation of the probability of transmission for an approximate double band model gave $p \sim \exp[-\pi E_G^{3/2} m^{1/2}/2\sqrt{2}\hbar|eF|]$ where E_G is the width of the gap separating the two bands, see Kane E O, J. Phys. Chem. Solids **12** (1959) 181.

7. Zener C, Proc. R. Soc. **145** (1934) 523.

8. Wannier G H, Phys. Rev. **117** (1960) 432.

9. Grecchi V, Maioli M, Sacchetti A, J. Phys. A: Math. Gen. **26** (1993) L379, and Grecchi V, Maioli M, Sacchetti A, Commun. Math. Phys. **159** (1994) 605.

10. Buslaev V and Dmitrieva L, Leningrad Math. J. **1** (1990) 287.

11. Kane E O and Blount E *Interband tunneling* in *Tunneling phenomena in solids*, ed. Burstein E and Lundqvist S (Plenum Press - New York, 1969) 79.

12. An example of such models is the Lamé potential $V(x) = 2t^2 \mathrm{sn}^2(x;t)$ where $\mathrm{sn}(x;t)$ is an Jacobian elliptic function with modulus $t \in (0,1)$; see Avron J, Ann. Phys. **143** (1982) 33.

13. Kohn W Phys. Rev. **115** (1959) 809.

14. A similar hypothesis appears also in adiabatic problems, see Joye A, J. Phys. A: Math. Gen. **26** (1993) 6517.

15. Grecchi V and Sacchetti A 1996 *Lifetime of the Wannier-Stark resonances and perturbation theory*, Commun. Math. Phys. (to be published).

16. Reed M and Simon B *Methods of Modern Mathematical Physics: IV Analysis of operators,* (Academic, New-York, 1978).

17. This method has been developed by Adams and Wannier [8] and it has been resumed by Nenciu G , Rev. Mod. Phys. **63** (1991) 91, for a large class of models.

18. Berry M V, J. Phys. A: Math. Gen. **15** (1982) 3693.

19. Korotyaev E *The estimates of periodic potentials in terms of effective masses,* (1996) preprint.

20. See §119 in Landau L and Lifsitz E *Quantum mechanics*, (Pergamon, Oxford, 1959).

21. In a 100Å—20Å$GaAs - Al_{0.3}Ga_{0.7}As$ superlattice model, discussed by means of the envelope function approximation, m plays the role of the effective mass (assumed constant here) given by $m = 0.067m_0$, where m_0 is the free—mass of the electron, and the potential $V(x)$ is approximated by a Krönig-Penney potential with barrier high $0.213eV$. For an electric field with strength $F = 20KV/cm$ the probability of transmission per period is $p = 0.4773 \times 10^{-11}$.

22. Grecchi V and Sacchetti A, work in progress.

23. A clear description of the time behavior of a metastable state in terms of resonant states is given by Simon B, Annals of Mathematics **97**

(1973) 247. For what concerns Stark type problems see Herbst I W, Commun. Math. Phys. **75** (1980) 197.

24. See the paper by Bastard G, Ferreira R, Chelles S and Voisin P, Phys. Rev. B **50** (1994) 4445, and the experimental results obtained by Schneider H, Grahn H T, Klitzing K v and Ploog K, Phys. Rev. Lett. **65** (1990) 2720.

25. Grecchi V and Sacchetti A, Ann. Phys. **241** (1995) 258.