Metastable Bloch Oscillators

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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 prefactor suggested by Kane and Blount, is definitely proved. Moreover, we give a new version of the acceleration theorem and the behavior of the Bloch oscillators in the adiabatic limit. [S0031-9007(97)03209-2]

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Our aim is to give a better description and understanding of the dynamics of an electron in a one-dimensional crystal moving under the effect of a homogeneous external field. In particular, this problem concerns at least three effects: the Bloch oscillators (BO) [1], the Wannier-Stark (WS) localization [2], and the Zener tunneling. 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 (hereafter called Bloch oscillator) is initially localized about a given value k_0 of the crystal momentum (quasimomentum) variable, then oscillations 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 has been observed in superlattices [4], but not in bulk materials [5].

On the other side, because of the tunneling effect, the state gradually goes into the other bands. Actually, this effect could destroy the Bloch oscillations [6]. The study of the transmission across a barrier created by a "tilted gap" goes back to Zener [7] and it was related to the transition between close levels in adiabatic problems.

Later, Wannier obtained stationary states for the single band approximated problem [8]. Recently, the existence of ladders of resonances associated to resonant states (hereafter called WS states) has been proved by means of the convergent perturbation series starting from the Wannier approximation, and their lifetime has been computed by means of the Fermi golden rule (FGR), that is, at the second perturbation order [9]. At this order a numerical prefactor equal to $(\pi/3)^2$ appears. However, the estimate that Buslaev and Dmitrieva [10] have given, 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. Let us also recall that, for what concerns the probability of transmission, Kane and Blount [11] proposed the elimination of the same numerical prefactor in the formula obtained by Kane himself [6].

Now, we discuss 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 a simplified model with two bands, one finite and the other one infinite [12], 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 that the crystal potential is symmetric [i.e., $V(-x) = V(x)$]. The crystal momentum representation of the WS Hamiltonian operator takes 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 they are both denoted 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. The first band function $\mathcal{E}_1(k)$ is a periodic function with period 1 and the second band function $\mathcal{E}_2(p)$ has the asymptotic behavior $\mathcal{E}_2(p) = (p - \frac{1}{2})^2[1 + O(p^{-1})]$ as p goes to infinity; moreover, they are analytic functions with branch points of square root type at $k_c = \frac{1}{2} + ir_c$ 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 spectrum of H_1 consists of one ladder of simple real eigenvalues $e_j(f) = \langle\mathcal{E}_1\rangle + 2\pi jf$, $j = 0, \pm1, \pm2, \ldots,$ where $\langle\mathcal{E}_1\rangle$ is the mean value of the first band function, with associated eigenvectors $\psi_j = (a_{1,j}, a_{2,j})$, where $a_{2,j} = 0$ and

$$a_{1,j}(k) = \exp\left[i2\pi jk + (i/f)\int_0^k [\mathcal{E}_1(q) - \langle\mathcal{E}_1\rangle]\,dq\right].$$

When we restore the coupling term $\tilde{X}$ then the ladder of real eigenvalues $e_j(f)$ becomes a ladder of resonances

$E_j(f) = E_0(f) + 2\pi j f$, $\Im E_0(f) < 0$, associated with WS states. Resonances are defined here as complex discrete eigenvalues, in the strip $f\Im\lambda < \Im z < 0$, of the nonsymmetric operator $H_f^\lambda = \mathcal{U}_\lambda H_f \mathcal{U}_\lambda^{-1}$, where $\mathcal{U}_\lambda$ is a one-parameter family of analytic distortions [14] and $\Im\lambda < 0$. For the sake of simplicity we drop λ if not necessary.

In order to compute exactly these resonances we introduce a technical hypothesis [15]: the two lines, starting from $\overline{k}_c$ with asymptotic direction $\pi/6$ and $5\pi/6$ and such that $\Im[\int_{\overline{k}_c}^p \Lambda(q)\,dq] = 0$ (anti-Stokes lines), belong to the complex strip $-r_c < \Im p < 0$. Under this hypothesis the FGR is true and we give now a sketch of the proof leaving to a forthcoming paper the detailed proof [16]. Let $E_j(f)$ be a resonance and let $\hat\psi_j^\lambda = (\hat a_{1,j}, \hat a_{2,j}^\lambda)$ be the associated wave function:

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

where

$$\hat a_{1,j}(k) = a_{1,j}(k)[1 + O(f)] \tag{2}$$

and $\|\hat a_{2,j}^\lambda\|_{L^2(R)} = O(f)$ as f goes to zero. By multiplying (1) by the vector $(\hat a_{1,j}, 0)$ and by using the first resolvent formula, 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

$$\rho_Z = -(i/f)\int_{\Re\overline{k}_c}^{\overline{k}_c} \Lambda(p)\,dp\,. \tag{3}$$

By means of the above hypothesis and the convergent perturbation series, by introducing the "semiclassical action" variable $s(p) = (1/f)\int_{\overline{k}_c}^p \Lambda(q)\,dq$ and by using a formula given by Berry [17], we obtain that $I(f) = \sum_{n=0}^\infty I_n(f)$ where this series is uniformly convergent for f small enough and where

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

Hence, it follows that $I(f) = i + o(1)$ as f goes to zero. Therefore we have shown, under a technical condition surely true for a class of double band models, the validity of the FGR for the WS problem where we replace the numerical prefactor $|I_0| = \pi/3$ by 1. The transition from $\pi/3$ to 1 goes as the Taylor series of the sine function computed at $\pi/6$.

There is evidence that the correct result is also given by the Adams-Wannier iteration scheme [18] 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 $(\alpha)_n = \alpha(\alpha+1)\cdots(\alpha+n-1)$.

Let us stress that (3) can 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.

Finally, going back to the true units, 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, using a recent result [19], ρ_Z can be directly written in terms of the periodic potential $V(x)$:

$$\rho_Z = \frac{m}{4|eF|\hbar^2}\int_0^d [V(x) - \langle V\rangle]^2\,dx\,, \tag{4}$$

$\langle V\rangle$ denotes the mean value of the crystal potential. Now, from [20] we have

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

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, so that the probability of transmission per period p has the leading behavior [21]

$$p \sim e^{-2\rho_Z} \quad \text{as } f \longrightarrow 0\,. \tag{5}$$

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., $\psi^0(k) = (a_1^0(k), 0)$, where $a_1^0(k)$ is a periodic f—independent smooth function with period $d/2\pi$. The projection $a_1^t(k)$ on the first band of the state $\psi^t(k)$ has the following time behavior

$$a_1^t(k) \sim a_{1,0}^t(k)\,(a_1^0/a_{1,0})\,(k - ft/\hbar) \tag{6}$$

for small f, for any t, $d_1 f^{-1}\ln(f^{-1}) < t < d_2/|\Im E_0(f)|$, where $d_1, d_2 > 0$ are independent of f, and $a_{1,0}^t(k) = e^{-iE_0 t/\hbar}a_{1,0}(k)$. Thus, we have BO, with period T_B and tunneling probability (5), and a new version of the acceleration theorem for $a_1^t(k)$ [3]. In this case we have a connection between T_B, the probability of transmission p, and the lifetime of the WS states (coinciding with the BO lifetime). The interval of validity of (6) contains a number of periods T_B of the order $e^{d_3/f}$ for some $d_3 > 0$.

In order to prove (6) we consider the time evolution of the state $\psi^t(k)$. By the spectral theorem and by performing an analytic complex distortion $\mathcal{U}_\lambda$ with $\Im\lambda < 0$, we have [23]

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

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 $\tilde{\Psi}_j^\lambda$. Therefore, the time behavior of the state ψ^t is described by means of a linear combination of the WS resonant states up to an error of the order $O(f^{-3}e^{t\Im\lambda f/\hbar})$, which can be neglected for $t > d_1 f^{-1}\ln(f^{-1})$. In particular, by projecting ψ^t on the first band we obtain a Fourier series for $a^t(k)$ which gives

$$a_1^t(k) = |c|^2 \sum_{j\in Z} \hat{a}_{1,j}(k) e^{-iE_j t/\hbar}[c_j + O(f)] \sim \hat{a}_{1,0}^t(k) \left[\sum_{j\in Z} c_j e^{idj(k - ft/\hbar)}\right]$$

for small f, where $c \equiv c(\lambda) = 1 + O(f)$ is a normalization constant independent of j, $\hat{a}_{1,j}(k) = e^{idjk}\hat{a}_{1,0}(k)$, $E_j = E_0 + fdj$, and $c_j = \langle e^{idjk}, a_1^0/\hat{a}_{1,0}\rangle_{L^2(\mathcal{B})}$ are the Fourier coefficients of the function $a_1^0(k)/\hat{a}_{1,0}(k)$.

Since f is small, it is relevant to consider the adiabatic behavior of BO, given for large t and $\tau = ft/\hbar$ fixed. The adiabatic behavior, obtained by means of a distributional limit, is given by

$$a_1^t(k) \sim a_1^{\tau,f}(k) = e^{i\pi/4} a_{1,0}(k) \sqrt{\pi f / |\mathcal{E}_1'(k)|} \times (a_1^0/a_{1,0})\,(k - \tau) \times [\delta(k - \tau/2) - i\delta(k - \tau/2 - \pi/d)]$$

for small f and $\tau d/2\pi$ not integer [otherwise $a_1^{\tau,f}(k) = a_1^0(k)$] and large enough ($\delta$ denotes the Dirac delta function). It directly follows from (6) because of the stationary phase effect. Therefore, we have a natural localization at two opposite points in the crystal momentum space. Each point moves with a velocity equal to one half of the value given by the acceleration theorem. 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 as above.

Let us end with a brief discussion of BO for a model with two (or more) finite bands [24]. As discussed in a previous paper [25], for certain classes of potentials we have a beating effect before the decay of the state when the two ladders of resonances cross. At such values of the electric field we have quasiperiodic 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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