Waves Dynamics in Disordered Media

TD 1: Bloch oscillations

March, 12, 2014

Abstract

In the presence of a static spatially periodic potential, quantum transport properties are strongly modified, with counter-intuitive behaviors such as the so-called Bloch oscillations.

In order to describe transport properties, we take a simple model where – in addition to a static spatially periodic potential – an homogeneous force is applied on the particles (modelling an electric field for charged particles or a gravitational field). The dynamics in the plane perpendicular to the field is unaffected and we can use a simple 1D model:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) - F(t)\hat{x} \tag{1}$$

with m the mass of the particle, $F(t)$ the time-dependent field and $V(x)$ the static potential with period a.

1 Accelerated frame

The applied field breaks the periodicity of the potential. It is however possible to recover spatial periodicity by moving to the accelarated frame. Starting from a state $|\psi(t)\rangle$ evolving with an arbitrary Hamiltonian $\hat{H}(t)$, one can perform the following unitary transformation:

$$|\tilde{\psi}(t)\rangle = \hat{U}(t)|\psi(t)\rangle \tag{2}$$

Show that $|\tilde{\psi}(t)\rangle$ obeys the Schroedinger equation with Hamiltonian:

$$\tilde{\hat{H}}(t) = \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t) + i\hbar\frac{\mathrm{d}\hat{U}(t)}{\mathrm{d}t}\hat{U}^\dagger(t) \tag{3}$$

The unitary operator (depending on the arbitrary function $p_0(t)$):

$$\hat{U}_1(t) = \mathrm{e}^{-ip_0(t)\hat{x}/\hbar} \tag{4}$$

is a translation operator in momentum space such that:

$$\hat{U}_1\hat{x}\hat{U}_1^\dagger = \hat{x}, \qquad \hat{U}_1\hat{p}\hat{U}_1^\dagger = \hat{p} + p_0(t) \tag{5}$$

Show, that for a convenient choice of $p_0(t)$, this unitary transformation transforms the Hamiltonian, eq. 1, into:

$$\hat{H}_1(t) = \frac{[\hat{p} - A(t)]^2}{2m} + V(\hat{x}) \tag{6}$$

which is spatially periodic.

By performing a second unitary transformation, a translation in configuration space:

$$\hat{U}_2(t) = \mathrm{e}^{-ix_0(t)\hat{p}/\hbar} \tag{7}$$

such that:

$$\hat{U}_2\hat{x}\hat{U}_2^\dagger = \hat{x} - x_0(t), \qquad \hat{U}_2\hat{p}\hat{U}_2^\dagger = \hat{p}, \tag{8}$$

show that one obtains, up to a global phase factor which can be eliminated by a third unitary transformation, an Hamiltonian:

$$\hat{H}_2(t) = \frac{\hat{p}^2}{2m} + V(\hat{x} - x_0(t)) \tag{9}$$

Show that this Hamiltonian is associated with the classical equation of motion in an accelerated frame.

2 Bloch theorem

The Hamiltonian $\hat{H}_2(t)$ being invariant by a translation by a in configuration space, one can use the (time-dependent) Bloch theorem which states the general solution of the Schroedinger equation can be chosen as a linear combination of solutions with a fixed quasi-momentum q of the form $\mathrm{e}^{iqx}u(x,t)$ where $u(x,t)$ is a spatially periodic function. For the original Hamiltonian $\hat{H}(t)$, show that it implies that the Bloch structure is preserved during time evolution, that is that an initial state:

$$\psi(x,0) = \mathrm{e}^{ixq_{\mathrm{initial}}}u(x,0) \tag{10}$$

will evolve to:

$$\psi(x,t) = \mathrm{e}^{ixq(t)}u(x,t) \tag{11}$$

where the time-dependent quasi-momentum is given by:

$$q(t) = q_{\mathrm{initial}} + \frac{1}{\hbar}\int_0^t F(t')\mathrm{d}t' \tag{12}$$

and the temporal evolution of u given by:

$$i\hbar\frac{\mathrm{d}|u(t)\rangle}{\mathrm{d}t} = \hat{H}_{\mathrm{periodic}}[q(t)]\ |u(t)\rangle \tag{13}$$

with:

$$\hat{H}_{\mathrm{periodic}}[q] = \frac{(\hat{p}+\hbar q)^2}{2m} + V(\hat{x}) \tag{14}$$

3 Adiabatic approximation

In order to solve eq. (13), some approximations must be performed. For a not-too-strong field, $q(t)$ varies slowly and the adiabatic approximation can be used: if the initial state $u(x,0)$ is a Bloch wave in the the first band (that is the ground state $\phi_{0,q_{\mathrm{initial}}}$ of eq. (14), the solution of the Schroedinger equation is given by

$$\psi(x,t) \approx \mathrm{e}^{ixq(t)}\phi_{0,q(t)}(x) \tag{15}$$

For a constant force, show that the temporal evolution is periodic with period:

$$\tau_{\mathrm{B}} = \frac{2\pi\hbar}{aF} \tag{16}$$

Give a physical interpretation of the corresponding energy $\hbar\omega_{\mathrm{B}} = \hbar 2\pi/\tau_{\mathrm{B}}$ in terms of the tilted lattice potential $V(x) - Fx$.

One now considers an initial wavapacket built by combining several Bloch waves $\phi_{0,q}(x)$. Show that the temporal evolution remains periodic in the adiabatic approximation. If the initial distribution in q is centered around a value $\overline{q}_{\mathrm{initial}}$ narrower than $2\pi/a$, the wavepacket will propagate with a group velocity:

$$\frac{\mathrm{d}\bar{x}}{\mathrm{d}t} = v_{\mathrm{g}}(t) = \frac{1}{\hbar}\left.\frac{\mathrm{d}E_{0,q}}{\mathrm{d}q}\right|_{q=\overline{q}(t)} \tag{17}$$

where $E_{0,q}$ is the dispersion relation in the first band (lowest eigenvalue of $\hat{H}_{\mathrm{periodic}}[q]$). Show that, in configuration space, the center of the wavepacket oscillates with amplitude:

$$L = \frac{\Delta}{F} \tag{18}$$

where Δ is the width of the first band. These oscillations are called Bloch oscillations.

What happens if the initial distribution in q is not narrower than $2\pi/a$?

4 Deep lattice

What happens for a deep lattice where $|V(x)| \gg \frac{\hbar^2}{ma^2}$?

5 Shallow lattice

Make a schematic plot of the band structure $E_{n,q}$ for a shallow lattice where $|V(x)| < \frac{\hbar^2}{ma^2}$? What is the amplitude of the Bloch oscillations? Show that they are very anharmonic for a very shallow lattice.

Figure 1 shows experimentally recorded velocity distributions of a cold atomic gas in an optical lattice exposed to a constant uniform force. Interpret these results in terms of Bloch oscillations? Which phenomenon takes place at $t = \tau_{\mathrm{B}}/2$? Among the three plots in the right part of the figure, which one corresponds to the shallowest lattice?

6 Beyond the adiabatic approximation

The previous approach predicts that there is zero long range transport whatever the F value, that is that the system is always an insulator. However, for $V(x) \to 0$, one should recover free particles where the transport is known to be ballistic. The next sections aim at understanding how to smoothly connect these pictures.

We first consider the situation where no disorder is present. Plot schematically the band structure in the limit of small $V(x)$. Show that the adiabatic approximation is likely

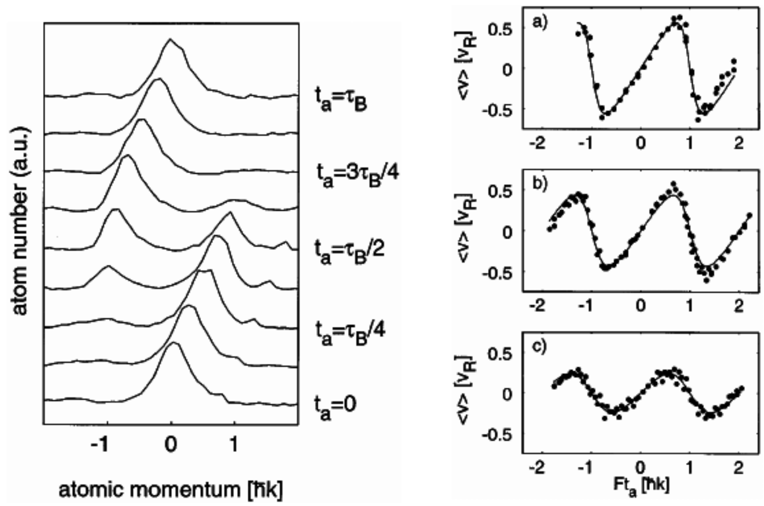

Figure 1: Bloch oscillations observed with a cold atomic gas. The left plot shows velocity distributions recorded at successive times and the right plot the average velocity of the wavepacket as a function of time, for various lattice strengths. From [2]

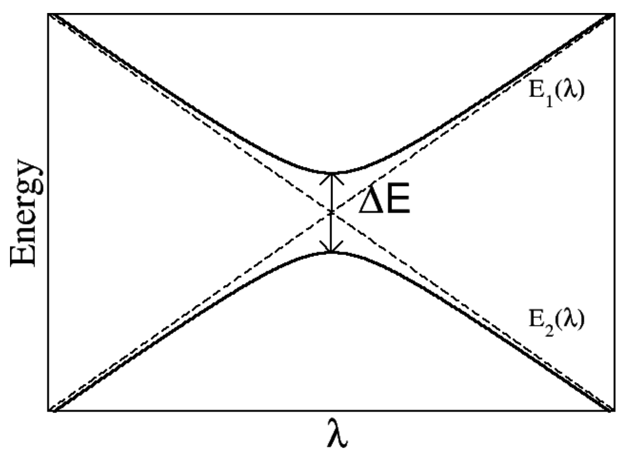

Figure 2: The Landau-Zener scenario. When crossing an avoided crossing by changing in time the parameter λ, the probability of staying in the same state is given by Eq. 20.

to fail at the edge of the Brillouin zone $q = \pm\pi/a$. For simplicity, we will consider a periodic potential:

$$V(x) = V_0 \sin^2(kx) \tag{19}$$

with $k = \pi/a$. In the limit of small V_0 (with respect to what?), show that the first band gap at the edge of the Brillouin zone has a width $V_0/2$. How do other band gaps scale with V_0?

One recalls the Landau-Zener formula, see Fig. 2: the probability of adiabatically following an avoided crossing (i.e. arrive on the lower branch and stay on it) is given by:

$$P = 1 - \exp\left(-\frac{\pi \Delta E^2}{2\hbar\alpha}\right) \tag{20}$$

where $\alpha = \frac{\mathrm{d}\lambda}{\mathrm{d}t}\frac{\mathrm{d}(E_2 - E_1)}{\mathrm{d}\lambda}$, with the slopes $\mathrm{d}E/\mathrm{d}t$ is evaluated far from the avoided crossing.

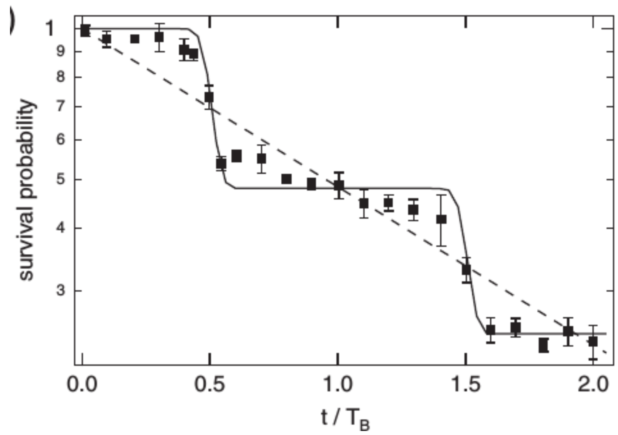

Figure 3: Probability of staying in the lowest band. From [3].

Show that the probability of crossing adiabatically the edge of the Brillouin zone is given by:

$$P(F) = 1 - \mathrm{e}^{-F_c/F} \tag{21}$$

with F_c the "critical" force given by:

$$F_c = \frac{\pi}{32}\frac{V_0^2}{E_\mathrm{r}}k \tag{22}$$

with $E_\mathrm{r} = \hbar^2k^2/2m$ the "recoil" of "Fermi" energy of the particle (for cold atoms and electrons respectively).

In figure 3, the experimentally measured probability of staying in the lowest band is shown vs. time for $V_0 = E_\mathrm{r}$ and $\hbar\omega_\mathrm{B} = 0.4E_\mathrm{r}$. Interpret these results.

Even if $F < F_c$, non-adiabatic processes will limit the lifetime of the of the Bloch oscillations. What will happen when particles cross daibatically the edge of the Brillouin zone? Show that a ballistic motion is eventually restored.

7 Effect of disorder; damping of the Bloch oscillations

Figure 4 shows Bloch oscillations of Strontium atoms under the influence of gravity. The force is weak enough for non-adiabatic transitions to be negligible. It also shows Bloch oscillations of electrons in a semiconductor superlattice under the influence of an electric field. These results show that the Bloch oscillations are damped.

In a (over)-simplified phenomenological model, one can assume that scattering events randomize the direction of the particle wavevector with a constant rate $1/\tau$. In the absence of scattering events, we will assume an harmonic dispersion relation $E_{0,q} \propto \cos(qa)$ and thus a group velocity $v \propto \sin(qa)$. Show that the average velocity correlation function is:

$$\overline{v(t')v(t+t')} = \overline{v}^2 \cos(\omega_\mathrm{B}t) \tag{23}$$

In the presence of scattering, it will become:

$$\overline{v(t')v(t+t')} = \overline{v}^2 \cos(\omega_\mathrm{B}t)\ \mathrm{e}^{-t/\tau} \tag{24}$$

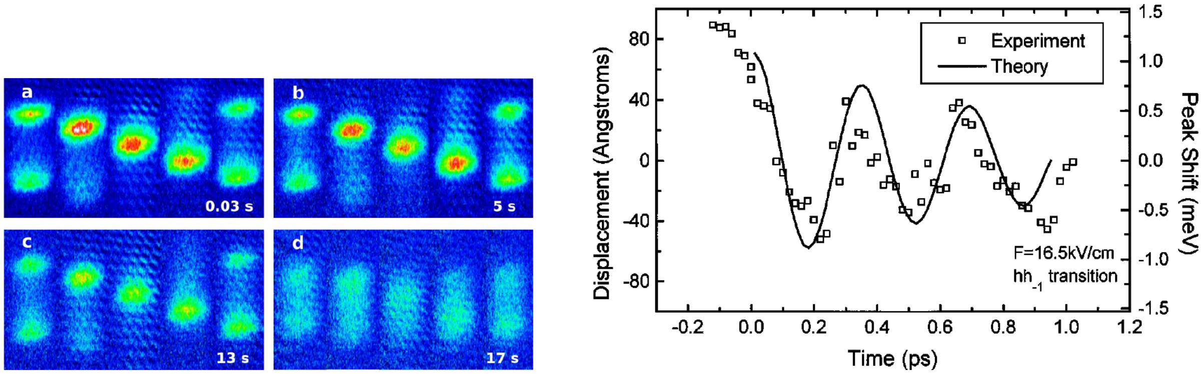

Figure 4: Left: Bloch oscillations observed with a cold Sr atomic gas. Successive images correspond to oscillation 1, 2900, 7500 and 9800. From [4]. Right: Bloch oscillations observed with electrons in a semiconductor superlattice. From [5].

Compute the diffusion constant and the conductivity of an electron gas. Show that one recovers the Drude formula when $\tau \ll \tau_{\mathrm{B}}$ and a reduced conductivity otherwise.

8 Observation of Bloch oscillations with electrons

In a good metal like Copper, Silver or Gold, the scattering time τ is of the order of 0.1 ps. Estimate the order of magnitude of the electric field required for observing Bloch oscillations. Suppose that this electric field produced a current according to the Drude formula. Estimte how much power would be dissipated per volume...

In semiconductors, the situation is better, but τ is still too short to observe Bloch oscillations. Explain why semiconductor superlattices make the observation easier (Hint: Eqs. (16) and (22); see [6] for a review paper).

For the experiment shown in fig. 4, the electric field was of the order of 10 kV/cm and the period of the superlattice of the order of 10 nm. Compare the theoretical predictions with the experimental observations.

References

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