FIP10601 – Text 6

Bloch electrons in the presence of external fields

After discussing the conduction band of a metal viewed as a Bloch-electron system in thermodynamic equilibrium at nonzero temperature, we turn now to its response to external applied fields. Time-varying fields are in general associated to electromagnetic radiation, and hence related to optical properties. In solids, they can be useful to probe the band structure. Here we will focus on static fields, which cause stationary response. We will begin by studying the effect of an applied electric field on the Bloch states, then we will present a quantum treatment of magnetic-field effects, and finish with the description of Bloch-electron dynamics in the *semiclassical approximation*.

Electric field – quantum treatment

In the presence of a *static* and *uniform* electric field $\mathbf{E}$, the Hamiltonian of a single electron is

$$\mathcal{H} = \frac{p^2}{2m} + V(\mathbf{r}) + e\mathbf{E}.\mathbf{r} \equiv \mathcal{H}_0 + e\mathbf{E}.\mathbf{r} \; . \tag{1}$$

By hypothesis, we know how to solve the energy-eigenvalue problem in the absence of field,

$$\mathcal{H}_0\psi_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_n(\mathbf{k})\psi_{n\mathbf{k}}(\mathbf{r}) \; . \tag{2}$$

Note that the term $\mathbf{E}.\mathbf{r}$ breaks the invariance under lattice translations.

Let us assume that the electric field is applied at time $t = 0$, when the electron was in a certain Bloch state $\psi_{n\mathbf{k}}(\mathbf{r})$. We then have an *initial condition*

$$\psi(\mathbf{r}, 0) = \psi_{n\mathbf{k}}(\mathbf{r}) \; , \tag{3}$$

and the time evolution is given by

$$\psi(\mathbf{r}, t) = \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}\psi(\mathbf{r}, 0) \; . \tag{4}$$

Let us see what is the effect of lattice translations on $\psi(\mathbf{r}, t)$.

$$T_{\mathbf{R}}\psi(\mathbf{r}, t) = T_{\mathbf{R}}\mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}\psi(\mathbf{r}, 0) = T_{\mathbf{R}}\mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}T_{\mathbf{R}}^{-1}T_{\mathbf{R}}\psi(\mathbf{r}, 0) \; . \tag{5}$$

It is easy to verify that

$$T_{\mathbf{R}}\mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}T_{\mathbf{R}}^{-1} = \mathrm{e}^{-\mathrm{i}T_{\mathbf{R}}\mathcal{H}T_{\mathbf{R}}^{-1}t/\hbar} \; , \tag{6}$$

and that

$$T_{\mathbf{R}}\mathcal{H}T_{\mathbf{R}}^{-1} = \mathcal{H} + e\mathbf{E}.\mathbf{R} \; . \tag{7}$$

Moreover, $\psi(\mathbf{r},0)$ obeys Bloch's theorem, i.e.,

$$T_{\mathbf{R}}\psi(\mathbf{r},0) = T_{\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{R}}\psi(\mathbf{r},0)\ , \tag{8}$$

so that,

$$\begin{aligned} T_{\mathbf{R}}\psi(\mathbf{r},t) &= \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}\mathrm{e}^{-\mathrm{i}e\mathbf{E}.\mathbf{R}t/\hbar}\mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{R}}\psi(\mathbf{r},0) \\ &= \mathrm{e}^{\mathrm{i}(\mathbf{k}-e\mathbf{E}t/\hbar).\mathbf{R}}\mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}\psi(\mathbf{r},0) \\ &= \mathrm{e}^{\mathrm{i}(\mathbf{k}-e\mathbf{E}t/\hbar).\mathbf{R}}\psi(\mathbf{r},t)\ . \end{aligned} \tag{9}$$

Therefore, $\psi(\mathbf{r},t)$ obeys Bloch's theorem with a *time-dependent wavevector*

$$\mathbf{k}(t) = \mathbf{k}(0) - \frac{e}{\hbar}\mathbf{E}t\ . \tag{10}$$

This result should be interpreted with caution because we are not solving the eigenvalue problem of the complete Hamiltonian, that is, $\psi(\mathbf{r},t)$ is **not** an eigenfunction of $\mathcal{H}$, although $\psi(\mathbf{r},0) = \psi_{n\mathbf{k}}(\mathbf{r})$ is an eigenfunction of $\mathcal{H}_0$. If we imagine that the electric field is *turned off* at time t, without causing an interband transition (adiabatic approximation), at subsequent times the electron will be found in an eigenstate of $\mathcal{H}_0$ corresponding to the wave vector $\mathbf{k}(t)$. Since we can choose the turn-off time arbitrarily, we can view the time evolution as if the electron were *continually visiting* the states of $\mathcal{H}_0$ in band n, with "its" wavevector "varying" in time according to the *equation of motion*

$$\hbar\dot{\mathbf{k}}(t) = -e\mathbf{E}\ . \tag{11}$$

Note that it *looks like* a classical equation of motion, but remember that $\hbar\dot{\mathbf{k}} \neq \dot{\mathbf{p}}$. Later on, we will see that the same equation of motion appears in a semiclassical approach that we will employ to study transport phenomena.

Magnetic field - quantum treatment

In the case of a magnetic field, we cannot employ the same development as for the electric field because the Hamiltonian transformation under a lattice translation is no longer a simple additive constant. This is due to the inclusion of a vector potential $\mathbf{A}(\mathbf{r})$ in the kinetic-energy term, with the magnetic field corresponding to a magnetic induction $\mathbf{B} = \nabla \times \mathbf{A}$. We will utilize an alternative *formal* procedure, described below.

We have seen that the eigenvalues of the translation operator $T_{\mathbf{R}}$ are $\mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{R}}$. But $T_{\mathbf{R}}$ changes the position dependence of any function from $\mathbf{r}$ to $\mathbf{r}+\mathbf{R}$. Since the generator of any translations is the momentum, we can write $T_{\mathbf{R}} = \mathrm{e}^{\mathrm{i}\mathbf{R}.\hat{\mathbf{p}}/\hbar}$ (where $\hat{\mathbf{p}}$ is the momentum **operator**), and we have

$$T_{\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{R}.\hat{\mathbf{p}}/\hbar}\psi_{n\mathbf{k}}(\mathbf{r}) = \psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = \mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r}) \tag{12}$$

On the other hand, similarly to what we did to introduce the Wannier functions, the periodicity of $\varepsilon_n(\mathbf{k})$ in the reciprocal lattice implies that we may write it as a Fourier series of the form

$$\varepsilon_n(\mathbf{k}) = \sum_i \varepsilon_{ni}\, \mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{R}_i}\,. \tag{13}$$

This can be viewed as an eigenvalue of an operator defined as

$$\hat{\varepsilon}_n(\hat{\mathbf{p}}) = \sum_i \varepsilon_{ni}\, \mathrm{e}^{\mathrm{i}\mathbf{R}_i.\hat{\mathbf{p}}/\hbar}\,, \tag{14}$$

which satisfies

$$\hat{\varepsilon}_n(\hat{\mathbf{p}})|n\mathbf{k}\rangle = \varepsilon_n(\mathbf{k})|n\mathbf{k}\rangle\,. \tag{15}$$

Now we can replace $\mathcal{H}$ by the *effective Hamiltonian*

$$\bar{\mathcal{H}} = \sum_n \hat{\varepsilon}_n(\hat{\mathbf{p}})\,, \tag{16}$$

since the two forms yield the same eigenvalue spectrum.

Note that the effective Hamiltonian $\bar{\mathcal{H}}$ can only be constructed **after** solving the original eigenvalue problem with $\mathcal{H}$, which depends on the lattice potential $V(\mathbf{r})$. This potential **does not** appear explicitly in $\bar{\mathcal{H}}$, which can be seen as "purely kinetic" but in a "curved space" that accounts for the effect of the lattice potential. This is consistent with $\hbar\mathbf{k}$ being referred to as *crystal momentum*.

The advantage of defining such an effective Hamiltonian is in the *natural* **assumption** that a magnetic field can be inserted through the substitution

$$\hat{\mathbf{p}} \to \hat{\mathbf{p}} + e\mathbf{A}(\hat{\mathbf{r}})\,, \tag{17}$$

extending to the effective Hamiltonian what is true to the original one.

Rather than trying to rigorously justify this substitution, we will apply it to a specific case and verify its consistency in a known limit.

Let us focus on a tight-binding band for a simple cubic lattice of lattice constant a, for which

$$\varepsilon(\mathbf{k}) = \varepsilon_0 - 2t\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right]\,. \tag{18}$$

We choose $\varepsilon_0 = 6t$ so that the band minimum at the BZ center corresponds to $\varepsilon = 0$. For $\mathbf{B}$ (of magnitude B) applied along the z axis, we can fix the *gauge* such that $\mathbf{A} = (0, Bx, 0)$. The effective Hamiltonian is then

$$\bar{\mathcal{H}} = 6t - 2t\left[\cos\left(-\mathrm{i}\,a\frac{\partial}{\partial x}\right) + \cos\left(-\mathrm{i}\,a\frac{\partial}{\partial y} + \frac{eBa}{\hbar}x\right) + \cos\left(-\mathrm{i}\,a\frac{\partial}{\partial z}\right)\right]\,. \tag{19}$$

Using $\psi(x,y,z) = \mathrm{e}^{\mathrm{i}k_z z}\,\mathrm{e}^{\mathrm{i}k_y y}\,\phi(x)$ as an *ansatz*, the energy-eigenvalue problem implies that $\phi(x)$ is determined by the equation

$$\phi(x+a) + \phi(x-a) + \left[\frac{\varepsilon - 6t}{t} + 2\cos\left(k_z a\right) + 2\cos\left(k_y a + \frac{eBa}{\hbar}x\right)\right]\phi(x) = 0\,. \tag{20}$$

It is easy to show (**EXERCISE**) that this last equation, when we rewrite t in terms of the *effective mass* m^* as $t = \hbar^2/2m^*a^2$, and then take the limit $a \to 0$, yields the differential equation

$$-\frac{\hbar^2}{2m^*}\phi'' + \frac{1}{2}m^*(\omega_c^*)^2(x - x_0)^2\phi = \left(\varepsilon - \frac{\hbar^2 k_z^2}{2m^*}\right)\phi \,, \tag{21}$$

where $\omega_c^* = eB/m^*$ is the effective cyclotron frequency, and

$$x_0 \equiv -\frac{\hbar k_y}{m^*\omega_c^*} \,. \tag{22}$$

Equation (21) is derived in many texts directly for a free electron model with a magnetic field as chosen above. Therefore, the consistency of Eq. (17) is checked in the sense that it reproduces the correct result for $a \to 0$, which is actually the free-electron limit. The energy eigenvalues obtained from Eq. (21) are

$$\varepsilon_{k_z,\nu} = \frac{\hbar^2 k_z^2}{2m^*} + \left(\nu + \frac{1}{2}\right)\hbar\omega_c^* \,, \qquad \nu = 0, 1, 2, \ldots, \tag{23}$$

where ν labels the so-called *Landau levels*. The harmonic-oscillator part defines circles of constant energy parallel to the k_xk_y plane, but with different energies as k_z varies. These levels are highly degenerate, since the total **number** of states must not change with field.

Going back to the tight-bind problem on a lattice, we just present a few comments on the solutions of Eq. (20). As only the motion in the k_xk_y plane is affected by the field, we will restrict ourselves to the case $k_z = 0$ for simplicity. In the tight-binding approach, electron positions along the x axis are integer multiples of the lattice parameter a. We then write Eq. (20) in the form

$$\phi(n+1) + \phi(n-1) + 2\cos(2\pi n\alpha - \delta)\,\phi(n) = \epsilon\phi(n) \,; \qquad n \text{ integer.} \tag{24}$$

This is a *finite-difference equation* which is known as Harper's equation. At this point, we have eliminated the additive constant $6t$, previously used to compare with the continuous limit, so that the eigenvalue ϵ is in the range $[-4, 4]$ (in units of the hopping parameter t). Furthermore, the lattice constant a has become the unit length, δ is a dimensionless parameter associated with k_y, and we define

$$\alpha \equiv Ba^2/(h/e) \,, \tag{25}$$

which is the ratio between the magnetic flux through a unit cell and the quantum of magnetic-flux h/e ($\simeq 4.14 \times 10^{-15}\,\mathrm{Tm}^2$).

Harper's equation was solved by D. R. Hofstadter in 1976 [Phys. Rev. B **14**, 2239 (1976)]. Figure 1 (similar to one that appears in the paper cited here) shows the energy spectrum as a function of α. The resulting pattern is known as *Hofstadter's butterfly*. It is actually a *fractal* pattern, only a part of which is shown in the figure. The range is restricted to $0 \le \alpha \le 1$, but the spectrum repeats itself with period 1. Physically relevant situations

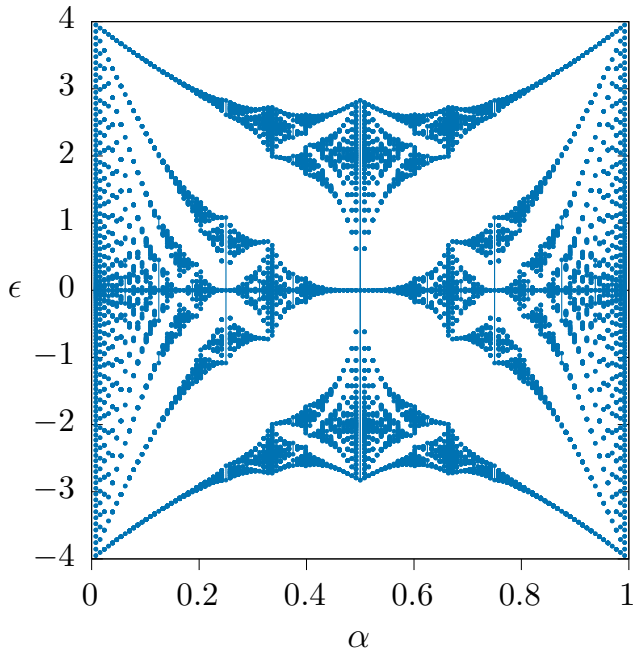

Figure 1: A version of the *Hofstadter's butterfly* for $\alpha = p/q$ with integer p, and $q = 128$.

involve small α, since $\alpha \sim 1$ corresponds to very intense magnetic fields. For $\alpha = 0$ we have the (continuous) tight-binding band. If we choose a rational $\alpha = p/q$, that band splits up into q sub-bands. They become Landau levels (zero-width sub-bands) in the continuum limit, but acquire finite widths because their high degeneracy is lifted by the lattice potential.

The above analysis did not take spin into account. We know that the electron spin is associated to an intrinsic magnetic moment. Thus, the full Hamiltonian should have a term describing the interaction of the spin with the magnetic field. This is relevant for an analysis of the magnetic response, i.e., the appearance of a magnetization induced by the applied field. Magnetic properties of solids will **not** be discussed in this course, being the subject of a more specific one. Hence, we will neglect the spin contribution here, and concentrate on the coupling of electric and magnetic fields with the electron charge only.

Dynamics of Bloch electrons – Semiclassical approximation

The preceding discussion focused on equilibrium properties of Bloch electrons subjected to a magnetic field. It was clear that resorting to an effective Hamiltonian is helpful, due to the difficulties inherent to a full quantum treatment of the lattice problem.

If we extend the effective-Hamiltonian method to take into account also the electric field,

we have

$$\bar{\mathcal{H}} = \sum_n \varepsilon_n(\hat{\mathbf{p}}/\hbar + e\mathbf{A}(\hat{\mathbf{r}})/\hbar) + e\phi(\hat{\mathbf{r}})\,, \tag{26}$$

where $\phi(\mathbf{r})$ is the scalar potential whose gradient gives the electric field.

We already mentioned the difficulties associated to the presence of a position-dependent vector-potential in the *kinetic* term. A usual approach is to connect the effective Hamiltonian $\bar{\mathcal{H}}$ with equations of motion that would be obtained in its **classical limit**.

From Classical Mechanics, we know that a particle of charge q in the presence of an electric field $\mathbf{E}$ and a magnetic induction $\mathbf{B}$ obeys the classical equation of motion is

$$m\dot{\mathbf{v}} = q\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right)\,, \tag{27}$$

where the right-hand side is the well-known *Lorentz force*, and the velocity is given by one of Hamilton's equations as

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \frac{\partial\mathcal{H}(\mathbf{r},\mathbf{p},t)}{\partial\mathbf{p}}\,. \tag{28}$$

Note that the left-hand side of Eq. (27) is the time derivative of the so called *kinetic momentum* $m\mathbf{v} = \mathbf{p} - q\mathbf{A}$, which defines the kinetic energy. From the derivation of the effective Hamiltonian, it is natural to associate the **kinectic momentum** with wavevectors of Bloch states, and these become time-dependent in the presence of external fields. Thus, Eq. (27) corresponds to

$$\hbar\dot{\mathbf{k}} = -e\left[\mathbf{E} + \mathbf{v}_n(\mathbf{k})\times\mathbf{B}\right]\,. \tag{29}$$

while Eq. (28) is consistent with our definition of velocity of a Bloch electron,

$$\dot{\mathbf{r}} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\,\varepsilon_n(\mathbf{k}) \equiv \mathbf{v}_n(\mathbf{k})\,. \tag{30}$$

In summary, the semiclassical approximation consists in associating a position $\mathbf{r}$ to a Bloch electron of wavevector $\mathbf{k}$. These quantities, which obey the above equations of motion, must be interpreted as indicating average values, that is, the centers of a wavepacket in wavevector space and in position space, respectively. This is done independently in each band, since any transition between bands would, of course, be an essentially quantum process, which cannot be described in the context of a semi-classical approximation. The **semi**-classical nature is evidenced in Eq. (30), where it is clear that the velocity depends on the solution of the **quantum**-mechanical problem in the absence of external fields.

Let us analyze the validity conditions of the semiclassical approximation for Bloch electrons.

- The above mentioned wavepacket has widths $\Delta\mathbf{k}$ and $\Delta\mathbf{r}$ in the respective spaces.
- Assigning a reasonably well-defined $\mathbf{k}$ implies that $|\Delta\mathbf{k}| \ll |\mathbf{K}_0|$, where $\mathbf{K}_0$ represents the smallest reciprocal-lattice vector, which limits the 1st BZ.
- Given that $|\mathbf{K}_0| \sim 1/a$, where a is a typical lattice parameter, we must have $\Delta\mathbf{r} \gg a$.

- Despite the notation in Eq. (29), the external fields may depend on $\mathbf{r}$, but the equation is **local**. This requires the characteristic distance for variations of the external fields to be large compared to the wavepacket width in **real** space. Denoting this characteristic distance by λ, we conclude that we must have $\lambda \gg |\Delta\mathbf{r}| \gg a$.

- We also have conservation of the band index. Without going into details, we can say that the absence of transitions between bands requires large *gaps* compared to the energy gained from external fields.

Note that it is important to take rigorously into account the lattice potential through the band energies $\varepsilon_n(\mathbf{k})$, even though the external fields are included by means of a *classical* force. A classical treatment of the lattice potential would violate the validity conditions stated above, since this potential varies in a characteristic distance of the order of a.

The equations of motion (29-30) will play an important role in our study of transport processes in metals, to be developed in the following Texts.