Dynamics of Electrons in Bands

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From Real-Space to k-Space Hamiltonian

Real-space Hamiltonian:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}), \quad V(\mathbf{r}+\mathbf{R}) = V(\mathbf{r}).$$

Bloch form of the wavefunction:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\, u_{n\mathbf{k}}(\mathbf{r}), \quad u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r}).$$

Substitute into $\hat{H}\psi = E\psi$ and factor out $e^{i\mathbf{k}\cdot\mathbf{r}}$:

$$\boxed{H(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\, \hat{H}\, e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{(\hat{\mathbf{p}}+\hbar\mathbf{k})^2}{2m} + V(\mathbf{r})}.$$

- $H(\mathbf{k})$ acts only on periodic functions $u_{n\mathbf{k}}(\mathbf{r})$.
- It is not a Fourier transform, but a unitary transformation shifting momentum: $\hat{\mathbf{p}} \to \hat{\mathbf{p}} + \hbar\mathbf{k}$.
- Solving $H(\mathbf{k})u_{n\mathbf{k}} = \varepsilon_n(\mathbf{k})u_{n\mathbf{k}}$ gives band energies $\varepsilon_n(\mathbf{k})$.

Bloch States and Crystal Momentum

For a periodic potential $V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\, u_{n\mathbf{k}}(\mathbf{r}), \quad u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

Define the k-space Hamiltonian:

$$H(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{(\hat{\mathbf{p}} + \hbar\mathbf{k})^2}{2m} + V(\mathbf{r}).$$

Crystal momentum: $\hbar\mathbf{k}$ labels irreducible representations of the translation group.

Expectation Value of the Momentum Operator

Apply the Hellmann–Feynman theorem to $H(\mathbf{k})$:

$$\frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}} = \langle u_{n\mathbf{k}} | \frac{\partial H(\mathbf{k})}{\partial \mathbf{k}} | u_{n\mathbf{k}} \rangle$$
$$= \frac{\hbar}{m} \langle u_{n\mathbf{k}} | \hat{\mathbf{p}} + \hbar \mathbf{k} | u_{n\mathbf{k}} \rangle .$$

Since $\hat{\mathbf{p}}\psi_{n\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}}(\hat{\mathbf{p}} + \hbar\mathbf{k})u_{n\mathbf{k}}$,

Result

$$\boxed{\langle \hat{\mathbf{p}} \rangle_{n\mathbf{k}} = \frac{m}{\hbar} \nabla_{\mathbf{k}} \varepsilon_n(\mathbf{k})}.$$

The **group velocity** is

$$\boxed{\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_n(\mathbf{k})}, \quad \langle \hat{\mathbf{p}} \rangle = m\mathbf{v}_n .$$

Electron Dynamics Under a Constant Electric Field

For a uniform field **E**, the semiclassical equations of motion are:

Semiclassical Equations

$$\hbar\dot{\mathbf{k}} = -e\mathbf{E},$$
$$\dot{\mathbf{r}} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon_n(\mathbf{k}).$$

Therefore,

$$\mathbf{k}(t) = \mathbf{k}_0 - \frac{e\mathbf{E}}{\hbar}t, \qquad \langle\hat{\mathbf{p}}\rangle(t) = m\mathbf{v}_n[\mathbf{k}(t)].$$

$\hbar\mathbf{k}$ is the **crystal momentum**, not a true mechanical momentum, but determines the velocity and band transport.

Bloch Oscillations in 1D

Tight-binding dispersion:

$$\varepsilon(k) = \varepsilon_0 - 2\gamma \cos(ka).$$

Then,

$$k(t) = k_0 - \frac{eE}{\hbar} t,$$

$$v(t) = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k} = \frac{2\gamma a}{\hbar} \sin(ka).$$

Bloch Frequency

$$\boxed{\omega_B = \frac{eEa}{\hbar}}$$

The motion is periodic with period $T_B = 2\pi/\omega_B$; real oscillations are damped by scattering or interband tunneling.

Visualization: Bloch Oscillations

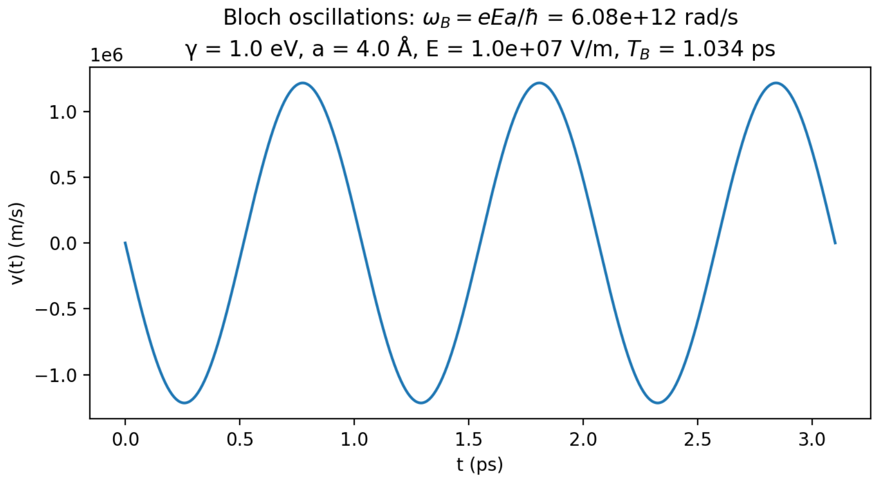

Figure: Example of velocity $v(t) = \frac{2\gamma a}{\hbar}\sin(k(t)a)$ for $\gamma = 1$ eV, $a = 4$ Å, and $E = 10^7$ V/m. The motion is periodic with $\omega_B = eEa/\hbar$.

Limitations of the Semiclassical Picture

- The semiclassical equations track only a **narrow wavepacket** centered at $\mathbf{k}(t)$.
- The field $-e\mathbf{E}\cdot\mathbf{r}$ actually **mixes Bloch states with different k** because it breaks translation symmetry.
- In the full Bloch basis:

$$\langle n\mathbf{k}|(-e\mathbf{E}\cdot\mathbf{r})|m\mathbf{k}'\rangle \propto ie\mathbf{E}\cdot\nabla_{\mathbf{k}}\delta(\mathbf{k}-\mathbf{k}') + e\mathbf{E}\cdot\mathbf{A}_{nm}(\mathbf{k})\delta(\mathbf{k}-\mathbf{k}'),$$

  showing explicit coupling between nearby **k**'s.
- The semiclassical approximation keeps only the **center of mass** motion: $\hbar\dot{\mathbf{k}} = -e\mathbf{E}$.
- Strong fields or long times cause k-mixing beyond this picture (Zener tunneling, Wannier–Stark localization).

Interband Dynamics: General Equations

Expand the wavefunction in cell-periodic Bloch states:

$$|\Psi(t)\rangle = \sum_n c_n(t) e^{\frac{i}{\hbar}\left[\hbar \mathbf{k}(t)\cdot\mathbf{r} - \int^t \varepsilon_n(\mathbf{k}(t'))dt'\right]} \left|u_{n\mathbf{k}(t)}\right\rangle ,$$

with $\hbar\dot{\mathbf{k}} = -e\mathbf{E}$. The coefficients evolve as:

$$i\hbar\dot{c}_n(t) = -e\mathbf{E}\cdot\sum_m \mathbf{A}_{nm}(\mathbf{k}(t))c_m(t),$$

where $\mathbf{A}_{nm}(\mathbf{k}) = i\langle u_{n\mathbf{k}}|\nabla_{\mathbf{k}} u_{m\mathbf{k}}\rangle$ is the **Berry connection**.

- Diagonal $\mathbf{A}_{nn}$: geometric (Berry) phase.
- Off-diagonal $\mathbf{A}_{n\neq m}$: interband coupling.
- Thus $\mathbf{E}$ drives transitions between bands through these matrix elements.

Landau–Zener Transitions and Breakdown

At an avoided crossing between bands separated by a gap $\Delta(\mathbf{k}_*)$:

Landau–Zener Probability

$$P_{\mathrm{LZ}} \approx \exp\left[-\frac{\pi\Delta^2}{2\hbar|e\mathbf{E}\cdot\Delta\mathbf{v}|}\right], \quad \Delta\mathbf{v} = \mathbf{v}_c - \mathbf{v}_v.$$

- Weak field $\Rightarrow P_{\mathrm{LZ}} \ll 1$: adiabatic motion within a band.
- Strong field $\Rightarrow$ Zener tunneling $v \to c$, damping Bloch oscillations.
- Leads to **Wannier–Stark localization** and ultimately **breakdown** at high E.

Example: In semiconductors, interband tunneling sets the threshold for dielectric breakdown.

Berry Curvature and Topology

The Berry curvature for band n:

$$\boldsymbol{\Omega}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}_{nn}(\mathbf{k}), \quad \mathbf{A}_{nn} = i\langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle.$$

Acts like a magnetic field in **k**-space.

- Integrating Ω_n over the Brillouin zone gives the **Chern number**:

$$C_n = \frac{1}{2\pi} \int_{BZ} \Omega_{n,z}(\mathbf{k})\, d^2k.$$

- $C_n = 0 \Rightarrow$ trivial band; $C_n \neq 0 \Rightarrow$ topologically nontrivial.
- Nontrivial topology implies obstruction to defining a global smooth phase.

Anomalous Velocity and Topological Bloch Oscillations

Semiclassical equations of motion including Berry curvature:

$$\boxed{\dot{\mathbf{r}} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon_n(\mathbf{k}) - \frac{e}{\hbar}\mathbf{E}\times\boldsymbol{\Omega}_n(\mathbf{k})}.$$

- The second term is the **anomalous velocity**.
- In topological bands, it produces a **transverse drift** during Bloch oscillations.
- Over one Bloch period, the displacement is:

$$\Delta\mathbf{r}_{\mathrm{anom}} \sim \frac{e}{\hbar}\int_0^{T_B}\mathbf{E}\times\boldsymbol{\Omega}_n(\mathbf{k}(t))\,dt.$$

- If the Berry curvature has nonzero winding (Chern number), this drift is quantized.

Topological Classification and Bloch Oscillation Behavior

Case	**Berry curvature**	**Topology**	**Bloch oscillations**
Trivial insulator	local $\Omega(\mathbf{k})$ may exist, net zero	smooth Bloch phases possible	purely longitudinal oscillations
Chern insulator / QHE	nonzero Chern number	topologically nontrivial	quantized transverse drift per period
TR-symmetric topological insulator	$\Omega(\mathbf{k})$ antisymmetric between spins	spin Chern number $\neq 0$	opposite drifts for opposite spins (spin current)

Topological bands thus yield **geometric Bloch oscillations**: motion encodes Berry phase structure.

Remarks

- The derivation assumes a single isolated band and slowly varying fields (adiabatic evolution).
- For multiple bands, interband transitions (Landau–Zener tunneling) can occur.
- Including Berry curvature adds an anomalous velocity term $-\frac{e}{\hbar}\mathbf{E} \times \boldsymbol{\Omega}_n$.
- Topologically nontrivial bands lead to quantized lateral motion or spin currents. γ, a, and E.