Why tight binding works

In tight binding one approximates the Bloch wave function as

\[ \psi_k = \frac{1}{R} \sum \left( \sum_n b_n \phi_n(\mathbf{r} - \mathbf{R}) \right) \]

One can show (see A+M, chpt 10, pgs 187-188) that the exact Bloch eigenstate can always be written in the form

\[ \psi_k(\mathbf{r}) = \frac{1}{R} \sum \left( \sum_n b_n \phi_n(\mathbf{r} - \mathbf{R}) \right) \]

for some suitable function \( \phi(\mathbf{r}) \). This \( \phi(\mathbf{r}) \) is called the Wannier function.

The tight binding approximation is then built on the assumption that the Wannier function \( \phi_1(\mathbf{r}) \) can be well approximated by a linear combination of atomic orbitals.

In principle, the complete set of eigenfunctions of the atomic Hamiltonian that form a complete basis set of functions in terms such that any function (and so in particular the Wannier function) can be written as a linear combination of these atomic eigenfunctions. But for this to be a complete basis, we need to include the continuum of ionized atomic eigenstates as well as the
discrete bound atomic orbitals $\Psi_n(r)$.

The tight binding approximation that consists of neglecting the ionized atomic eigenstates when trying to expand the Wannier function $\phi(r)$. It works well when $\phi(r)$ is well localized or when $\phi(r)$ decays quickly to zero as $|r| \to \infty$. 
Spin-orbit interaction

We have seen in both the weak potential approx and the tight binding approx, that there may remain degeneracies in the band structure at certain points of high symmetry (for example in prob. 3 of HW 4).

An example would be the absence of the expected energy gap at the top and bottom faces of the 1st BZ for hcp crystals, due to the vanishing of the geometric structure factor $S_K$ on these faces.

In such case, in the heavier elements, the degeneracy may be lifted (i.e an energy gap appear) due to the effects of the spin-orbit interaction.

In principle there is always an interaction between the intrinsic electron spin and the magnetic moment $\mu$ and its motion in the electric field of the ions.

$$\mathcal{H}_{50} = g \mu \cdot (\vec{r} \times \vec{E})$$

$\vec{B}$ in local rest frame of electron

$\vec{E}$ is from ionic potential
If one includes $S_{1s0}$ in the single-electron Hamiltonian, one can no longer ignore the coupling between electron spin state and real space wave function (as we have been doing). One needs to consider linear combinations of both different spatial orbitals and spin states, thus doubling the number of functions used in the tight binding expansion for $\Psi$. When one includes $S_{1s0}$, one finds that symmetry induced band degeneracies can be lifted. This effect is most noticeable in heavier elements where the cubic electric field is stronger.
Semi-classical Approx for dynamics of electrons in periodic potential

Same idea as we used in Sommerfeld model.

Imagine constructing wave packets of Bloch states to localize electrons. To each electron assign position \( \vec{r} \), crystal momentum \( \vec{p} \), band index \( n \).

Semi-classical equations of motion tell how \( \vec{r} \), \( \vec{p} \), \( n \) evolve in time in presence of applied \( \vec{E} \) and \( \vec{H} \) fields, un-between collisions. Then a relaxation approximation will be used to average over effect of collisions modify semi-classical equations to include average effect of collisions.

+) Wave packet approx good only when applied fields vary slowly over dimensions of size of primitive cell.

\( \Rightarrow \) (localize crystal momentum well on scale of 1st BZ
\( \Rightarrow \) wave packet in \( \vec{r} \)-space extends over a few primitive cells)

+) Quantum effects are handled entirely through the band structure \( E_n(\vec{p}) \) which we take as given function that describes wave functions. All effects of quantum mechanics or periodic potential (which varies rapidly on scale of primitive cell) is taken into account in fully quantum mechanical way by use of the Bloch states \( E_n(\vec{p}) \). Externally slowly varying fields are treated in semi-classical way.
Collisions can not be with static periodic cons. Their effect already included in $E_n (\tau)$.

In the absence of collisions, $N, \overrightarrow{\tau}, \overrightarrow{n}$ evolve as

1) band index $i$ is constant. No interband transitions
   Good when field strengths are not too large
   See appendix J)
   \[ E \leq E_\tau \ll \left( E_{gap} (\vec{k}) \right)^2 / \varepsilon_F \] = "electric breakdown" when fail
   \[ H \ll \left( E_{gap} (\vec{k}) \right)^2 / \varepsilon_F \] = "magnetic breakdown" when fail.

2) $\overrightarrow{n}$ always true in metals, can fail in insulators + semiconductors

3) possible in strong $\overrightarrow{H}$ fields

Also need $\{ \tau \gg \varepsilon \}$

\[
\overrightarrow{\dot{\tau}} = \overrightarrow{\nabla} (E_n) = \frac{1}{\hbar} \frac{\partial E_n}{\partial \overrightarrow{k}}
\]

\[
\hbar \overrightarrow{k} = -e \left[ \overrightarrow{E} (\overrightarrow{k}, t) + \frac{1}{c} \overrightarrow{\nabla} (\overrightarrow{k}) \times \overrightarrow{H} (\overrightarrow{k}, t) \right]
\]

3) States $\overrightarrow{k}$ and $\overrightarrow{k} + \overrightarrow{K}$ are equivalent when $\overrightarrow{K}$ is reciprocal lattice vector.

In equilibrium, states occupied with Fermi function

\[
\frac{1}{C_e (\overrightarrow{E_n})} = \frac{1}{e^{(\overrightarrow{E_n} - \mu)/k_B T} + 1}
\]

*) $\overrightarrow{k}$ is not total momentum, $\overrightarrow{p}$ is given by total force
   (includes con. potential) $\overrightarrow{p}$ is seen as applied force only.
Lessons to believe Semi classical equations: For more see references given in text.

\[ \vec{p} = \vec{p}_n(\vec{k}) \]

is just definition of momentum

+ we derived earlier that \( \vec{p}_n(\vec{k}) = \frac{1}{\hbar} \frac{\partial \epsilon}{\partial \vec{k}} \)

We show that equ for \( \vec{p} \) is consistent with energy conservation.

For motion in an electric field \( \vec{E} = -\nabla \phi \) the electrostatic potential \( \phi_n(\vec{k}(t)) \) to be constant: bond energy + electrostatic energy = constant

\[ \Rightarrow \frac{d}{dt} \left[ \phi_n(\vec{k}(t)) + e \phi(\vec{r}(t)) \right] = 0 \]

\[ \Rightarrow \frac{d \phi_n}{dt} \vec{k} - e \nabla \phi \cdot \frac{d \vec{r}}{dt} = 0 \]

plug in \( \vec{r} = \vec{r}_e \) semi classical

\[ \text{true when } \vec{r}_e = -e \vec{E} \]

Although when \( \vec{H} = c \)

Could also have piece \( \nabla \times \vec{B} \)

although we haven't shown that only possible such piece \( \vec{E} \)

\[ \text{Consequences: Filled bands do not contribute to transport properties.} \]

\[ \text{electric current } \vec{j} = -e \int \frac{d^3k}{8\pi^2} \frac{1}{\hbar} \frac{2 \epsilon}{2 \hbar} \]

\[ \text{thermal current } \vec{j}_c = \frac{1}{3} \int \frac{d^3k}{8\pi^2} \frac{\epsilon \frac{2 \epsilon}{2 \hbar}}{\epsilon} = \frac{1}{3} \int \frac{d^3k}{8\pi^2} \frac{2 \epsilon^2}{2 \hbar} \]

\[ \vec{B} \]
\[ \frac{\partial^2 \psi}{\partial k^2} = -\frac{1}{2} \psi(k) \]

**Proof:**

If the crystal has inversion symmetry, \( \psi(k) = \psi(-k) \),

\[ \psi^2(k) = \psi^2(-k) \Rightarrow \frac{\partial^2 \psi}{\partial k^2} = -\frac{1}{2} \psi(k) \]

so the integrand integrates to zero over the first Brillouin Zone.

\[ \int_0^1 \psi(k) \, dk = 0 \]

Actually the statement is true more generally, even if no inversion symmetry. Gradient of any periodic function also integrates to zero over unit cell. See text.

\( \psi(k) \) is periodic in transition by \( k \)

Therefore current is carried only by partially full bands. Conduction electrons in Drude model should be just electrons in partially full bands.

**Motion in DC \( \vec{E} \) fields**

\[ \vec{v}(t) = \vec{v}(0) - \vec{e} \frac{\vec{E} t}{k} \]

in general \( \vec{v} \neq \vec{k} \)

so only when \( \vec{v} \) is in constant near band minimum is \( \vec{v} \parallel \vec{k} \)

Near band max (near zone edge) \( \vec{v} = \vec{\omega} \times \vec{k} \)

As electron approaches zone edge it slows down and goes in next...