Why tight binding works

In tight binding one approximates the Block wavefunction as

$$\psi_k = \sum_R e^{i\vec{k}\cdot\vec{R}} \left(\sum_n b_n \phi_n(\vec{r}-\vec{R}) \right)$$

↑ atomic orbitals

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

$$\psi_k(\vec{r}) = \sum_R e^{i\vec{k}\cdot\vec{R}} \phi(\vec{r}-\vec{R})$$

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

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

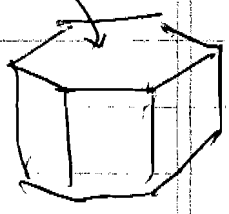
In principle the complete set of eigenfunctions of the atomic Hamiltonian H_{at} form a complete basis set of functions such that any function (and so in particular the Wannier function) can be written as a linear combination of these atomic eigenfunctions. But for this to be a complete basis we need to include the continuum of ionized atomic eigenstates as well as the

discrete bound atomic orbitals $\varphi_n(\vec{r})$.

The tight binding approximation thus consists of neglecting the ionized atomic eigenstates when trying to expand the Wannier function $\phi(\vec{r})$. It works well when $\phi(\vec{r})$ is well localized i.e. when $\phi(\vec{r})$ decays quickly to zero as $|\vec{r}| \to \infty$.

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 (ie 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 with~~ ~~its~~ magnetic moment $\vec{\mu}$ (due to intrinsic spin) and its motion in the electric field of the ions

$$\delta H_{so} \simeq g \vec{\mu} \cdot (\vec{v} \times \vec{E})$$

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

$\vec{E}$ is from ionic potential

If one includes δH_{SO} 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 ψ_k.

When one includes δH_{SO} one finds that symmetry induced band degeneracies can be lifted.

This effect is most noticeable in heavier elements where the ionic electric field $\vec{E}$ 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 $\vec{k}$, band index n. Semiclassical equations of motion tell how $\vec{r}$, $\vec{k}$, n evolve in time in presence of applied $\vec{E}$ and $\vec{H}$ fields, inbetween collisions. Then a relaxation approximation will be used to ~~average over effect of collisions~~ modify semiclassical equations to include average effect of collisions.

*) Wave packet approx good only when applied fields vary slowly over dimensions of size of primitive cell.
~~(~~(localize crystal momentum well on scale of 1st BZ
⇒ wave packet in $\vec{r}$-space extends over a few primitive cells)

*) Quantum effects are handled entirely through the band structure $E_n(\vec{k})$ which we take as given function ~~does describes does~~ ~~includes 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 $E_n(\vec{k})$. External slowly varying fields are treated in semi classical way.

* Collisions can not be with static periodic cons. Their effec already included in $\varepsilon_n(\vec{k})$.

In the absence of collisions, n, $\vec{k}$, $\vec{r}$ evolve as

1) band index is constant. No interband transitions
Good when field strengths are not too large

(see Appendix J) i) $eEa \ll [\varepsilon_{gap}(\vec{k})]^2/\varepsilon_F$ "electric breakdown" when fail

ii) $\hbar\omega_c \ll [\varepsilon_{gap}(\vec{k})]^2/\varepsilon_F$ "magnetic breakthrough" when fails

i) ~~usually~~ always true in metals, can fail in insulator + semiconductors

ii) possible in strong $\vec{H}$ fields

Also need $\begin{cases} \hbar\omega \ll \varepsilon_{gap} & \text{– photon cannot excite to higher band} \\ \lambda \gg a & \text{slowly varying fields} \end{cases}$

2) $\vec{r}$ and $\vec{k}$ evolve just like classical particle if we took $\hbar\vec{k}$ as ordinary momentum (which it is not)

$$\dot{\vec{r}} = \vec{v}_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\vec{k})}{\partial \vec{k}}$$

$$\hbar\dot{\vec{k}} = -e\left[\vec{E}(\vec{r},t) + \frac{1}{c}\vec{v}_n(\vec{k}) \times \vec{H}(\vec{r},t)\right]$$

3) States $\vec{k}$ and $\vec{k}+\vec{K}$ are equivalent when $\vec{K}$ is reciprocal lattice vector.
In equilibrium, states occupied with fermi function $f(\varepsilon_n(\vec{k})) = \dfrac{1}{e^{(\varepsilon_n(\vec{k})-\mu)/kT}+1}$

*) $\hbar\vec{k}$ is not total momentum. $\dot{\vec{p}}$ is given by total force (includes coin potential) $\hbar\dot{\vec{k}}$ is given by applied force only.

Reasons to believe Semi classical equations: For more see references given in text

$\dot{\vec{r}} = \vec{v}_n(k)$ ← just definition of velocity
+ we derived earlier that $\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}}$

We show that eqn for $\dot{\vec{k}}$ is consistent with energy conservation
For motion in ~~the~~ electric field $\vec{E} = -\vec{\nabla}\phi$ ← electrostatic potential
expect $\varepsilon_n(\vec{k}(t)) - e\phi(\vec{r}(t))$ to be constant = band energy + electrostatic energy = constant

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

$$\Rightarrow \frac{d\varepsilon_n}{d\vec{k}} \cdot \frac{d\vec{k}}{dt} - e\vec{\nabla}\phi \cdot \frac{d\vec{r}}{dt} = 0$$

plug in $\hbar\dot{\vec{k}}$ = semi class eqn

or $\hbar\vec{v}\cdot\dot{\vec{k}} = -\vec{v}\cdot e\vec{E}$ ⇒ consistent

~~was~~ true when $\hbar\dot{\vec{k}} = -e\vec{E}$ ~~although~~ when $\vec{H} = 0$
Could also have piece ~~to~~ $\frac{e}{c}\vec{v}\times\vec{H}$
although we haven't shown that only possible such piece is $-\frac{e}{c}\vec{v}_n \times \vec{H}$

Consequences: Filled bands do not contribute to transport properties.

electric current $\vec{j} = -e\int_{BZ}\frac{d^3k}{4\pi^3}\frac{1}{\hbar}\frac{\partial\varepsilon}{\partial\vec{k}}$

thermal current $j_\varepsilon = \frac{1}{T}\int_{BZ}\frac{d^3k}{4\pi^3}\frac{\varepsilon}{\hbar}\frac{\partial\varepsilon}{\partial\vec{k}} = \frac{1}{2}\int\frac{d^3k}{4\pi^3}\frac{1}{\hbar}\frac{\partial}{\partial\vec{k}}($

$\vec{j} = \vec{j}_\varepsilon = 0$ for filled bands

Proof:

If crystal has inversion symmetry $\varepsilon(k) = \varepsilon(-k)$,

$\varepsilon^2(k) = \varepsilon^2(-k) \Rightarrow \frac{d}{dk}\varepsilon^2(k) = -\frac{d}{dk}\varepsilon^2(-k)$

$\frac{d}{dk}\varepsilon^2(k) = -\frac{d}{dk}\varepsilon^2(-k)$ so these are odd functions

so $\int$ over 1st BZ vanishes.

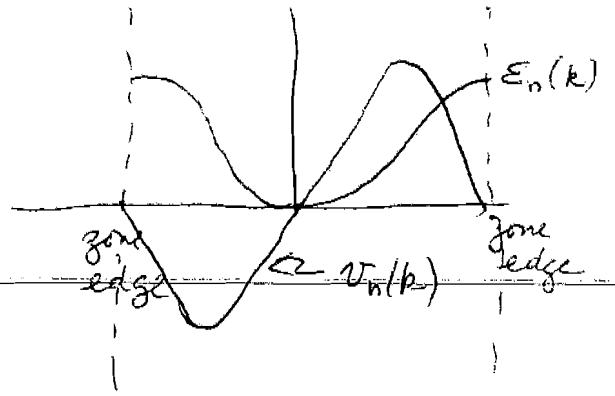
Actually ~~proof~~ this is true more generally, even if no inversion symmetry. Gradient of any periodic function also integrates to zero over unit cell. See text

$\varepsilon(k)$ is periodic in translation by $\vec{K}$

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

Motion in DC $\vec{E}$ fields

$$\vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}}{\hbar}t$$ in general $\vec{v} \not\propto \vec{k}$



Since so only when $\vec{k}$ is ~~in center of~~ near band minimum is $\vec{v} \propto \vec{k}$

Near band max (near zone edge) $\vec{v} \propto -\vec{k}$

As electron approaches zone edge, it slows down and goes in reverse due to scattering at Bragg plane