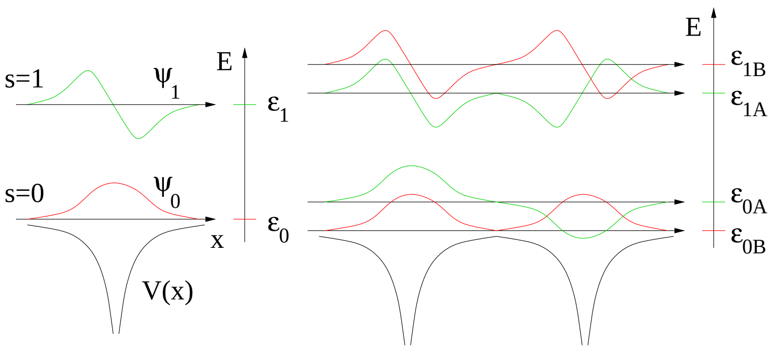
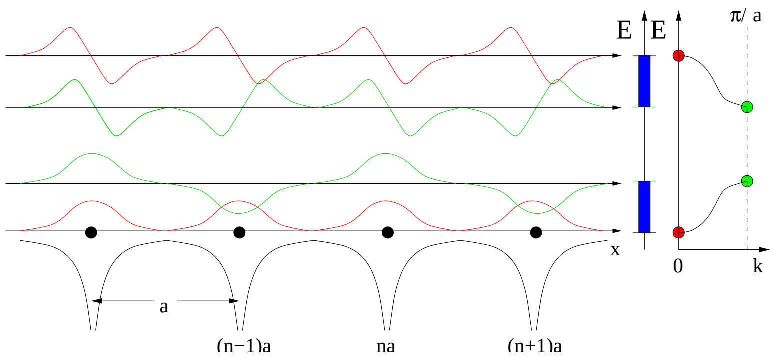
Lecture VI: Tight-binding and the Mott transition

According to band picture of non-interacting electrons, a 1/2-filled band of states is metallic. But strong Coulomb interaction of electrons can lead to a condensation or crystallisation of the electron gas into a solid, magnetic, insulating phase — Mott transition. Here we employ the second quantisation to explore the basis of this phenomenon.

▷ <u>‘Atomic Limit’ of crystal</u>

How do atomic orbitals broaden into band states? `Transparencies`





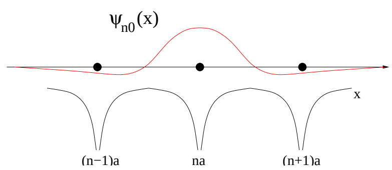
Weak overlap of tightly bound states $\mapsto$ narrow band:

Bloch states $|\psi_{ks}\rangle$, band index s, $k \in [-\pi/a, \pi/a]$

Bloch states can be used to define <u>†‘Wannier basis’</u>

cf. discrete Fourier decomposition

$$|\psi_{ns}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{k\in[-\pi/a,\pi/a]}^{\text{B.Z.}} e^{-ikna}|\psi_{ks}\rangle, \qquad |\psi_{ks}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikna}|\psi_{ns}\rangle, \qquad k = \frac{2\pi}{Na}m$$



In ‘atomic limit’, Wannier states $|\psi_{ns}\rangle$ mirror atomic orbital $|s\rangle$ on site n

Field operators associated with Wannier basis: $\overbrace{|\psi_{ns}\rangle}^{c^\dagger_{ns\sigma}|\Omega\rangle} = \int dx \overbrace{|x\rangle}^{c^\dagger_\sigma(x)|\Omega\rangle} \overbrace{\langle x|\psi_{ns}\rangle}^{\psi_{ns}(x)}$

$$c^\dagger_{ns\sigma} \equiv \int dx\ \psi_{ns}(x) c^\dagger_\sigma(x)$$

and using completeness (exercise) $\sum_{ns} \psi^*_{ns}(x')\psi_{ns}(x) = \delta(x-x')$

$$c^\dagger_\sigma(x) = \sum_{ns} \psi^*_{ns}(x) c^\dagger_{ns\sigma}, \qquad [c_{ns\sigma}, c^\dagger_{n's'\sigma'}]_+ = \delta_{\sigma\sigma'}\delta_{nn'}\delta_{ss'}$$

i.e. operators $c^\dagger_{ns\sigma}/c_{ns\sigma}$ create/annihilate electrons at site n in band s with spin σ

▷ In atomic limit, bands are well-separated in energy. If electron densities are low, one may project onto lowest band $s = 0$

Transforming to Wannier basis, interacting electron Hamiltonian takes form

$$\boxed{\hat{H} = \sum_{mn\sigma} t_{mn} c^\dagger_{m\sigma} c_{n\sigma} + \sum_{mnrs\sigma\sigma'} U_{mnrs} c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{r\sigma'} c_{s\sigma'}}$$

where "hopping" matrix elements: $t_{mn} = \langle\psi_m|\hat{H}^{(0)}|\psi_n\rangle = t^*_{nm}$
and "interaction parameters"

$$U_{mnrs} = \frac{1}{2}\int dx \int dx' \psi^*_m(x)\psi^*_n(x') \frac{e^2}{|x-x'|}\psi_r(x')\psi_s(x)$$

(For lowest band) representation is exact:
but, in atomic limit, matrix elements decay exponentially with separation

(i) "Tight-binding" approximation:

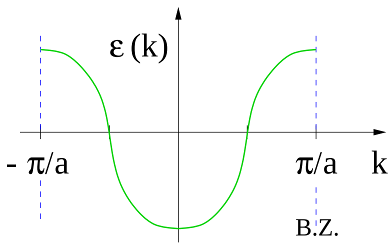
$$t_{mn} = \begin{cases} \epsilon & m = n \\ -t & mn \text{ neighbours} \\ 0 & \text{otherwise} \end{cases}, \qquad \hat{H}^{(0)} \simeq \sum_{n\sigma} \epsilon\ c^\dagger_{n\sigma} c_{n\sigma} - t \sum_{n\sigma}\left(c^\dagger_{n+1\sigma} c_{n\sigma} + \text{h.c.}\right)$$

In discrete Fourier basis: $c^\dagger_{n\sigma} = \dfrac{1}{\sqrt{N}} \sum_{k\in[-\pi/a,\pi/a]}^{\text{B.Z.}} e^{ikna} c^\dagger_{k\sigma}$

$$-t\sum_{n\sigma}^{N}\left(c^\dagger_{n+1\sigma}c_{n\sigma} + \text{h.c.}\right) = -t\sum_{kk'\sigma} \overbrace{\frac{1}{N}\sum_n e^{i(k-k')na}}^{\delta_{kk'}} e^{ika} c^\dagger_{k\sigma} c_{k'\sigma} + \text{h.c.} = -2t\sum_{k\sigma}\cos(ka)\ c^\dagger_{k\sigma}c_{k\sigma}$$

$$\boxed{\hat{H}^{(0)} = \sum_{k\sigma}(\epsilon - 2t\cos ka) c^\dagger_{k\sigma} c_{k\sigma}}$$

As expected, as $k \to 0$, spectrum becomes free electron-like:
$\epsilon_k \to \epsilon - 2t + t(ka)^2 + \cdots$ (with $m^* = 1/2a^2t$)



(ii) Interaction

- Focusing on lattice sites $m \neq n$:
  1. Direct terms $U_{mnnm} \equiv V_{mn}$ — couple to density fluctuations: $\sum_{m\neq n} V_{mn}\hat{n}_m\hat{n}_n$
     $\rightsquigarrow$ potential for charge density wave instabilities
  2. Exchange coupling $J^F_{mn} \equiv U_{mnmn}$ (exercise — see lecture handout)

$$\sum_{m\neq n,\sigma\sigma'} U_{mnmn} c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{m\sigma'} c_{n\sigma} = -2\sum_{m\neq n} J^F_{mn}\left(\hat{\mathbf{S}}_m\cdot\hat{\mathbf{S}}_n + \frac{1}{4}\hat{n}_m\hat{n}_n\right), \qquad \hat{\mathbf{S}}_m = \frac{1}{2}c^\dagger_{m\alpha}\sigma_{\alpha\beta}c_{m\beta}$$

  i.e. weak ferromagnetic coupling ($J_F > 0$) cf. Hund's rule in atoms

  spin alignment $\mapsto$ symmetric spin state and asymmetric spatial state — lowers p.e.

  But, in atomic limit, both t_{mn} and J^F_{mn} exponentially small in separation $|m-n|a$

- 'On-site' Coulomb or 'Hubbard' interaction

$$\sum_{n\sigma\sigma'} U_{nnnn} c^\dagger_{n\sigma} c^\dagger_{n\sigma'} c_{n\sigma'} c_{n\sigma} = U\sum_n \hat{n}_{n\uparrow}\hat{n}_{n\downarrow}, \qquad U \equiv 2U_{nnnn}$$

▷ Minimal model for strong interaction: Hubbard Hamiltonian

$$\boxed{\hat{H} = -t\sum_{n\sigma}(c^\dagger_{n+1\sigma}c_{n\sigma} + \text{h.c.}) + U\sum_n \hat{n}_{n\uparrow}\hat{n}_{n\downarrow}}$$

...could have been guessed on phenomenological grounds

`Transparencies on Mott-Insulators and the Magnetic State`