Solution for one e^-: $\psi^\dagger_{e/o} = \frac{1}{\sqrt{2}}(\psi^\dagger_A \pm \psi^\dagger_B)$

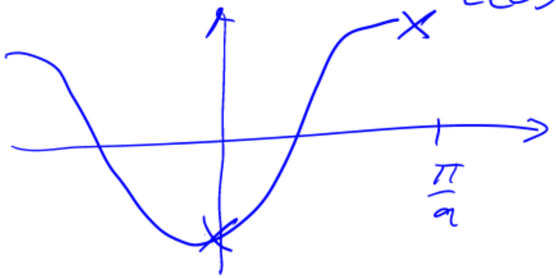
$e \rightarrow k=0$

$o \rightarrow k=\frac{\pi}{a}$

The Hydrogen molecule (now $2e^-$)

Tight binding: $H = -t \sum_{\sigma=\uparrow,\downarrow} \left(\psi^\dagger_{A,\sigma}\psi_{B,\sigma} + \psi^\dagger_{B,\sigma}\psi_{A,\sigma} \right) = -t \sum_{\sigma=\uparrow\downarrow} (\psi^\dagger_{e\sigma}\psi_{e\sigma} - \psi^\dagger_{o\sigma}\psi_{o\sigma})$

$\varepsilon_{e/o} = \mp t$



for $2e^-$: 2 spins, two orbitals

4 single electron basis functions

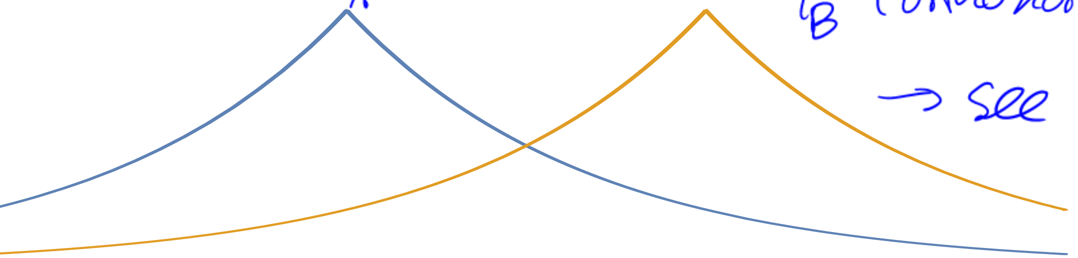
double occupancy forbidden, odd under exchange, e.g. $\psi^\dagger_{A\uparrow}\psi^\dagger_{A\uparrow} = 0$

→ only six possible 2 electron basis states (for s-orbitals) $\psi^\dagger_{A\sigma_1}\psi^\dagger_{B\sigma_2}|0\rangle$

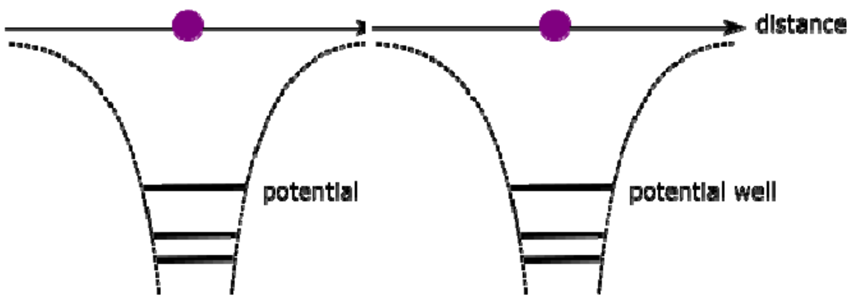
or $\psi^\dagger_{A\uparrow}\psi^\dagger_{A\downarrow}|0\rangle$

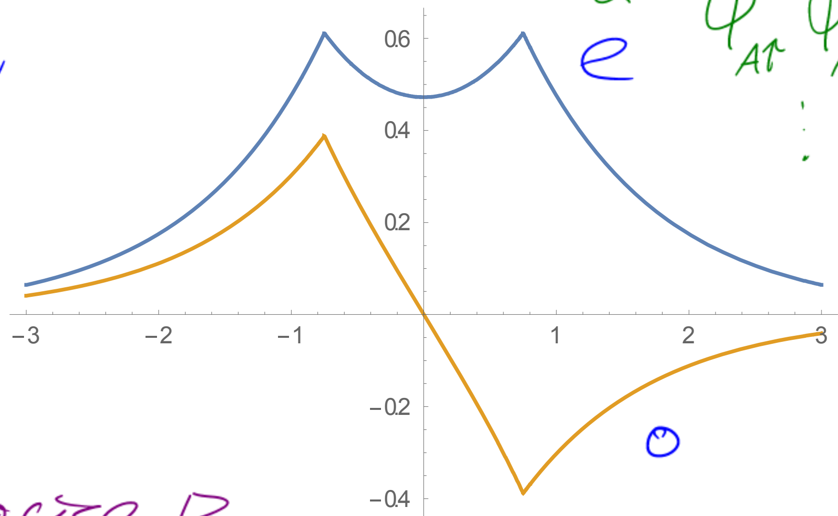
⋮

ψ_A ψ_B (orthonormalized)



→ see exercise 11





see exercise 13

Double occupation in lowest orbital

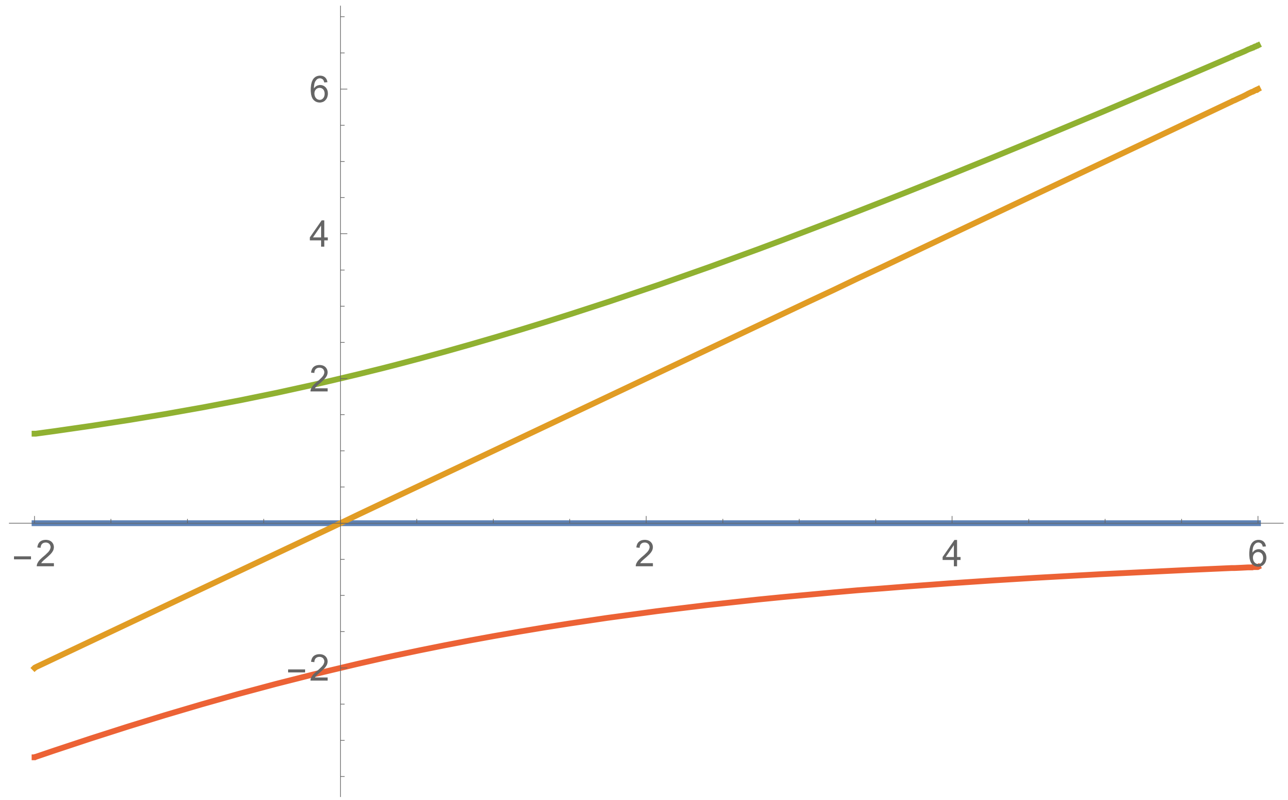
Non-interacting ground state $\left|GS\right\rangle = \Psi^{\dagger}_{e,\uparrow}\Psi^{\dagger}_{e,\downarrow}\left|0\right\rangle$

Heitler London ansatz $\left|HL\right\rangle = \frac{1}{\sqrt{2}}\left(\Psi^{\dagger}_{A,\uparrow}\Psi^{\dagger}_{B,\downarrow} + \Psi^{\dagger}_{B,\uparrow}\Psi^{\dagger}_{A,\downarrow}\right)\left|0\right\rangle$

Minimal Interacting model

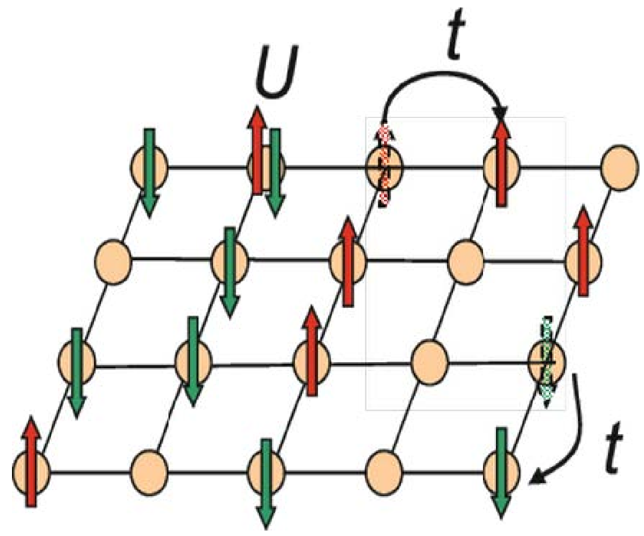
$$H = -t\sum_{\sigma=\uparrow,\downarrow}\left(\psi^{\dagger}_{A,\sigma}\psi_{B,\sigma} + \psi^{\dagger}_{B,\sigma}\psi_{A,\sigma}\right) + U\left(n_{A,\uparrow}n_{A,\downarrow} + n_{B,\uparrow}n_{B,\downarrow}\right)$$

Interacting Eigenvalues



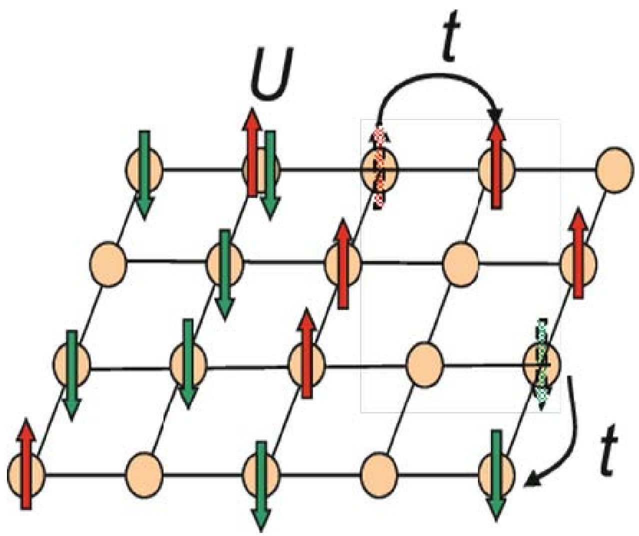
The Hubbard model

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \psi^{\dagger}_{i,\sigma} \psi_{j,\sigma} + U \sum_{j} n_{j,\uparrow} n_{j\downarrow}$$



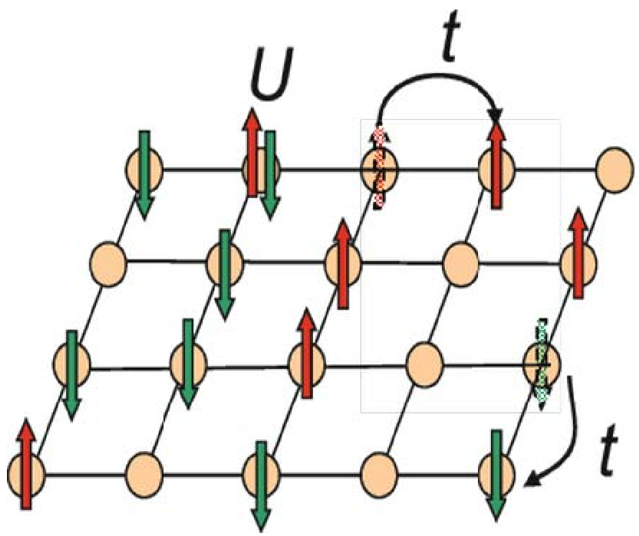
The Hubbard model: U=0 limit

$$H = -t\sum_{\langle i,j\rangle}\sum_{\sigma=\uparrow,\downarrow}\psi^{\dagger}_{i,\sigma}\psi_{j,\sigma} + U\sum_{j} n_{j,\uparrow} n_{j\downarrow}$$



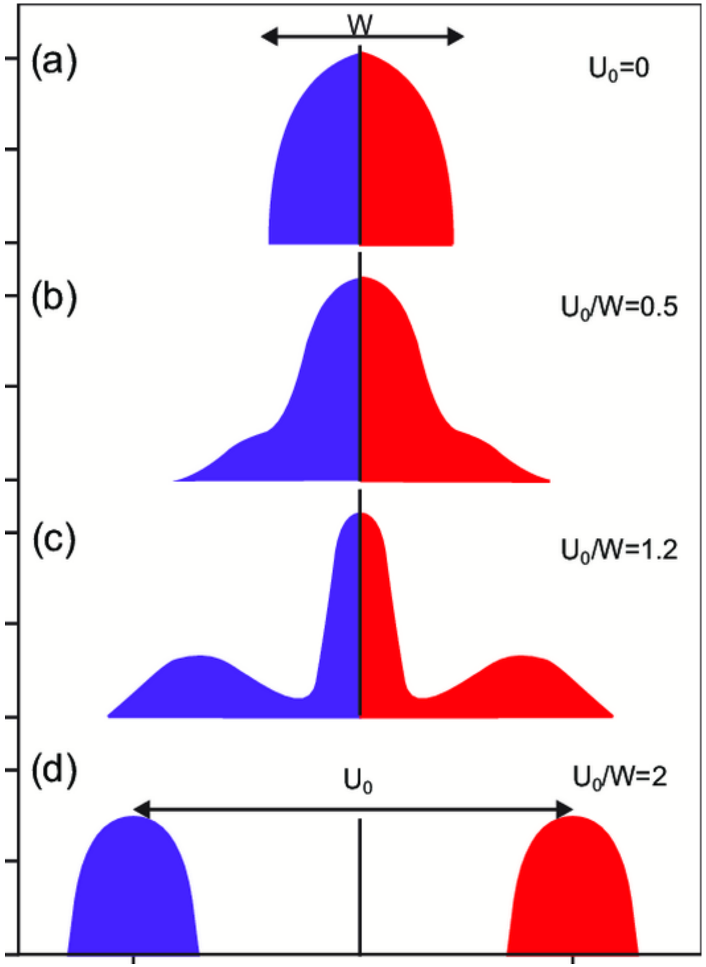
The Hubbard model: t=0 limit

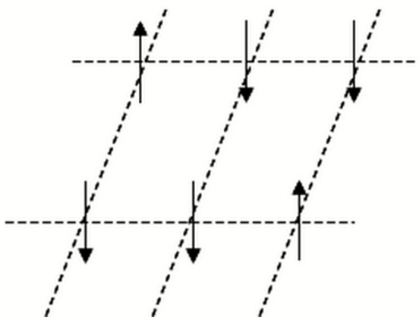
$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \psi^{\dagger}_{i,\sigma} \psi_{j,\sigma} + U \sum_{j} n_{j,\uparrow} n_{j\downarrow}$$

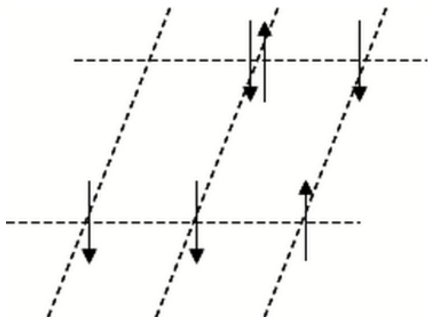


The Hubbard model: Phase transition at "half-filling" $\langle n \rangle = 1$

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \psi^{\dagger}_{i,\sigma} \psi_{j,\sigma} + U \sum_{j} n_{j,\uparrow} n_{j\downarrow}$$







General approach: perturbation theory

General: $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$ known: $\hat{H}_0 |\alpha_0\rangle = \varepsilon_\alpha^0 |\alpha_0\rangle$

Ansatz: $|\alpha\rangle \approx |\alpha_0\rangle + |\alpha_1\rangle$ with $\hat{H}|\alpha\rangle = (\varepsilon_\alpha^0 + \varepsilon_\alpha^1 + \varepsilon_\alpha^2 + \ldots)|\alpha\rangle$

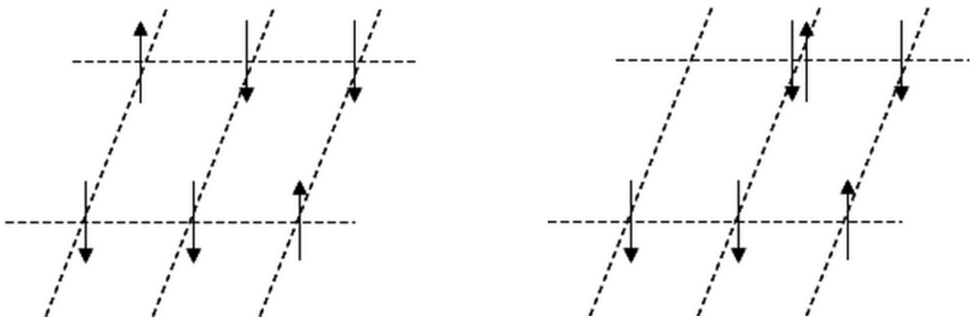
Gives: $|\alpha_1\rangle = \sum_{b \neq \alpha} \frac{|\beta_0\rangle\langle\beta_0|\lambda\hat{H}_1|\alpha_0\rangle}{\varepsilon_\alpha^0 - \varepsilon_\beta^0}$

$$\varepsilon_\alpha^1 = \langle\alpha_0|\lambda\hat{H}_1|\alpha_0\rangle$$

$$\varepsilon_\alpha^2 = \langle\alpha_0|\lambda\hat{H}_1|\alpha_1\rangle$$

The Hubbard model: Magnetic correlations in the Mott phase

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \psi^{\dagger}_{i,\sigma} \psi_{j,\sigma} + U \sum_{j} n_{j,\uparrow} n_{j\downarrow}$$



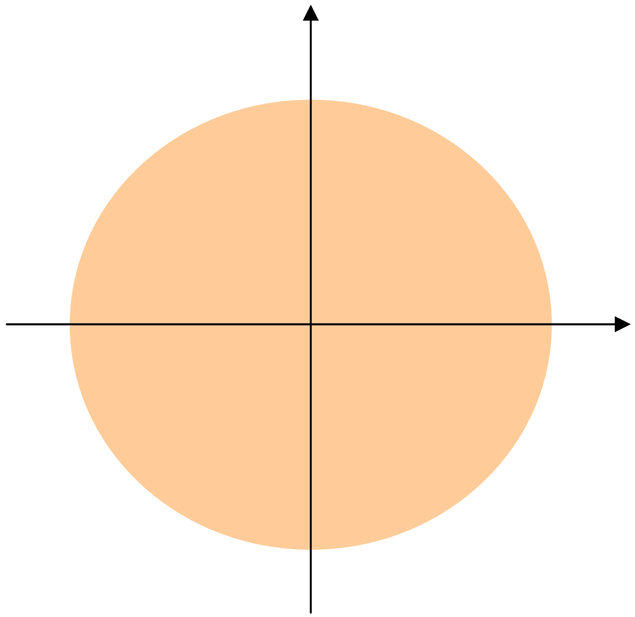
General interacting models: Fermi liquid

$$\hat{c}^\dagger(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{r}\; e^{i\vec{k}\cdot\vec{r}}\, \hat{\Psi}^\dagger(\vec{r})$$

$$\widehat{H}_{\text{int}} = \sum_{\sigma_1,\sigma_2} \int d^3\vec{r}_1 d^3\vec{r}_2\; \hat{\Psi}^\dagger_{\sigma_1}(\vec{r}_1)\hat{\Psi}^\dagger_{\sigma_2}(\vec{r}_2) V(\vec{r}_1 - \vec{r}_2)\hat{\Psi}_{\sigma_2}(\vec{r}_2)\hat{\Psi}_{\sigma_1}(\vec{r}_1)$$

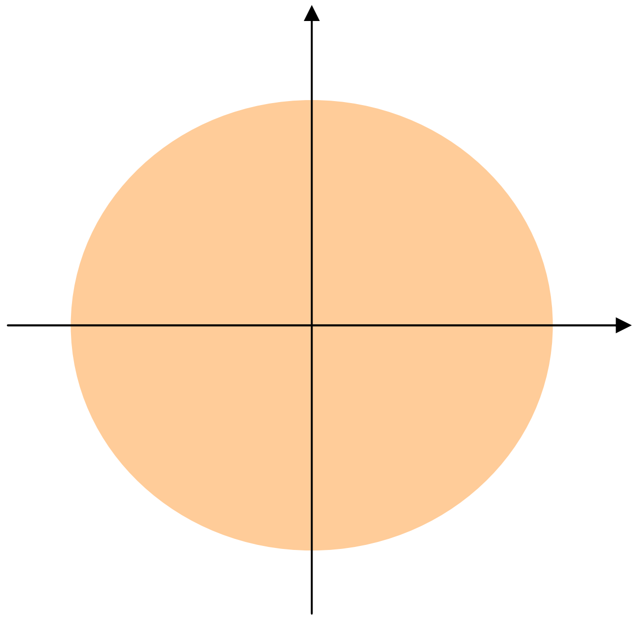
Scattering in k-space

$$\hat{H}_{\text{int}} = \frac{1}{(2\pi)^3} \sum_{\sigma_1,\sigma_2} \int d^3\vec{k}_1 d^3\vec{k}_2\, d^3\Delta\vec{k}\; c^\dagger_{\sigma_1}(\vec{k}_1) c^\dagger_{\sigma_2}(\vec{k}_2) \tilde{V}(\Delta\vec{k}\,) c_{\sigma_2}(\vec{k}_2 - \Delta\vec{k}) c_{\sigma_1}(\vec{k}_1 + \Delta\vec{k})$$



Stability of the excitations

Decay probability using two constraints



Effective lifetime and correlations

$$c_{\sigma}^{\dagger}(\vec{k},t) = e^{itH/\hbar} c_{\sigma}^{\dagger}(\vec{k})$$