We can use different bases for the one-particle states; $|\lambda\rangle$ can refer to

$|\vec{x}\rangle$; $|\vec{k}\rangle$ (spinless)

$|\vec{x}\sigma\rangle$; $|\vec{k}\sigma\rangle$ (spinfull), etc.

$|\lambda\rangle$ has to be a complete set:

$\mathbb{1} = \sum_\lambda |\lambda\rangle\langle\lambda|$, so a basis transformation to $|\mu\rangle$ can be done:

$$|\mu\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\mu\rangle = \sum_\lambda \langle\lambda|\mu\rangle\, |\lambda\rangle$$

To get the transformation behavior of a_λ^+:

$$|\lambda\rangle = a_\lambda^+ |0\rangle \; ; \; |\mu\rangle = a_\mu^+ |0\rangle$$

$$a_\mu^+ |0\rangle = |\mu\rangle = \sum_\lambda \langle\lambda|\mu\rangle\, |\lambda\rangle = \sum_\lambda \underbrace{\langle\lambda|\mu\rangle}_{\langle\mu|\lambda\rangle^*} a_\lambda^+ |0\rangle$$

so: $a_\mu^+ = \sum_\lambda \langle\lambda|\mu\rangle\, a_\lambda^+$, and $a_\mu = \sum_\lambda \langle\mu|\lambda\rangle\, a_\lambda$

Important: position vs. momentum rep:

$\hat{p} = -i\hbar\partial_x \rightsquigarrow \psi_p(x) = e^{ipx/\hbar} = \langle x|p\rangle$

Fourier transform!

Representation of operators:

One-body operators (using state notation):

$$\hat{U}\,|\lambda_1, \lambda_2, \dots \lambda_N\rangle = \sum_i \hat{u}_i\,|\lambda_1, \lambda_2, \dots, \lambda_N\rangle$$

($\hat{u}_i$: acts on i^{th} particle)

assume $\hat{u}$ is diagonal in $|\lambda\rangle$ basis: $\hat{u}_i|\lambda_i\rangle = u_{\lambda_i}|\lambda_i\rangle$

(or $\hat{u}|\lambda\rangle = u_\lambda|\lambda\rangle$)

Then: $\hat{U}\,|\lambda_1, \dots, \lambda_N\rangle = \sum_i u_{\lambda_i}\,|\lambda_1, \dots, \lambda_N\rangle$.

Rewrite this in our number basis:

$$\hat{U}\,|n_1, n_2, \dots\rangle = \sum_\lambda \hat{n}_\lambda u_\lambda\,|n_1, n_2, \dots\rangle$$

($\hat{n}_\lambda$: operator that gives n_λ)

$\hat{n}_\lambda = a_\lambda^\dagger a_\lambda$, so we have $\hat{U} = \sum_\lambda u_\lambda \hat{n}_\lambda$

$$= \sum_\lambda \langle\lambda|\hat{U}|\lambda\rangle a_\lambda^\dagger a_\lambda$$

We can transform to an arbitrary basis:

$$\hat{U} = \sum_{\mu,\nu} \langle\mu|\hat{U}|\nu\rangle\, a_\mu^\dagger a_\nu$$

Important one-body operators:

$\hat{N} = \sum_\lambda \hat{n}_\lambda = \sum_\lambda a_\lambda^\dagger a_\lambda$: total number of particles

$\hat{T} = \sum_n \hat{p}_n^2/2m$: total kin. energy

($\sum_n$: sum over particles)

In general, for a two-body operator, one finds:

$$\hat{V} = \sum_{\lambda,\lambda';\nu,\nu'} \langle \lambda\lambda' | \hat{V} | \nu\nu' \rangle \, a^+_\lambda a^+_{\lambda'} a_{\nu'} a_\nu$$

Note ordering of primes important for fermionic case!

$$\langle \lambda\lambda' | \hat{V} | \nu\nu' \rangle =: V_{\lambda\lambda';\nu\nu'}$$

Look at diagonal case:

$$\hat{V} | \lambda_1 \lambda_2 \rangle = \underbrace{\langle \lambda_1 \lambda_2 | \hat{V} | \lambda_1 \lambda_2 \rangle}_{V_{\lambda_1\lambda_2}} | \lambda_1 \lambda_2 \rangle$$

On general state: $\hat{V} | \lambda_1, \lambda_2, \ldots, \lambda_N \rangle = \sum_{[i,j]\ (\text{all pairs})} V_{\lambda_i\lambda_j} | \lambda_1, \ldots, \lambda_N \rangle$

In occ. number representation:

$$\hat{V} | n_1, n_2, \ldots \rangle = \sum_{\lambda,\lambda'} (\#\text{pairs } \lambda,\lambda') \, V_{\lambda\lambda'} | n_1, n_2, \ldots \rangle$$

$$(\#\text{pairs } \lambda,\lambda') := P_{\lambda\lambda'} = \frac{1}{2}(\hat{n}_\lambda \hat{n}_{\lambda'} - \delta_{\lambda\lambda'} \hat{n}_\lambda), \text{ so,}$$

one finds

$$\hat{V} = \frac{1}{2} \sum_{\lambda,\lambda'} V_{\lambda,\lambda'} \, a^+_\lambda a^+_{\lambda'} a_{\lambda'} a_\lambda$$ (check order of primes!)

Creation operators in position rep: (continuum)

$|\lambda\rangle = |\vec{r}\rangle$; we typically write: $a^+_{\vec{r}} = \hat{\phi}^+(\vec{r})$ bosons

$= \hat{\psi}^+(r)$ fermions

often: skip the hat

In momentum space:

$$\hat{\phi}^+(\vec{r}) = \int \frac{d^d p}{(2\pi)^d} \underbrace{e^{-i\vec{p}\cdot\vec{r}}}_{\langle \vec{p}|\vec{r}\rangle = \langle \vec{r}|\vec{p}\rangle^*} a^+_p$$

$$a^+_p = \int d^d r\, e^{i\vec{p}\cdot\vec{r}}\, \hat{\phi}^+(\vec{r})$$

$(\hbar = 1)$

$\left[\hat{p} = -i\hbar\,\partial/\partial x \right.$
$\left. \psi_p(x) = e^{ipx/\hbar} = \langle x|p\rangle \right]$

Electron system in a solid:

One particle contribution: $\propto$ kinetic energy, interaction w/ ions

+ electron-electron interaction:

$$H = H_0 + V_{ee}$$

$$H_0 = \int d^d r\, \psi^+_\sigma(\vec{r}) \left(\frac{p^2}{2m} + \underbrace{V(\vec{r})}_{\text{periodic background of ions}} \right) \psi_\sigma(\vec{r}) \qquad V(\vec{r}+a\vec{e}_i) = V(\vec{r})$$

$$V_{ee} = \frac{1}{2}\iint d^d r\, d^d r'\, V_{ee}(\vec{r}-\vec{r}')\, \psi^+_\sigma(r)\, \psi^+_{\sigma'}(r')\, \psi_{\sigma'}(r')\, \psi_\sigma(r)$$

(sum over $\sigma = \uparrow, \downarrow$ implied).

Very general Hamiltonian!

We have e^- in periodic potential, so wave functions are Bloch waves:

$$\psi_{k,n}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{k,n}(\vec{r})$$

n: band index (# atoms in unit cell)

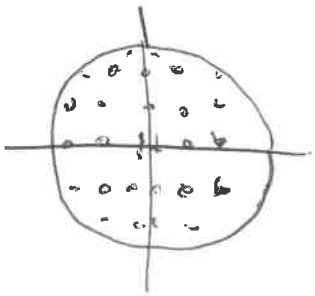
$k_i \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ for cubic lattice

If we assume that the electrons are nearly free, (metal!)
we can ignore lattice potential and set $u_{k,n} = 1$

The electrons effectively screen each other, so the effective interaction is approx. zero!

So the Hamiltonian becomes: $H = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} a^+_{k\sigma} a_{k\sigma}$

The ground state follows from Pauli principle:
States have energy $\varepsilon_k = \hbar^2/2m$, fill them uniformly,
the cutoff is the Fermi energy $E_F = \frac{\hbar^2 k_F^2}{2m}$
Allowed momenta: $k_i = \frac{\pm\pi n_i}{L}$



Ground state:

$$|\Omega\rangle = \prod_{\substack{|k|<k_F \\ \sigma}} a^+_{k\sigma} |0\rangle$$

How do we make an excitation:

Take e^- with $\varepsilon \sim \varepsilon_F$, and move it to an orbital with $\varepsilon > \varepsilon_F$: can create an excitation w/ arbitrary low energy.

For the system, $|\Omega\rangle$ acts as the new vacuum. So, what are the operators $c_{k\sigma}$ s.t. $c_{k\sigma}|\Omega\rangle = 0$?

$$c_{k\sigma} = \begin{cases} a_{k\sigma} & k > k_F \\ a^\dagger_{k\sigma} & k \leq k_F \end{cases} \qquad c^\dagger_{k\sigma} = \begin{cases} a^\dagger_{k\sigma} & k > k_F \\ a_{k\sigma} & k \leq k_F \end{cases}$$

Show: $c_{k\sigma}$'s satisfy fermion comm. relations!

Consider opposite limit: electrons tightly bound to atoms.

Use a basis that reflects this: Wannier.

$$\psi_{\vec{R}_i,n}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{k \in BZ} e^{-i\vec{k}\cdot\vec{R}_i} \psi_k(\vec{r})$$

↳ Bloch.

(atomic orbitals, if atoms are far apart).

Transformation between real space and Wannier:

$$a_\sigma^\dagger(\vec{r}) = \sum_i \psi_{R_i}^*(\vec{r})\, a_{i\sigma}^\dagger$$

(lattice site label)

Together, we find: $a_{k\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} a_{i\sigma}^\dagger$

In these terms, the one particle H_0 becomes:

$$H_0 = \sum_{k,\sigma} \varepsilon_k a_{k\sigma}^\dagger a_{k\sigma} = \frac{1}{N} \sum_{i,i',k,\sigma} e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_{i'})} \varepsilon_k a_{i\sigma}^\dagger a_{i'\sigma}$$

$$:= \sum_{i,i'} t_{i,i'} a_{i\sigma}^\dagger a_{i\sigma}$$

$$t_{i,i'} = \frac{1}{N} \sum_k e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_{i'})} \varepsilon_k \quad \text{: hopping elements}$$

H_0: describes hopping from one site to another!

What is the form of the interaction term?

$$\hat{V}_{ee} = \sum_{\substack{i,i' \\ j,j'}} U_{ii'jj'}\, a^{\dagger}_{i\sigma}\, a^{\dagger}_{i'\sigma'}\, a_{j'\sigma}\, a_{j\sigma}$$

$$V_{ee} \rightsquigarrow U_{ii'jj'} = \frac{1}{2}\int d^d r\, d^d r'\, \psi^{\alpha}_{R_i}(\vec{r})\, \psi^{*}_{R_{i'}}(\vec{r}')\, \psi_{R_{j'}}(\vec{r}')\, \psi_{R_j}(\vec{r}) \times V(\vec{r}-\vec{r}')$$

What are the important terms?

* Direct: $U_{ii'ii'} = V_{ii'} \quad i \neq i'$

$$\rightsquigarrow \sum_{i \neq i'} V_{ii'}\, \hat{n}_i\, \hat{n}_{i'} \qquad \hat{n}_i = \sum_{\sigma} a^{\dagger}_{i\sigma} a_{i\sigma}$$

Coulomb interaction between electrons.

* Exchange: gives magnetic coupling!

$$U_{ijji} = J^{F}_{ij}$$

$$\hat{V}_{ee} \rightsquigarrow \sum_{i \neq j} U_{ijji}\, a^{\dagger}_{i\sigma}\, a^{\dagger}_{j\sigma'}\, a_{j\sigma'}\, a_{j\sigma}$$

Using a spin operator: $\vec{S}_i = \frac{1}{2}\, a^{\dagger}_{i\sigma}\, \vec{\sigma}_{\sigma\sigma'}\, a_{i\sigma}$, one gets:

($\vec{\sigma}$: Pauli matrices)

$$V_{ee} \rightsquigarrow -2 \sum_{i \neq j} J^{F}_{ij} \left(\vec{S}_i \cdot \vec{S}_j + \frac{1}{4}\, \hat{n}_i\, \hat{n}_j \right)$$

Coulomb is repulsive $\to J^F_{ij} > 0$, gives a ferromagnetic spin interaction!

$$\left(\vec{\tau}_{\alpha\beta} \cdot \vec{\tau}_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta} \right)$$

Local (Hubbard) term:

$$V_{ee} \rightsquigarrow \sum_{i,\sigma\sigma'} U''^{U_2}_{iiii} \, a^+_{i\sigma} a^+_{i\sigma'} a_{i\sigma'} a_{i\sigma}$$

$$= \sum_{i,\sigma\sigma'} \frac{U_i}{2} \left(\hat{n}_{i\sigma}\hat{n}_{i\sigma'} - \hat{n}_{i\sigma}\delta_{\sigma\sigma'} \right)$$

$$= \cancel{0} \sum_i U_i \, \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

On-site term, dominates if atoms are far ~~apart~~ apart.

(t_{ij}, J^F_{ij} small)