SECOND QUANTIZATION

Aim of these notes is to introduce the method of second quantization (2ndQ), i.e., a formulation based on the algebra of ladder operators $\hat{a}, \hat{a}^{\perp}$

- Why the need of second quantization (2ndQ)
- The formalism of 2ndQ

1. DRAWBACKS OF 1st QUANTIZATION

Motivations of a 2Q approach:

(i.e. drawbacks of 1Q approach to many-body problems)

Refresh:

- Quantum mechanical indistinguishability of identical particles

$$\psi(\vec{r}_1,...,\vec{r}_j,..,\vec{r}_k,...,\vec{r}_N) = \lambda\psi(\vec{r}_1,...,\vec{r}_k,..,\vec{r}_j,...,\vec{r}_N) = \lambda^2\psi(\vec{r}_1,...,\vec{r}_j,..,\vec{r}_k,...,\vec{r}_N)$$

$\Rightarrow$ $\lambda^2 = 1$, or $\lambda = \pm 1$ for bosons/fermions

requires symmetrization of many-body wave function in 1Q
(→ complications, especially in the presence of interactions)

- 1stQ tailor-made for problems with fixed particle number *N*

1stQ APPROACH TO MANY-BODY QUANTUM MECHANICS

Consider the set of eigenfunctions $|\psi_\lambda\rangle = |\lambda\rangle$ of a single-particle Hamiltonian $\hat{H}_{\text{sp}}$

$$\hat{H}_{\text{sp}}|\psi_\lambda\rangle = \varepsilon_\lambda|\psi_\lambda\rangle$$

or the set

$$\{\psi_\lambda(\vec{r}) = \langle\vec{r}|\psi_\lambda\rangle = \langle\vec{r}|\lambda\rangle\}$$

The quantum mechanics for a system on *N* particles in 1Q is based on the observation that any *N*-particles wave function can be built from the complete, orthonormal basis $\{\psi_\lambda(\vec{r})\}$

2-PARTICLES WAVE FUNCTION

A two-particles wave function (normalized) reads

$$\begin{cases} \psi^{\mathrm{F/B}}_{\lambda_{\nu_1},\lambda_{\nu_2}}(\vec{r}_1,\vec{r}_2) = \dfrac{1}{\sqrt{2}}\mathcal{N}\left[\psi_{\lambda_{\nu_1}}(\vec{r}_1)\psi_{\lambda_{\nu_2}}(\vec{r}_2) \mp \psi_{\lambda_{\nu_2}}(\vec{r}_1)\psi_{\lambda_{\nu_1}}(\vec{r}_2)\right] \\ \mathcal{N} = \dfrac{1}{\prod_\lambda \sqrt{n_\lambda!}} \end{cases}$$

F/B: Fermions/Bosons

Where n_λ is the number of times the state $|\lambda\rangle$ appears in the set $\{|\lambda_{\nu_1}\rangle, |\lambda_{\nu_2}\rangle\}$. In Dirac representation,

$$|\lambda_{\nu_1}, \lambda_{\nu_2}\rangle_{\mathrm{F/B}} = \frac{\mathcal{N}}{\sqrt{2}}\left[|\lambda_{\nu_1}\rangle \otimes |\lambda_{\nu_2}\rangle \mp |\lambda_{\nu_2}\rangle \otimes |\lambda_{\nu_1}\rangle\right]$$

➡ Generic 2-body wave function reads (cf. H_2 molecule)

$$\psi^{\mathrm{F/B}}(\vec{r}_1,\vec{r}_2) = \sum_{\nu_1\nu_2} B_{\nu_1\nu_2}\psi^{\mathrm{F/B}}_{\lambda_{\nu_1},\lambda_{\nu_2}}(\vec{r}_1,\vec{r}_2)$$

1stQ 3-BODY WAVE FUNCTION

For the 3-particles wave function (normalized) one introduces the determinant/permanent for fermions/bosons

$$Example: \lambda_{\nu_1} = \lambda_1, \lambda_{\nu_2} = \lambda_2, \lambda_{\nu_3} = \lambda_3$$

$$\psi^{F/B}_{\lambda_1,\lambda_2,\lambda_3}(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \frac{\mathcal{N}}{\sqrt{3!}} \begin{vmatrix} \psi_{\lambda_1}(\vec{r}_1) & \psi_{\lambda_1}(\vec{r}_2) & \psi_{\lambda_1}(\vec{r}_3) \\ \psi_{\lambda_2}(\vec{r}_1) & \psi_{\lambda_2}(\vec{r}_2) & \psi_{\lambda_2}(\vec{r}_3) \\ \psi_{\lambda_3}(\vec{r}_1) & \psi_{\lambda_3}(\vec{r}_2) & \psi_{\lambda_3}(\vec{r}_3) \end{vmatrix}_{\mp}, \quad \mathcal{N} = \frac{1}{\prod_\lambda \sqrt{n_\lambda!}}$$

$|\,|_-$ determinant, $|\,|_+$ permament (= no sign change)

or

$$|\lambda_1,\lambda_2,\lambda_3\rangle_{F/B} = \frac{1}{\sqrt{3!}}\mathcal{N}[|\lambda_1\rangle\otimes|\lambda_2\rangle\otimes|\lambda_3\rangle \mp |\lambda_1\rangle\otimes|\lambda_3\rangle\otimes|\lambda_2\rangle$$

$$\mp|\lambda_2\rangle\otimes|\lambda_1\rangle\otimes|\lambda_3\rangle \mp |\lambda_3\rangle\otimes|\lambda_2\rangle\otimes|\lambda_1\rangle + |\lambda_2\rangle\otimes|\lambda_3\rangle\otimes|\lambda_1\rangle$$

$$+|\lambda_3\rangle\otimes|\lambda_1\rangle\otimes|\lambda_2\rangle]$$

3-BODY WAVE FUNCTION

Generic 3-body wave function reads

$$\psi^{\mathrm{F/B}}(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \sum_{\nu_1,\nu_2,\nu_3} B_{\lambda_{\nu_1}\lambda_{\nu_2}\lambda_{\nu_3}} \psi^{\mathrm{F/B}}_{\lambda_{\nu_1},\lambda_{\nu_2},\lambda_{\nu_3}}(\vec{r}_1,\vec{r}_2,\vec{r}_3)$$

1Q *N*-BODY WAVE FUNCTION

The *N*-particles wave function (normalized) is

$$\left|\lambda_{\nu_1},\lambda_{\nu_2},\ldots\lambda_{\nu_N}\right\rangle = \frac{1}{\sqrt{N!}}\frac{1}{\sqrt{\prod_{\lambda=0}^{\infty} n_\lambda!}}\sum_P(-\xi)^{(1-\mathrm{par}\,P)/2}\left|\lambda_{P_1}\right\rangle\otimes\ldots.\otimes\left|\lambda_{P_N}\right\rangle$$

Where:

- $\xi = \pm$ for fermions / bosons
- n_λ total number of particles in state λ ($n_\lambda = 0,1$ for fermions)
- $\sum_P$ sum over all permutations of the q-numbers $\{\lambda_{\nu_1},\ldots,\lambda_{\nu_N}\}$
- $\mathrm{par}\,P$ parity of the permutation P

(= 1 or –1 for even/odd number of transpositions)

2. THE FORMALISM OF 2nd Q

The so-called second quantized representation, or occupation number representation, is based on:

- Particle´s indistinguishability
- Observation that determinants or permanents of single particle states form a basis for the Hilbert space of *N*-particle states

Idea: It must be simpler to formulate a representation where one just counts how many particles are in each single particle state

THE FORMALISM OF 2nd Q

In the occupation nr. representation the basis states for an *N*-particle system are obtained by listing the occupation nr. of each basis state:

N-particle basis states

$$\left\{ \left| n_{\lambda_1}, n_{\lambda_2}, \ldots \right\rangle \right\}; \quad \sum_j n_{\lambda_j} = N$$

Sum over j determined by the dimension M of single particle Hilbert space

We introduce the nr. operators $\hat{n}_{\lambda_i} \left| n_{\lambda_i} \right\rangle = n_{\lambda_i} \left| n_{\lambda_i} \right\rangle$

Note: In the following, when speaking about the state $\left| n_{\lambda_1}, n_{\lambda_2}, \ldots \right\rangle$ it is convenient to think that the quantum numbers $\{\lambda_j\}$ are ordered (e.g. $\lambda_i = x_i$, $x_1 < x_2 < \ldots x_n$)

THE FORMALISM OF 2nd Q

N-fermion basis states

$$
\begin{array}{llllll}
0 & |0,0,0,..\rangle & & & & \\
1 & |1,0,0,..\rangle & |0,1,0,..\rangle & |0,0,1,..\rangle & ... \\
2 & |1,1,0,..\rangle & |1,0,1,..\rangle & |0,1,1,..\rangle & .... \\
\vdots & \vdots & \vdots & \vdots &
\end{array}
$$

N-boson basis states

$$
\begin{array}{llllll}
0 & |0,0,0,..\rangle & & & & \\
1 & |1,0,0,..\rangle & |0,1,0,..\rangle & |0,0,1,..\rangle & ... \\
2 & |2,0,0,..\rangle & |0,2,0,..\rangle & |1,1,0,..\rangle & .... \\
\vdots & \vdots & \vdots & \vdots &
\end{array}
$$

CREATION AND DESTRUCTION OPERATORS

To construct this more efficient formulation, we begin with some abstract definitions:

i) Introduce a reference state $|0\rangle$ called vacuum state

ii) Introduce a set of operators $\hat{a}_\lambda$, and their adjoint $\hat{a}_\lambda^\perp$, such that

$$\hat{a}_\lambda |0\rangle = 0$$

$$\mathcal{N}\prod_{i=1}^{N} \hat{a}^\perp_{\lambda_{\nu_i}} |0\rangle = \mathcal{N}\, \hat{a}^\perp_{\lambda_{\nu_1}}\, \hat{a}^\perp_{\lambda_{\nu_2}} \ldots \hat{a}^\perp_{\lambda_{\nu_N}} |0\rangle = |\lambda_{\nu_1}, \lambda_{\nu_2}, \ldots, \lambda_{\nu_N}\rangle, \quad \mathcal{N}^{-1} = \sqrt{\prod_\lambda n_\lambda !}$$

with n_λ the number of times the state $|\lambda\rangle$ appears in the set $\{|\lambda_{\nu_1}\rangle, \ldots, |\lambda_{\nu_N}\rangle\}$

$$|n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle$$

$$n_\lambda = \begin{cases} 0,1 & \text{fermions} \\ 0,1,2,\ldots & \text{bosons} \end{cases}$$

COMMUTATION RELATIONS

iii) In order to take care of the symmetry of the wave functions, the operators $\hat{a}_\lambda$, $\hat{a}_\lambda^\perp$ fulfill the commutation relations

$$[\hat{a}_\lambda, \hat{a}_\mu^\perp]_\xi \equiv \hat{a}_\lambda \hat{a}_\mu^\perp + \xi \hat{a}_\mu^\perp \hat{a}_\lambda = \delta_{\mu\lambda} \qquad (*)$$

ξ = +/- fermions/bosons

$$[\hat{a}_\lambda, \hat{a}_\mu]_\xi = [\hat{a}_\lambda^\perp, \hat{a}_\mu^\perp]_\xi = 0 \qquad (**)$$

- To understand (**), observe that:

$$|\lambda, \mu\rangle = \mathcal{N} \hat{a}_\lambda^\perp \hat{a}_\mu^\perp |0\rangle, \quad |\mu, \lambda\rangle = \mathcal{N}\, \hat{a}_\mu^\perp \hat{a}_\lambda^\perp |0\rangle = -\xi |\lambda, \mu\rangle \Rightarrow (**)$$

- For (*) observe that:

$$\delta_{\lambda\mu} = \langle 0 | \hat{a}_\lambda \hat{a}_\mu^\perp | 0 \rangle = \langle 0 | (-\xi)\, \hat{a}_\mu^\perp \hat{a}_\lambda + [\hat{a}_\lambda, \hat{a}_\mu^\perp]_\xi | 0 \rangle = \langle 0 | [\hat{a}_\lambda, \hat{a}_\mu^\perp]_\xi | 0 \rangle$$

COMPLETENESS OF 2Q APPROACH

Under these prescriptions:

Any *N*-body wave function can be generated by the application of a set of *N* independent creation operators $\hat{a}_\lambda^\perp$ to a unique vacuum state

FOCK SPACE

iv) Define now by $\mathcal{F}_N$ the Hilbert space of states with fixed particle number *N*; i.e., the linear span of all states

$$\left| \lambda_{\nu_1}, \lambda_{\nu_2}, ..., \lambda_{\nu_N} \right\rangle.$$

v) Call Fock space $\mathcal{F}$ the full space containing all many-body states

$$\mathcal{F} \equiv \oplus_{N=1}^{\infty} \mathcal{F}_N$$

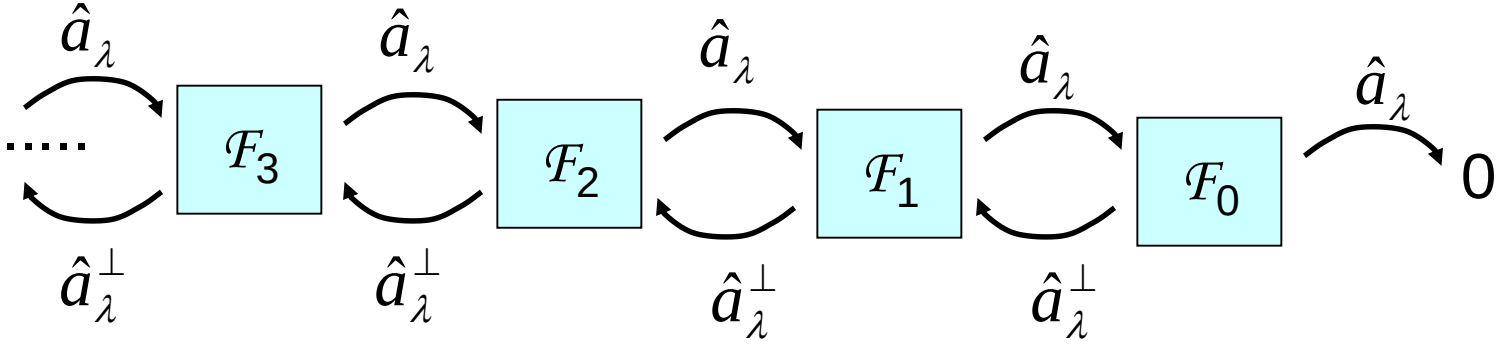
⟶ While the operator algebra of $\hat{a}_\lambda, \hat{a}_\lambda^\perp$ does not close in individual $\mathcal{F}_N$, it does in $\mathcal{F}$

FOCK SPACE II

Note: bosons vs fermions

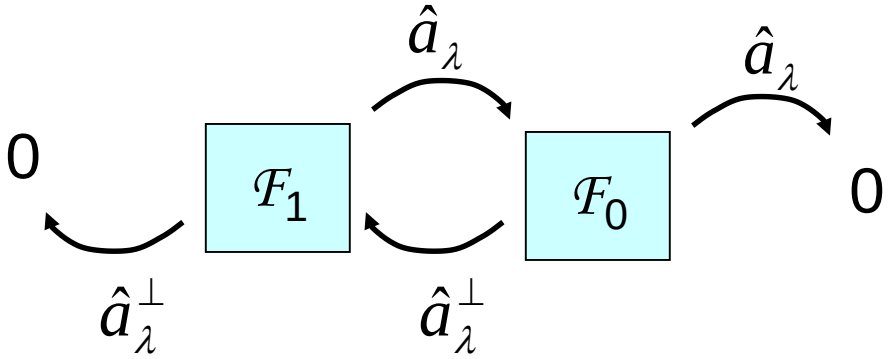
Let us repeatedly apply the same destruction / creation operators $\hat{a}_\lambda, \hat{a}_\lambda^\perp$

bosons



fermions

$$\left(\hat{a}_\lambda^\perp\right)^2 = \left(\hat{a}_\lambda\right)^2 = 0$$



OCCUPATION NUMBER OPERATOR

vi) Define the occupation number operator $\hat{n}_\lambda = \hat{a}_\lambda^\perp \hat{a}_\lambda$

$$\Rightarrow \quad \hat{n}_\lambda (\hat{a}_\lambda^\perp)^n \left|0\right\rangle = n (\hat{a}_\lambda^\perp)^n \left|0\right\rangle$$

i.e., $(\hat{a}_\lambda^\perp)^n \left|0\right\rangle$ is eigenstate of $\hat{n}_\lambda$

Moreover,

$$\hat{n}_\lambda \left| \lambda_{\nu_1}, \lambda_{\nu_2}, ..., \lambda_{\nu_N} \right\rangle = \mathcal{N} \hat{a}_\lambda^\perp \hat{a}_\lambda \prod_{i=1}^{N} \hat{a}_{\lambda_{\nu_i}}^\perp \left|0\right\rangle = \sum_{i=1}^{N} \delta_{\lambda \lambda_{\nu_i}} \left| \lambda_{\nu_1}, ..., \lambda_{\nu_N} \right\rangle$$

NOTE: CHANGE OF BASIS

$$I = \sum_{\lambda} |\lambda\rangle\langle\lambda| \Rightarrow \quad |\tilde{\lambda}\rangle = \sum_{\lambda} |\lambda\rangle\langle\lambda|\tilde{\lambda}\rangle = \sum_{\lambda} \hat{a}_{\lambda}^{\perp}|0\rangle\langle\lambda|\tilde{\lambda}\rangle = \hat{a}_{\tilde{\lambda}}^{\perp}|0\rangle$$

i.e.,

$$\hat{a}_{\tilde{\lambda}}^{\perp} = \sum_{\lambda} \hat{a}_{\lambda}^{\perp}\langle\lambda|\tilde{\lambda}\rangle, \quad \hat{a}_{\tilde{\lambda}} = \sum_{\lambda} \hat{a}_{\lambda}\langle\tilde{\lambda}|\lambda\rangle$$

Example: Transformation from the coordinate to the momentum representation for a 1d system of length *L*

$$\hat{a}_{\tilde{\lambda}} = \hat{a}(x), \quad \hat{a}_{\lambda} = \hat{a}_k$$

$$\hat{a}(x) = \sum_k \hat{a}_k \langle x|k\rangle = \frac{1}{\sqrt{L}} \sum_k \hat{a}_k e^{ikx}$$

$$\hat{a}_k = \int_0^L \mathrm{d}x \langle k|x\rangle \hat{a}(x) = \frac{1}{\sqrt{L}} \int_0^L \mathrm{d}x e^{-ikx} \hat{a}(x)$$

NOTE: OPERATORS

In 2ndQ every operator can be expressed in terms of the creation and annhilation operators.

ONE- AND TWO-BODY OPERATORS

In particular:

- 1-body operators

$$\hat{O}_1 = \sum_{i=1}^{N} \hat{o}_{1,i} = \sum_{\lambda,\mu} o_{\mu\lambda} \hat{a}_\mu^\perp \hat{a}_\lambda$$

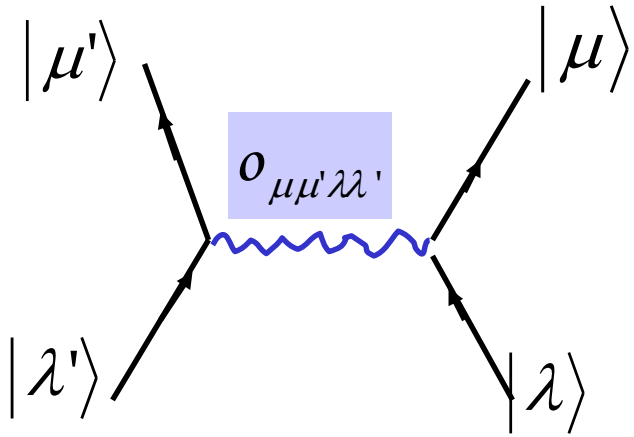
$$o_{\mu\lambda} = \langle \mu | \hat{o}_1 | \lambda \rangle$$

matrix elements from 1stQ

- 2-body operators

$$\hat{O}_2 = \frac{1}{2} \sum_{j,k \neq j=1}^{N} \hat{o}_{2,jk} = \frac{1}{2} \sum_{\lambda\lambda'\mu\mu'} o_{\mu\mu'\lambda\lambda'} \hat{a}_\mu^\perp \hat{a}_{\mu'}^\perp \hat{a}_{\lambda'} \hat{a}_\lambda$$

$$o_{\mu\mu'\lambda\lambda'} = \langle \mu | \langle \mu' | \hat{o}_2 | \lambda \rangle | \lambda' \rangle,$$



- matrix elements from 1stQ
- non symmetrized form!
- order of indices relevant for fermion operators

3. REPRESENTATION FOR 1-BODY OPERATORS IN 1stQ

One-body operators $\hat{O}_1$ acting in the *N*-particle Hilbert space $\mathcal{F}_N$ read

$$\hat{O}_1 = \sum_{i=1}^{N} \hat{o}_{1,i}$$

with $\hat{o}_{1,i}$ an ordinary operator acting on particle i

Example: local operators

- Kinetic operator $\hat{T} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2M} = -\sum_{i=1}^{N} \frac{\hbar^2 \hat{\nabla}_i^2}{2M} = \sum_{i=1}^{N} \hat{t}_i$
- One particle potential operator $\hat{V} = \sum_{i=1}^{N} v(\hat{\vec{r}}_i) = \sum_{i=1}^{N} \hat{v}_i$

In general

$$\hat{o}_1 = \sum_{\lambda_1,\lambda_2} o_{\lambda_1\lambda_2} |\lambda_1\rangle\langle\lambda_2|,$$

$$o_{\lambda_1\lambda_2} = \langle\lambda_1|\hat{o}_1|\lambda_2\rangle = \int d\vec{r}_i \psi^*_{\lambda_1}(\vec{r}_i) o_1(\vec{r}_i) \psi_{\lambda_2}(\vec{r}_i)$$

in position representation

1-BODY OPERATORS IN 2ndQ

Consider a 1-body operator that is diagonal in the basis $|\lambda\rangle$, i.e.,

$$\hat{O}_1 = \sum_{i=1}^{N} \hat{o}_{1,i} \quad \text{with} \quad \hat{o}_1 = \sum_{\lambda} o_\lambda |\lambda\rangle\langle\lambda|, \quad o_\lambda = \langle\lambda|\hat{o}_1|\lambda\rangle$$

$$\langle \lambda_{\nu_1'}, \lambda_{\nu_2'}, ..., \lambda_{\nu_N'} | \hat{O}_1 | \lambda_{\nu_1}, \lambda_{\nu_2}, ..., \lambda_{\nu_N} \rangle$$

$$= \langle \lambda_{\nu_1'}, \lambda_{\nu_2'}, ..., \lambda_{\nu_N'} | \sum_{i=1}^{N} \sum_{\lambda_i} o_{\lambda_i} |\lambda_i\rangle\langle\lambda_i| \lambda_{\nu_1}, \lambda_{\nu_2}, ..., \lambda_{\nu_N} \rangle$$

$$\langle \lambda_{\nu_1'}, \lambda_{\nu_2'}, ..., \lambda_{\nu_N'} | \sum_{i=1}^{N} \sum_{\lambda_i} o_{\lambda_i} \delta_{\lambda_i, \lambda_{\nu_i}} | \lambda_{\nu_1}, \lambda_{\nu_2}, ..., \lambda_{\nu_N} \rangle$$

$$= \langle \lambda_{\nu_1'}, \lambda_{\nu_2'}, ..., \lambda_{\nu_N'} | \sum_{\lambda} o_\lambda \hat{n}_\lambda | \lambda_{\nu_1}, \lambda_{\nu_2}, ..., \lambda_{\nu_N} \rangle$$

$$\hat{n}_\lambda | \lambda_{\nu_1}, \lambda_{\nu_2}, ..., \lambda_{\nu_N} \rangle = \sum_{i=1}^{N} \delta_{\lambda \lambda_{\nu_i}} | \lambda_{\nu_1}, ..., \lambda_{\nu_N} \rangle$$

$$\hat{O}_1 = \sum_{\lambda} o_\lambda \hat{n}_\lambda = \sum_{\lambda} \langle\lambda|\hat{o}_1|\lambda\rangle \hat{a}_\lambda^\dagger \hat{a}_\lambda$$

1-BODY OPERATORS IN 2ndQ II

$$\hat{O}_1 = \sum_{\lambda} o_\lambda \hat{n}_\lambda = \sum_{\lambda} \langle \lambda | \hat{o}_1 | \lambda \rangle \hat{a}^\perp_\lambda \hat{a}_\lambda$$

In a generic basis $|\tilde{\lambda}\rangle$ using

$$\hat{a}_{\tilde{\lambda}} = \sum_{\lambda} \hat{a}_\lambda \langle \tilde{\lambda} | \lambda \rangle, \quad \hat{a}^\perp_{\tilde{\lambda}} = \sum_{\lambda} \hat{a}^\perp_\lambda \langle \lambda | \tilde{\lambda} \rangle$$

$$\hat{a}_\lambda = \sum_{\tilde{\eta}} \hat{a}_{\tilde{\eta}} \langle \lambda | \tilde{\eta} \rangle, \quad \hat{a}^\perp_\lambda = \sum_{\tilde{\nu}} \hat{a}^\perp_{\tilde{\nu}} \langle \tilde{\nu} | \lambda \rangle$$

one finds

$$\hat{O}_1 = \sum_{\tilde{\nu},\tilde{\eta}} o_{\tilde{\nu}\tilde{\eta}} \hat{a}^\perp_{\tilde{\nu}} \hat{a}_{\tilde{\eta}}$$

1-body operators in 2ndQ are composed of products of creation and annihilation operators, weighted by the appropriate matrix element of the operator calculated in 1stQ

LOCAL 1-BODY OPERATORS: KINETIC ENERGY

Local operators defined on single particle states described by the coordinate $\vec{r}_i$

$$\hat{T} = \sum_{i=1}^{N} \hat{t}_i = -\sum_{i=1}^{N} \frac{\hbar^2}{2M} \hat{\nabla}^2_{\vec{r}_i} = \sum_{\lambda,\mu} t_{\mu\lambda} \hat{a}^{\perp}_{\mu} \hat{a}_{\lambda}$$

Kinetic energy

i) Position representation

$$t_{\mu\lambda} = \langle \mu | \hat{t} | \lambda \rangle = \int d\vec{r} \int d\vec{r}' \langle \mu | \vec{r} \rangle \langle \vec{r} | \hat{t} | \vec{r}' \rangle \langle \vec{r}' | \lambda \rangle$$

$t(\vec{r})$

$$= \int d\vec{r} \int d\vec{r}' \psi^*_{\mu}(\vec{r}) \langle \vec{r} | \hat{t} | \vec{r}' \rangle \psi_{\lambda}(\vec{r}') = \int d\vec{r} \psi^*_{\mu}(\vec{r}) \left(-\frac{\hbar^2}{2M} \hat{\nabla}^2_{\vec{r}} \right) \psi_{\lambda}(\vec{r})$$

$$\Rightarrow \hat{T} = \sum_{\lambda,\mu} t_{\mu\lambda} \hat{a}^{\perp}_{\mu} \hat{a}_{\lambda} = \int d\vec{r} \left(\sum_{\mu} \psi^*_{\mu}(\vec{r}) \hat{a}^{\perp}_{\mu} \right) t(\vec{r}) \left(\sum_{\lambda} \psi_{\lambda}(\vec{r}) \hat{a}_{\lambda} \right)$$

$$= \boxed{\int d\vec{r} \hat{a}^{\perp}(\vec{r}) t(\vec{r}) \hat{a}(\vec{r})}$$

same form as for matrix elements with

$$\psi(\vec{r}_i) \to \hat{a}(\vec{r}_i), \quad \psi^*(\vec{r}_i) \to \hat{a}^{\perp}(\vec{r}_i)$$

KINETIC ENERGY II

ii) Momentum representation

$$\hat{T} = \int d\vec{r}\,\hat{a}^{\perp}(\vec{r})\,t(\vec{r})\,\hat{a}(\vec{r}) = -\frac{1}{V}\sum_{\vec{k}}\sum_{\vec{k}'}\int d\vec{r}\,e^{-i\vec{k}\cdot\vec{r}}\,\hat{a}^{\perp}_{\vec{k}}\,\frac{\hbar^2}{2M}\nabla^2_{\vec{r}}\,e^{i\vec{k}'\cdot\vec{r}}\,\hat{a}_{\vec{k}'}$$

$$= -\sum_{\vec{k}}\frac{\hbar^2 k^2}{2M}\underbrace{\hat{a}^{\perp}_{\vec{k}}\hat{a}_{\vec{k}}}$$

$$\hat{a}^{\perp}(\vec{r}) = \sum_{\vec{k}}\left\langle \vec{r}\middle|\vec{k}\right\rangle^{*}\hat{a}^{\perp}_{\vec{k}} = \frac{1}{\sqrt{V}}\sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}}\,\hat{a}^{\perp}_{\vec{k}}$$

$$\frac{1}{V}\int d\vec{r}\,e^{i\vec{k}\cdot\vec{r}} = \delta_{\vec{k},0}$$

i.e.,

$$\hat{T} = -\sum_{\vec{k}}\frac{\hbar^2 k^2}{2M}\hat{n}_{\vec{k}}$$

since $\hat{t}$ is diagonal in *k*-space

LOCAL 1 BODY OPERATORS: DENSITY OPERATOR

$$n(\vec{r}) = |\psi(\vec{r})|^2 = \int d\vec{r}\,'\psi^*(\vec{r}\,')\delta(\vec{r}-\vec{r}\,')\psi(\vec{r}\,')$$

probability density to find a particle in $\vec{r}$

$$\Rightarrow \quad \hat{n}_{tot} = \sum_{i=1}^{N} \hat{n}_i = \sum_{i=1}^{N} \delta(\vec{r} - \hat{\vec{r}}_i)$$

Density operator

i) Position representation

$$\hat{n}_{tot} = \sum_{\mu\lambda} \rho_{\mu\lambda} \hat{a}_\mu^\perp \hat{a}_\lambda = \sum_{\mu\lambda} \left(\int d\vec{r}\,' \psi_\mu^*(\vec{r}\,') \delta(\vec{r}-\vec{r}\,') \psi_\lambda(\vec{r}\,') \right) \hat{a}_\mu^\perp \hat{a}_\lambda = \boxed{\hat{a}^\perp(\vec{r})\hat{a}(\vec{r})}$$

ii) Momentum representation

$$\hat{n}_{tot}(\vec{r}) = \hat{a}^\perp(\vec{r})\hat{a}(\vec{r}) = \frac{1}{V}\sum_{\vec{k},\vec{k}'} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}\, \hat{a}_{\vec{k}}^\perp \hat{a}_{\vec{k}'} = \frac{1}{V}\sum_{\vec{k}',\vec{q}} e^{-i\vec{q}\cdot\vec{r}}\, \hat{a}_{\vec{k}'+\vec{q}}^\perp \hat{a}_{\vec{k}'}$$

$$\hat{n}_{tot}(\vec{r}) = \frac{1}{V}\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}}\, \hat{\rho}_{\vec{q}}; \quad \hat{\rho}_{\vec{q}} = \sum_{\vec{k}} \hat{a}_{\vec{k}}^\perp \hat{a}_{\vec{k}+\vec{q}}$$

$\vec{q} = \vec{k} - \vec{k}'$

momentum transfer

LOCAL 1 BODY OPERATORS: NUMBER OPERATOR

$$\hat{N} = \int d\vec{r}\,\hat{n}_{tot}(\vec{r})$$ Number operator

i) Position representation

$$\hat{N} = \int d\vec{r}\;\hat{a}^{\perp}(\vec{r})\hat{a}(\vec{r})$$

ii) Momentum representation

$$\hat{N} = \frac{1}{V}\int d\vec{r}\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}}\,\hat{\rho}_{\vec{q}} = \hat{\rho}_{\vec{q}=0} = \sum_{\vec{k}} \hat{a}^{\perp}_{\vec{k}}\hat{a}_{\vec{k}} = \sum_{\vec{k}} \hat{n}_{\vec{k}}$$

Note: 1 body Hamiltonian

$$\hat{H} = \sum_{\lambda} \varepsilon_{\lambda}\hat{a}^{\perp}_{\lambda}\hat{a}_{\lambda} + const = \sum_{\lambda} \varepsilon_{\lambda}\hat{n}_{\lambda} + const.$$

SPIN OPERATOR

$$\vec{S} = \sum_{i=1}^{N} \hat{\vec{s}}_{1,i} = \frac{\hbar}{2} \sum_{i=1}^{N} \hat{\vec{\sigma}}_{1,i}$$

Total spin operator for *N* electrons

In 1stQ single spin is expressed with the vector of Pauli matrices

$$\hat{\vec{\sigma}}_1 = \{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}$$

in basis

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle; \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle$$

To obtain the 2ndQ form, pull out the spin explicitly: $\mu = \{\alpha, \sigma\}$

$$\vec{S} = \frac{\hbar}{2} \sum_{\alpha\alpha'\sigma\sigma'} \langle \alpha' | \langle \sigma' | \vec{\sigma}_1 | \sigma \rangle | \alpha \rangle \hat{a}^{\perp}_{\alpha'\sigma'} \hat{a}_{\alpha\sigma} = \frac{\hbar}{2} \sum_{\alpha\sigma\sigma'} \langle \sigma' | \vec{\sigma}_1 | \sigma \rangle \hat{a}^{\perp}_{\alpha\sigma'} \hat{a}_{\alpha\sigma}$$

where $\hat{a}^{\perp}, \hat{a}$ are fermionic operators

SPIN OPERATOR II

One has, with, $\left\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\right\} = \left\{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}$

$$\begin{cases} \left\langle \sigma' \middle| \hat{\vec{\sigma}}_x \middle| \sigma \right\rangle = \delta_{\sigma,-\sigma'} \\ \left\langle \sigma' \middle| \hat{\vec{\sigma}}_y \middle| \sigma \right\rangle = i\delta_{\sigma,-\sigma'}(\delta_{\sigma,\uparrow} - \delta_{\sigma,\downarrow}) \\ \left\langle \sigma' \middle| \hat{\vec{\sigma}}_z \middle| \sigma \right\rangle = \delta_{\sigma,\sigma'}(\delta_{\sigma,\uparrow} - \delta_{\sigma,\downarrow}) \end{cases}$$

yielding

$$\hat{\vec{S}} = \frac{\hbar}{2}\sum_{\alpha}\left[(\hat{a}^{\perp}_{\alpha\downarrow}\hat{a}_{\alpha\uparrow} + \hat{a}^{\perp}_{\alpha\uparrow}\hat{a}_{\alpha\downarrow}), i(\hat{a}^{\perp}_{\alpha\downarrow}\hat{a}_{\alpha\uparrow} - \hat{a}^{\perp}_{\alpha\uparrow}\hat{a}_{\alpha\downarrow}), (\hat{a}^{\perp}_{\alpha\uparrow}\hat{a}_{\alpha\uparrow} - \hat{a}^{\perp}_{\alpha\downarrow}\hat{a}_{\alpha\downarrow})\right]$$

$\hat{a}^{\perp}, \hat{a}$ fermionic operators

4. REPRESENTATION OF TWO-BODY OPERATORS

Since only 2 particles are involved in a pair interaction process, a general two-body operator $\hat{O}_2$ can be completely characterized in terms of its action on two-particle states

- Consider the matrix element

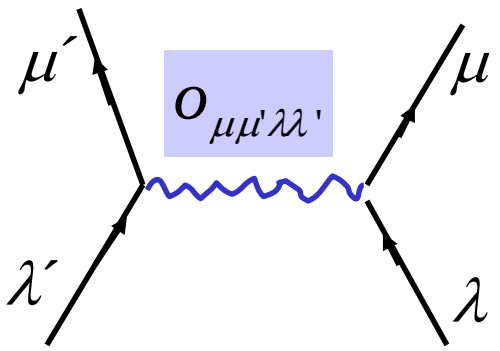
$$o_{\mu,\mu';\lambda,\lambda'} = \langle \mu | \langle \mu' | \hat{o}_2 | \lambda \rangle | \lambda' \rangle$$

Non symmetrized

- Compute

$$\langle \mu_1 \mu_2 \ldots \mu_N | \hat{O}_2 | \lambda_1 \lambda_2 \ldots \lambda_N \rangle$$

$$\Rightarrow \quad \hat{O}_2 = \frac{1}{2} \sum_{\lambda\lambda'\mu\mu'} o_{\mu\mu'\lambda\lambda'} \hat{a}^{\perp}_{\mu} \hat{a}^{\perp}_{\mu'} \hat{a}_{\lambda'} \hat{a}_{\lambda}$$

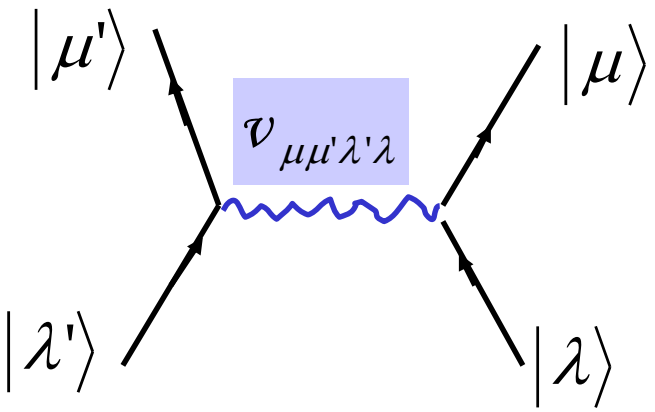


2-BODY OPERATOR: COULOMB INTERACTION

Coulomb interaction is an operator defined on two single particle states described by the coordinates $\vec{r}_j, \vec{r}_k$

$$\hat{H}_{ee} = \hat{V}_{ee} = \frac{1}{2}\sum_{j,k\neq j}^{N}\hat{v}_{ee,jk} = \frac{1}{2}\sum_{j,k\neq j}^{N} v_{ee}(\hat{\vec{r}}_j - \hat{\vec{r}}_k)$$

2ndQ: $$\hat{V}_{ee} = \frac{1}{2}\sum_{\mu\mu'\lambda\lambda'}^{\infty} v_{\mu\mu'\lambda\lambda'}\hat{a}_{\mu}^{\perp}\hat{a}_{\mu'}^{\perp}\hat{a}_{\lambda'}\hat{a}_{\lambda}$$



i) Position representation

$$\hat{V}_{ee} = \frac{1}{2}\sum_{\mu\mu'\lambda\lambda'}^{\infty}\left(\int d\vec{r}\int d\vec{r}'\psi_{\mu}^{*}(\vec{r})\psi_{\mu'}^{*}(\vec{r}')v_{ee}(\vec{r}-\vec{r}')\psi_{\lambda'}(\vec{r}')\psi_{\lambda}(\vec{r})\right)\hat{a}_{\mu}^{\perp}\hat{a}_{\mu'}^{\perp}\hat{a}_{\lambda'}\hat{a}_{\lambda}$$

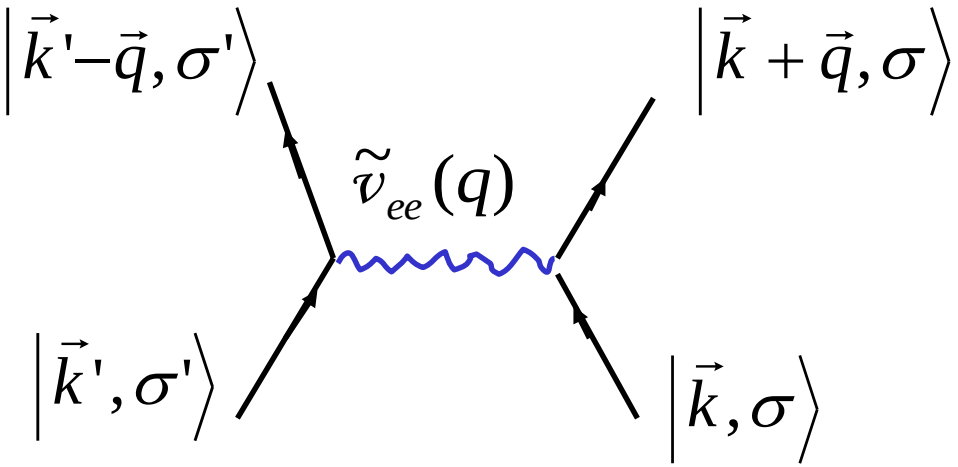
$$= \frac{1}{2}\int d\vec{r}\int d\vec{r}'\hat{a}^{\perp}(\vec{r})\hat{a}^{\perp}(\vec{r}')v_{ee}(\vec{r}-\vec{r}')\hat{a}(\vec{r}')\hat{a}(\vec{r})$$

COULOMB INTERACTION II

ii) Momentum representation

Coulomb interaction can be seen as a scattering process with momentum transfer *q* mediated by $\tilde{v}_{ee}(q)$

$$\hat{V}_{ee} = \frac{1}{2V}\sum_{\vec{q}} \tilde{v}_{ee}(\vec{q})\hat{\rho}_{\vec{q}}\hat{\rho}_{-\vec{q}} = \frac{1}{2V}\sum_{\vec{q}}\sum_{\vec{k},\vec{k}',\sigma\sigma'} \tilde{v}_{ee}(\vec{q})\hat{a}^{\perp}_{\vec{k}+\vec{q},\sigma}\hat{a}^{\perp}_{\vec{k}'-\vec{q},\sigma'}\hat{a}_{\vec{k}',\sigma'}\hat{a}_{\vec{k},\sigma}$$



$$\tilde{v}_{ee}(\vec{q}) = \int d\vec{r} e^{i\vec{q}\cdot\vec{r}}\frac{e^2}{r} = \lim_{\eta\to 0}\int d\vec{r} e^{i\vec{q}\cdot\vec{r}}e^{-\eta r}\frac{e^2}{r} = \frac{4\pi e^2}{q^2}$$

5 EXAMPLE: FREE ELECTRON GAS

We start from considering the e-dynamics in the absence of ee and ei interactions:

➡ Free electron gas described by the Hamiltonian

$$\hat{T}_{el} = \hat{H}_e^0 = \sum_{\vec{k},\sigma} \frac{\hbar^2 k^2}{2m} \hat{a}^{\perp}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} = \sum_{\vec{k}} \varepsilon_k \hat{n}_{\vec{k}}$$

- Allowed momentum values $k_i = \frac{2\pi}{L_i} n_i, \quad n_i \in Z, \quad V = L_x L_y L_z$
- σ spin degree of freedom
- $\hat{a}_{\vec{k}\sigma} |0\rangle = 0, \qquad \prod_{i=1}^{N} \hat{a}^{\perp}_{\vec{k}_i\sigma_i} |0\rangle = \left| \vec{k}_1\sigma_1, \vec{k}_2\sigma_2, ..., \vec{k}_N\sigma_N \right\rangle$

where the action of $\hat{a}^{\perp}_{\vec{k}_i\sigma_i}$ has been ordered: $\left|\vec{k}_1\right| \le \left|\vec{k}_2\right| \le ... \left|\vec{k}_N\right|$

GROUND STATE OF FREE E-GAS

$T = 0$ + Pauli principle: Ground state of noninteracting electrons is obtained upon filling all single particle states up to an energy ε_F

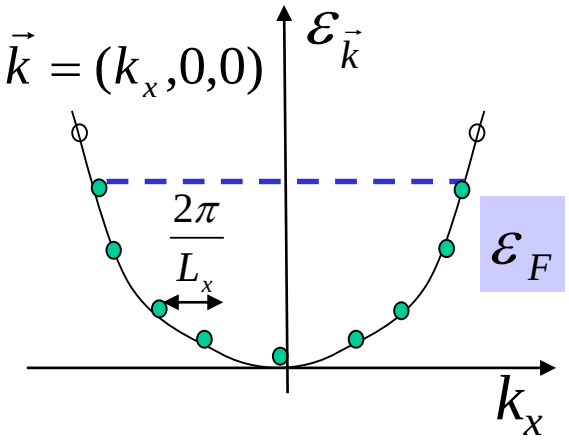
This ground state is denoted as Fermi sea (Fermi sphere in 3d):

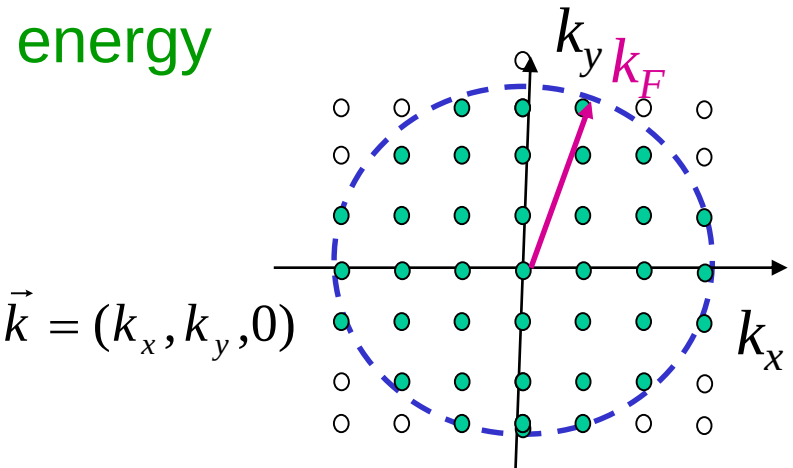
$$\left|FS\right\rangle \equiv \hat{a}^{\perp}_{\vec{k}_1\uparrow}\hat{a}^{\perp}_{\vec{k}_1\downarrow}....\hat{a}^{\perp}_{\vec{k}_{N/2}\uparrow}\hat{a}^{\perp}_{\vec{k}_{N/2}\downarrow}\left|\Omega\right\rangle = \left|\vec{k}_1\uparrow,\vec{k}_1\downarrow,...,\vec{k}_{N/2}\uparrow,\vec{k}_{N/2}\downarrow\right\rangle$$

$$\varepsilon_{\vec{k}_1} \le \varepsilon_{\vec{k}_2} \le ... \le \varepsilon_{\vec{k}_{N/2}}, \quad \varepsilon_{\vec{k}_{N/2}} \equiv \varepsilon_F \equiv \frac{\hbar^2 k_F^2}{2m} \qquad (N = \text{even})$$

Fermi energy

Fermi momentum





FERMI MOMENTUM k_F

As a first exercise, we calculate the relation between the macroscopic quantity $n_e = N/V$ (e-density), and the microscopic quantity k_F

i) $$k_i = \frac{2\pi}{L_i} n_i, \quad n_i \in Z$$

➡ one state fills the volume $$\frac{2\pi}{L_x}\frac{2\pi}{L_y}\frac{2\pi}{L_z} = \frac{(2\pi)^3}{V}$$ in k-space

hence $$\sum_{\vec{k}\sigma} \to \sum_{\sigma} \frac{V}{(2\pi)^3} \int d\vec{k}$$

ii) $$N = \langle FS | \hat{N} | FS \rangle = \langle FS | \sum_{\vec{k}\sigma} \hat{n}_{\vec{k}\sigma} | FS \rangle = \sum_{\sigma} \frac{V}{(2\pi)^3} \int d\vec{k} \langle FS | \hat{n}_{\vec{k}\sigma} | FS \rangle$$

FERMI MOMENTUM k_F II

iii) $\hat{n}_{\vec{k}\,\sigma}\,|FS\rangle = \begin{cases} |FS\rangle & \text{for } |\vec{k}| \le k_F \\ 0 & \text{otherwise} \end{cases}$

$$\Rightarrow N_e = \sum_\sigma \frac{V}{(2\pi)^3}\int d\vec{k}\,\theta(k_F - |\vec{k}|)\langle FS|FS\rangle$$

$$= \frac{2V}{(2\pi)^3}\int_0^{k_F} dk k^2 \int_{-1}^{1} d(\cos\theta)\int_0^{2\pi} d\varphi\, 1 = \frac{V}{3\pi^2}k_F^3$$

$$\Rightarrow \boxed{k_F^3 = 3\pi^2 n_e}$$

EXAMPLE : Cu

Alkali metals, Au, Ag, Cu, 1 valence electron per elementary unit cell (core electrons do not contribute explicitly).
→ Concentration of conduction electrons = atom concentration

Example: Cu, 4 atoms per FCC unit cell, configuration ($3d_{10}\,4s_1$)

$$a_{Cu}^{FCC} = 3.61\text{Å}, \quad n_{Cu} = 8.45 \cdot 10^{22}\, cm^{-3} \longrightarrow k_F = 13.6\, nm^{-1};$$

yielding: $\varepsilon_F = 7.03\, eV \Rightarrow T_F = \varepsilon_F / k_B = 81600K$ Fermi T

$$v_F = \frac{\hbar k_F}{m} = 1.57 \times 10^6\, m/s = 0.005c$$ Fermi v

- Melting temperature of Copper ~ 10^3 K

  ⟶ Cu is a degenerate Fermi system even near melting

GROUND STATE ENERGY

We move on by calculating the ground state energy

$$E^{(0)} = \langle FS | \hat{H}_e^0 | FS \rangle = \langle FS | \sum_{\vec{k}\sigma} \frac{\hbar^2 k^2}{2m} \hat{n}_{\vec{k}\sigma} | FS \rangle$$

$$= \frac{2V}{(2\pi)^3} \frac{\hbar^2}{2m} \int d\vec{k} k^2 \theta(k_F - |\vec{k}|)$$

$$= \frac{2V}{(2\pi)^3} \frac{\hbar^2}{2m} 4\pi \int_0^{k_F} dk k^4 = \frac{V}{5\pi^2} \frac{\hbar^2}{2m} k_F^5 = \frac{3}{5} N_e \varepsilon_F$$

➡ Kinetic energy per particle

$$\frac{E^{(0)}}{N_e} = \frac{3}{5} \frac{\hbar^2}{2m} k_F^2 = \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2 n_e)^{2/3}$$

High kinetic energy. Repulsive contribution to binding energy of materials