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NON - RELATIVISTIC
QUANTUM THEORY
OF
MANY - PARTICLE
SYSTEMS

I 1) BOSONS & FERMIONS

I 2) FREE ELECTRON GAS

I 3) SECOND QUANTIZATION

↳ BOSONS

↳ FERMIONS

↳ HOMOGENEOUS ELECTRON GAS
 (JELLIUM MODEL)

1) BOSONS & FERMIONS

↳ 2 PARTICLE STATE :
 ↗ ONE PARTICLE IN STATE a : ψ_a
 ↘ SECOND PARTICLE IN STATE b : ψ_b

* CLASSICAL PHYSICS : PARTICLES CAN BE DISTINGUISHED

$$\psi(\vec{r}_1, \vec{r}_2) = \psi_a(\vec{r}_1) \psi_b(\vec{r}_2)$$

* IN QUANTUM PHYSICS : PARTICLES ARE INDISTINGUISHABLE

2 WAYS TO TAKE CARE OF THIS

$$\psi_{\pm}(\vec{r}_1, \vec{r}_2) = A \left[\psi_a(\vec{r}_1) \psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1) \psi_a(\vec{r}_2) \right]$$

↑
NORMALIZATION

+ : WAVE FUNCTION IS SYMMETRIC w.r.t.

INTERCHANGE $1 \leftrightarrow 2$: BOSONS

- : WAVE FUNCTION IS ANTI-SYMMETRIC w.r.t.

INTERCHANGE $1 \leftrightarrow 2$: FERMIONS

↳ 'DEEP CONNECTION' (RELATIVISTIC QUANTUM FIELD THEORY)
 BETWEEN SYMMETRY OF WF & SPIN

SPIN - STATISTICS THEOREM

BOSONS (SYMM. UNDER $1 \leftrightarrow 2$) HAVE INTEGER SPIN

FERMIONS (ANTISYMM UNDER $1 \leftrightarrow 2$) HAVE HALF INTEGER SPIN

↳ PAULI EXCLUSION PRINCIPLE

2 FERMIONS CANNOT OCCUPY SAME STATE !

if $\psi_b = \psi_a$

$$\psi_-(\vec{r}_1, \vec{r}_2) = A \cdot [\psi_a(\vec{r}_1)\psi_a(\vec{r}_2) - \psi_a(\vec{r}_1)\psi_a(\vec{r}_2)] = 0$$

↳ EXCHANGE OPERATOR P

$$P \psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_2, \vec{r}_1)$$

$$P^2 = 1$$

FOR 2 IDENTICAL PARTICLES ($m_1 = m_2$, $V(\vec{r}_1, \vec{r}_2) = V(\vec{r}_2, \vec{r}_1)$)

↓
 $[P, H] = 0$

∴ EIGENSTATES OF H ARE EITHER SYMMETRIC OR ANTISYMM w.r.t $1 \leftrightarrow 2$

$$\psi_{\pm}(\vec{r}_1, \vec{r}_2) = \begin{matrix} \text{+} \\ \text{-} \end{matrix} \psi_{\pm}(\vec{r}_2, \vec{r}_1)$$

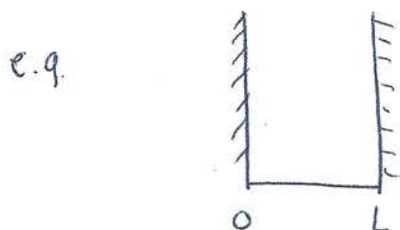
→ BOSONS
 → FERMIONS

• EXCHANGE FORCES

2 PARTICLES IN 1 DIM $\Psi_a(x)$ STATE a

$\Psi_b(x)$ STATE b

$a \neq b$



↳ DISTINGUISHABLE: $\Psi(x_1, x_2) = \Psi_a(x_1) \Psi_b(x_2)$

↳ BOSONS: $\Psi_+(x_1, x_2) = \frac{1}{\sqrt{2}} [\Psi_a(x_1) \Psi_b(x_2) + \Psi_b(x_1) \Psi_a(x_2)]$

↳ FERMIONS: $\Psi_-(x_1, x_2) = \frac{1}{\sqrt{2}} [\Psi_a(x_1) \Psi_b(x_2) - \Psi_b(x_1) \Psi_a(x_2)]$

WHAT IS $\langle \rangle$ OF $(x_1 - x_2)^2$ DISTANCE² BETWEEN 1 & 2

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2 \langle x_1 x_2 \rangle$$

↳ DISTINGUISHABLE

$$\begin{aligned} \langle x_1^2 \rangle &= \int dx_1 \cdot x_1^2 |\Psi_a(x_1)|^2 \underbrace{\int dx_2 |\Psi_b(x_2)|^2}_1 \\ &= \langle x^2 \rangle_a \end{aligned}$$

$$\langle x_2^2 \rangle = \langle x^2 \rangle_b$$

$$\langle x_1 x_2 \rangle = \langle x \rangle_a \langle x \rangle_b$$

1

↳ IDENTICAL PARTICLES

$$\begin{aligned}
 \langle x_1^2 \rangle &= \frac{1}{2} \left\{ \int dx_1 x_1^2 |\Psi_a(x_1)|^2 \int dx_2 |\Psi_b(x_2)|^2 \right. \\
 &\quad + \int dx_1 x_1^2 |\Psi_b(x_1)|^2 \int dx_2 |\Psi_a(x_2)|^2 \\
 &\quad \pm \int dx_1 x_1^2 \Psi_a^*(x_1) \Psi_b(x_1) \int dx_2 \Psi_b^*(x_2) \Psi_a(x_2) \\
 &\quad \left. \pm \int dx_1 x_1^2 \Psi_b^*(x_1) \Psi_a(x_1) \int dx_2 \underbrace{\Psi_a^*(x_2) \Psi_b(x_2)}_0 \right\} \\
 &= \frac{1}{2} \left\{ \langle x^2 \rangle_a + \langle x^2 \rangle_b + 0 + 0 \right\}
 \end{aligned}$$

$\langle x_2^2 \rangle = \langle x_1^2 \rangle$ IDENTICAL!

$$\begin{aligned}
 \langle x_1 x_2 \rangle &= \frac{1}{2} \left\{ 2 \langle x \rangle_a \langle x \rangle_b \right. \\
 &\quad \pm \int dx_1 x_1 \Psi_a^*(x_1) \Psi_b(x_1) \int dx_2 x_2 \Psi_b^*(x_2) \Psi_a(x_2) \\
 &\quad \left. \pm \int dx_1 x_1 \underbrace{\Psi_b^*(x_1) \Psi_a(x_1)}_{\langle x \rangle_{ba}} \int dx_2 x_2 \underbrace{\Psi_a^*(x_2) \Psi_b(x_2)}_{\langle x \rangle_{ab}} \right\}
 \end{aligned}$$

$\langle x_1 x_2 \rangle = \langle x \rangle_a \langle x \rangle_b \pm |\langle x \rangle_{ab}|^2$

∴ DISTINGUISHABLE PARTICLES

$$\langle (x_1 - x_2)^2 \rangle_d = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2 \langle x \rangle_a \langle x \rangle_b$$

∴ IDENTICAL PARTICLES

$$\langle (x_1 - x_2)^2 \rangle_{\pm} = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2 \langle x \rangle_a \langle x \rangle_b \mp 2 |\langle x \rangle_{ab}|^2$$

$$\langle (x_1 - x_2)^2 \rangle_{\pm} = \langle (x_1 - x_2)^2 \rangle_d \mp 2 |\langle x \rangle_{ab}|^2$$

INDUCES

A CORRELATION
BETWEEN
PARTICLES.

(EXCHANGE 'FORCE')

→ 'ATTRACTION' FOR BOSONS

PULLS THEM CLOSER TOGETHER

$\langle (x_1 - x_2)^2 \rangle$ DECREASES

→ 'REPULSIVE' FOR FERMIONS

PUSHES THEM FURTHER APART

$\langle (x_1 - x_2)^2 \rangle$ INCREASES

TOTAL WF INCLUDES SPIN ∇ \rightarrow COVALENT BOND

2) FREE ELECTRON GAS (SOMMERFELD)

↳ FREE PARTICLES (e^-) IN A BOX

$$V(x, y, z) = \begin{cases} 0 & \begin{array}{l} 0 < x < l_x \\ \& 0 < y < l_y \\ \& 0 < z < l_z \end{array} \\ \infty & \text{OTHERWISE} \end{cases}$$

(3D ANALOGON OF INFINITE SQUARE WELL POT.)

↳ $-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi$ WITHIN BOX

$$\psi(x, y, z) = X(x) Y(y) Z(z)$$

$$\begin{cases} -\frac{\hbar^2}{2m} \nabla^2 X = E_x X \\ -\frac{\hbar^2}{2m} \nabla^2 Y = E_y Y \\ -\frac{\hbar^2}{2m} \nabla^2 Z = E_z Z \end{cases} \quad E = E_x + E_y + E_z$$

$$k_x \equiv \frac{\sqrt{2m E_x}}{\hbar}, \quad k_y \equiv \frac{\sqrt{2m E_y}}{\hbar}, \quad k_z \equiv \frac{\sqrt{2m E_z}}{\hbar}$$

↳ SOLUTIONS

$$\begin{cases} X(x) = A_x \sin(k_x x) + B_x \cos(k_x x) \\ Y(y) = A_y \sin(k_y y) + B_y \cos(k_y y) \\ Z(z) = A_z \sin(k_z z) + B_z \cos(k_z z) \end{cases}$$

↳ BOUNDARY CONDITION

$$\rightsquigarrow X(0) = Y(0) = Z(0) = 0$$

$$\Rightarrow B_x = B_y = B_z = 0$$

$$\rightsquigarrow X(l_x) = Y(l_y) = Z(l_z) = 0$$

$$\Rightarrow k_x = \frac{n_x \pi}{l_x}, \quad k_y = \frac{n_y \pi}{l_y}, \quad k_z = \frac{n_z \pi}{l_z}$$

$$n_x, n_y, n_z = 1, 2, 3, \dots$$

$$\psi_{n_x n_y n_z} = C \sin\left(\frac{n_x \pi}{l_x} x\right) \sin\left(\frac{n_y \pi}{l_y} y\right) \sin\left(\frac{n_z \pi}{l_z} z\right)$$

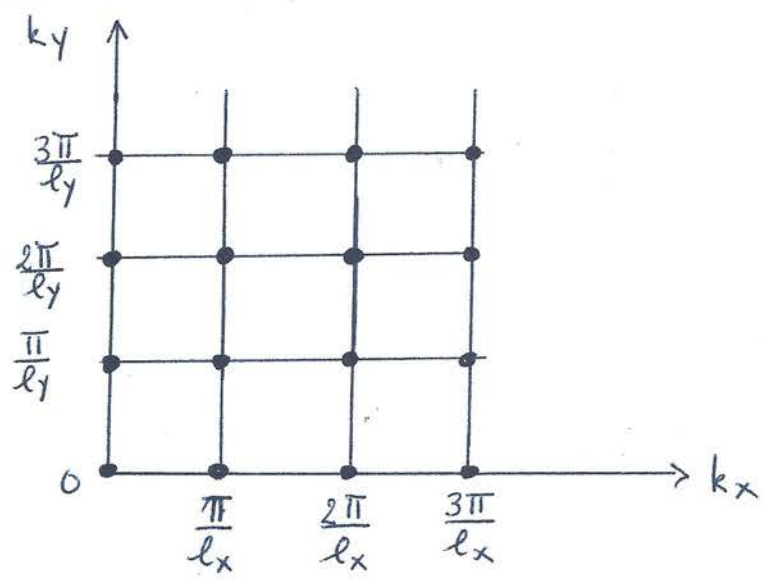
NORMALIZATION

$$C = \sqrt{\frac{8}{l_x l_y l_z}}$$

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2} \right) = \frac{\hbar^2 k^2}{2m}$$

WAVEVECTOR $\vec{k} = (k_x, k_y, k_z)$

↳ RECIPROCAL SPACE (IN 3D)



EACH POINT IN GRID CORRESPONDS
TO A STATIONARY STATE

↓
OCCUPIES A VOLUME (CELL) IN RECIPROCAL SPACE

$$\frac{\pi^3}{l_x l_y l_z} = \frac{\pi^3}{V}$$

INVERSELY PROPORTIONAL
TO PHYSICAL VOLUME

"k-SPACE"

↳ N ATOMS
EACH ATOM: q FREE e⁻ (q=1,2) } ∴ TOTAL Nq FREE e⁻

Nq FREE e⁻ IN BOX

WILL FILL LEVELS ACCORDING TO PAULI PRINCIPLE

2 (BOTH SPIN ORIENTATIONS) CAN OCCUPY A STATIONARY STATE



e^- OCCUPY A FINITE VOLUME IN k -SPACE

ONE OCTANT OF SPHERE OF RADIUS k_F \Rightarrow FERMI SURFACE

$$\frac{1}{8} \cdot \frac{4}{3} \pi k_F^3 = \frac{Nq}{2} \cdot \left(\frac{\pi^3}{V} \right)$$

\downarrow
 # e^- PAIRS OF $\uparrow \downarrow$ THAT OCCUPY STATIONARY STATES
 \hookrightarrow VOLUME IN k -SPACE OCCUPIED BY 1 STATIONARY STATE



$$k_F = (3 \rho \pi^2)^{1/3}$$

\rightarrow DETERMINES FERMI SURFACE

$$\underline{\underline{\rho = \frac{Nq}{V}}}$$

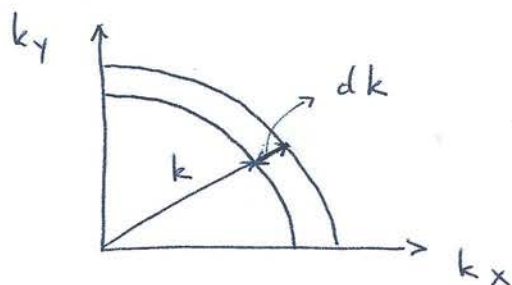
FREE e^- DENSITY
(# FREE e^- / UNIT VOLUME)

FERMI ENERGY : ENERGY OF MOST ENERGETIC e^-

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m} (3 \rho \pi^2)^{2/3}$$

e.g. Cu : $E_F \approx 7. \text{eV}$

↳ TOTAL ENERGY OF e^- GAS



↳ # e^- IN SHELL $k, k+dk$

$$\text{SPIN} \rightarrow \frac{2 \left[\frac{1}{8} (4\pi k^2) dk \right]}{\left[\frac{\pi^3}{V} \right]} = \frac{V}{\pi^2} k^2 dk.$$

↳ VOLUME IN k -SPACE
OF 1 STATE

↳ ENERGY OF SHELL $k, k+dk$

$$dE = \frac{\hbar^2 k^2}{2m} \frac{V}{\pi^2} k^2 dk.$$

↳ TOTAL ENERGY

$$E_{\text{tot}} = \frac{\hbar^2 V}{2m \pi^2} \int_0^{k_F} dk k^4$$

$$\boxed{E_{\text{tot}} = \frac{\hbar^2 V}{10 \pi^2 m} k_F^5} = \frac{\hbar^2 (3\pi^2 N)^{5/3}}{10 \pi^2 m} V^{-2/3}$$

$$= \left(\frac{3}{5} E_F \right) \cdot N$$

↳ PRESSURE OF e^- ON WALLS

E_{tot} PLAY ROLE OF INTERNAL ENERGY U
(cf. ORDINARY GAS)

if V INCREASES U DECREASE

$$dU = - \underset{\substack{\uparrow \\ \text{PRESSURE OF WALLS.}}}{P} dV$$

$$dE_{tot} = - \frac{2}{3} \frac{E_{tot}}{V} dV$$

↓
PRESSURE $P = \frac{2}{3} \frac{E_{tot}}{V}$

$$P = \frac{2}{3} \frac{\hbar^2 k_F^5}{10 \pi^2 m} = \frac{(3\pi^2)^{2/3} \hbar^2}{5m} \rho^{5/3}$$

↓
'DEGENERACY PRESSURE' (QM: $\sim \hbar^2$)
DUE TO EXCLUSION PRINCIPLE

(PREVENTS SOLIDS FROM COLLAPSING)

3) SECOND QUANTIZATION

SCHRÖDINGER EQ. FOR N-PARTICLE SYSTEM WITH INTERACTIONS

$$H = \sum_{i=1}^N H_0(x_i) + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N V(x_i, x_j)$$

KINETIC ENERGY + EXTERNAL FIELDS (1 BODY OPERATOR)
 e.g.

POTENTIAL ENERGY OF INTERACTION BETWEEN PARTICLES (2 BODY OPERATOR)

e.g. COULOMB POTENTIAL $\frac{e^-}{|\vec{r}_i - \vec{r}_j|} \frac{e^-}{\vec{r}_j}$

$$V(\vec{r}_i, \vec{r}_j) = + \frac{q_i q_j}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}$$

WAVE FUNCTION FOR N-PARTICLE SYSTEM

$$\Psi(x_1, \dots, x_N; t)$$

$$H \Psi(x_1, \dots, x_N; t) = i\hbar \frac{\partial}{\partial t} \Psi(x_1, \dots, x_N; t)$$

EXPANSION IN COMPLETE SET OF SINGLE PARTICLE W.F.

$$H_0(i) \psi_{\alpha_i}(x_i) = E_i \psi_{\alpha_i}(x_i)$$

α_i : QUANTUM NUMBER FOR PARTICLE i (e.g. $\alpha_i = 1, 2, 3, \dots$)

e.g. HOMOGENEOUS SYSTEM

$\psi_{\alpha_i}(x_i) \rightarrow$ PLANE WAVES IN LARGE BOX WITH PERIODIC BOUNDARY CONDITIONS

$$\Psi(x_1 \dots x_N; t) = \sum_{\alpha_1 \dots \alpha_N} C(\alpha_1 \dots \alpha_N; t) \Psi_{\alpha_1}(x_1) \dots \Psi_{\alpha_N}(x_N)$$

NORMALIZATION $\xrightarrow{\text{QUANTUM NUMBERS}}$ $\sum_{\alpha_1 \dots \alpha_N} |C(\alpha_1 \dots \alpha_N; t)|^2 = 1$

• SCHRÖDINGER EQ.

$$i\hbar \frac{\partial}{\partial t} \sum_{\alpha_1' \dots \alpha_N'} C(\alpha_1' \dots \alpha_N'; t) \Psi_{\alpha_1'}(x_1) \dots \Psi_{\alpha_N'}(x_N)$$

$$= \sum_{\alpha_1' \dots \alpha_N'} C(\alpha_1' \dots \alpha_N'; t) \sum_{k=1}^N H_0(x_k) \Psi_{\alpha_1'}(x_1) \dots \Psi_{\alpha_N'}(x_N)$$

$$+ \sum_{\alpha_1' \dots \alpha_N'} C(\alpha_1' \dots \alpha_N'; t) \frac{1}{2} \sum_{k, \ell=1}^N V(x_k, x_\ell) \Psi_{\alpha_1'}(x_1) \dots \Psi_{\alpha_N'}(x_N)$$

⇓ MULTIPLY ON LEFT WITH $\int dx_1 \dots \int dx_N \Psi_{\alpha_1}^*(x_1) \dots \Psi_{\alpha_N}^*(x_N)$

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1 \dots \alpha_N; t)$$

$$= \sum_{k=1}^N \sum_{\alpha_k'} C(\alpha_1 \dots \alpha_{k-1} \underline{\alpha_k'} \alpha_{k+1} \dots \alpha_N, t) \int dx_k \Psi_{\alpha_k'}^*(x_k) H_0(x_k) \Psi_{\alpha_k'}(x_k)$$

$$+ \frac{1}{2} \sum_{k, \ell} \sum_{\alpha_k'} \sum_{\alpha_\ell'} C(\alpha_1 \dots \alpha_{k-1} \underline{\alpha_k'} \alpha_{k+1} \dots \alpha_{\ell-1} \underline{\alpha_\ell'} \alpha_{\ell+1} \dots \alpha_N, t) \int dx_k \int dx_\ell \Psi_{\alpha_k'}^*(x_k) \Psi_{\alpha_\ell'}^*(x_\ell) V(x_k, x_\ell) \Psi_{\alpha_k'}(x_k) \Psi_{\alpha_\ell'}(x_\ell)$$



✓ SET OF QUANTUM NUMBERS $\alpha_1 \dots \alpha_N$
DIFF. EQ. FOR COEFFICIENTS $C(\alpha_1 \dots \alpha_N; t)$

⇒ COUPLED SET OF DIFFERENTIAL EQUATIONS
COMPLICATED !

• SYMMETRY CONDITION ; IDENTICAL PARTICLES

SYMMETRY OF MANY-PARTICLE W.F. UNDER $i \leftrightarrow j$

$$\Psi(\dots x_i \dots x_j \dots; t) = \pm \Psi(\dots x_j \dots x_i \dots; t)$$

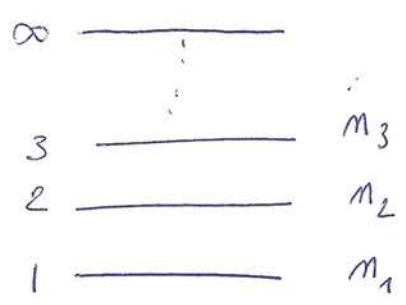
+ ⇒ SYMMETRIC (BOSONS)
- ⇒ ANTI-SYMMETRIC (FERMIONS)



$$C(\dots \alpha_i \dots \alpha_j \dots; t) = \pm C(\dots \alpha_j \dots \alpha_i \dots; t)$$

• BOSONS

EVERY SINGLE PARTICLE ENERGY LEVEL CAN BE MULTIPLE OCCUPIED $\alpha_i = 1, 2, 3, \dots$



m_i : OCCUPATION NUMBER OF STATE i
FOR BOSONS $m_i = 0, 1, 2, 3, \dots$
 $\sum_i m_i = N$

$$C(12123412\dots; t)$$

$$= C(\underbrace{1\dots 1}_{n_1}, \underbrace{2\dots 2}_{n_2}, \dots; t)$$

↳ NORMALIZATION CONDITION

$$1 = \sum_{\alpha_1 \dots \alpha_N} |C(\alpha_1 \dots \alpha_N; t)|^2$$

$$= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \dots \sum_{n_{\infty}=0}^{\infty} |\tilde{C}(n_1 \dots n_{\infty}; t)|^2 \cdot \frac{N!}{n_1! \dots n_{\infty}!}$$

REARRANGEMENTS OF N PARTICLES SUCH THAT

n_1	OCCUPY STATE	1
n_2	"	2
	⋮	
n_{∞}	"	∞

DEFINE $\parallel f(n_1 \dots n_{\infty}; t) \equiv \tilde{C}(n_1 \dots n_{\infty}; t) \left(\frac{N!}{n_1! n_2! \dots n_{\infty}!} \right)^{1/2}$

NORMALIZATION

$$\sum_{n_1 \dots n_{\infty}} |f(n_1 \dots n_{\infty}; t)|^2 = 1$$

PROBABILITY TO HAVE

n_1	PARTICLES IN STATE	1
n_2	"	2
	"	
n_{∞}	"	∞

$$\sum_{i=1}^{\infty} n_i = N$$

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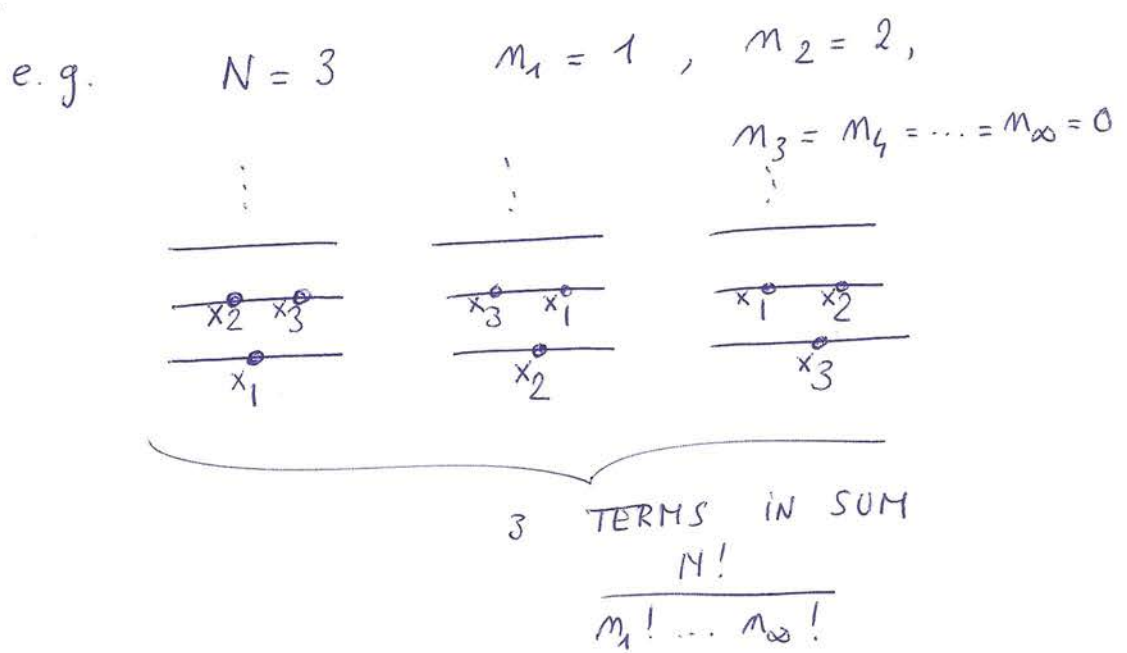
$$\hookrightarrow \underline{\Phi}(x_1, \dots, x_N; t) = \sum_{\alpha_1, \dots, \alpha_N} C(\alpha_1, \dots, \alpha_N; t) \Psi_{\alpha_1}(x_1) \dots \Psi_{\alpha_N}(x_N)$$

$$= \sum_{\alpha_1, \dots, \alpha_N} \tilde{C}(m_1, \dots, m_\infty; t) \Psi_{\alpha_1}(x_1) \dots \Psi_{\alpha_N}(x_N)$$

$$= \sum_{m_1, \dots, m_\infty} f(m_1, \dots, m_\infty; t) \cdot \left(\frac{m_1! \dots m_\infty!}{N!} \right)^{1/2}$$

$$\sum_{\substack{\alpha_1, \dots, \alpha_N \\ (m_1, \dots, m_\infty)}} \Psi_{\alpha_1}(x_1) \dots \Psi_{\alpha_N}(x_N)$$

SUM OVER ALL QUANTUM NUMBERS
GIVEN A SET OF OCCUPATION NUMBERS



$$\underline{\Phi}_{m_1, \dots, m_\infty}(x_1, \dots, x_N) \equiv \left(\frac{m_1! \dots m_\infty!}{N!} \right)^{1/2} \sum_{\substack{\alpha_1, \dots, \alpha_N \\ (m_1, \dots, m_\infty)}} \Psi_{\alpha_1}(x_1) \dots \Psi_{\alpha_N}(x_N)$$

FOR $N=3$ $m_1 = 1, m_2 = 2$
 $m_3 = m_4 = \dots = m_\infty = 0$

$$\begin{aligned} & \bar{\Phi}_{1200\dots 0}(x_1, x_2, x_3) \\ &= \frac{1}{\sqrt{3}} \left\{ \psi_1(x_1) \psi_2(x_2) \psi_2(x_3) \right. \\ & \quad + \psi_1(x_2) \psi_2(x_3) \psi_2(x_1) \\ & \quad \left. + \psi_1(x_3) \psi_2(x_1) \psi_2(x_2) \right\} \end{aligned}$$

NORMALIZATION

$$\int dx_1 \dots \int dx_N \left| \bar{\Phi}_{m_1 \dots m_\infty}(x_1 \dots x_N) \right|^2 = 1$$

$$\Psi(x_1 \dots x_N; t) = \sum_{m_1 \dots m_\infty} f(m_1 \dots m_\infty; t) \bar{\Phi}_{m_1 \dots m_\infty}(x_1 \dots x_N)$$

SUM OVER
OCCUPATION
NUMBERS

COORDINATE SPACE
WAVEFUNCTION

FOR N BOSON STATE

OCCUPATION NUMBER REPRESENTATION (BOSONS)

↳ INTRODUCE TIME-INDEPENDENT STATE VECTOR

$$|m_1 \dots m_\infty\rangle$$

STATE WITH	m_1	PARTICLES	IN STATE	1
	m_2	"	"	2
	m_∞	"	"	∞

↳ ORTHONORMALITY

$$\langle m'_1 \dots m'_\infty | m_1 \dots m_\infty \rangle = \delta_{m'_1 m_1} \dots \delta_{m'_\infty m_\infty}$$

↳ COMPLETENESS:

$$\sum_{m_1 \dots m_\infty} |m_1 \dots m_\infty\rangle \langle m_1 \dots m_\infty| = \mathbb{1}$$

↳ CORRESPONDENCE
WAVE FUNCTION

STATE VECTOR

$$\Psi(x_1 \dots x_N; t) \iff |\underline{\Psi}(t)\rangle$$

$$\Phi_{m_1 \dots m_\infty}(x_1 \dots x_N) \iff |m_1 \dots m_\infty\rangle$$

$$|\underline{\Psi}(t)\rangle = \sum_{m_1 \dots m_\infty} f(m_1 \dots m_\infty; t) |m_1 \dots m_\infty\rangle$$

↳ CREATION & ANNIHILATION OPERATORS

\downarrow
 c_i^+
 c_i (TIME-INDEPENDENT)
 IDENTICAL TO HARMONIC OSCILLATOR

DEFINE $\left\{ \begin{array}{l} [c_i, c_j^+] = \delta_{ij} \\ [c_i, c_j] = 0 \\ [c_i^+, c_j^+] = 0 \end{array} \right.$
 $[A, B] \equiv AB - BA$

⇓

$\left\{ \begin{array}{l} c_i^+ c_i |m_i\rangle = m_i |m_i\rangle \\ c_i |m_i\rangle = \sqrt{m_i} |m_i - 1\rangle \\ c_i^+ |m_i\rangle = \sqrt{m_i + 1} |m_i + 1\rangle \end{array} \right.$
 $m_i = 0, 1, 2, \dots$

$c_i^+ c_i$: HERMITIAN OPERATOR
 \downarrow
 REAL EIGENVALUES m_i
 $\left. \begin{array}{l} \} \\ \} \end{array} \right\}$
 NUMBER OPERATOR.

↳ $\hat{H} |\Psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle$

$= \sum_{m_1 \dots m_\infty} i\hbar \frac{\partial f(m_1 \dots m_\infty, t)}{\partial t} |m_1 \dots m_\infty\rangle$

↳ (H_0) TERM

$$i\hbar \frac{\partial}{\partial t} C(\alpha_1 \dots \alpha_N; t)$$

$$= \sum_{k=1}^N \sum_{\alpha'_k} C(\alpha_1 \dots \alpha_{k-1} \alpha'_k \alpha_{k+1} \dots \alpha_N; t) \\ \cdot \langle \alpha_k | H_0 | \alpha'_k \rangle$$

$$= \sum_{k=1}^N \sum_{\alpha'_k} \tilde{C}(m_1 \dots (m_{\alpha'_k} - 1) \dots (m_{\alpha'_k} + 1) \dots m_\infty; t) \\ \cdot \langle \alpha_k | H_0 | \alpha'_k \rangle$$

⇓ REPLACE SUM OVER PARTICLES
BY SUM OVER STATES.

$$= \sum_{\alpha_k} \sum_{\alpha'_k} m_{\alpha'_k} \tilde{C}(m_1 \dots (m_{\alpha'_k} - 1) \dots (m_{\alpha'_k} + 1) \dots m_\infty; t) \\ \cdot \langle \alpha_k | H_0 | \alpha'_k \rangle$$

↓ SIMPLIFY NOTATION

$$= \sum_i \sum_j m_i \left(\frac{m_1! \dots (m_i - 1)! \dots (m_j + 1)! \dots m_\infty!}{N!} \right)^{1/2}$$

$$\cdot f(m_1 \dots m_i - 1 \dots m_j + 1 \dots m_\infty, t)$$

$$\langle i | H_0 | j \rangle$$

$$\begin{aligned}
&= \sum_i n_i \left(\frac{n_1! \dots n_i! \dots n_\infty!}{N!} \right)^{1/2} f(n_1 \dots n_i \dots n_\infty; t) \langle i | H_0 | i \rangle \\
&+ \sum_{i \neq j} n_i \left(\frac{n_1! \dots (n_i-1)! \dots (n_j+1)! \dots n_\infty!}{N!} \right)^{1/2} \\
&\quad \cdot f(n_1 \dots n_i-1 \dots n_j+1 \dots n_\infty; t) \langle i | H_0 | j \rangle
\end{aligned}$$

$$\circ \circ \quad i\hbar \frac{\partial}{\partial t} f(n_1 \dots n_\infty, t)$$

$$= \sum_i n_i f(n_1 \dots n_i \dots n_\infty; t) \langle i | H_0 | i \rangle$$

$$+ \sum_{i \neq j} n_i^{1/2} (n_j+1)^{1/2} f(n_1 \dots n_i-1 \dots n_j+1 \dots n_\infty; t) \langle i | H_0 | j \rangle$$

\Downarrow

$$\hat{H}_0 | \Psi \rangle = \sum_{n_1 \dots n_\infty} i\hbar \frac{\partial}{\partial t} f(n_1 \dots n_\infty; t) | n_1 \dots n_\infty \rangle$$

$$= \sum_{n_1 \dots n_\infty} \left\{ \sum_i n_i f(n_1 \dots n_i \dots n_\infty; t) \langle i | H_0 | i \rangle \right.$$

$$+ \left. \sum_{i \neq j} n_i^{1/2} (n_j+1)^{1/2} f(n_1 \dots n_i-1 \dots n_j+1 \dots n_\infty; t) \langle i | H_0 | j \rangle \right\}$$

$$| n_1 \dots n_\infty \rangle$$

IN 2^0 TERM

$$n'_i = n_i - 1$$

$$\Downarrow$$

$$n'_j = n_j + 1$$

IDENTIFY EACH TERM IN SUM $\sum_{m_1 \dots m_\infty}$ (DROP ' IN 2^0 TERM)

$$\hat{H}_0 | m_1 \dots m_\infty \rangle$$

$$= \left\{ \sum_i n_i \langle i | H_0 | i \rangle | m_1 \dots m_\infty \rangle \right.$$

$$\left. + \sum_{i \neq j} (n_i + 1)^{1/2} (n_j)^{1/2} \langle i | H_0 | j \rangle | \dots n_i + 1 \dots n_j - 1 \dots \rangle \right\}$$

$$= \left\{ \sum_i c_i^\dagger c_i \langle i | H_0 | i \rangle \right.$$

$$\left. + \sum_{i \neq j} c_i^\dagger c_j \langle i | H_0 | j \rangle \right\} | m_1 \dots m_\infty \rangle$$

$$\circ \circ \quad \hat{H}_0 | m_1 \dots m_\infty \rangle$$

$$= \sum_{i,j} \langle i | H_0 | j \rangle c_i^\dagger c_j | m_1 \dots m_\infty \rangle$$

$$\hat{H}_0 = \sum_{i,j} \langle i | H_0 | j \rangle c_i^\dagger c_j$$

HAMILTONIAN H_0 IN SECOND QUANTIZATION

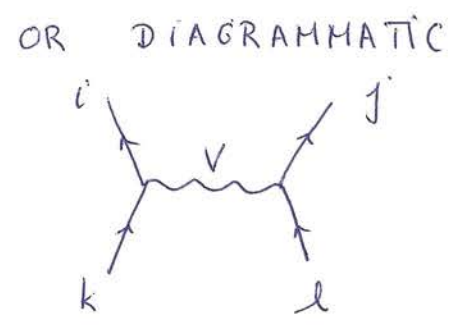
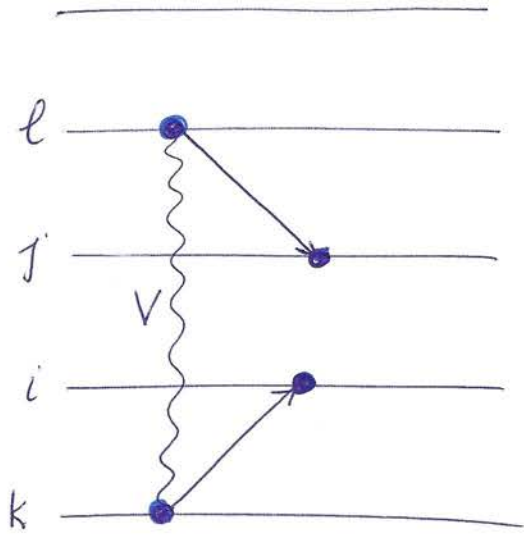
↳ (V) TERM

CAN BE DONE IN AN ANALOGOUS WAY

$$\hat{H} = \sum_{i,j} \langle i | H_0 | j \rangle c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl} \langle ij | V | kl \rangle c_i^\dagger c_j^\dagger c_l c_k$$

TOTAL HAMILTONIAN IN 2^o QUANTIZATION

INTERPRETATION INTERACTION TERM



DUE TO V : 2 PARTICLES ANNIHILATED IN STATE k, l
 & CREATED IN STATE i, j

OCCUPATION NUMBER REPRESENTATION (FERMIONS)

C(... alpha_i ... alpha_j ...; t) = - C(... alpha_j ... alpha_i ...; t)

psi_i : m_i = 0, 1 (PAULI PRINCIPLE)

psi(x_1, ..., x_N; t) = sum_{m_1, ..., m_infinity = 0}^1 f(m_1, ..., m_infinity; t) phi_{m_1, ..., m_infinity}(x_1, ..., x_N)
phi_{m_1, ..., m_infinity}(x_1, ..., x_N) = (m_1! ... m_infinity! / N!)^1/2 | psi_alpha_1(x_1) ... psi_alpha_1(x_N) ... psi_alpha_N(x_1) ... psi_alpha_N(x_N) |
SLATER DETERMINANT
alpha_1 ... alpha_N QUANTUM NUMBERS OF N OCCUPIED STATES ORDERED SUCH THAT alpha_1 < alpha_2 < ... < alpha_N

=> e.g. N=2

phi_{110...0}(x_1, x_2) = 1/sqrt(2) { psi_1(x_1) psi_2(x_2) - psi_1(x_2) psi_2(x_1) }

=> e.g. N=3

phi_{1110...0}(x_1, x_2, x_3) = 1/sqrt(6) { psi_1(x_1) psi_2(x_2) psi_3(x_3) - psi_1(x_1) psi_2(x_3) psi_3(x_2) + psi_1(x_2) psi_2(x_3) psi_3(x_1) - psi_1(x_2) psi_2(x_1) psi_3(x_3) + psi_1(x_3) psi_2(x_1) psi_3(x_2) - psi_1(x_3) psi_2(x_2) psi_3(x_1) }

$$\hookrightarrow |\Psi(t)\rangle = \sum_{n_1 \dots n_\infty = 0}^1 f(n_1 \dots n_\infty; t) |n_1 \dots n_\infty\rangle$$

ANTI-COMMUTATORS $n_i = 0, 1$
FOR FERMIONS

$$\{A, B\} \equiv [A, B]_+ \equiv AB + BA$$

ANTI-COMMUTATION RULES FOR CREATION / ANNIHILATION OPERATORS

DEFINE

$$\begin{cases} \{c_i, c_j^+\} = \delta_{ij} \\ \{c_i, c_j\} = 0 \\ \{c_i^+, c_j^+\} = 0 \end{cases}$$

↓

⇒ if $i = j$

$$\{c_i, c_i\} = 0 \Rightarrow c_i^2 = 0$$

$$\{c_i^+, c_i^+\} = 0 \Rightarrow c_i^{+2} = 0$$

$(c_i^+)^2 |0\rangle = 0$ ONE CANNOT CREATE
2 PARTICLES IN SAME
QUANTUM STATE
(PAULI PRINCIPLE).

~> NUMBER OPERATOR $N_i \equiv c_i^\dagger c_i$

$$\{c_i, c_i^\dagger\} = 1 \Rightarrow c_i^\dagger c_i = 1 - c_i c_i^\dagger$$

⇓

$$\begin{aligned}
(c_i^\dagger c_i)^2 &= (1 - c_i c_i^\dagger)(1 - c_i c_i^\dagger) \\
&= 1 - 2c_i c_i^\dagger + c_i c_i^\dagger c_i c_i^\dagger \\
&= 1 - 2c_i c_i^\dagger + c_i (1 - c_i c_i^\dagger) c_i^\dagger \\
&= 1 - c_i c_i^\dagger \\
&= c_i^\dagger c_i
\end{aligned}$$

∴ $N_i^2 = N_i$ ⇒ EIGENVALUES $m_i = 0, 1$

$$N_i |m_i\rangle = m_i |m_i\rangle$$

$$\begin{aligned}
c_i^\dagger |0\rangle &= |1\rangle & c_i |1\rangle &= |0\rangle \\
\uparrow & \quad \uparrow \\
\text{STATE } i & \quad \text{STATE } i
\end{aligned}$$

$$\begin{aligned}
c_i^\dagger |1\rangle &= 0 & c_i |0\rangle &= 0
\end{aligned}$$

~> ANTI-COMMUTATORS : IMPORTANT TO KEEP TRACK OF SIGNS !

DEFINE

$$|m_1 \dots m_\infty\rangle = (c_1^\dagger)^{m_1} (c_2^\dagger)^{m_2} \dots (c_\infty^\dagger)^{m_\infty} |0\rangle$$

e.g. ANNIHILATE PARTICLE IN STATE s ($m_s = 1$)

$$c_s |m_1 \dots m_s \dots m_\infty\rangle = \underbrace{(-1)^{S_s}}_{\substack{\Downarrow \\ \text{PHASE FACTOR}}} (c_1^+)^{m_1} \dots \underbrace{c_s (c_s^+)}_{1 - c_s^+ c_s} \dots (c_\infty^+)^{m_\infty} |0\rangle$$

$$S_s = m_1 + \dots + m_{s-1}$$

e.g. CREATE PARTICLE IN STATE s ($m_s = 0$)

$$c_s^+ |m_1 \dots 0 \dots m_\infty\rangle = (-1)^{S_s} (c_1^+)^{m_1} \dots c_s^+ \dots (c_\infty^+)^{m_\infty} |0\rangle$$

$$c_s | \dots m_s \dots \rangle = \begin{cases} (-1)^{S_s} \sqrt{m_s} | \dots m_s - 1 \dots \rangle, & \text{if } m_s = 1 \\ 0, & \text{if } m_s = 0 \end{cases}$$

$$c_s^+ | \dots m_s \dots \rangle = \begin{cases} (-1)^{S_s} \sqrt{m_s + 1} | \dots m_s + 1 \dots \rangle, & \text{if } m_s = 0 \\ 0, & \text{if } m_s = 1 \end{cases}$$

$$c_s^+ c_s | \dots m_s \dots \rangle = m_s | \dots m_s \dots \rangle$$

SAME FORM AS FOR BOSONS

EXCEPT FOR PHASE FACTOR ∇

↳ HAMILTONIAN (FERMIONS) IN SECOND QUANTIZED FORM

$$\hat{H} = \sum_{i,j} \langle i | H_0 | j \rangle c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl} \langle ij | V | kl \rangle c_i^\dagger c_j^\dagger c_l c_k$$

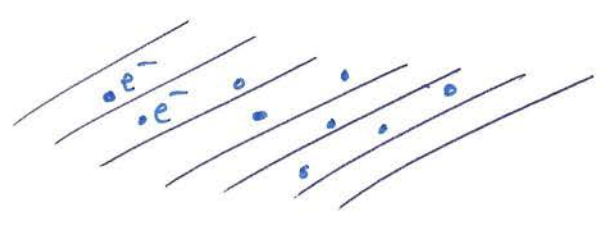
↑
ORDERING
IMPORTANT !

CHECK ORDERING

• HOMOGENEOUS ELECTRON GAS (JELLIUM MODEL)

↳ FIRST APPROXIMATION TO A METAL OR A PLASMA

∴ INTERACTING e⁻ GAS PLACED IN A UNIFORMLY DISTRIBUTED POSITIVE BACKGROUND (IONS)



TOTAL SYSTEM IS ELECTRICAL NEUTRAL.

↳ SYSTEM IN LARGE CUBICAL BOX OF LENGTH L (AT END OF CALCULATION L → ∞). V = L³

e⁻ WAVE FUNCTION $\Psi_{\vec{k}, \lambda}(\vec{x}) = \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{x}} \chi_{\lambda}$
↑
SPIN PROJ $\lambda = \pm \frac{1}{2}$

$\chi_{\lambda = +\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\chi_{\lambda = -\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

PERIODIC BOUNDARY CONDITION $k_i = \frac{2\pi}{L} n_i$
 $i = x, y, z$
 $n_i = 0, \pm 1, \pm 2, \dots$

↳ TOTAL : N ELECTRONS IN BOX OF VOLUME V

AT END $\left. \begin{matrix} N \rightarrow \infty \\ V \rightarrow \infty \end{matrix} \right\} n \equiv \frac{N}{V} \text{ STAYS CONSTANT}$

↳ HAMILTONIAN

$$\rightarrow H = H_{el} + H_b + H_{el-b}$$

↑ ↑ ↑
 ELECTRON BACKGROUND e⁻ BACKGROUND INTERACTION

$$\rightsquigarrow H_{el} = \sum_{i=1}^N \frac{p_i^2}{2m} + \underbrace{\frac{1}{2} e^2 \sum_{i \neq j} \frac{e^{-\mu |\bar{r}_i - \bar{r}_j|}}{|\bar{r}_i - \bar{r}_j|}}_{e^- \text{ REPULSION}}$$

$e^{-\mu |r|}$ INTRODUCED FOR CONVERGENCE
 AT END : $\mu \rightarrow 0$

$$\rightsquigarrow H_b = \frac{1}{2} e^2 \int d^3\bar{x} \int d^3\bar{x}' \underbrace{m(\bar{x}) m(\bar{x}')}_{\uparrow} \frac{e^{-\mu |\bar{x} - \bar{x}'|}}{|\bar{x} - \bar{x}'|}$$

DENSITY OF POSITIVELY CHARGED BACKGROUND PARTICLES.

$$\rightsquigarrow H_{el-b} = - \sum_{i=1}^N \int d^3\bar{x} m(\bar{x}) \frac{e^{-\mu |\bar{x} - \bar{r}_i|}}{|\bar{x} - \bar{r}_i|}$$

↑
 ATTRACTIVE INTERACTION BETWEEN e⁻ AND BACKGROUND

UNIFORM BACKGROUND $m(\bar{x}) = \frac{N}{V}$

$$\begin{aligned}
H_b &= \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \int d^3\bar{x} \int d^3\bar{x}' \frac{e^{-\mu|\bar{x}-\bar{x}'|}}{|\bar{x}-\bar{x}'|} \\
&= \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \cdot V \int d^3\bar{r} \frac{e^{-\mu|\bar{r}|}}{|\bar{r}|} \\
&= \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \cdot V \cdot 4\pi \underbrace{\int_0^\infty d\tau \tau e^{-\mu\tau}}_{\frac{1}{\mu^2}} \quad (\text{LIMIT } L \rightarrow \infty) \\
&= \frac{1}{2} e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2} \\
&\hookrightarrow \text{DIVERGES IN LIMIT } \mu \rightarrow 0.
\end{aligned}$$

$$\begin{aligned}
H_{el-b} &= - e^2 \frac{N}{V} \sum_{i=1}^N \int d^3\bar{x} \frac{e^{-\mu|\bar{x}-\bar{r}_i|}}{|\bar{x}-\bar{r}_i|} \\
&\quad \downarrow \text{TRANSLATIONAL INVARIANCE} \\
&= - e^2 \frac{N^2}{V} \int d^3\bar{r} \frac{e^{-\mu|\bar{r}|}}{|\bar{r}|} \\
&= - e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2}
\end{aligned}$$

$$\circ \circ \quad H = -\frac{1}{2} e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2} + H_{el}$$

→ \hat{H}_{el} IN SECOND QUANTIZATION

e^- STATES CHARACTERIZED BY $i = \bar{k}, s$

• KINETIC ENERGY

$$\hat{T} = \sum_{i,j} \langle i | T | j \rangle c_i^\dagger c_j$$

↓

$$\hat{T} = \sum_{\bar{k}, s} \sum_{\bar{k}', s'} \langle \bar{k}, s | T | \bar{k}', s' \rangle c_{\bar{k}, s}^\dagger c_{\bar{k}', s'}$$

$$\langle \bar{k}, s | T | \bar{k}', s' \rangle$$

$$= \int d^3 \bar{x} \psi_{\bar{k}, s}^*(\bar{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \psi_{\bar{k}', s'}(\bar{x})$$

$$= \frac{\hbar^2}{2mV} \underbrace{\eta_s^\dagger \eta_{s'}}_{\delta_{ss'}} \int d^3 \bar{x} e^{-i\bar{k} \cdot \bar{x}} \bar{k}'^2 e^{i\bar{k}' \cdot \bar{x}}$$

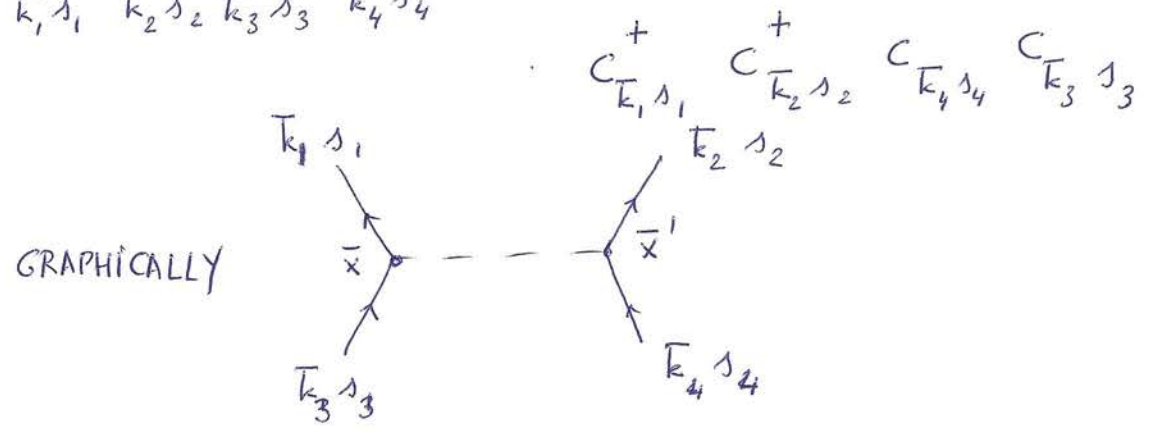
$$= \frac{\hbar^2 \bar{k}'^2}{2mV} \underbrace{\delta_{ss'}}_{\delta_{\bar{k}\bar{k}'}} \int d^3 \bar{x} e^{i(\bar{k}' - \bar{k}) \cdot \bar{x}}$$

$$V \cdot \delta_{\bar{k}\bar{k}'}$$

$$\therefore \hat{T} = \sum_{\bar{k}, s} \frac{\hbar^2 \bar{k}^2}{2m} c_{\bar{k}, s}^\dagger c_{\bar{k}, s}$$

POTENTIAL ENERGY

$$\hat{V} = \frac{1}{2} \sum_{\vec{k}_1, \sigma_1} \sum_{\vec{k}_2, \sigma_2} \sum_{\vec{k}_3, \sigma_3} \sum_{\vec{k}_4, \sigma_4} \langle \vec{k}_1, \sigma_1, \vec{k}_2, \sigma_2 | V | \vec{k}_3, \sigma_3, \vec{k}_4, \sigma_4 \rangle$$



$$\langle \vec{k}_1, \sigma_1, \vec{k}_2, \sigma_2 | V | \vec{k}_3, \sigma_3, \vec{k}_4, \sigma_4 \rangle$$

$$= \frac{1}{V^2} \int d^3 \vec{x} \int d^3 \vec{x}' e^{-i(\vec{k}_1 - \vec{k}_3) \cdot \vec{x}} e^{-i(\vec{k}_2 - \vec{k}_4) \cdot \vec{x}'}$$

$$\cdot e^2 \frac{e^{-\mu |\vec{x} - \vec{x}'|}}{|\vec{x} - \vec{x}'|} \cdot \underbrace{\eta_{\sigma_1}^+ \eta_{\sigma_2}^+}_{\delta_{\sigma_1 \sigma_3}} \underbrace{\eta_{\sigma_3} \eta_{\sigma_4}}_{\delta_{\sigma_2 \sigma_4}}$$

(SPIN DOES NOT CHANGE)

↳ INTERACTION IS SPIN-INDEPENDENT

↓ $\vec{y} \equiv \vec{x} - \vec{x}'$
ELIMINATE \vec{x}

$$= \frac{1}{V^2} \cdot e^2 \delta_{\sigma_1 \sigma_3} \delta_{\sigma_2 \sigma_4} \int d^3 \vec{x}' e^{-i(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4) \cdot \vec{x}'}$$

$$\cdot \int d^3 \vec{y} \frac{e^{-\mu |\vec{y}|}}{|\vec{y}|} e^{-i(\vec{k}_1 - \vec{k}_3) \cdot \vec{y}}$$

$$= \frac{1}{V^2} e^2 \sum_{s_1 s_3} \sum_{s_2 s_4} V \sum_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4}$$

MOMENTUM
CONSERVATION
(UNIFORM SYSTEM)

$$\int d^3 \vec{y} \frac{e^{-\mu y}}{y} e^{-i(\vec{k}_1 - \vec{k}_3) \cdot \vec{y}}$$

$$2\pi \int_0^\infty dy y e^{-\mu y} \int_{-1}^1 d\cos\theta e^{i|\vec{k}_1 - \vec{k}_3| y \cos\theta}$$

$$\frac{1}{-i|\vec{k}_1 - \vec{k}_3| y} \left(e^{-i|\vec{k}_1 - \vec{k}_3| y} - e^{i|\vec{k}_1 - \vec{k}_3| y} \right)$$

$$\frac{2\pi}{i|\vec{k}_1 - \vec{k}_3|} \int_0^\infty dy \left\{ \begin{array}{l} e^{(i|\vec{k}_1 - \vec{k}_3| - \mu) y} \\ - e^{-(i|\vec{k}_1 - \vec{k}_3| + \mu) y} \end{array} \right\}$$

$$= \frac{2\pi}{i|\vec{k}_1 - \vec{k}_3|} \cdot \left\{ -\frac{1}{i|\vec{k}_1 - \vec{k}_3| - \mu} + \frac{1}{-i|\vec{k}_1 - \vec{k}_3| - \mu} \right\}$$

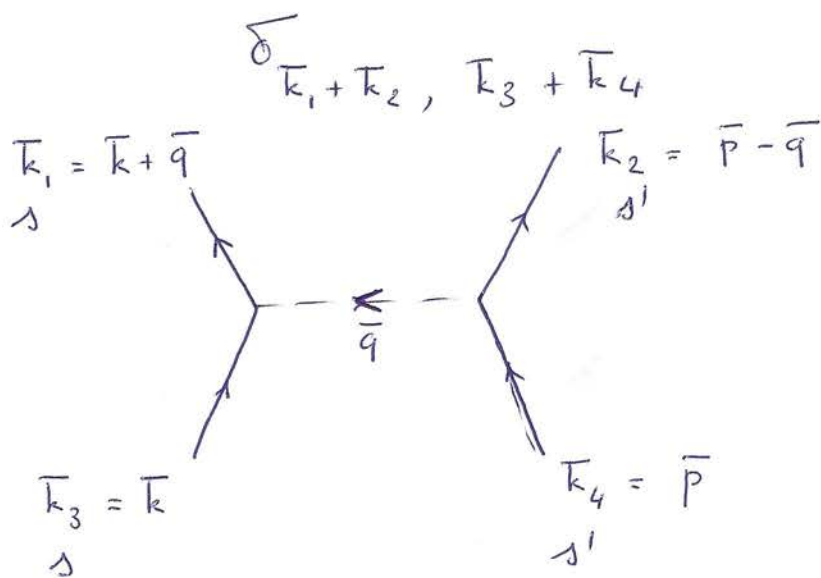
$$\frac{2i|\vec{k}_1 - \vec{k}_3|}{|\vec{k}_1 - \vec{k}_3|^2 + \mu^2}$$

$$= \frac{4\pi}{|\vec{k}_1 - \vec{k}_3|^2 + \mu^2}$$

∞
∞

$$\hat{V} = \frac{e^2}{2V} \sum_{\vec{k}_1} \sum_{\vec{k}_2} \sum_{\vec{k}_3} \sum_{\vec{k}_4} \sum_{s_1 s_2} \sum_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4} \frac{4\pi}{|\vec{k}_1 - \vec{k}_3|^2 + \mu^2} \begin{matrix} + \\ C_{\vec{k}_1 s_1} \end{matrix} \begin{matrix} + \\ C_{\vec{k}_2 s_2} \end{matrix} \begin{matrix} + \\ C_{\vec{k}_4 s_2} \end{matrix} \begin{matrix} + \\ C_{\vec{k}_3 s_1} \end{matrix}$$

SIMPLIFY USING MOMENTUM CONSERVATION



$$\therefore \hat{V} = \frac{e^2}{2V} \sum_{s, s'} \sum_{\vec{k}} \sum_{\vec{p}} \sum_{\vec{q}} \frac{4\pi}{|\vec{q}|^2 + \mu^2}$$

$$\cdot c_{\vec{k}+\vec{q}, s}^+ c_{\vec{p}-\vec{q}, s'}^+ c_{\vec{p}, s'} c_{\vec{k}, s}$$

↓ DIVERGES FOR $|\vec{q}| = 0$ (WHEN $\mu \rightarrow 0$)

$$\therefore \text{SPLIT } \sum_{\vec{q}} \dots = (\vec{q}=0 \text{ TERM}) + \sum_{\vec{q} \neq 0} \dots$$

$$\hat{V} = \frac{e^2}{2V} \sum_{s, s'} \frac{4\pi}{\mu^2} \cdot \sum_{\vec{p}} \sum_{\vec{k}} c_{\vec{k}, s}^+ c_{\vec{p}, s'}^+ c_{\vec{p}, s'} c_{\vec{k}, s}$$

+ TERM WITH $\vec{q} \neq 0$

USE

$$\begin{aligned}
 & C_{\bar{k}\lambda}^+ C_{\bar{p}\lambda'}^+ C_{\bar{p}\lambda'} C_{\bar{k}\lambda} \\
 &= C_{\bar{k}\lambda}^+ C_{\bar{p}\lambda'}^+ (-C_{\bar{k}\lambda} C_{\bar{p}\lambda'}) \\
 &= -C_{\bar{k}\lambda}^+ (\delta_{\lambda\lambda'} \delta_{\bar{k}\bar{p}} - C_{\bar{k}\lambda} C_{\bar{p}\lambda'}) C_{\bar{p}\lambda'} \\
 &= -\delta_{\lambda\lambda'} \delta_{\bar{k}\bar{p}} C_{\bar{k}\lambda}^+ C_{\bar{k}\lambda} + (C_{\bar{k}\lambda}^+ C_{\bar{k}\lambda}) (C_{\bar{p}\lambda'}^+ C_{\bar{p}\lambda'})
 \end{aligned}$$

$$\Rightarrow \hat{V} = \frac{e^2}{2V} \frac{4\pi}{\mu^2} (\hat{N}^2 - \hat{N})$$

+ TERM WITH $\bar{q} \neq 0$

WITH PARTICLE NUMBER OPERATOR $\hat{N} = \sum_{\bar{k}\lambda} C_{\bar{k}\lambda}^+ C_{\bar{k}\lambda}$

⇓

FOR SYSTEMS WITH FIXED N

$$\hat{N}^2 - \hat{N} \rightsquigarrow \text{EIGENVALUE } N(N-1)$$

$$\text{FIRST TERM } \frac{e^2}{2V} N^2 \frac{4\pi}{\mu^2} - \frac{e^2}{2V} N \frac{4\pi}{\mu^2}$$

CANCELS

ENERGY PER e^-

$$H_b + H_{el-b}$$

$$\sim \frac{1}{V} \xrightarrow{V \rightarrow \infty} 0$$

→ TOTAL ENERGY $\hat{H} = \hat{H}_{el} + \hat{H}_b + \hat{H}_{el-b}$

$$\hat{H} = \sum_{\vec{k}, s} \frac{\hbar^2 \vec{k}^2}{2m} C_{\vec{k}, s}^+ C_{\vec{k}, s}$$

$$+ \frac{e^2}{2V} \sum_{\vec{k}} \sum_{\vec{p}} \sum_{\vec{q} \neq 0} \sum_{s, s'} \frac{4\pi}{q^2} C_{\vec{k}+\vec{q}, s}^+ C_{\vec{p}-\vec{q}, s'}^+ C_{\vec{p}, s'} C_{\vec{k}, s}$$

↑
 WE TOOK LIMIT $\mu \rightarrow 0$
 (FIRST $V \rightarrow \infty$, THEN $\mu \rightarrow 0$)
 \Downarrow
 INFINITE TERMS CANCEL
 IN THERMODYNAMIC LIMIT
 (ELECTRIC NEUTRALITY)

→ DIMENSIONLESS VARIABLES

κ_0 : INTERPARTICLE SPACING' $\frac{V}{N} \equiv \frac{4}{3} \pi \kappa_0^3$

a_0 : "BOHR RADIUS"
 (DUE TO COULOMB INTERACTION) $a_0 \equiv \frac{\hbar^2}{me^2}$

κ_s : DIMENSIONLESS $\kappa_s \equiv \frac{\kappa_0}{a_0}$

$\tilde{V} \equiv \frac{V}{\kappa_0^3}$

$\tilde{\vec{k}} \equiv \kappa_0 \vec{k}$ $\tilde{\vec{p}} \equiv \kappa_0 \vec{p}$ $\tilde{\vec{q}} \equiv \kappa_0 \vec{q}$

o
o o

$$\hat{H} = \frac{e^2}{a_0 n_s^2} \left\{ \sum_{\tilde{k}, s} \frac{1}{2} \tilde{k}^2 c_{\tilde{k}, s}^+ c_{\tilde{k}, s} \right. \\ \left. + \frac{n_s}{2V} \sum_{\tilde{k}} \sum_{\tilde{p}} \sum_{\tilde{q} \neq 0} \sum_{s, s'} \frac{4\pi}{\tilde{q}^2} c_{\tilde{k} + \tilde{q}, s}^+ c_{\tilde{p} - \tilde{q}, s'}^+ c_{\tilde{p}, s'} c_{\tilde{k}, s} \right\}$$

IN LIMIT $n_s \rightarrow 0$ (HIGH DENSITY LIMIT)

POTENTIAL BECOMES A SMALL PERTURBATION



EXERCISE: CALCULATE GROUND STATE ENERGY

OF HIGH DENSITY e^- GAS.

IN 1st ORDER PERTURBATION THEORY