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COLD GASES

Complementary lectures and exercises
for Yvan Castin's Lectures

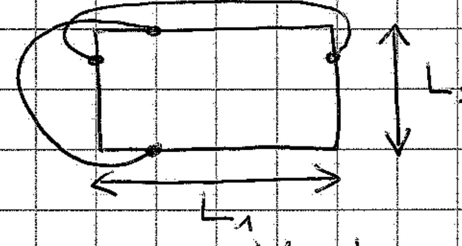
Let us take $\hbar = m = k_B = 1$.

Part 1: Coherence and correlations. Wick's Theorem. Ideal gas

(I) Definitions and notations

$$\eta = \begin{cases} +1 & \text{if we consider a gas of identical } \underline{\text{bosons}} \\ -1 & \text{"} \qquad \underline{\text{fermions}} \end{cases}$$

$(|u_\alpha\rangle)_\alpha$ denotes an orthonormal basis (ONB) of the single-particle Hilbert space.
In all applications, we consider the simple case of a <u>homogeneous system</u>, i.e. a box in d dimensions, with periodic boundary conditions.
For $d = 2$:



$\vec{r} = (x_1, x_2)$

The "volume" is $V = L_1 \times \cdots \times L_d$
Periodic boundary conditions mean that $x_i = 0$ is equivalent to $x_i = L_i$ for $i \in \{1, .., d\}$.
In this homogeneous case, a useful ONB is:

$$\alpha = \vec{k}, \quad u_{\vec{k}}(\vec{r}) = \langle \vec{r} | u_{\vec{k}} \rangle = \frac{1}{\sqrt{V}} e^{i \vec{k}\cdot\vec{r}},$$

$$\vec{k} = (k_1, \ldots, k_d), \quad k_i = \frac{2\pi}{L_i} n_i, \quad n_i \in \mathbb{Z}$$

The thermodynamic limit (t.l.) is:
N = Number of atoms $\to \infty$, $V \to \infty$, $\rho = \frac{N}{V}$ fixed
(and $\frac{L_i}{L_j}$ fixed)

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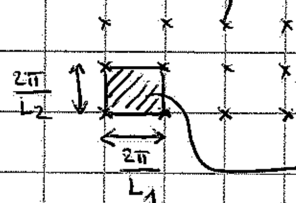
Exercise 1: Show that (S.t.):

$$\sum_{\vec{k}} F(\vec{k}) \underset{t.l.}{\sim} \frac{V}{(2\pi)^d} \int d^d\vec{k} \; F(\vec{k})$$

(assuming $F(\vec{k})$ is regular)

Solution For $d=2$, this is clear from the picture:



area $= \dfrac{(2\pi)^2}{L_1 L_2} = \dfrac{(2\pi)^2}{V}$.

More formally: $\dfrac{(2\pi)^d}{V} \sum_{\vec{k}} F(\vec{k}) = \sum_{n_1=-\infty}^{+\infty} \left(\dfrac{2\pi}{L_1}\right) \cdots \sum_{n_d=-\infty}^{+\infty} \left(\dfrac{2\pi}{L_d}\right) F\left(\dfrac{2\pi}{L_1} n_1, \ldots, \dfrac{2\pi}{L_d} n_d\right)$

$$\xrightarrow[t.l.]{} \int_{-\infty}^{+\infty} dk_1 \ldots \int_{-\infty}^{+\infty} dk_d \; F(k_1, \ldots, k_d). \qquad \boxtimes$$

We note $\sigma \in S_n$ if σ is a permutation of $\{1, \ldots, n\}$. $\varepsilon(\sigma)$ is the signature.

Example: $\sigma \in S_2$, $\sigma(1) = 2$, $\sigma(2) = 1$
$\Rightarrow \varepsilon(\sigma) = -1$.

Definition: $\varepsilon_\eta(\sigma) = \begin{cases} 1 & \text{if } \eta = +1 \text{ (bosons)} \\ \varepsilon(\sigma) & \text{if } \eta = -1 \text{ (fermions)} \end{cases}$

(II) Reminder on Second Quantization

We denote by $\mathcal{E}_N$ the N-particle Hilbert space.
It is generated by the (unnormalized) states of the form: $\sum_{\sigma \in S_N} \varepsilon_\eta(\sigma) \; |u_{\alpha_{\sigma(1)}}\rangle \otimes \cdots \otimes |u_{\alpha_{\sigma(N)}}\rangle$.

(These states are indeed symmetric / antisymmetric for bosons / fermions, i.e. for $\eta = +1 / -1$)

The Fock space is then defined by:

$$\mathcal{E} = \mathcal{E}_0 \overset{\perp}{\oplus} \mathcal{E}_1 \overset{\perp}{\oplus} \cdots \overset{\perp}{\oplus} \mathcal{E}_N \overset{\perp}{\oplus} \cdots$$

where $\mathcal{E}_0 = \mathbb{C} \cdot |0\rangle$ and $|0\rangle$ is called vacuum.

The number operator is given by: $\hat{N}|\psi\rangle = N|\psi\rangle$ if $|\psi\rangle \in \mathcal{E}_N$.

Definition: (i) $a^+_{|u_{\alpha_1}\rangle}$ is the operator defined by:

- $a^+_{|u_{\alpha_1}\rangle} |0\rangle = |u_{\alpha_1}\rangle$
- $a^+_{|u_{\alpha_1}\rangle} \left(|u_{\alpha_2}\rangle \otimes \dots \otimes |u_{\alpha_N}\rangle \right) = \frac{\sqrt{N}}{N!} \sum_{\sigma \in S_N} \varepsilon_?(\sigma) |u_{\alpha_{\sigma(1)}}\rangle \otimes \dots \otimes |u_{\alpha_{\sigma(N)}}\rangle$

(ii) For any single particle state $|u\rangle$, $a^+_{|u\rangle}$ is then defined by imposing that $|u\rangle \longmapsto a^+_{|u\rangle}$ is linear, i.e.:
$$a^+_{|u\rangle} = a^+_{\left(\sum_\alpha |\alpha\rangle\langle\alpha|u\rangle\right)} = \sum_\alpha \langle\alpha|u\rangle \, a^+_{|\alpha\rangle}.$$

Notations: $|\alpha\rangle = |u_\alpha\rangle$, $a^+_\alpha = a^+_{|\alpha\rangle}$, $\psi^+(\vec{r}) = a^+_{|\vec{r}\rangle}$.

In a box, one thus has:
$$\psi^+(\vec{r}) = \sum_{\vec{k}} \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} a^+_{\vec{k}}.$$

Definition: An ONB of the Fock space $\mathcal{E}$ is given by the following "Fock states":

- For Fermions: $|\alpha_1, \dots, \alpha_N\rangle \equiv a^+_{\alpha_1} \dots a^+_{\alpha_N} |0\rangle$
- For Bosons: if $n_\alpha \in \mathbb{N}$ and $\sum_\alpha n_\alpha < \infty$,
$$|(n_\alpha)\rangle \equiv \prod_\alpha \frac{1}{\sqrt{n_\alpha!}} (a^+_\alpha)^{n_\alpha} |0\rangle$$

Property:

- For Fermions: $a^+_{\alpha_1} |\alpha_2, \dots, \alpha_N\rangle = |\alpha_1, \dots, \alpha_N\rangle$
$$a_{\alpha_0} |\alpha_1, \dots, \alpha_N\rangle = \begin{cases} 0 & \text{if } \alpha_0 \notin \{\alpha_1, \dots, \alpha_N\}; \\ (-1)^{i+1} |\alpha_1, \dots, \alpha_{i-1}, \alpha_{i+1}, \dots, \alpha_N\rangle & \text{if } \alpha_0 = \alpha_i. \end{cases}$$

- For Bosons:
$$a^+_\beta |(n_\alpha)\rangle = \sqrt{n_\beta + 1} \, |(n'_\alpha)\rangle \text{ with } n'_\alpha = n_\alpha + \delta_{\alpha\beta}$$
$$a_\beta |(n_\alpha)\rangle = \sqrt{n_\beta} \, |(n'_\alpha)\rangle \text{ with } n'_\alpha = n_\alpha - \delta_{\alpha\beta}$$

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We do not give the proof neither of this basic property, nor of the following one. (They are simple but lengthy. See e.g. Y. Castin, "Cours de Mécanique Quantique", unpublished)

<u>Expression of an observable</u>

	1st quantization	2nd quantization
1-body observable	$\mathcal{B} = \sum_{i=1}^{\hat{N}} B(i)$	$\mathcal{B} = \sum_{\alpha,\beta} \langle u_\alpha \vert B(1) \vert u_\beta \rangle a^\dagger_\alpha a_\beta$
2-body observable	$\mathcal{C} = \sum_{1 \leq i < j \leq \hat{N}} C(i,j)$	$\mathcal{C} = \sum_{\alpha\beta\gamma\delta} \langle u_\alpha \vert \langle u_\beta \vert C(1,2) \vert u_\gamma \rangle \vert u_\delta \rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$

<u>Examples</u>: $B(i) = V_{ext}(\hat{\vec{r}}_i)$; or $B(i) = \dfrac{\hat{\vec{p}}_i^{\,2}}{2m}$

$C(i,j) = V_{int}(\hat{\vec{r}}_i - \hat{\vec{r}}_j)$.

[The $B(i)$'s must be the same operator acting on different particles. Similarly for the $C(i,j)$'s]

III ρ, g_1 and g_2

In classical mechanics, a natural definition of the particle <u>density</u> is: $\rho(\vec{r}; \vec{r}_1, \ldots, \vec{r}_N) = \sum_{i=1}^{N} \delta(\vec{r}_i - \vec{r})$. Indeed, the number of particles in a volume W is then simply $\int_W d\vec{r}\ \rho(\vec{r}; \vec{r}_1, \ldots, \vec{r}_N)$.

Defining in first quantization

$$\hat{\rho}(\vec{r}) \equiv \rho(\vec{r}; \hat{\vec{r}}_1, \ldots, \hat{\vec{r}}_N) = \sum_{i=1}^{\hat{N}} \delta(\hat{\vec{r}}_i - \vec{r}),$$

the postulates of Quantum Mechanics (*) imply that $\langle \hat{\rho}(\vec{r}) \rangle \equiv \rho(\vec{r})$ is the average result of many measurements. More precisely, the mean number of particles in W is: $\int_W d\vec{r}\ \langle \hat{\rho}(\vec{r}) \rangle$.

<u>Exercise 2</u>: S.t. in 2nd quantization:

$$\hat{\rho}(\vec{r}) = \Psi^\dagger(\vec{r})\Psi(\vec{r})$$

(*) C. Cohen-Tannoudji, B. Diu, F. Laloë, "Mécanique Quantique", Volume 1, Paragraph III B 5.

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<u>Solution</u>: Applying the above reminder for $\mathcal{B} = \hat{\rho}(\vec{x})$ and the "basis" $|\vec{x}\rangle$ gives:

$$\hat{\rho}(\vec{x}) = \int_V d\vec{x}_\alpha \int_V d\vec{x}_\beta \underbrace{\langle \vec{x}_\alpha | \delta(\vec{\hat{x}}_1 - \vec{x}) | \vec{x}_\beta \rangle}_{\delta(\vec{x}_\beta - \vec{x}) \langle \vec{x}_\alpha | \vec{x}_\beta \rangle} \psi^+(\vec{x}_\alpha)\, \psi(\vec{x}_\beta)$$

$$\underline{\hat{\rho}(\vec{x})} = \psi^+(\vec{x})\, \psi(\vec{x}). \qquad \boxtimes$$

Thus: $\boxed{\rho(\vec{x}) = \langle \psi^+(\vec{x}) \psi(\vec{x}) \rangle}$.

<u>Definition</u>: $\boxed{g_1(\vec{x}, \vec{x}') \equiv \langle \psi^+(\vec{x}) \psi(\vec{x}') \rangle}$ is called First order <u>coherence function</u>.

<u>Remark</u>: $g_1(\vec{x}, \vec{x}) = \rho(\vec{x})$.

<u>Definition</u>: In classical mechanics, it is natural to define a <u>pair distribution function</u> $\rho_2(\vec{x}, \vec{x}'; \vec{x}_1, \ldots, \vec{x}_N)$ by:

(The number of pairs (i, j) with $i \neq j$ such that $\begin{cases} \vec{x}_i \in W \\ \vec{x}_j \in W' \end{cases}$ ~~or $\begin{cases} \vec{x}_j \in W \\ \vec{x}_i \in W' \end{cases}$~~ equals:

$$\int_W d\vec{x} \int_{W'} d\vec{x}' \; \rho_2(\vec{x}, \vec{x}'; \vec{x}_1, \ldots, \vec{x}_N).$$

<u>Exercice 3</u>: S.t. the observable corresponding to $\rho_2(\vec{x}, \vec{x}'; \vec{x}_1 - \vec{x}_N)$ writes: $\hat{\rho}_2(\vec{x}, \vec{x}') = \psi^+(\vec{x}) \psi^+(\vec{x}') \psi(\vec{x}') \psi(\vec{x})$

<u>Solution</u>: The above equation is satisfied if we take:

$$\rho_2(\vec{x}, \vec{x}'; \vec{x}_1 \ldots \vec{x}_N) = \sum_{i \neq j} \delta(\vec{x}_i - \vec{x})\, \delta(\vec{x}_j - \vec{x}')$$

Thus, in first quantization:

$$\hat{\rho}_2(\vec{x}, \vec{x}') = \sum_{i \neq j} \delta(\hat{\vec{x}}_i - \vec{x})\, \delta(\hat{\vec{x}}_j - \vec{x}')$$

and in 2^{nd} quantization; applying the reminder for $\mathcal{C} = \hat{\rho}_2$:

$$\hat{\rho}_2(\vec{x}, \vec{x}') = \int d\vec{x}_\alpha \int d\vec{x}_\beta \int d\vec{x}_\gamma \int d\vec{x}_\delta \langle \vec{x}_\alpha, \vec{x}_\beta | \delta(\hat{\vec{x}}_1 - \vec{x}) \delta(\hat{\vec{x}}_2 - \vec{x}') | \vec{x}_\gamma, \vec{x}_\delta \rangle$$
$$\times\, \psi^+(\vec{x}_\alpha)\, \psi^+(\vec{x}_\beta)\, \psi(\vec{x}_\delta)\, \psi(\vec{x}_\gamma)$$
$$= \psi^+(\vec{x})\, \psi^+(\vec{x}')\, \psi(\vec{x}')\, \psi(\vec{x})$$

IV <u>Simple Gedankenexperiment to measure g_1</u>

The following is a very simplified version of real "atom-laser" experiments, first reported in: Bloch, Hänsch and Esslinger; Nature <u>403</u>, 166 (2000).

Consider atoms with two internal (hyperfine) states denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$.

Define $\psi^+_\uparrow(\vec{x}) \equiv a^+_{(|\vec{x}\rangle\otimes|\uparrow\rangle)}$

and $d^+_\downarrow \equiv a^+_{(|\phi\rangle\otimes|\downarrow\rangle)}$ where $\phi(\vec{x})$ is some fixed normalized wavefunction [e.g. $\phi = \frac{1}{\sqrt{V}}$ in a box]

- For $t<0$, all atoms are in state $|\uparrow\rangle$ and the Hamiltonian H_0 does not act on the internal state [e.g. $H_0 = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{\vec{x}_i} + \sum_{i<j} V(\hat{\vec{x}}_i - \hat{\vec{x}}_j)$]

- At $t=0$, the gas is in state $|\Psi(0)\rangle = |\Psi_0\rangle\otimes|\uparrow\uparrow\cdots\uparrow\rangle$ (where Ψ_0 is a function of $(\vec{x}_1,\dots,\vec{x}_N)$.)
- For $t>0$, the Hamiltonian becomes $H = H_0 + H_1$ with $H_1 = \Gamma\cdot\left[d^+_\downarrow(\psi_\uparrow(\vec{x}) + \psi_\uparrow(\vec{x}')) + h.c.\right]$
(this models an electromagnetic field which couples resonantly $|\vec{x}\rangle\otimes|\uparrow\rangle$ and $|\vec{x}'\rangle\otimes|\uparrow\rangle$ to $|\phi\rangle\otimes|\downarrow\rangle$)
- At a <u>short</u> time $t=\delta t$, one measures the number of atoms in state $|\phi\rangle\otimes|\downarrow\rangle$, given by the observable $\hat{n}_d \equiv d^+_\downarrow d_\downarrow$, and one averages over many experiments.

The result is: $\langle\hat{n}_d(\delta t)\rangle = \langle\Psi(\delta t)|\,\hat{n}_d\,|\Psi(\delta t)\rangle$

where $|\Psi(\delta t)\rangle = \exp(-iH\delta t)|\Psi(0)\rangle$

$$\simeq \left[1 - i(H_0+H_1)\delta t\right]|\Psi(0)\rangle.$$

<u>Exercise 4:</u> S.t. $\langle\hat{n}_d(\delta t)\rangle \simeq (\Gamma\cdot\delta t)^2\left[\rho(\vec{x}) + \rho(\vec{x}') + 2\,\mathrm{Re}\, g_1(\vec{x},\vec{x}')\right]$

where $g_1(\vec{x},\vec{x}') \equiv \langle\Psi(0)|\,\psi^+_\uparrow(\vec{x})\psi_\uparrow(\vec{x}')\,|\Psi(0)\rangle = \langle\Psi_0|\psi^+(\vec{x})\psi(\vec{x}')|\Psi_0\rangle$

and $\rho(\vec{x}) \equiv \langle\Psi(0)|\psi^+_\uparrow(\vec{x})\psi_\uparrow(\vec{x})|\Psi(0)\rangle = \langle\Psi_0|\psi^+(\vec{x})\psi(\vec{x})|\Psi_0\rangle$.

<u>Solution:</u> $\hat{n}_d|\Psi(\delta t)\rangle \simeq \hat{n}_d[-iH_1\delta t]\cdot|\Psi(0)\rangle$ (since H_0 does not change the internal state). Moreover

$$\hat{n}_d|\Psi(\delta t)\rangle \simeq \hat{n}_d\cdot\left[-i\Gamma\delta t\, d^+_\downarrow\right](\psi_\uparrow(\vec{x}) + \psi_\uparrow(\vec{x}'))|\Psi(0)\rangle$$
$$= -i\Gamma\delta t\cdot d^+_\downarrow(\psi_\uparrow(\vec{x}) + \psi_\uparrow(\vec{x}'))|\Psi(0)\rangle.$$

Similarly: $\langle\hat{n}_d(\delta t)\rangle = \langle\Psi(0)|(i\Gamma\delta t)d_\downarrow(\psi^+_\uparrow(\vec{x}) + \psi^+_\uparrow(\vec{x}'))$
$\times(-i\Gamma\delta t)\,d^+_\downarrow(\psi_\uparrow(\vec{x}) + \psi_\uparrow(\vec{x}'))|\Psi(0)\rangle$

and the result follows. $\square$

V Reminder: Statistical operator (also called density matrix)

① **Definition:** A system which is in state $|\psi_n\rangle$ with probability P_n can be conveniently represented by a "statistical operator" $\hat\rho \equiv \sum_n P_n |\psi_n\rangle\langle\psi_n|$. The average result of many measurements of an observable $\hat A$ is then

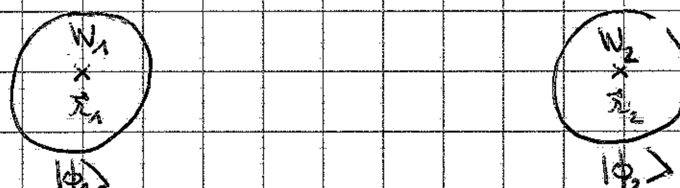
$$\langle \hat A\rangle = \sum_n P_n \langle\psi_n|\hat A|\psi_n\rangle = \mathrm{Tr}(\hat\rho\hat A).$$

(In particular $\sum_n P_n = \mathrm{Tr}\,\hat\rho = 1$).

(Note: We assumed $\langle\psi_n|\psi_n\rangle = 1$.)

Remark: The above Gedankenexperiment generalizes to this case: if the system is in a statistical mixture represented by $\hat\rho$ at $t=0$, then the average result of the experiment is still given by Exercise 4's formula, with $\langle . \rangle = \mathrm{Tr}(\hat\rho\, .)$, and $g_1(\vec x, \vec x') = \mathrm{Tr}(\hat\rho\,\psi^+(\vec x)\psi(\vec x'))$

② Example with 1 particle:



Consider two wavefunctions $\phi_1(\vec x)$ and $\phi_2(\vec x)$ such that $\phi_i(\vec x) = 0$ if $\vec x \notin W_i$, where W_1 and W_2 are two non-overlapping regions centered at $\vec x_1$ and $\vec x_2$.

ⓘ If $\hat\rho = \frac{1}{2}|\phi_1\rangle\langle\phi_1| + \frac{1}{2}|\phi_2\rangle\langle\phi_2|$, then

$$g_1(\vec x_1, \vec x_2) = \mathrm{Tr}\left(\hat\rho\,\psi^+(\vec x_1)\psi(\vec x_2)\right) = \sum_{i=1}^{2}\frac{1}{2}\langle\phi_i|\psi^+(\vec x_1)\psi(\vec x_2)|\phi_i\rangle.$$

Exercise 5: S.t. for 1 particle in state $|\phi\rangle$,

$$\boxed{\langle\phi|\psi^+(\vec x)\psi(\vec x')|\phi\rangle = \phi^*(\vec x)\,\phi(\vec x')}$$

Solution: One possible way (among others) is to first show that $\psi^+(\vec x)\psi(\vec x') = \sum_{i=1}^{\hat N}(|\vec x\rangle\langle\vec x'|)_i$, by applying the Reminder with $\mathcal{B} = \sum_{i=1}^{\hat N}\hat B(i)$ and $\hat B(i) = (|\vec x\rangle\langle\vec x'|)_i$:

$$\mathcal{B} = \int d\vec x_\alpha\, d\vec x_\beta\, \langle\vec x_\alpha|\vec x\rangle\langle\vec x'|\vec x_\beta\rangle\,\psi^+(\vec x_\alpha)\psi(\vec x_\beta)$$
$$= \psi^+(\vec x)\psi(\vec x').$$

The result follows. ☐

Coming back to our example we get:

$$g_1(\vec{r}_1, \vec{r}_2) = \frac{1}{2} \sum_{i=1}^{2} \phi_i^*(\vec{r}_1)\,\phi_i(\vec{r}_2) = 0.$$

(ii) If the particle is in the pure state $|\phi\rangle = \frac{|\phi_1\rangle + |\phi_2\rangle}{\sqrt{2}}$ [i.e. $\hat{\rho} = |\phi\rangle\langle\phi|$] then

$$g_1(\vec{r}_1, \vec{r}_2) = \phi^*(\vec{r}_1)\,\phi(\vec{r}_2) = \frac{1}{2}\,\phi_1^*(\vec{r}_1)\phi_2(\vec{r}_2) \neq 0.$$

(3) Thermal equilibrium in the Grand Canonical ensemble (G.C.E)

In this case $\hat{\rho} = \frac{1}{Z} \exp\left[-\beta(\hat{H} - \mu\hat{N})\right]$ ($\beta = T^{-1}$).

If we call $|\ell\rangle$ the (many-body) eigenstates of $\hat{H}$, E_ℓ their energies and N_ℓ their particle numbers:

$$\hat{\rho} = \frac{1}{Z} \sum_\ell e^{-\beta(E_\ell - \mu N_\ell)}\, |\ell\rangle\langle\ell|,$$ and thus

$$\langle A \rangle = Z^{-1} \sum_\ell e^{-\beta(E_\ell - \mu N_\ell)} \langle \ell | A | \ell \rangle.$$

(4) Ideal gas in the G.C.E.

If we call $|u_\alpha\rangle$ and ε_α the eigenvectors and eigenenergies of the single-particle hamiltonian $h^{(1)}$, then the hamiltonian of the ideal gas is

$$H = \sum_{i=1}^{\hat{N}} h^{(i)} = \sum_\alpha \varepsilon_\alpha\, a_\alpha^\dagger a_\alpha = \sum_\alpha \varepsilon_\alpha \hat{n}_\alpha.$$

It's eigenstates are the Fock states, and one finds (see George Batrouni's Lectures):

$$\langle \hat{n}_\alpha \rangle = \frac{1}{e^{\beta(\varepsilon_\alpha - \mu)} - \eta} \quad ; \quad \langle a_\alpha^\dagger a_{\alpha'} \rangle = 0 \text{ if } \alpha \neq \alpha'.$$

In the rest of these complementary lectures, we restrict to the homogeneous case, where

$$\alpha = \vec{k}, \quad \varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} = \frac{k^2}{2}.$$

(VI) Reminder: Wick's Theorem

Definition: Let C_{2n} denote the set of all permutations $\sigma \in S_{2n}$ satisfying:

$$\begin{cases} \sigma(1) = 1 \\ \forall k \in \{1, \ldots, n-1\},\ \sigma(2k+1) = \mathrm{Min}\left(\{1, \ldots, 2n\} \setminus \{\sigma(1), \ldots, \sigma(2k)\}\right) \end{cases}$$

(We call contraction such a permutation)

Example : $C_4 = \{\sigma \in S_4 \,/\, \sigma(1) = 1 \text{ and } \sigma(3) = \mathrm{Min}\left(\{1,2,3,4\} \setminus \{\sigma(1), \sigma(2)\}\right)\}$
$= \{\sigma_1, \sigma_2, \sigma_3\}$ where :

i	$\sigma_1(i)$	$\sigma_2(i)$	$\sigma_3(i)$
1	1	1	1
2	2	3	4
3	3	2	2
4	4	4	3

Theorem [For a proof, see Y. Castin, Lectures at les Houches in 2003, J. Phys. IV France 116, 89 (2004) and cond-mat/0407118; Appendix A]

Consider :

- $\eta = \pm 1$
- $\hat{a}_\alpha$'s obeying bosonic or fermionic commutation relations:

$$a_\alpha a_\beta^\dagger - \eta\, a_\beta^\dagger a_\alpha = \delta_{\alpha\beta}$$
$$a_\alpha a_\beta - \eta\, a_\beta a_\alpha = 0$$

- A statistical operator $\hat{\rho} = Z^{-1} e^{-\sum_\alpha \nu_\alpha a_\alpha^\dagger a_\alpha}$ with $\nu_\alpha > 0$ if $\eta = +1$ (and $\mathrm{Tr}\,\rho = 1$)
- $\langle \hat{A} \rangle = \mathrm{Tr}\,(\hat{\rho}\hat{A})$
- Operators $\hat{b}_1, \dots, \hat{b}_k$ which are linear combinations of a_α's and $(a_\alpha^\dagger)$'s.

Then :

$$\langle b_1 b_2 \dots b_k \rangle = \begin{cases} 0 \text{ if } k \text{ is odd} ; \\ \sum_{\sigma \in C_k} \varepsilon_\eta(\sigma) \langle b_{\sigma(1)} b_{\sigma(2)} \rangle \dots \langle b_{\sigma(k-1)} b_{\sigma(k)} \rangle \\ \text{if } k \text{ is even} \end{cases}$$

Example : $\langle b_1 b_2 b_3 b_4 \rangle = \langle b_1 b_2 \rangle \langle b_3 b_4 \rangle + \eta \langle b_1 b_3 \rangle \langle b_2 b_4 \rangle + \langle b_1 b_4 \rangle \langle b_2 b_3 \rangle$.

VII g_1 and g_2 for the ideal gas in the non-degenerate regime

In the following we consider an ideal gas at thermal equilibrium in the G.C.E. with parameters T, μ.

Exercise 6 : S.t. $g_1(\vec{x},\vec{x}') = \frac{1}{V} \sum_{\vec{k}} e^{-i\vec{k}\cdot(\vec{x}-\vec{x}')} \langle n_{\vec{k}} \rangle$

Solution : Using the previous results :
$$g_1(\vec{x},\vec{x}') = \langle \Psi^+(\vec{x})\Psi(\vec{x}') \rangle = \left\langle \left(\sum_{\vec{k}} \frac{e^{-i\vec{k}\cdot\vec{x}}}{\sqrt{V}} a^+_{\vec{k}}\right)\left(\sum_{\vec{k}'} \frac{e^{i\vec{k}'\cdot\vec{x}'}}{\sqrt{V}} a_{\vec{k}'}\right)\right\rangle$$
gives the result. $\square$

Remark : It follows that $\rho(\vec{x}) = g_1(\vec{x},\vec{x})$ is independent of $\vec{x}$, as expected for a homogeneous system.

We now consider the so-called non-degenerate regime defined by : $\boxed{-\beta\mu \gg 1}$ and $\boxed{\mu < 0}$

(Recall that $\mu \leq 0$ is always true for bosons)

In this regime, one has
$$\langle n_{\vec{k}} \rangle = \frac{1}{e^{\beta\frac{k^2}{2}} e^{-\beta\mu} - \eta} \simeq e^{-\beta\frac{k^2}{2}} e^{\beta\mu}$$
because $e^{\beta\frac{k^2}{2}} e^{-\beta\mu} \geq e^{-\beta\mu} \ggg 1$.

We shall do this approximation in the following.

Exercise 7 : S.t.
$$g_1(\vec{x},\vec{x}') \underset{t.l.}{\simeq} e^{\beta\mu}\left(\frac{T}{2\pi}\right)^{\frac{d}{2}} e^{-\frac{|\vec{x}-\vec{x}'|^2 T}{2}}$$

Solution : $g_1(\vec{x},\vec{x}') \simeq \frac{1}{V}\sum_{\vec{k}} e^{-i\vec{k}\cdot(\vec{x}-\vec{x}')} e^{-\beta\frac{k^2}{2}} e^{\beta\mu}$

$$\xrightarrow[t.l.]{} \frac{1}{(2\pi)^d} \underbrace{\int d\vec{k}\, e^{-i\vec{k}\cdot(\vec{x}-\vec{x}')} e^{-\frac{k^2}{2T}}}_{=\,(2\pi T)^{d/2} e^{-\frac{|\vec{x}-\vec{x}'|^2 T}{2}}} \cdot e^{\beta\mu} \;. \square$$

Thus we have :
$$\rho = g_1(\vec{x},\vec{x}) = e^{\beta\mu}\left(\frac{T}{2\pi}\right)^{d/2}.$$
Setting $R = |\vec{x}-\vec{x}'|$: $\boxed{g_1(R) = \rho\, e^{-\frac{R^2 T}{2}}}$

In terms of the de Broglie wavelength
$$\lambda_{dB} \equiv \sqrt{\frac{2\pi}{T}} \quad \left(\text{i.e. } \lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{m k_B T}}\right)$$
we have :
$$\rho \cdot (\lambda_{dB})^d = e^{\beta\mu} \ll 1.$$

This shows that the non-degenerate regime is a nearly-classical regime (small $\hbar$, or high T). One indeed recovers the classical results, for example:

Exercise 8: S.t. $\langle H \rangle \simeq \frac{d}{2} \langle N \rangle T$

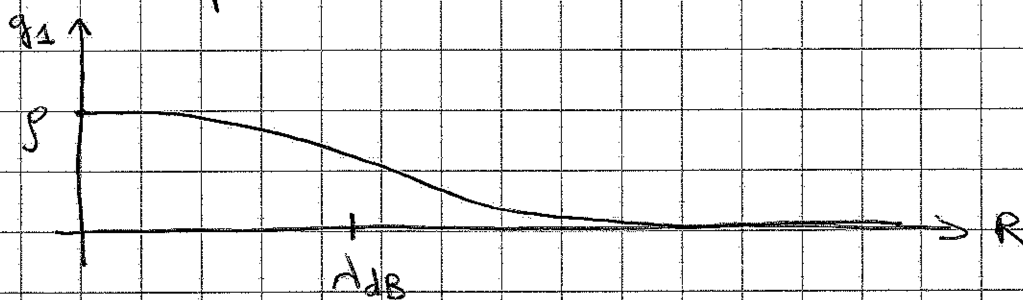
Solution:

$$\langle H \rangle = \sum_{\vec{k}} \varepsilon_k \langle n_k \rangle \simeq \sum_{\vec{k}} \frac{k^2}{2} \cdot e^{-\beta \frac{k^2}{2}} e^{\beta\mu}$$

$$\xrightarrow{t.l.} \frac{V}{(2\pi)^d} \int d\vec{k} \cdot \frac{k^2}{2} \cdot e^{-\beta k^2/2} e^{\beta\mu}$$

$$= \frac{1}{2} e^{\beta\mu} \cdot V \cdot \left(\frac{T}{2\pi}\right)^{d/2} \cdot d \cdot T = \frac{d}{2} \rho V T = \frac{d}{2} \langle N \rangle T . \ \square$$

We have found:



Exercise 9: S.t. $g_2(\vec{x}, \vec{x}') = \rho^2 + \eta \, |g_1(\vec{x}, \vec{x}')|^2$

Solution: From Wick's Theorem:

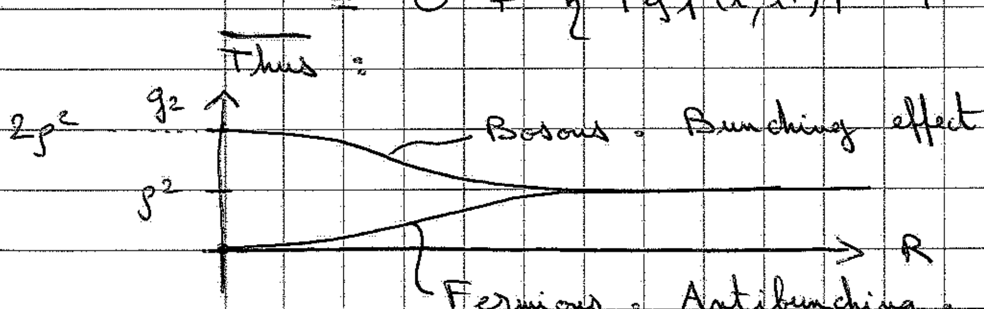
$$g_2(\vec{x}, \vec{x}') = \langle \psi^+(\vec{x}) \psi^+(\vec{x}') \psi(\vec{x}') \psi(\vec{x}) \rangle$$

$$= \langle \psi^+(\vec{x})\psi^+(\vec{x}') \rangle \langle \psi(\vec{x}')\psi(\vec{x}) \rangle + \eta \langle \psi^+(\vec{x})\psi(\vec{x}') \rangle \langle \psi^+(\vec{x}')\psi(\vec{x}) \rangle$$

$$+ \langle \psi^+(\vec{x})\psi(\vec{x}) \rangle \langle \psi^+(\vec{x}')\psi(\vec{x}') \rangle$$

$$= 0 + \eta \, |g_1(\vec{x}, \vec{x}')|^2 + \rho^2 . \ \square$$

Thus:



Remark: The classical gas is recovered in the limit $\lambda_{dB} \to 0$, where $g_1 \to 0$ (no coherence) and $g_2 \to \rho^2$ (no correlations between the particle's positions).

Warning: The result of Exercice 9 breaks down in presence of a BEC. See Yvan Castin's Lectures.