Fock Space

$\mathcal{H}_n$ = Hilbert space of n particles

$\hookrightarrow L^2_{s/a}(\Omega^n)$

$\mathcal{F} = \bigoplus_{n \geq 0} \mathcal{H}_n \quad , \quad \mathcal{H}_0 = \mathbb{C}$

Ψ

$\{ \underline{\Psi}^{(0)}, \underline{\Psi}^{(1)} \ldots \} : \underline{\Psi}^{(n)} \in \mathcal{H}_n$

$\langle \underline{\Psi}, \Phi \rangle_{\mathcal{F}} = \sum_{n \geq 0} \langle \underline{\Psi}^{(n)}, \Phi^{(n)} \rangle_{\mathcal{H}_n}$

$\{ \underline{\Psi}^{(n)} \}_{n \geq 0}$ $\quad \hookrightarrow \{ \Phi^{(n)} \}_{n \geq 0}$

$(\mathcal{N}\underline{\Psi})^{(n)} = n\,\underline{\Psi}^{(n)}$ number operator

domain $\underline{\Psi} \in \mathcal{F}$: $\sum_{n \geq 0} n^2 \|\underline{\Psi}^{(n)}\|^2_{\mathcal{H}_n} < \infty$

Vectors with n particles are eigenvectors of $\mathcal{N}$

↳ $\underline{\Psi}^{(n)} \in \mathcal{F}$

$\{0, \dots \underline{\Psi}^{(n)}, 0 \dots\}$

$\Omega = \{1, 0, \dots\}$ vacuum vector creation and annihilation op. in bosonic Fock space

$f \in \mathcal{H}_1$

$$(a(f)\,\Psi)^{(n)}(x_1 \dots x_n) = \sqrt{n+1}\int \overline{f(x)}\,\Psi^{(n+1)}(x, x_1 \dots x_n)\,dx$$

$a(f)$ is the annihilation operator

$$a(f): \mathcal{H}_{n+1} \longrightarrow \mathcal{H}_n \rightsquigarrow a(f): \mathcal{F} \longrightarrow \mathcal{F}$$

$$(a^*(f)\,\Psi)^{(n)}(x_1 \dots x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} f(x_j)\,\Psi^{(n-1)}(x_1 \dots \cancel{x_j} \dots x_n)$$

creation operator

$a^*(f)$ is the adjoint of $a(f)$

$$[a(f), a(g)] = [a^*(f), a^*(g)] = 0$$

$$[a(f), a^*(g)] = \langle f, g \rangle_{\mathcal{H}_1}$$

canonical commutation relations (CCR)

creation and annihilation operators in the fermionic space

$$(a(f)\,\underline{\Psi})^{(n)}(x_1,\dots,x_n) = \sqrt{n+1}\int dx\,\overline{f(x)}\,\underline{\Psi}^{(n+1)}(x_1 \dots x_n, x)$$

$$(a^*(f)\,\underline{\Psi})^{(n)}(x_1 \dots x_n) = \frac{1}{\sqrt{n}}\sum_{j=1}^{n}(-1)^{j-1} f(x_j)\,\underline{\Psi}^{(n-1)}(x_1 \dots \cancel{x_j} \dots x_n)$$

$$\{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0, \quad \{a^*(f), a(g)\} = \langle f, g\rangle_{\mathcal{H}_1}$$

(CAR)

$\{A, B\} = AB + BA$ anticommutator

$$\Rightarrow a^*(f)^2 = 0 \quad \forall f \in \mathcal{H}_1$$ Pauli principle

$$\| a(f)\Psi \|^2_{\mathcal{F}} = \langle a(f)\Psi, a(f)\Psi \rangle_{\mathcal{F}}$$

$$= \langle \Psi, \underbrace{a^*(f)a(f)}_{\{a^*(f), a(f)\} - a(f)a^*(f)} \Psi \rangle_{\mathcal{F}}$$

$$= \|f\|^2_{\mathcal{H}_1} \|\Psi\|^2_{\mathcal{F}} - \langle \Psi, a(f)a^*(f)\Psi \rangle_{\mathcal{F}}$$

$$= \|f\|^2 \|\Psi\|^2 - \underbrace{\| a^*(f)\Psi \|^2_{\mathcal{F}}}_{\geq 0} \leq \|f\|^2_{\mathcal{H}_1} \|\Psi\|^2_{\mathcal{F}}$$

$\rightsquigarrow$ $a(f)$ bdd in fermionic case!

$x \in \Omega \subset \mathbb{R}^d$

$$(a_x \Psi)^{(n)}(x_1 \dots x_n) = \sqrt{n+1}\; \Psi^{(n+1)}(x, x_1 \dots x_n)$$

the adjoint would be formally $a^*_x = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \delta(x - x_j)\, \Psi^{(n-1)}(x_1 \dots \cancel{x_j} \dots x_n)$

which is not a densely defined operator

In the sense of quadratic form

$$\langle \Phi, a_x \Psi \rangle_{\mathcal{F}} = \langle a^*_x \Phi, \Psi \rangle_{\mathcal{F}}$$

$$a(f) = \int dx \, a_x \overline{f(x)}$$

$$a^*(f) = \int dx \, a^*_x f(x)$$

$f \in \mathcal{H}_1$

a_x, a^*_x operator-valued distribution

$[a_x, a^*_y] = \delta(x,y)$, $[a_x, a_y] = [a^*_x, a^*_y] = 0$ bosonic

$\{a_x, a^*_y\} = \delta(x-y)$, $\{a_x, a_y\} = \{a^*_x, a^*_y\} = 0$ fermionic

$$\langle \underline{\Psi}, \int dx\, a_x^* a_x \Phi \rangle_{\mathcal{F}} = \int dx \, \langle \underline{\Psi}, a_x^* a_x \Phi \rangle_{\mathcal{F}}$$

$$= \int dx \, \langle a_x \underline{\Psi}, a_x \Phi \rangle_{\mathcal{F}}$$

$$= \langle \underline{\Psi}, \mathcal{N} \underline{\Phi} \rangle_{\mathcal{F}}$$

$$\rightsquigarrow \mathcal{N} = \int dx \, a_x^* a_x$$

Let O one-particle operator

$$(d\Gamma(O)\,\underline{\Psi})^{(n)} = O^{(n)}\,\underline{\Psi}^{(n)}$$

$$\hookrightarrow \sum_{j=1}^{n} O^{(n)}_j = \sum_{j=1}^{n} \mathbb{1} \otimes \cdots \otimes \underbrace{O}_{j\text{-th position}} \otimes \cdots \otimes \mathbb{1}$$

$d\Gamma(O)$ the second quantization of O

In general even if O is bounded $d\Gamma(O)$ is not

ex $\mathcal{N} = d\Gamma(1)$

$\left(\text{but } |\langle \underline{\Psi}, d\Gamma(O)\,\underline{\Psi}\rangle| \leq \|O\|\, |\langle \underline{\Psi}, \mathcal{N}\,\underline{\Psi}\rangle| \right)$

Assume $\mathcal{O}$ has integral kernel $\mathcal{O}(x;y)$

$$\langle \Phi, d\Gamma(\mathcal{O})\Psi\rangle_{\mathcal{F}} = \sum_{n\geq 1} \sum_{j=1}^{n} \langle \Phi^{(n)}, \mathcal{O}_j^{(n)} \Psi^{(n)}\rangle_{\mathcal{H}_n}$$

$$= \sum_{n\geq 1} \sum_{j} \int dx_1 .. dx_n \, \Phi^{(n)}(x_1 .. x_n) \int dy \, \mathcal{O}(x_j; y) \Psi^{(n)}(x_1 .. \, y \, .. x_n)$$

$$= \sum_{n\geq 1} n \int dx_1 .. dx_n \, \Phi^{(n)}(x_1 .. x_n) \int dy \, \mathcal{O}(x_1, y) \, \Psi^{(n)}(y, x_2 .. x_n)$$

$$= \sum_{n\geq 1} \int dx_1 \, dy \, (a_{x_1}\Phi)^{(n-1)}(x_2 .. x_n) \, (a_y \Psi)^{(n-1)}(x_2, .. x_n) \, \mathcal{O}(x;y)$$

$$= \int dx \, dy \, \mathcal{O}(x;y) \langle a_x \Phi, a_y \Psi\rangle_{\mathcal{F}}$$

$$d\Gamma(O) = \int dx\, dy\; O(x;y)\, a_x^* a_y$$

O k-particle operator $\quad d\Gamma(O) = \sum_{\{i_1 \ldots i_k\}} O^{(n)}_{i_1 \ldots i_k} \Psi^{(n)}$

$$d\Gamma(O) = \int dx_1 \ldots dx_k\, dy_1 \ldots dy_k\; O(x_1 \ldots x_k; y_1 \ldots y_k)\, a_{x_1}^* \ldots a_{x_k}^* a_{y_1} \ldots a_{y_k}$$

$$H_N = \sum_{j=1}^{N} h_j + \sum_{i<j} V(x_i - x_j)$$

$$d\Gamma(H) = \int dx\,dy\; h(x,y)\, a^*_x a_y + \frac{1}{2}\int dx\,dy\; V(x-y)\, a^*_x a^*_y a_x a_y$$

if $h = -\Delta \rightsquigarrow \nabla_x a^*_x \nabla_y a_y$

$\{\varphi_j\}$ onb of $\mathcal{H}_1$

$\{P_n^s(\varphi_{j_1} \otimes \dots \otimes \varphi_{j_n})\}$ or $\{P_n^a(\varphi_{j_1} \otimes \dots \otimes \varphi_{j_n})\}$

onb of $\mathcal{H}_n$ in bosonic/fermionic case

$\{P_n^s(\varphi_{j_1} \otimes \dots \otimes \varphi_{j_n})\}_{n \geq 1}$ $\{P_n^a(\varphi_{j_1} \otimes \dots \otimes \varphi_{j_n})\}_{n \geq 0}$

onb of $\mathcal{F}$ in bosonic/fermionic case

The generic element of the basis can be written as

$$\frac{1}{\sqrt{n_{i_1}! \dots n_{i_M}!}} a^*(\varphi_{i_1})^{n_{i_1}} \dots a^*(\varphi_{i_M})^{n_{i_M}} \Omega \rightsquigarrow |n_{i_1} \dots n_{i_M}\rangle$$

this basis is known as the occupation number basis

$M = 1, 2 \dots, \quad 1 \leq i_1 < i_2 < \dots < i_M$

rmk $\quad n_{i_j} \in \{0, 1, 2, \dots\}$ for bosons

$n_{i_j} \in \{0, 1\}$ for fermions

$\mathcal{O}$ one-particle op

$$d\Gamma(\mathcal{O}) = \sum_{i,j} \langle \varphi_i, \mathcal{O}\varphi_j \rangle a_i^* a_j$$

$\hookrightarrow a^*(\varphi_i)$

$\mathcal{O}$ two particle operator

$$d\Gamma(\mathcal{O}) = \sum_{ijkl} \langle \varphi_i \otimes \varphi_j, \mathcal{O}\varphi_k \otimes \varphi_l \rangle a_i^* a_j^* a_k a_l$$

$$\rightsquigarrow d\Gamma(H) = \sum_{i,j} \langle \varphi_i, h\varphi_j \rangle + \frac{1}{2} \sum_{ijkl} \langle \varphi_i \otimes \varphi_j, V\varphi_k \otimes \varphi_l \rangle a_i^* a_j^* a_k a_l$$

$T=0$ equilibrium states minimisers of

$$\langle \Psi_N, H_N \Psi \rangle$$

$T>0$?

Let ρ density matrix

$$S(\rho) = -\operatorname{Tr}(\rho \log \rho)$$

$$\rho = \sum_j \lambda_j \, |\Psi_{N,j}\rangle\langle\Psi_{N,j}|$$

$\rightsquigarrow$ by Spectral Theorem

$$\rho \log \rho = \sum_j \lambda_j \log \lambda_j \, |\Psi_{N,j}\rangle\langle\Psi_{N,j}|$$

$$S(\rho) = - \sum_j \lambda_j \log \lambda_j$$

In particular if $\rho = |\Psi_N\rangle\langle\Psi_N| \iff S(\rho) = 0$

$T > 0$ $$F(T;\rho_N) = \mathrm{Tr}(H_N \rho_N) - T S(\rho_N)$$

free energy

we look for minimizers of F

↳ Gibbs state

Note that if $T=0$ the minimizer is a pure state

and we recover $\langle \Psi_N, H_N \Psi_N \rangle$

The Gibbs state is

$$\rho_c = \frac{e^{-\beta H_N}}{Z_c(\beta)} \quad , \quad Z_c(\beta) = \mathrm{Tr}\left(e^{-\beta H_N}\right)$$

↳ canonical partition function

$$\beta = \frac{1}{T}$$

$$S(\rho_c) = \frac{1}{T}\mathrm{Tr}(H_N \rho_c) + \log(Z_c(\beta))$$

There are cases in which we can't consider the number of particle fixed

chemical potential

$$(\mathcal{H} - \mu \mathcal{N}) - TS$$

$\hookrightarrow \mathcal{H} = d\Gamma(H)$

$$\rho_{GC} = \frac{e^{-\beta(\mathcal{H} - \mu \mathcal{N})}}{Z_{GC}(\beta, \mu)} \, , \qquad Z_{GC}(\beta, \mu) = \mathrm{Tr}\left(e^{-\beta(\mathcal{H} - \mu \mathcal{N})}\right)$$

$$S(\rho_{GC}) = \beta \, \mathrm{Tr}\left(\rho_{GC} (\mathcal{H} - \mu \mathcal{N})\right) + \log\left(Z_{GC}(\beta, \mu)\right)$$

The grand potential

$$\Omega(\beta, \mu) = -\frac{1}{\beta} \log \left(Z_{GC}(\beta, \mu) \right)$$

$$N := \langle \mathcal{N} \rangle_{\rho_{GC}} = \mathrm{Tr}\left(\mathcal{N} \rho_{GC} \right) = \frac{\mathrm{Tr}\left(\mathcal{N} e^{-\beta(\mathcal{H} - \mu \mathcal{N})} \right)}{\mathrm{Tr}\left(e^{-\beta(\mathcal{H} - \mu \mathcal{N})} \right)}$$

$$= -\left(\frac{\partial \Omega(\beta, \mu)}{\partial \mu} \right)$$

$$E := \langle \mathcal{H} \rangle_{\rho_{GC}} = \mathrm{Tr}\left(\mathcal{H} \rho_{GC} \right) = \left(\frac{\partial (\beta \Omega)}{\partial \beta} \right)_{\beta \mu}$$

$\hookrightarrow$ $\beta\mu$ held const in taking derivatives