

Partie IV Fonctions de Green à T finie

23. Résultats principaux 2^{ème} quantification

1. Espace de Fock, opérateurs de création-annihilation

1. Fermions

2. Bosons

3. Opérateur nombre

2. Changement de base

1. $|\vec{r}\rangle$ et $|\vec{k}\rangle$

3. Opérateurs à 1 corps

4. Opérateurs à 2 corps

5. 2^{ème} quant. et représentation de Heisenberg

24. Motivation pour la déf. de la fonction de Green G^R

✓ 1. ARPES vs $A(k, \omega)$

✓ 2. Déf. de G^R et lien avec précédente

3. Exemple pour H quadratique

25. Représentation d'interaction et produit chronologique

23.1.3 Fermions

$$a_{\alpha_i}^{\dagger} a_{\alpha_i} (a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} \dots a_{\alpha_i}^{\dagger} \dots a_{\alpha_p}^{\dagger}) |0\rangle$$

$$a^{\dagger} a a^{\dagger} = a^{\dagger} [1 + a a]$$

$$[\hat{n}_{\alpha_i}, a_{\alpha_i}^{\dagger}] = a_{\alpha_i}^{\dagger}$$

$$[\hat{n}_{\alpha_i}, a_{\alpha_i}] = -a_{\alpha_i}$$

$$\begin{aligned}
 & |\alpha_i \alpha_j \dots \alpha_k \dots \alpha_l \dots \alpha_m \rangle \\
 &= - |\alpha_i \alpha_j \dots \alpha_l \dots \alpha_k \dots \alpha_m \rangle \\
 & a_{\alpha_i}^+ a_{\alpha_j}^+ \dots a_{\alpha_k}^+ \dots a_{\alpha_l}^+ \dots a_{\alpha_m}^+ |0\rangle
 \end{aligned}$$

23.1.2 Bosons

$$|\alpha_i \alpha_j\rangle = |\alpha_j \alpha_i\rangle$$

$$[a_{\alpha_i}^\dagger, a_{\alpha_j}^\dagger] = 0 = [a_{\alpha_i}, a_{\alpha_j}]$$

$$[a_{\alpha_i}, a_{\alpha_j}^\dagger] = \delta_{ij}$$

$$[a^\dagger a, a^\dagger] = a^\dagger a a^\dagger - a^\dagger a^\dagger a$$

$$= a^\dagger (1 + a^\dagger a) - a^\dagger a^\dagger a$$

$$= a^\dagger$$

$$[\hat{n}_{\alpha_i}, a_{\alpha_i}^\dagger] = a_{\alpha_i}^\dagger$$

$$[\hat{n}_{\alpha_i}, a_{\alpha_i}] = -a_{\alpha_i}$$

$$a_{\alpha_i}^\dagger a_{\alpha_i}^\dagger a_{\alpha_j}^\dagger \dots |0\rangle$$

3. Opérateur nombre

"Théorème" sur les commutateurs d'opérateurs d'échelle

$$\text{Soit } [\hat{n}, a^\dagger] = B a^\dagger$$

Si $|n\rangle$ est état propre de \hat{n} , i.e. $\hat{n}|n\rangle = n|n\rangle$

alors

$$\hat{n}(a^\dagger|n\rangle) = (n+B)(a^\dagger|n\rangle)$$

↑
valeur propre.

Preuve

$$(\hat{n}a^\dagger - a^\dagger\hat{n})|n\rangle = B(a^\dagger|n\rangle)$$

$$[\hat{n}, a^\dagger] = B a^\dagger$$

$$a^+ |n\rangle = C |n+1\rangle$$

$$\langle n | a a^+ |n\rangle = |C|^2 \langle n+1 | n+1\rangle$$

$$\langle n | 1 + a^+ a |n\rangle = n+1 \langle n | n\rangle$$

$$C = \sqrt{n+1}$$

$$|\alpha_1 \alpha_2 \dots \alpha_n\rangle = \frac{1}{\sqrt{\prod_i n_i!}} a_{\alpha_1}^+ a_{\alpha_2}^+ \dots a_{\alpha_n}^+ |0\rangle$$

$$a^+ |0\rangle = |1\rangle$$

$$(a^+)^2 |0\rangle = \sqrt{2} |2\rangle$$

$$(a^+)^3 |0\rangle = \sqrt{3} \sqrt{2} |3\rangle$$

23.2 Changement de base.

$$|\mu_m\rangle = \sum_i |\alpha_i\rangle \langle \alpha_i | \mu_m \rangle$$

$$c_{\mu_m}^+ = \sum_i a_{\alpha_i}^+ \langle \alpha_i | \mu_m \rangle$$

$$c_{\mu_n} = \sum_i \langle \mu_n | \alpha_i \rangle a_{\alpha_i}$$

$$\left[\left\{ c_{\mu_m}, c_{\mu_n}^+ \right\} \right] = \sum_{i,j} \langle \mu_n | \alpha_i \rangle \underbrace{\left\{ a_{\alpha_i}, a_{\alpha_j}^+ \right\}}_{\delta_{ij}} \langle \alpha_j | \mu_m \rangle$$
$$= \langle \mu_m | \mu_n \rangle$$

Transfo. unitaire
 \Leftrightarrow
Transfo. canonique
préserve
anticomm.

1. Base $|r\rangle$ et $|k\rangle$

Fermeture $\int d^3r |r\rangle\langle r| = \mathbb{I}$

$$\sum_k |k\rangle\langle k| = \mathbb{I}$$

$$\langle r|k\rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \quad \langle k|r\rangle = \frac{1}{\sqrt{V}} e^{-i\mathbf{k}\cdot\mathbf{r}} \quad \leftarrow$$

$$\Psi^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k c_k^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}}$$

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k e^{i\mathbf{k}\cdot\mathbf{r}} c_k$$

$$\begin{aligned} \langle r|r'\rangle &= \sum_k \langle r|k\rangle\langle k|r'\rangle = \frac{1}{V} \sum_k e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \\ &= \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \delta(\mathbf{r}-\mathbf{r}') \end{aligned}$$

$$\{\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\} = \delta(\mathbf{r}-\mathbf{r}')$$

$$\langle k|k'\rangle = \int d^3r \langle k|r\rangle\langle r|k'\rangle = \frac{1}{V} \int d^3r e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}$$

$$\{c_k, c_{k'}^\dagger\} = \delta_{\mathbf{k}, \mathbf{k}'}$$

23.3 Opérateurs à 1 corps

$$\left[V(R_1) + V(R_2) + V(R_3) \right] |r'\rangle |r\rangle |r''\rangle = \left[\underline{V(r') + V(r) + V(r'')} \right] |r'\rangle |r\rangle |r''\rangle$$

$$\sum_{i=1}^N V(R_i) |r, r', r'' \dots\rangle = \left(V(r) + V(r') + V(r'') + \dots \right) |r, r', r''\rangle$$

$$\sum_n \hat{U}_{\alpha_n} |\alpha_i, \alpha_j, \dots, \alpha_h\rangle = \left(U_{\alpha_i} + U_{\alpha_j} + U_{\alpha_h} + \dots \right) |\alpha_i, \alpha_j, \dots, \alpha_h\rangle$$

$$= \sum_n U_{\alpha_n} \hat{n}_{\alpha_n} |\alpha_i, \alpha_j, \dots, \alpha_h\rangle$$

$$\sum_i a_i^\dagger \langle \alpha_i | U | \alpha_j \rangle a_j \quad \rightsquigarrow \langle \alpha_i | \mu_n \rangle c_m$$

U_{α_n}

Base quelconque

$$\sum_m \sum_n c_{\mu_m}^\dagger \langle \mu_m | U | \mu_n \rangle c_{\mu_n}$$

Examples: $\int d^3r \Psi^\dagger(r) V(r) \Psi(r)$ ←

$$\sum_k c_k^\dagger \langle k | \frac{\hbar^2}{2m} | k \rangle c_k = \sum_k \int d^3r \Psi^\dagger(r) \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\hbar^2}{2m} \int d^3r' \frac{1}{\sqrt{V}} e^{-i\mathbf{k}\cdot\mathbf{r}'} \Psi(r')$$

$$= \int d^3r \Psi^\dagger(r) \left(-\frac{\nabla^2}{2m} \right) \Psi(r)$$

23.4 Opérateurs à 2 corps.

$$V_{r,r'} + V_{r,r''} + V_{r',r''} |r, r', r''\rangle$$

$$\frac{1}{2} \sum_{\mu=1}^N \sum_{\nu=1}^N U_{\mu\nu} |\alpha_i, \alpha_j, \dots, \alpha_k\rangle$$

$$\langle \alpha_1 | \langle \alpha_2 | \langle \alpha_3 | \dots \rangle$$

$$\frac{1}{2} \sum_m \sum_n \langle \alpha_m | \langle \alpha_n | U | \alpha_m \rangle | \alpha_n \rangle \left(\hat{n}_{\alpha_m} \hat{n}_{\alpha_n} - \delta_{mn} \hat{n}_{\alpha_n} \right) |\alpha_i, \alpha_j, \dots, \alpha_k\rangle$$

$$\frac{1}{2} \int d^3r d^3r' V(r-r') \left[\psi^\dagger(r) \psi(r) \psi^\dagger(r') \psi(r') - \delta(r-r') \psi^\dagger(r') \psi(r') \right]$$

$$\frac{1}{2} \int d^3r d^3r' V(r-r') \psi^\dagger(r) \psi^\dagger(r') \psi(r') \psi(r)$$

$\langle \alpha | \langle \beta | V | \gamma' \rangle | \beta \rangle c_a^\dagger c_b^\dagger c_c c_d$ order normal

$$V(\overbrace{R_1 - R_2}) \downarrow |r\rangle \downarrow |r'\rangle$$

$$= V(r - r') |r\rangle |r'\rangle$$

$$\langle r | \langle r' | \underbrace{V(r - r') |r\rangle |r'\rangle}$$

23.5 Repr. d'Heisenberg 2nd quant.

$$C_h(t) = e^{\uparrow iHt} C_h e^{-iHt \uparrow}$$

Cas particulier $H = \sum_k \epsilon_k c_k^\dagger c_k + c^\dagger c^\dagger c c$

$$i \frac{\partial}{\partial t} C_h(t) = -[H, C_h(t)] = -\sum_{k'} \epsilon_{k'} [\hat{n}_{k'}(t), C_h(t)] = \epsilon_h C_h(t)$$

$$\rightarrow C_h(t) = e^{-i\epsilon_h t} C_h$$

$$[A, BC] = [A, B]C + B[A, C] = (\cancel{AB - BA})C + B(\cancel{AC - CA})$$

$$[A, BC] = \{A, B\}C - B\{A, C\} \leftarrow$$

$$= (\cancel{AB + BA})C - B(\cancel{AC + CA})$$

24. Motiver G^R N-corps et lien avec avant

$$\langle n | \langle h | \langle 0 | - \sum_{\vec{h}'} \vec{j}_{\vec{h}'} \cdot \vec{A}_{-\vec{h}'} | m \rangle | 0 \rangle | 1 \rangle_{em}$$

\uparrow syst. \uparrow detect \uparrow photon
 \uparrow -1 photo. \uparrow $g = h' = 0$

$$\vec{A}_{\vec{h}} \propto (a_{\vec{h}}^+ + a_{-\vec{h}}) \hat{e}_{\vec{h}}$$

$$\vec{j}_{\vec{h}'} = - \sum_{\vec{p}} \vec{p} c_{\vec{p}}^+ c_{\vec{p} + \vec{h}'}$$

$$\langle n | c_{\vec{h}'} | m \rangle \left(\langle h | c_{\vec{h}'}^+ | 0 \rangle \frac{\hbar_{||}}{m} \langle 0 | \vec{A} | h \rangle_{em} \right)$$

$$\frac{d^2 \sigma}{d\Omega d\omega} \propto \sum_{\vec{m}} \sum_n e^{-\beta E_n} |\langle m | c_{\vec{h}'} | n \rangle|^2 \delta(\omega - (E_m - E_n))$$

$$k_{||} = E_n - \mu N_n$$

Can reponse à diffusion electron $c_{\vec{h}'} \rightarrow \vec{p}$

$$\int dt e^{i(\omega - E_m + E_n)t}$$

$$\frac{d^2 \sigma}{d\Omega d\omega} \propto \int dt e^{i\omega t} \langle c_{\vec{h}'}^+ c_{\vec{h}'}(t) \rangle \propto A(k, \omega) f(\omega)$$

24.2 Def. Green N-corps:

$$\langle r | \hat{G}^R(t) | r' \rangle = -i \langle r | e^{-iH(t-t')} | r' \rangle \theta(t-t') \quad \begin{matrix} \Psi(r',t') = \int \Psi(r,t) G^R(r,t; r',t') \\ \Psi(r,t) \end{matrix}$$

"Tentation"

$$\langle \Omega | G^R_{(t-t')} | \Omega \rangle = -i \langle \Omega | \Psi(-) e^{-iH(t-t')} \Psi^\dagger(r') | \Omega \rangle \theta(t-t')$$

↑ f.o.d. ↑ f.o.d. si: $H|\Omega\rangle = 0$

$$\Psi^\dagger(r',t') \cdot e^{iHt'} \Psi^\dagger(r') e^{-iHt'}$$

$$= -i \langle \Omega | \Psi(r,t) \Psi^\dagger(r',t') | \Omega \rangle \theta(t-t')$$

Pas géniale

à la place [,] ↖ Bosons

$$G^R(r,t; r',t') = -i \langle \{ \Psi(r,t), \Psi^\dagger(r',t') \} \rangle \theta(t-t')$$

↑ moyennes thermiques

Cas à 1 seule particule: $H = \sum_n E_n a_n^\dagger a_n$

$$\Psi(r,t) = \sum_n \langle r | n \rangle a_n(t) = \sum_n \varphi_n(r) a_n e^{-iE_n t}$$

$$\Psi^\dagger(r',t') = \sum_m a_m^\dagger(t') \langle m | r' \rangle = \sum_m \varphi_m^*(r') a_m^\dagger e^{iE_m t'}$$

$$\{ \Psi(r,t), \Psi^\dagger(r',t') \} = \sum_n \varphi_n(r) \varphi_n^*(r') e^{-iE_n(t-t')}$$

$$G^R(r,t; r',t') = -i \sum_n \varphi_n(r) \varphi_n^*(r') e^{-iE_n(t-t')} \theta(t-t')$$

$$\int d(t-t') G^R e^{i\omega(t-t')} = \sum_n \frac{\varphi_n(-) \varphi_n^*(r')}{\omega + i\eta - E_n} = G^R(\omega)$$

