ECHANIKA KWANTOWA II B – ĆWICZENIA 4 — 24.10.2017

Notacja liczby obsadzeń

$$|\alpha_1 \dots \alpha_N\rangle \longrightarrow |n_1 n_2 n_3 \dots\rangle$$ ← istotne jest uporządkowanie bazy!

↑ obsadzenie stanu α_1, itd.

Bozony: $n_i \in \mathbb{N} \cup \{0\}$

$$a_i |n_1 \dots n_i \dots\rangle = \sqrt{n_i}\, |n_1 \dots (n_i - 1) \dots\rangle$$

$$a_i^\dagger |n_1 \dots n_i \dots\rangle = \sqrt{n_i + 1}\, |n_1 \dots (n_i + 1) \dots\rangle$$

Fermiony: $n_i = 0, 1$ (zakaz Pauliego)

$$a_i |n_1 \dots n_i \dots\rangle = (-1)^{\Sigma_i}\, n_i\, |n_1 \dots (n_i - 1) \dots\rangle$$

$$a_i^\dagger |n_1 \dots n_i \dots\rangle = (-1)^{\Sigma_i} (1 - n_i)\, |n_1 \dots (n_i + 1) \dots\rangle,$$

gdzie $(-1)^{\Sigma_i} = (-1)^{\overbrace{n_1 + n_2 + \dots + n_{i-1}}}$ ↑ ilość koniecznych przestawień

① Policz dla fermionów:

•) $a_5 |11111100\dots\rangle = (-1)^4\, 1\, |11110100\dots\rangle =$

$= |11110100\dots\rangle$

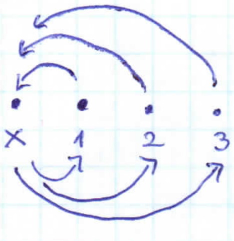
••) $a_4^\dagger |1110110\dots\rangle = (-1)^3 (1-0)\, |1111100\dots\rangle =$

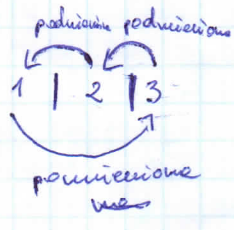
$= -|1111100\dots\rangle$

•••) $a_2^\dagger a_3 a_1^\dagger a_2 a_3^\dagger a_1 |1100\dots\rangle = a_2^\dagger a_3 a_1^\dagger a_2 a_3^\dagger |010\dots\rangle =$

$= -a_2^\dagger a_3 a_1^\dagger a_2 |0110\dots\rangle = -a_2^\dagger a_3 a_1^\dagger |0010\dots\rangle =$

$= -a_2^\dagger a_3 |1010\dots\rangle = +a_2^\dagger |100\dots\rangle = -|1100\dots\rangle$





operator wymiany cząstek

) Znajdź transformatę Fouriera potencjału Yukawy:

$$V_Y(\vec{r}) = \frac{\tilde{e}^2}{r} e^{-\kappa r} \qquad (\kappa > 0)$$

Wykonaj przejście graniczne $\kappa \to 0$ w której dostajemy transformację Fouriera dla potencjału kulombowskiego.

Rozwiązanie:

$$\tilde{V}_Y(\vec{k}) = \int V_Y(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} d^3r = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \int_0^{\infty} dr\, r^2 \frac{\tilde{e}^2 e^{-\kappa r}}{r} e^{-ikr\cos\theta} \sin\theta =$$

$$= \left\{ \begin{array}{l} u = \cos\theta \\ du = -\sin\theta\, d\theta \end{array} \right\} = -2\pi\tilde{e}^2 \int_{+1}^{-1} du \int_0^{\infty} dr\, r e^{-\kappa r} e^{-ikru} =$$

$$= 2\pi\tilde{e}^2 \int_0^{\infty} r e^{-\kappa r} \left[-\frac{1}{ikr} e^{-ikru} \right]_{-1}^{1} dr = 2\pi\tilde{e}^2 \int_0^{\infty} dr\, \cancel{r} e^{-\kappa r} \cdot$$

$$\cdot \left[-\frac{1}{ik\cancel{r}} e^{-ikr} + \frac{1}{ik\cancel{r}} e^{ikr} \right] = \frac{2\pi\tilde{e}^2}{ik} \int_0^{\infty} dr \left[e^{(ik-\kappa)r} - e^{-(ik+\kappa)r} \right] =$$

$$= \frac{2\pi\tilde{e}^2}{ik} \left[\frac{e^{-(ik+\kappa)r}}{\kappa + ik} - \frac{e^{(ik-\kappa)r}}{\kappa - ik} \right]_0^{\infty} =$$

$$= \frac{2\pi\tilde{e}^2}{ik} \left[-\frac{1}{\kappa + ik} + \frac{1}{\kappa - ik} \right] = \frac{2\pi\tilde{e}^2}{ik} \frac{-\cancel{\kappa} + ik + \cancel{\kappa} + ik}{k^2 + \kappa^2} = \frac{4\pi\tilde{e}^2}{k^2 + \kappa^2}$$

$$\frac{4\pi\tilde{e}^2}{k^2 + \kappa^2} \xrightarrow[\kappa \to 0]{} \frac{4\pi\tilde{e}^2}{k^2} = \tilde{V}_c(\vec{k})$$

transformata Fouriera dla potencjału kulombowskiego

) Posługując się ~~liczbą~~ reprezentacją liczby obsadzeń pokaż, że $[a_k, a_l]_+ = 0$, oraz $[a_k, a_l^+]_+ = \delta_{kl}$ dla fermionów.

$$(a_k a_l + a_l a_k) | \ldots n_k \ldots n_l \ldots \rangle \qquad \Sigma_k = n_1 + \ldots + n_{k-1}$$

$$a_l a_k | \ldots n_k \ldots n_l \ldots \rangle = n_k (-1)^{\Sigma_k} a_l | \ldots n_k - 1 \ldots n_l \ldots \rangle =$$

$$= (-1)^{\Sigma_k + \Sigma_l - 1} n_k n_l | \ldots n_k - 1 \ldots n_l - 1 \ldots \rangle$$

$$a_k a_l | \ldots n_k \ldots n_l \ldots \rangle = (-1)^{\Sigma_l} n_l a_k | \ldots n_k \ldots n_l - 1 \ldots \rangle =$$

$$= (-1)^{\Sigma_l + \Sigma_k} n_k n_l | \ldots n_k - 1 \ldots n_l - 1 \ldots \rangle$$

$$(a_k a_l + a_l a_k) | \ldots n_k \ldots n_l \ldots \rangle = (-1)^{\Sigma_l + \Sigma_k} \cancel{(-1)} (\underbrace{n_k n_l - n_l n_k}_{=0}) | \ldots n_k - 1 \ldots n_l - 1 \ldots \rangle$$

$$\Rightarrow [a_k, a_l]_+ = 0$$

$k \neq l$

$$(a_k a_l^+ + a_l^+ a_k) | \ldots n_k \ldots n_l \ldots \rangle$$

$$a_k a_l^+ | \ldots n_k \ldots n_l \ldots \rangle = (-1)^{\Sigma_l} (1 - n_l) a_k | \ldots n_k \ldots n_l + 1 \ldots \rangle =$$

$$= (-1)^{\Sigma_l + \Sigma_k} (1 - n_l) n_k | \ldots n_k - 1 \ldots n_l + 1 \ldots \rangle$$

$$a_l^+ a_k | \ldots n_k \ldots n_l \ldots \rangle = (-1)^{\Sigma_k} n_k a_l^+ | \ldots n_k - 1 \ldots n_l \ldots \rangle =$$

$$= (-1)^{\Sigma_k + \Sigma_l - 1} n_k (1 - n_l) | \ldots n_k - 1 \ldots n_l + 1 \ldots \rangle$$

$$(a_k a_l^+ + a_l^+ a_k) | \ldots n_k \ldots n_l \ldots \rangle = (-1)^{\Sigma_k + \Sigma_l} (\underbrace{n_k (1 - n_l) - n_k (1 - n_l)}_{=0}) | \ldots n_k - 1 \ldots n_l + 1 \ldots \rangle$$

$$\Rightarrow [a_k, a_l^+]_+ = 0, \quad k \neq l$$

$l = k$

$(a_k a_k^+ + a_k^+ a_k)|\ldots n_k \ldots\rangle =$

$$a_k a_k^+ |\ldots n_k \ldots\rangle = (-1)^{\Sigma_k} (1-n_k)\, a_k |\ldots n_k+1 \ldots\rangle =$$

$$= (-1)^{\Sigma_k + \Sigma_k} (1-n_k)(1+n_k)|\ldots n_k \ldots\rangle =$$

$$= \underbrace{(-1)^{2\Sigma_k}}_{= 1} (1-n_k)(1+n_k)|\ldots n_k \ldots\rangle$$

$$a_k^+ a_k |\ldots n_k \ldots\rangle = (-1)^{\Sigma_k} n_k\, a_k^+ |\ldots n_k-1 \ldots\rangle =$$

$$= (-1)^{2\Sigma_k} n_k(1-(n_k-1))|\ldots n_k \ldots\rangle =$$

$$= n_k(2-n_k)|\ldots n_k \ldots\rangle$$

$$(a_k a_k^+ + a_k^+ a_k)|\ldots n_k \ldots\rangle = (-1)^{2\Sigma_k}(2n_k - n_k^2 + 1 - n_k^2)|\ldots n_k \ldots\rangle =$$

$$\underset{n_k = 0,1}{=} |\ldots n_k \ldots\rangle$$

zatem $\quad [a_k, a_l^+]_+ = \delta_{kl}$.

Operatory pola

Operatory kreacji i anihilacji w reprezentacji położeniowej nazywane są operatorami pola:

$$[\hat{\psi}(x), \hat{\psi}(y)]_{-\zeta} = [\hat{\psi}^+(x), \hat{\psi}^+(y)]_{-\zeta} = 0$$

$$[\hat{\psi}(x), \hat{\psi}^+(y)]_{-\zeta} = \delta(x-y)$$

Możemy je wyrazić w bazie $\{|\alpha\rangle\}$ jako:

$$\hat{\psi}^+(x) = \sum_\alpha \langle\alpha|x\rangle a_\alpha^+ = \sum_\alpha \phi_\alpha^*(x)\, a_\alpha^+$$

$$\hat{\psi}(x) = \sum_\alpha \langle x|\alpha\rangle a_\alpha = \sum_\alpha \phi_\alpha(x)\, a_\alpha$$

④ Zapisać w drugiej kwantyzacji poniższe operatory dla układu elektronów:

(a) operator spinu

$$\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}} \quad , \quad \vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\} = \underbrace{\left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}}_{\text{macierze Pauliego}}$$

Baza: $\{ |\alpha\rangle = |\mu\sigma\rangle = |\mu\rangle|\sigma\rangle \}$

$|\mu\rangle$ – może to być np. $\vec{k}$; $|\sigma\rangle$ – stan spinowy

Dla wielu cząstek

$$\hat{\vec{S}} = \int d^3r\, \hat{\psi}^+_\alpha(r)\, \hat{\vec{S}}\, \hat{\psi}_{\alpha'}(r) = \sum_{\alpha\alpha'} \int \phi^*_\alpha(\vec{r})\, \hat{\vec{S}}\, \phi_{\alpha'}(\vec{r})\, d^3r\ a^+_{\alpha} a_{\alpha'} =$$

$$= \sum_{\alpha\alpha'} \int d^3r\, \langle\alpha|r\rangle\, \hat{\vec{S}}\, \langle r|\alpha'\rangle\, a^+_\alpha a_{\alpha'} = \sum_{\substack{\mu\mu' \\ \sigma\sigma'}} \langle\mu|\langle\sigma| \underbrace{\int d^3r\, |r\rangle\langle r|}_{\mathbb{1}}\, \hat{\vec{S}}\, |\sigma'\rangle|\mu'\rangle\, a^+_{\sigma\mu} a_{\sigma'\mu'}$$

$$= \sum_{\substack{\mu\mu' \\ \sigma\sigma'}} \underbrace{\langle\mu|\mu'\rangle}_{\delta_{\mu\mu'}} \langle\sigma|\hat{\vec{S}}|\sigma'\rangle\, a^+_{\mu\sigma} a_{\mu'\sigma'} = \sum_{\mu,\sigma\sigma'} \langle\sigma|\hat{\vec{S}}|\sigma'\rangle\, a^+_{\mu\sigma} a_{\mu\sigma'} =$$

$$= \frac{\hbar}{2}\sum_\mu \left[\left(a^+_{\mu\uparrow}a_{\mu\downarrow} + a^+_{\mu\downarrow}a_{\mu\uparrow}\right),\ i\left(a^+_{\mu\downarrow}a_{\mu\uparrow} - a^+_{\mu\uparrow}a_{\mu\downarrow}\right),\ \left(a^+_{\mu\uparrow}a_{\mu\uparrow} - a^+_{\mu\downarrow}a_{\mu\downarrow}\right) \right]$$

~~(b) operator gęstości:~~

$$\cancel{\hat{n}(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i)}$$

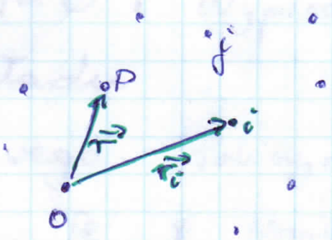
$$\cancel{\hat{n}(\vec{k}) = \sum \int d^3r'\, \hat{\psi}^+_{\vec{k}}(\vec{r}')\, \delta(\vec{r} - \vec{r}')\, \hat{\psi}_{\vec{k}'}(\vec{r}') =}$$

$$\cancel{= \sum_{\vec{k}\vec{k}'} \int d^3r' \langle\vec{k}|\vec{r}'\rangle\, \delta(\vec{r} - \vec{r}')\, \langle\vec{r}'|\vec{k}'\rangle\, a^+_{\vec{k}} a_{\vec{k}'} =}$$

$$\cancel{= \sum_{\vec{k}\vec{k}'} \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}} \frac{1}{\sqrt{V}} e^{+i\vec{k}'\cdot\vec{r}}\, a^+_{\vec{k}} a_{\vec{k}'}}$$

(b) operator gęstości w reprezentacji pędowej

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



$$\hat{n}(\vec{r}) = \int d^3 r' \, \hat{\Psi}^+(\vec{r}') \, \delta(\vec{r} - \vec{r}') \, \hat{\Psi}(\vec{r}') =$$

$$= \hat{\Psi}^+(\vec{r}) \, \hat{\Psi}(\vec{r})$$

$$\hat{n}(\vec{k}) = \int d^3 r \, e^{-i\vec{k}\cdot\vec{r}} \sum_{k'k''} \langle \vec{k}' | \vec{r} \rangle \langle \vec{r} | \vec{k}'' \rangle \, a^+_{k'} a_{k''} =$$

$$= \int d^3 r \sum_{k'k''} \frac{1}{\Omega_0} e^{-i\vec{k}'\cdot\vec{r}} \, e^{i\vec{k}''\cdot\vec{r}} \, a^+_{k'} a_{k''} =$$

$$= \sum_{k'k''} \underbrace{\frac{1}{V} \int d^3 r \, e^{i(\vec{k}'' - \vec{k} - \vec{k}')\cdot\vec{r}}}_{\delta_{\vec{k}'' - \vec{k} - \vec{k}' = 0}} \, a^+_{k'} a_{k''} =$$

$$= \sum_{\vec{q}} a^+_{\vec{q}} \, a_{\vec{q}+\vec{k}}$$

(c) operator energii kinetycznej w reprezentacji położeniowej:

$$\hat{T} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m} \nabla_i^2$$

$$\hat{T} = \underbrace{\int d^3 r \, \hat{\Psi}^+(\vec{r}) \left(-\frac{\hbar^2}{2m} \nabla_i^2\right) \hat{\Psi}(\vec{r})} = \sum_{\mu\mu'} \underbrace{\phi^*_{\mu}(\vec{r}) \left(-\frac{\hbar^2}{2m} \nabla^2\right) \phi_{\mu'}(\vec{r})}_{t_{\mu\mu'}} \, a^+_{\mu} a_{\mu'} =$$

$$= \sum_{\mu\mu'} t_{\mu\mu'} \cancel{(\vec{r})} \, a^+_{\mu} a_{\mu'}$$