QMII - cv10 Formalismus II. kvantování

(OPAKOVÁNÍ)

1 částice: $\mathcal{H}^{(1)}$, $|m\rangle$

N-částic: $\mathcal{H}^{(N)} = \mathcal{H}^{(1)} \otimes \dots \otimes \mathcal{H}^{(1)}$, $|m_1 m_2 \dots m_N\rangle$

nerozlišitelnost: $\supset \mathcal{H}^{(N)}_{S/A}$, $|N_1 N_2 \dots\rangle = \eta \hat{S} |m_1 \dots m_N\rangle = \frac{(a_1^+)^{N_1}}{\sqrt{N_1!}} \frac{(a_2^+)^{N_2}}{\sqrt{N_2!}} \dots |0\rangle$

Fock: $\mathcal{H}_F = \bigoplus_N \mathcal{H}^{(N)}_{S/A}$

kreační/anihilační operátory:

- Bosony: $[\hat{a}_m, \hat{a}_m] = [\hat{a}^+_m, \hat{a}^+_m] = 0$ $\quad [\hat{a}_m, a^+_m] = \delta_{mm}$
- Fermiony: $\{\hat{a}_m, \hat{a}_m\} = \{\hat{a}^+_m, \hat{a}^+_m\} = 0$ $\quad \{a_m, a^+_m\} = \delta_{mm}$

- jednočásticový operátor:

$\hat{C}$ $\qquad \hat{C}^{(i)} = \hat{I} \otimes \dots \otimes \hat{C} \dots \otimes \hat{I} \rightarrow \hat{\mathbf{C}} = \sum_i \hat{C}^{(i)} = \sum_{mm} \langle m | \hat{C} | m \rangle \hat{a}^+_m \hat{a}_m$

- dvoučásticový operátor:

$\hat{C}^{(12)}$ na $\mathcal{H}^{(2)}$ $\longrightarrow$ $\hat{\mathbf{C}} = \sum_{i<j} \hat{C}^{(ij)} = \frac{1}{2} \sum_{kl} \sum_{mm} \langle kl | \hat{C}^{(12)} | mm \rangle \hat{a}^+_k \hat{a}^+_l \hat{a}_m \hat{a}_m$

ÚLOHA 1: • najít komutační relace $[\hat{a}^+_k \hat{a}_l, \hat{a}_m]$ a $[\hat{a}^+_k \hat{a}_l, \hat{a}^+_m]$

pro 1) BOSONY 2) FERMIONY

1) i 2) vyjde $[a^+_k a_l, a_m] = -\delta_{mk} a_l$ $\qquad [a^+_k a_l, a^+_m] = \delta_{lm} a^+_k$

3) necht' $H = \sum_k \epsilon_k \hat{a}^+_k \hat{a}_k$ najděte $\hat{a}^{+(H)}_k(t)$, $\hat{a}^{(H)}_k(t)$

$$i\hbar \partial_t A = i\hbar \partial_t \{ \underbrace{e^{+\frac{i}{\hbar}Ht}}_{H} A \underbrace{e^{-\frac{i}{\hbar}Ht}}_{-H} \} = i\hbar \frac{i}{\hbar} (HA - AH) = AH - HA$$

$$i\hbar \partial_t A^{(H)} = [A^{(H)}, H] \quad \text{pro} \quad a^{(H)}_k$$

$$i\hbar \partial_t \hat{a}^{(H)}_k(t) = [a_k, \sum_m \epsilon_m a^+_m a_m] = \sum_m \epsilon_m \underbrace{[a_k, a^+_m}_{\delta_{km}} a_m] = \epsilon_k a^{(H)}_k$$

$\delta_{km} a_m$

4)

$\rightarrow$ $t=0$ $\quad a^{(H)}_k(t=0) = a_k$

$$\rightarrow \quad \hat{a}^{(H)}_k(t) = \hat{a}_k \exp\{-\frac{i}{\hbar}\epsilon_k t\} \checkmark$$

$$\hat{a}^{+(H)}_k(t) = \hat{a}^+_k \exp\{+\frac{i}{\hbar}\epsilon_k t\} \checkmark$$

5) ve Fockově prostoru $|\{N_i\}\rangle \equiv |N_1 N_2 \dots\rangle \in \mathcal{H}^{(N)}_{S/A}$ $\quad N = \sum_i N_i$

a) vypočtěte $\langle \{N_i\} | \hat{a}_k \hat{a}^+_m | \{N_i\} \rangle$ $\qquad a_k|0\rangle = 0$

b) $\langle \{N_i\} | \hat{a}_k \hat{a}_l \hat{a}^+_m \hat{a}^+_n | \{N_i\} \rangle$ $\qquad \hat{N}_k |\{N_i\}\rangle = N_k |\{N_i\}\rangle$, $\hat{N}_k = a^+_k a_k$

potom: $\langle \{N_i\} | \underbrace{a_k^+ a_m} | \{N_i\} \rangle = \delta_{km} \langle \{N_i\} | \underbrace{\hat{a}_k^+ \hat{a}_k}_{\hat{N}_k \to N_k} | \{N_i\} \rangle =$

$\langle \{N_i\} \Big| \begin{matrix} N_k \to N_k + 1 \\ N_m \to N_m - 1 \end{matrix} \Big\rangle = 0$ ... nespárované $a_k^+ a_m$

$= \delta_{km} N_k \underbrace{\langle \{N_i\} | \{N_i\} \rangle}_{1} = N_k \delta_{km} \leftarrow$

5a) $\langle \{N_i\} | a_k a_m^+ | \{N_i\} \rangle = \langle \{N\} | \delta_{km} \pm a_m^+ a_k | \{N\} \rangle$

Bosony $= a_m^+ a_k + [a_k, a_m^+] = a_m^+ a_k + \delta_{km}$

Ferm. $\delta_{km} = \{a_k, a_m^+\} = a_k a_m^+ + a_m^+ a_k \longrightarrow a_k a_m^+ = \delta_{km} - a_m^+ a_k$

$$\begin{aligned} AB &= BA + [A, B] \\ AB &= -BA + \{A, B\} \end{aligned}$$

$N_k = 0, 1$

Fermi $\delta_{km}(1 - N_k)$ not N_k

$= \delta_{km} \pm \langle \{N_i\} | a_m^+ a_k | \{N_i\} \rangle = \delta_{km}(1 \pm N_k)$

Bosony $\delta_{km}(N_k + 1)$

5b)

$\langle \{N_i\} | \hat{a}_k \hat{a}_l \hat{a}_m^+ \hat{a}_n^+ | \{N_i\} \rangle =$

poznámka $= 0$ pokud nejsou spárovány $a^+ \leftrightarrow a$

$\delta_{km} \delta_{ln} \langle \{N\} | \hat{a}_k \hat{a}_l \hat{a}_l^+ \hat{a}_k^+ | \{N\} \rangle + \delta_{kn} \delta_{lm} \langle \{N\} | \hat{a}_k \hat{a}_l \hat{a}_k^+ \hat{a}_l^+ | \{N\} \rangle$

$\pm \hat{a}_l \hat{a}_k \hat{a}_l^+ \hat{a}_k^+$ $\qquad$ $\delta_{lk} \pm a_k^+ a_l$

$\delta_{kl} \pm a_l^+ a_k$ $\qquad$ $1 + N_l$

$= \delta_{kn} \delta_{lm} \delta_{kl} \langle \{N\} | \pm \hat{a}_l \hat{a}_l^+ + \hat{a}_l \hat{a}_l^+ | \{N\} \rangle$

$\delta_{kn} \delta_{lm} \langle \{N\} | \underbrace{\hat{a}_l a_l^+}_{1 \pm N_l} \underbrace{a_k a_k^+}_{1 \pm N_k} | \{N\} \rangle \pm \delta_{km} \delta_{ln} \langle \{N\} | \underbrace{a_k a_k^+}_{1 \pm N_k} \underbrace{a_l a_l^+}_{1 \pm N_l} | \{N\} \rangle$

$= \delta_{kn} \delta_{lm} \delta_{kl} (1 \pm 1)(1 + N_l) + (\delta_{kn} \delta_{lm} \pm \delta_{km} \delta_{lm})(1 \pm N_k)(1 \pm N_l)$

Úloha 2: Hubbardův model

①—②—③- - -—Ⓓ

elektrony ~ fermion + spin 1/2

$\mathcal{H}^{(1)} \equiv \mathbb{C}^D \otimes \mathbb{C}^2$

$\uparrow$ D kvantteček, $\uparrow$ spin

$\mathcal{H}^{(1)}$ ~ $|ms\rangle$ $\quad m=1,2,\dots D$, $\quad s=+,-$ ~ $S_z = \pm\frac{\hbar}{2}$

$\mathcal{H}_F = \mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)} \oplus \mathcal{H}^{(2)}_A \oplus \dots$

$\mathcal{H}^{(0)}$ ~ $|0\rangle$

$|ms\rangle = a^+_{ms}|0\rangle$

$\{a_{ms}, a_{m's'}\} = \{a^+_{ms}, a^+_{m's'}\} = 0 \qquad \{a_{ms}, a^+_{m's'}\} = \delta_{mm'}\delta_{ss'}$

--- $\hat{N}_{ms} \equiv \hat{a}^+_{ms}\hat{a}_{ms}$

Hamiltonián

$$\boxed{\hat{H} = \underbrace{-t\sum_{m=1}^{D}\sum_s \left(\hat{a}^+_{ms}\hat{a}_{m+1,s} + \hat{a}^+_{m+1,s}\hat{a}_{ms}\right)}_{\text{1-částicový operátor}} + U\sum_m \underbrace{\hat{N}_{m+}}_{0,1}\underbrace{\hat{N}_{m-}}_{0,1}}$$

coulomb. repulze $|\{N_{ms}\}\rangle$

① pro $U=0$ $\hat{H}$ je 1-část. operátor

na $\mathcal{H}^{(1)}$ $\hat{C} \equiv \hat{h} = -t\sum_m \left(|m\rangle\langle m+1| + |m+1\rangle\langle m|\right) \otimes I_{spin}$

Fock: $\hat{H} = \sum_{ms}\sum_{m's'} \langle ms|\hat{h}|m's'\rangle a^+_{ms} a_{m's'}$

$\langle ms|\hat{h}|m's'\rangle = -t\,\delta_{ss'}\sum_m \left(\delta_{mm}\delta_{m'm+1} + \delta_{mm+1}\delta_{mm'}\right)$

$= -t\,\delta_{ss'}\left(\delta_{m'm+1} + \delta_{mm'+1}\right)$

$= -t\sum_s\sum_{mm'}\left(\delta_{m'm+1} + \delta_{mm'+1}\right) a^+_{ms} a_{m's}$

$= -t\sum_{sm} a^+_{ms} a_{m+1s} - t\sum_{sm'} a^+_{m'+1} a_{m's}$

přezn. sčít indx ~ $m' \to m$

② ověřte, že $|\psi_{ks_0}\rangle \equiv \sum_m e^{ikm} a^+_{ms_0}|0\rangle$ jsou vle. stavy $\hat{H}|\psi_{ks}\rangle = E(k)|\psi_{ks}\rangle$ a najděte $E(k)$

člen s U je pro $N=1$ 0

$\hookrightarrow -t\sum_m\sum_s \left(a^+_{ms}a_{m+1s} + a^+_{m+1s}a_{ms}\right)\sum_m e^{ikm} a^+_{ms_0}|0\rangle$

$$= -t \sum_n \sum_s \sum_m e^{ik} \Big[a^\dagger_{ns} \underbrace{a_{n+1 s}\, a^\dagger_{m s_0}}_{\delta_{s s_0}\delta_{m\, n+1} - \cancel{a^\dagger_{ms} a_{n+1 s}}} + a^\dagger_{n+1 s} \underbrace{a_{ns}\, a^\dagger_{m s_0}}_{\delta_{s s_0}\delta_{mn} - \cancel{a^\dagger a}} \Big] |0\rangle$$

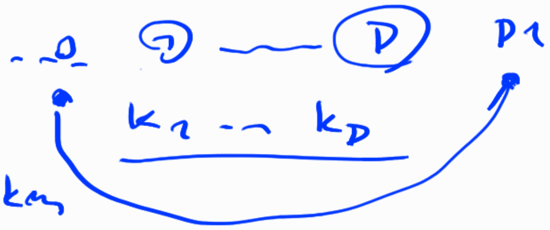
$$= -t \sum_n \sum_m e^{ikm} \Big(\delta_{m\, n+1}\, a^\dagger_{\underbrace{n}_{\substack{m-1\\ l}} s_0} + \delta_{nm}\, a^\dagger_{\underbrace{n+1}_{\substack{m+1\\ l}} s_0} \Big) |0\rangle$$

$$= -t \Big(\sum_m e^{ik\overset{l+1}{m}} a^\dagger_{m-1\, s_0} |0\rangle \Big) - t \Big(\sum_m e^{ik\overset{l-1}{m}} a^\dagger_{m+1\, s_0} |0\rangle \Big)$$

$$= -t \sum_l \Big(e^{i(l+1)k} + e^{i(l-1)k} \Big) a^\dagger_{l s_0} |0\rangle$$

$$= \underbrace{-t\left(e^{ik} + e^{-ik}\right)} \underbrace{\sum_l e^{ilk} a^\dagger_{l s_0} |0\rangle}_{|\psi_k\rangle} = E(k)\,|\psi_k\rangle$$

$$\boxed{E(k) = -2t \cos k}$$



e^{ikm} e^{-ikm}