Solution – Problem Set   Second Quantization

1. Commutator algebra

$$
\begin{aligned}
[AB, C] &= ABC - CAB \\
&= ABC - ACB + ACB - CAB \\
&= A(BC - CB) + (AC - CA)B \\
&= A[B,C] + [A,C]B
\end{aligned}
\tag{1}
$$

or:
$$
\begin{aligned}
[AB, C] &= ABC - CAB \\
&= ABC + ACB - ACB - CAB \\
&= A(BC + CB) - (AC + CA)B \\
&= A\{B,C\} - \{A,C\}B
\end{aligned}
\tag{2}
$$

Similarly: $[A, BC] \overset{(3)}{=} [A,B]C + B[A,C] \overset{(4)}{=} \{A,B\}C - B\{A,C\}$

2. Diagonal Hamiltonian

i) $H = \sum_k \varepsilon_k b_k^\dagger b_k$, with $\{b_k, b_{k'}^\dagger\} = \delta_{kk'}$, $\{b_k, b_{k'}\} = 0$, $\{b_k^\dagger, b_{k'}^\dagger\} = 0$

Then $[H, b_k^\dagger] = \sum_{k'} \varepsilon_{k'} [b_{k'}^\dagger b_{k'}, b_k^\dagger] \overset{(1.2)}{=} \varepsilon_k b_k^\dagger$

ii) This means that $b_k^\dagger$ is a ladder operator, that maps an eigenstate of H with energy E, onto another eigenstate with energy $E + \varepsilon_k$:

if $H|E\rangle = E|E\rangle$, then

$$H b_k^\dagger |E\rangle = (\underbrace{H b_k^\dagger - b_k^\dagger H}_{\varepsilon_k b_k^\dagger} + b_k^\dagger \underbrace{H)|E\rangle}_{E|E\rangle} = (\varepsilon_k + E)\, b_k^\dagger |E\rangle$$

Hence: $b_k^\dagger |E\rangle \equiv |E + \varepsilon_k\rangle$.

iii) ③

It follows that eigenstates of H have the following general form:

$$|E\rangle = \mathcal{N} \sum_{\{n_{k_1}, n_{k_2}, \dots\}} b_{k_1}^{\dagger\, n_{k_1}} b_{k_2}^{\dagger\, n_{k_2}} \dots \underbrace{|0\rangle}_{\text{empty state, } b_k|0\rangle = 0 \ \forall k}$$

normalization

with energy $\quad E = \sum_k n_k \varepsilon_k$

where $\begin{cases} n_k \in \{0,1\} & \text{for fermions} \quad (\text{because } b^{\dagger 2} = 0) \\ n_k \in \{0,1,2,\dots\} & \text{for bosons.} \end{cases}$

To prove this, check (literally!) that $\quad [H, b_k^{\dagger n}] = n\varepsilon_k b_k^{\dagger n}$.

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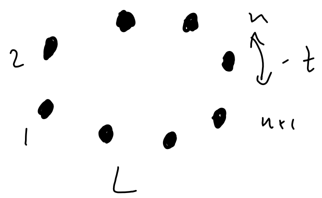
3. Tight-binding chain

④



(i)

$$H = -t \sum_{n=1}^{L} \left(a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1} \right) \quad , \text{ with } a_{L+n} = a_n \ \forall n \tag{1}$$

Ansatz for creator of eigenstate: $\quad b_k^\dagger = \underbrace{\frac{1}{L^{1/2}}}_{\text{normalization}} \sum_{n=1}^{L} e^{ikn} a_n^\dagger$

to be compatible with translational invariance, we need also

$$b_k^\dagger = \frac{1}{L^{1/2}} \sum_{n=1}^{L} e^{ik(n+L)} \underbrace{a_{n+L}}_{=a_n} \qquad \Longrightarrow \text{ we need } 1 = e^{ikL}$$

k must have the form $k = \frac{2\pi m_k}{L}$, $\quad m_k = 0, \dots, L-1$

⑤

(ii) $$\{b_k, b_{k'}^\dagger\} = \frac{1}{L}\sum_{n,n'} e^{-ikn} e^{ik'n'} \underbrace{\{a_n, a_{n'}^\dagger\}}_{\delta_{nn'}}$$

$$= \frac{1}{L}\underbrace{\sum_{n=1}^{L} e^{-i(k-k')n}}_{= \begin{cases} L & \text{if } k=k' \\ 0 & \text{if } k\neq k' \end{cases}}$$

(since $\sum_{m=1}^{L} e^{2\pi i m/L} = 0$)

Similarly, but more trivially, $\{b_k, b_{k'}\} = 0$ since $\{a_n, a_{n'}\} = 0$ and likewise for creation operators.

(iii) $$a_n^\dagger = \frac{1}{L^{1/2}}\sum_{m_k=1}^{L} e^{-ikn} \underbrace{b_k^\dagger}_{\frac{1}{L^{1/2}}\sum_{n'} e^{ikn'} a_{n'}^\dagger}$$

$$= \frac{1}{L}\sum_{n'} a_{n'}\, L\,\delta_{nn'} = a_n^\dagger$$

⑥

(iv) $$[H, b_k^\dagger] = -t\sum_{n=1}^{L} \frac{1}{L^{1/2}}\sum_{n'} e^{ikn'} \underbrace{\left[\left(a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}\right), a_{n'}^\dagger\right]}_{a_{n+1}^\dagger\,\delta_{nn'} + a_{n'-1}^\dagger\,\delta_{n+1\,n'}}$$

$$= -t\sum_{n'=1}^{L} e^{ikn'}\frac{1}{L^{1/2}}\Big(\underbrace{a_{n'+1}^\dagger}_{n'+1\to n} + \underbrace{a_{n'-1}^\dagger}_{n'-1\to n}\Big)$$

shift: $n'\pm 1 \to n'$

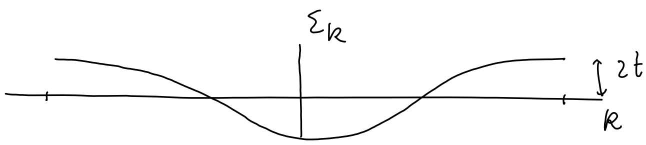
recall: $a_{N+1} = a_1$
$a_0 = a_N$

$$= -t\sum_{n=1}^{L} \frac{1}{L^{1/2}}\, e^{ikn}\left(a_n^\dagger e^{-ik} + a_n e^{+ik}\right)$$

$$= \underbrace{-2t\cos k}_{\varepsilon_k}\ \underbrace{\sum_{n=1}^{L}\frac{1}{L^{1/2}}\, e^{ikn}\, a_n^\dagger}_{b_k^\dagger}$$

$$= \varepsilon_k\, b_k^\dagger$$

$\Longrightarrow$ Eigenenergies: $\varepsilon_k = -2t\cos k$



(iv) 7

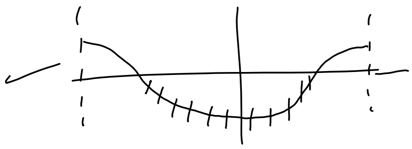
$$H = -t \sum_{n=1}^{L} \left(a^{\dagger}_{n+1} a_n + a^{\dagger}_n a_{n+1} \right)$$

$$= -t \sum_{n=1}^{L} \sum_{kk'} \frac{1}{L} \left(e^{-ik(n+1)} e^{ik'n} + e^{-ikn} e^{ik'(n+1)} \right) b^{\dagger}_k b_{k'}$$

use $\displaystyle \frac{1}{L} \sum_{n=1}^{L} e^{-in(k-k')} = \delta_{kk'}$

$$= -t \sum_k \underbrace{\left(e^{-ik} + e^{ik} \right)}_{2\cos k} b^{\dagger}_k b_k$$

$$= \sum_k \underbrace{(-2t \cos k)}_{\varepsilon_k} b^{\dagger}_k b_k$$



(v) Half-filling: $\displaystyle |g\rangle = \prod_{k<0} c^{\dagger}_k |0\rangle$

<u>Fermionic Repr. of spin</u> 8

$$S_i = \frac{\hbar}{2} \sum_{n\mu\mu'} c^{\dagger}_{n\mu} \sigma^i_{\mu\mu'} c_{n\mu'} \qquad i = x, y, z$$

$$[S_i, S_j] = \frac{\hbar}{4} \sum_{n\mu\mu'} \sum_{\bar n \bar\mu \bar\mu'} \sigma^i_{\mu\mu'} \sigma^j_{\bar\mu\bar\mu'} \underbrace{\left[c^{\dagger}_{n\mu} c_{n\mu'}, c^{\dagger}_{\bar n\bar\mu} c_{\bar n\bar\mu'} \right]}_{①}$$

$$① = \left(c^{\dagger}_{n\mu} \delta_{\mu'\bar\mu} c_{n\bar\mu'} - c^{\dagger}_{\bar n\bar\mu} \delta_{\bar\mu'\mu} c_{n\mu'} \right) \delta_{n\bar n}$$

$\bar\mu \leftrightarrow \mu, \ \bar\mu' \leftrightarrow \mu'$

$$= \frac{\hbar}{4} \sum_n \underbrace{\left(\sigma^i_{\mu\mu'} \sigma^j_{\mu'\bar\mu'} - \sigma^j_{\mu\mu'} \sigma^i_{\mu'\bar\mu'} \right)}_{[\sigma^i, \sigma^j]_{\mu\bar\mu'} = 2\varepsilon^{ijk} \sigma^k_{\mu\bar\mu'}} c^{\dagger}_{n\mu} c_{n\bar\mu'}$$

$$= \varepsilon^{ijk} \frac{\hbar}{2} \sum_n c^{\dagger}_{n\mu} \sigma^k_{\mu\mu'} c_{n\mu'} = \varepsilon^{ijk} \hbar S^k \qquad \square$$