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27.01.2017 **Advanced Quantum theory 12. Exercise**

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H17) a) $t_{ij} = \langle i | \hat{t} | j \rangle$, $\hat{t} = \sum_{i,j} t_{ij} |i\rangle\langle j|$

Operator for N-particle system?

For N-Particle System: $\hat{T} = \sum_{\alpha=1}^{N} \hat{t}_\alpha = \sum_{ij} t_{ij} \underbrace{\sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha}_{(*)}$

One "easily" sees that

$$|k\rangle_\alpha {}_\alpha\langle j | i_1, \dots, i_\alpha, \dots, i_N\rangle = |i_1, \dots, k, \dots, i_N\rangle \delta_{i_\alpha, j}$$

where $|a\rangle_\alpha$ only operates on state α and the other states are represented by 1's in the operator like this: $\sum_b |b\rangle\langle b| \otimes \dots \otimes$

Now, we let this operate on a symmetrized state:

$$S_+ |i_1, \dots, i_\alpha, \dots, i_N\rangle = |n_1, n_2, \dots\rangle$$
$$= \frac{1}{\sqrt{N!}} \sum_{P \in S_N} P |i_1, \dots, i_\alpha, \dots, i_N\rangle \frac{1}{\sqrt{n_1! n_2! \dots}}$$

k=j case?

So we take a look at (*) for the new variables k, j, for reasons of clarity:

$$\sum_\alpha |k\rangle_\alpha {}_\alpha\langle j| S_+ |i_1, \dots, i_\alpha, \dots, i_N\rangle \left(= \sum_\alpha |k\rangle_\alpha {}_\alpha\langle j | n_1, \dots, n_k, \dots, n_j, \dots\rangle \right)$$

$$= \sum_\alpha |k\rangle_\alpha {}_\alpha\langle j| \frac{1}{\sqrt{N!}} \sum_{P \in S_N} P |i_1, \dots, i_\alpha, \dots, i_N\rangle \frac{1}{\sqrt{n_1! n_2! \dots}}$$

Swap sums and put $\sqrt{n_1! n_2! \dots}$ in front of sum?

$$= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \dots}} \sum_{P \in S_N} \sum_\alpha P |k\rangle_\alpha {}_\alpha\langle j | i_1, \dots, i_\alpha, \dots, i_N\rangle$$

$$= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \dots}} \sum_{P \in S_N} \sum_\alpha P |i_1, \dots, k, \dots, i_N\rangle \delta_{i_\alpha, j}$$

Counts the amounts of j's in the multi-particle sum

$$= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \dots}} \sum_{P \in S_N} n_j P |i_1, \dots, k, \dots, i_N\rangle$$

$$= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \dots (n_k+1)! \dots (n_j-1)! \dots}} \frac{\sqrt{n_k+1}}{\sqrt{n_j}} \sum_{P \in S_N} n_j P |i_1, \dots, k, \dots, i_N\rangle$$

$$= \sqrt{n_k+1} \sqrt{n_j} \frac{1}{\sqrt{N!}} \sum_{P \in S_N} P |i_1, \dots, k, \dots, i_N\rangle \frac{1}{\sqrt{n_1! \dots (n_k+1)! \dots (n_j-1)! \dots}}$$

$$= \sqrt{n_k+1} \sqrt{n_j} S_+ |i_1, \dots, k, \dots, i_N\rangle = \sqrt{n_k+1} \sqrt{n_j} |n_1, \dots, n_k+1, \dots, n_j-1, \dots\rangle$$

why not apply a_k^+ first? Different result?

Comparing this to $a_k^+ a_j S_+ |i_1, \dots, i_\alpha, \dots, i_N\rangle = a_k^+ a_j |n_1, \dots, n_N\rangle$

$$= a_k^+ \sqrt{n_j} |n_1, \dots, n_k, \dots, n_j - 1, \dots\rangle = \sqrt{n_k+1} \sqrt{n_j} |n_1, \dots, n_k+1, \dots, n_j-1, \dots\rangle$$

yields $\sum_\alpha^N |i\rangle_\alpha \langle j| = a_i^+ a_j$ and therefore $\hat{T} = \sum t_{ij} a_i^+ a_j$

why $\alpha \neq \beta$?

b) Two particle operator: $\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} \hat{f}^{(2)}(x_\alpha, x_\beta)$

Important if Completeness relation multiplied in middle or end?

multiply with 1's

$$\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} \sum_{i,j} |i,j\rangle_{\alpha,\beta\ \alpha\beta}\langle i,j|\, \hat{f}^{(2)}(x_\alpha, x_\beta) \sum_{k,l} |k,l\rangle_{\alpha\beta\ \alpha\beta}\langle k,l|$$

$$= \frac{1}{2} \sum_{i,j,k,l} \sum_{\alpha \neq \beta} f_{i,j,k,l}\, |i,j\rangle_{\alpha,\beta\ \alpha\beta}\langle k,l| = \frac{1}{2} \sum_{i,j,k,l} f_{ijkl} \underbrace{\sum_{\alpha \neq \beta} |i\rangle_\alpha |j\rangle_\beta\, {}_\alpha\langle k|\, {}_\beta\langle l|}_{(*)}$$

Why is $f_{ijkl} = {}_{\alpha\beta}\langle i,j| f^{(2)} |k,l\rangle_{\alpha\beta}$ equal for all α, β?

In this case, we take a look at $(*)$; again with $i \equiv m$ for reasons of clarity

$$\sum_{\alpha \neq \beta} |m\rangle_\alpha |j\rangle_\beta\, {}_\alpha\langle k|\, {}_\beta\langle l|\, n_1, n_2 \ldots\rangle = \sum_{\alpha \neq \beta} |m\rangle_\alpha |j\rangle_\beta\, {}_\alpha\langle k|\, {}_\beta\langle l|\, S_+ |i_1, \ldots, i_\alpha, \ldots, i_\beta, \ldots i_N\rangle$$

Order of α, β doesn't matter?

analogously to a)

$$= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \ldots}} \sum_{P \in S_N} P \sum_{\alpha \neq \beta} |m\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta\, |i_1, \ldots, i_\alpha, \ldots, i_\beta \ldots i_N\rangle$$

$$= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \ldots}} \sum_{P \in S_N} P \sum_{\alpha \neq \beta} |i_1, \ldots, m, \ldots, j, \ldots, i_N\rangle\, \delta_{k, i_\alpha}\, \delta_{l, i_\beta}$$

$k = i_\alpha$ and $l = i_\beta$ at the same time?

$$= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \ldots}} \sum_{P \in S_N} n_k n_l\, P\, |i_1, \ldots, m, \ldots, j, \ldots, i_N\rangle$$

$$= \frac{1}{\sqrt{N!}} \frac{1 \cdot \frac{\sqrt{n_m+1}}{\sqrt{n_k}} \cdot \frac{\sqrt{n_j+1}}{\sqrt{n_l}}}{\sqrt{n_1! \ldots (n_m+1)! \ldots (n_k-1)! \ldots (n_j+1)! \ldots (n_l-1)! \ldots}}\, n_k n_l \sum_{P \in S_N} P\, |i_1, \ldots, m, \ldots, j, \ldots, i_N\rangle$$

$$= \sqrt{n_m+1}\sqrt{n_k}\sqrt{n_j+1}\sqrt{n_l}\, \frac{1}{\sqrt{N!}} \sum_{P \in S_N} P\, |i_1, \ldots, m, \ldots, j, \ldots, i_N\rangle \frac{1}{\sqrt{n_1! \ldots (n_m+1)! \ldots (n_k-1)! \ldots (n_j+1)! \ldots (n_l-1)!}}$$

$$= \sqrt{n_m+1}\sqrt{n_k}\sqrt{n_j+1}\sqrt{n_l}\, S_+ |i_1, \ldots, m, \ldots, j, \ldots, i_N\rangle$$

$$= \sqrt{n_m+1}\sqrt{n_k}\sqrt{n_j+1}\sqrt{n_l}\, |n_1, \ldots, n_m+1, \ldots, n_k-1, \ldots, n_j+1, \ldots, n_l-1 \ldots\rangle$$

What if $k = l$ or $m = j$ or any other the same? Why not different order of a's?

Comparing this to $a_m^\dagger a_j^\dagger a_k a_l |n_1, n_2, \ldots\rangle = a_m^\dagger a_j^\dagger a_k a_l S_+ |i_1, \ldots, i_N\rangle$

$$= a_m^\dagger a_j^\dagger \sqrt{n_k}\sqrt{n_l}\, |n_1, \ldots, n_m, \ldots, n_k-1, \ldots, n_j, \ldots, n_l-1, \ldots\rangle$$

$$= \sqrt{n_m+1}\sqrt{n_j+1}\sqrt{n_k}\sqrt{n_l}\, |n_1, \ldots, n_m+1, \ldots, n_k-1, \ldots, n_j+1, \ldots, n_l-1, \ldots\rangle$$

Yields $\sum_{\alpha \neq \beta} |i\rangle_\alpha |j\rangle_\beta\, {}_\alpha\langle k|\, {}_\beta\langle l| = a_i^\dagger a_j^\dagger a_k a_l$ (with $i \equiv m$) and therefore

$$\hat{F} = \frac{1}{2} \sum_{i,j,k,l} f_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l = \frac{1}{2} \sum_{i,j,k,l} \langle i,j| f^{(2)} |k,l\rangle\, a_i^\dagger a_j^\dagger a_k a_l$$

There's an easier way!

$$\sum_{\alpha \neq \beta} \sum_{ijkl} |i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta = \sum_{\alpha, \beta} |i\rangle_\alpha \langle k|_\alpha |j\rangle_\beta \langle l|_\beta - \sum_\alpha |i\rangle_\alpha \langle k_\alpha | j\rangle_\alpha \langle l|_\alpha$$

H18)

a) $[\hat{a}_i\hat{a}_j, \hat{a}_k] = \hat{a}_i\underbrace{[\hat{a}_j, \hat{a}_k]}_{0} + \underbrace{[\hat{a}_i, \hat{a}_k]}_{0}\hat{a}_j = 0$

Order of applying a_i, a_j, a_k important?

$[\hat{a}_i^+\hat{a}_j^+, \hat{a}_k^+] = \hat{a}_i^+\underbrace{[\hat{a}_j^+, \hat{a}_k^+]}_{0} + \underbrace{[\hat{a}_i^+, \hat{a}_k^+]}_{0}\hat{a}_j^+ = 0$

Can you prove $[a_i, a_j] = 0$ etc or assumption?

$[\hat{a}_i\hat{a}_j, \hat{a}_k^+] = \hat{a}_i\underbrace{[\hat{a}_j, \hat{a}_k^+]}_{\delta_{jk}} + \underbrace{[\hat{a}_i, \hat{a}_k^+]}_{\delta_{ik}}\hat{a}_j = \hat{a}_i\delta_{jk} + \delta_{ik}\hat{a}_j$

$[\hat{a}_i^+\hat{a}_j^+, \hat{a}_k] = \hat{a}_i^+\underbrace{[\hat{a}_j^+, \hat{a}_k]}_{-[\hat{a}_k, \hat{a}_j^+] = -\delta_{kj}} + \underbrace{[\hat{a}_i^+, \hat{a}_k]}_{-[\hat{a}_k, \hat{a}_i^+] = -\delta_{ki}}\hat{a}_j^+ = -\hat{a}_i^+\delta_{kj} - \delta_{ki}\hat{a}_j^+$

b) $\hat{N} = \sum_i \hat{a}_i^+\hat{a}_i \quad ; \quad \hat{H} = \sum_{i,j} \underbrace{t_{ij}}_{\langle i|\hat{T}|j\rangle} \hat{a}_i^+\hat{a}_j + \frac{1}{2}\sum_{i,j,k,l} \underbrace{V_{ijkl}}_{\langle ij|\hat{V}|kl\rangle} \hat{a}_i^+\hat{a}_j^+\hat{a}_k\hat{a}_l$

$l \in [\ldots]$? $m \in [\ldots]$?

$0 \overset{!}{=} [\hat{N}, \hat{H}] = [\sum_m \hat{a}_m^+\hat{a}_m, \sum_{i,j} t_{ij}\hat{a}_i^+\hat{a}_j + \frac{1}{2}\sum_{i,j,k,l} V_{ijkl}\hat{a}_i^+\hat{a}_j^+\hat{a}_k\hat{a}_l]$

$= \sum_m \Big\{ \underbrace{[\hat{a}_m^+\hat{a}_m, \sum_{i,j} t_{ij}\hat{a}_i^+\hat{a}_j]}_{(1)} + \frac{1}{2}\underbrace{[\hat{a}_m^+\hat{a}_m, \sum_{i,j,k,l} V_{ijkl}\hat{a}_i^+\hat{a}_j^+\hat{a}_k\hat{a}_l]}_{(2)} \Big\}$

How to use a) for this?

Taking a look at (1) first yields:

$[\hat{a}_m^+\hat{a}_m, \sum_{i,j} t_{ij}\hat{a}_i^+\hat{a}_j] = \sum_{i,j} t_{ij}[\hat{a}_m^+\hat{a}_m, \hat{a}_i^+\hat{a}_j] = \sum_{i,j} t_{ij}\{\hat{a}_m^+[\hat{a}_m, \hat{a}_i^+\hat{a}_j] + [\hat{a}_m^+, \hat{a}_i^+\hat{a}_j]\hat{a}_m\}$

$= \sum_{i,j} t_{ij}\{\hat{a}_m^+(\hat{a}_i^+\underbrace{[\hat{a}_m, \hat{a}_j]}_{0} + \underbrace{[\hat{a}_m, \hat{a}_i^+]}_{\delta_{mi}}\hat{a}_j) + (\hat{a}_i^+\underbrace{[\hat{a}_m^+, \hat{a}_j]}_{-\delta_{mj}} + \underbrace{[\hat{a}_m^+, \hat{a}_i^+]}_{0}\hat{a}_j)\hat{a}_m\}$

$= \sum_{i,j} t_{ij}\{\hat{a}_m^+\delta_{mi}\hat{a}_j - \hat{a}_i^+\delta_{mj}\hat{a}_m\} \left(= \sum_j t_{mj}\hat{a}_m^+\hat{a}_j - \sum_i t_{im}\hat{a}_i^+\hat{a}_m\right)$

Are we allowed to apply δ_{mi} without sum over m?

We thus get:

$\sum_m [\hat{a}_m^+\hat{a}_m, \sum_{i,j} t_{ij}\hat{a}_i^+\hat{a}_j] \overset{\text{rename sums from above}}{=} \sum_m \left(\sum_k (t_{mk}\hat{a}_m^+\hat{a}_k - t_{km}\hat{a}_k^+\hat{a}_m)\right)$

$= \sum_m\sum_k t_{mk}\hat{a}_m^+\hat{a}_k - \sum_{m'}\sum_{k'} t_{m'k'}\hat{a}_{m'}^+\hat{a}_{k'} = 0$

$k \equiv m'$, $m \equiv k'$ in half of the sum

Now we only have to take care of (2):

$$\frac{1}{2}\Big[\hat{a}_m^+\hat{a}_m, \sum_{i,j,k,l} V_{ijkl}\,\hat{a}_i^+\hat{a}_j^+\hat{a}_k\hat{a}_l\Big] = \frac{1}{2}\sum_{i,j,k,l} V_{ijkl}\,[\hat{a}_m^+\hat{a}_m, \hat{a}_i^+\hat{a}_j^+\hat{a}_k\hat{a}_l]$$

$$= \frac{1}{2}\sum_{i,j,k,l} V_{ijkl}\Big\{(\hat{a}_i^+\hat{a}_j^+)[\hat{a}_m^+\hat{a}_m, a_k a_l] + [\hat{a}_m^+\hat{a}_m, \hat{a}_i^+\hat{a}_j^+](\hat{a}_k\hat{a}_l)\Big\}$$

$$= \frac{1}{2}\sum_{i,j,k,l} V_{ijkl}\Big\{\hat{a}_i^+\hat{a}_j^+\Big(\hat{a}_m^+\underbrace{[\hat{a}_m, \hat{a}_k\hat{a}_l]}_{=0,\text{ see a)}} + \underbrace{[\hat{a}_m^+, \hat{a}_k\hat{a}_l]}_{=-[\hat{a}_k\hat{a}_l, \hat{a}_m^+] = -(\hat{a}_k\delta_{lm} + \delta_{km}\hat{a}_l)}\hat{a}_m\Big)$$

$$+ \Big(\hat{a}_m^+\underbrace{[\hat{a}_m, \hat{a}_i^+\hat{a}_j^+]}_{-[\hat{a}_i^+\hat{a}_j^+, \hat{a}_m] = \hat{a}_i^+\delta_{jm} + \delta_{im}\hat{a}_j^+} + \underbrace{[\hat{a}_m^+, \hat{a}_i^+\hat{a}_j^+]}_{=0,\text{ see a)}}\hat{a}_m\Big)\hat{a}_k\hat{a}_l\Big\}$$

$$= \frac{1}{2}\sum_{i,j,k,l} V_{ijkl}\Big\{-\hat{a}_i^+\hat{a}_j^+(\hat{a}_k\delta_{lm} + \delta_{km}\hat{a}_l)\hat{a}_m + \hat{a}_m^+(\hat{a}_i^+\delta_{jm} + \delta_{im}\hat{a}_j^+)\hat{a}_k\hat{a}_l\Big\}$$

We thus get:

$$\sum_m \frac{1}{2}\Big[\hat{a}_m^+\hat{a}_m, \sum_{i,j,k,l} V_{ijkl}\,\hat{a}_i^+\hat{a}_j^+\hat{a}_k\hat{a}_l\Big]$$

$$= \frac{1}{2}\Big\{-\sum_{i,j,k,m} V_{ijkm}\,\hat{a}_i^+\hat{a}_j^+\hat{a}_k\hat{a}_m - \sum_{i,j,m,l} V_{ijml}\,\hat{a}_i^+\hat{a}_j^+\hat{a}_l\hat{a}_m$$

$$+ \sum_{i,m,k,l} V_{imkl}\,\hat{a}_m^+\hat{a}_i^+\hat{a}_k\hat{a}_l + \sum_{m,j,k,l} V_{mjkl}\,\hat{a}_m^+\hat{a}_j^+\hat{a}_k\hat{a}_l\Big\}$$

$[\hat{a}_i^+, \hat{a}_j^+] = 0$, $[\hat{a}_k, \hat{a}_l] = 0$

$$\overset{\downarrow}{=} \frac{1}{2}\Big\{-\sum_{i,j,k,m} V_{ijkm}\,\hat{a}_j^+\hat{a}_i^+\hat{a}_k\hat{a}_m - \sum_{i,j,m,l} V_{ijml}\,\hat{a}_i^+\hat{a}_j^+\hat{a}_m\hat{a}_l$$

$$+ \sum_{i,m,k,l} V_{imkl}\,\hat{a}_m^+\hat{a}_i^+\hat{a}_k\hat{a}_l + \sum_{m,j,k,l} V_{mjkl}\,\hat{a}_m^+\hat{a}_j^+\hat{a}_k\hat{a}_l\Big\}$$

renaming $m \mapsto j'$, $l \mapsto m'$ and $m \mapsto i'$, $k \mapsto m'$ in 2nd sum

$$\overset{\downarrow}{=} \frac{1}{2}\Big\{-\sum_{i,j,k,m} \hat{a}_j^+\hat{a}_i^+\hat{a}_k\hat{a}_m - \sum_{i,j,m,l} V_{ijml}\,\hat{a}_i^+\hat{a}_j^+\hat{a}_m\hat{a}_l$$

$$+ \sum_{i,j',k,m'} V_{ij'km'}\,\hat{a}_j^+\hat{a}_i^+\hat{a}_k\hat{a}_{m'} + \sum_{i',j,m',l} V_{i'jm'l}\,\hat{a}_i^+\hat{a}_j^+\hat{a}_m\hat{a}_l\Big\}$$

$$= 0$$

$\Rightarrow [\hat{N}, \hat{H}] = 0$, which has the physical meaning of particle conservation ✓