Second Quantization $\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$

Edward Lu, RPI, 3/12

Idea of Second Quantization

- First Quantization
  - Fixed number of particles (e.g. electrons)
- Second Quantization
  - Unfixed number of particles (e.g. electrons)
  - We want to use sparse matrices as opposed to using a differential operator
    - Large matrices can store more and be faster
    - Creation and annihilation matrices

Tensor Product Representation

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv \text{unoccupied} \quad \text{and} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \text{occupied}$$

- Example
  - |101>, where 1 is occupied, 0 unoccupied
- One to one correspondence with each possible state

Example result is (00000100)^T

Creation and Annihilation Operators

$$a_p^\dagger : \mathcal{F} \to \mathcal{F} \; ; \; |s_1, ..., s_n\rangle \mapsto (-1)^{\sigma(p)}(1 - s_p)|s_1, ...s_{p-1}, 1 - s_p, s_{p+1}, ..., s_n\rangle$$

$$a_p : \mathcal{F} \to \mathcal{F} \; ; \; |s_1, ..., s_n\rangle \mapsto (-1)^{\sigma(p)} s_p |s_1, ...s_{p-1}, 1 - s_p, s_{p+1}, ..., s_n\rangle$$

- Creates/Annihilates at p-th index
- Annihilation: $\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ = a
- Creation: a^+
  $\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$

Example

- a_2

Anticommutator relations

$$[a_p, a_q]_+ = [a_p^\dagger, a_q^\dagger]_+ = 0 \quad \text{and} \quad [a_p, a_q]_+ = \delta_{p,q}. \tag{10}$$

Can be proved by properties of tensor products

Normal ordering

Definition

- Writing an operator string $\hat{O}$ on normal-ordered form $\left\{\hat{O}\right\}$ corresponds to moving all creation operators to the left and all annihilation operators to the left *as if they all anticommuted, e.g.*

$$\{a_p a_q\} = a_p a_q; \quad \left\{a_p^\dagger a_q^\dagger\right\} = a_p^\dagger a_q^\dagger$$

$$\left\{a_p^\dagger a_q\right\} = a_p^\dagger a_q; \quad \left\{a_p a_q^\dagger\right\} = -a_q^\dagger a_p$$

- A more complicated example is

$$\left\{a_s a_r a_p^\dagger a_q a_t^\dagger a_u^\dagger\right\} = \left\{a_p^\dagger a_s a_r a_q a_t^\dagger a_u^\dagger\right\} = -\left\{a_p^\dagger a_t^\dagger a_s a_r a_q a_u^\dagger\right\} = a_p^\dagger a_t^\dagger a_u^\dagger a_s a_r a_q$$

- The vacuum expectation value of a normal-ordered operator string is zero

$$\left\langle vac \left| \left\{\hat{O}\right\} \right| vac \right\rangle = 0$$

Example

$$\left\{a_s a_r a_p^\dagger a_q a_t^\dagger a_u^\dagger\right\} = \left\{a_p^\dagger a_s a_r a_q a_t^\dagger a_u^\dagger\right\} = -\left\{a_p^\dagger a_t^\dagger a_s a_r a_q a_u^\dagger\right\} = a_p^\dagger a_t^\dagger a_u^\dagger a_s a_r a_q$$

Contraction

- A **contraction** is defined as

$$\overbrace{xy} = xy - \{xy\}$$

- There are four possible combinations

$$\begin{aligned}
\overbrace{a_p^\dagger a_q^\dagger} &= a_p^\dagger a_q^\dagger - \left\{a_p^\dagger a_q^\dagger\right\} = a_p^\dagger a_q^\dagger - a_p^\dagger a_q^\dagger = 0 \\
\overbrace{a_p a_q} &= a_p a_q - \{a_p a_q\}_v = a_p a_q - a_p a_q = 0 \\
\overbrace{a_p^\dagger a_q} &= a_p^\dagger a_q - \left\{a_p^\dagger a_q\right\} = a_p^\dagger a_q - a_p^\dagger a_q = 0 \\
\overbrace{a_p a_q^\dagger} &= a_p a_q^\dagger - \left\{a_p a_q^\dagger\right\} = a_p a_q^\dagger + a_q^\dagger a_p = \delta_{pq}
\end{aligned}$$

- The only non-zero contraction occurs when an annihilation operator appears to the left of a creation operator.

Example of One-electron expectation (energy)

Wick's theorem

An operator string may be written as a linear combination of normal-ordered strings.

$$
\begin{aligned}
ABC\ldots XYZ &= \{ABC\ldots XYZ\} \\
&+ \sum_{\text{singles}} \left\{ \contraction{}{A}{}{B} ABC\ldots XYZ \right\} \\
&+ \sum_{\text{doubles}} \left\{ \contraction{}{A}{BC\ldots}{X} \contraction[2ex]{A}{B}{C\ldots X}{Y} ABC\ldots XYZ \right\} \\
&+ \ldots
\end{aligned}
$$

Only fully contracted terms contribute to vacuum expectation values.