Review single-particle states

- Notation $|\ldots\rangle$
- … list of quantum numbers associated with a CSCO
- Normalization $\langle\alpha|\beta\rangle = \delta_{\alpha,\beta}$
- Continuous quantum numbers
  - Example $\langle \boldsymbol{r}, m_s | \boldsymbol{r}', m_s' \rangle = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta_{m_s,m_s'}$
- Completeness $\sum_{\alpha} |\alpha\rangle\langle\alpha| = 1$

Consequences for two-particle states

- CVS for two particles: product space
- Notation $|\alpha_1\alpha_2) = |\alpha_1\rangle|\alpha_2\rangle$
- Orthogonality $(\alpha_1\alpha_2|\alpha_1'\alpha_2') = \delta_{\alpha_1,\alpha_1'}\delta_{\alpha_2,\alpha_2'}$
- Completeness $\sum_{\alpha_1\alpha_2} |\alpha_1\alpha_2)(\alpha_1\alpha_2| = 1$

Exchange degeneracy for identical particles

- Consider $\alpha_1 \neq \alpha_2$
- Then $|\alpha_2\alpha_1) \neq |\alpha_1\alpha_2)$
- All states $|\alpha_1\alpha_2)$

  $|\alpha_2\alpha_1)$

  $c_1|\alpha_1\alpha_2) + c_2|\alpha_2\alpha_1)$

  yield α_1 for one particle and α_2 for the other upon measurement
- Yet, unclear which state describes this system and therefore inconsistent with quantum postulates
- Consider permutation operator

$$P_{12}|\alpha_1\alpha_2) = |\alpha_2\alpha_1)$$

  with $P_{12} = P_{21} \text{ and } P_{12}^2 = 1$

- Hamiltonian for two particles is symmetric for 1 ⇔ 2

Development

- Typical Hamiltonian $H = \frac{\boldsymbol{p}_1^2}{2m} + \frac{\boldsymbol{p}_2^2}{2m} + V(|\boldsymbol{r}_1 - \boldsymbol{r}_2|)$
- Consider operator acting on particle 1 and corresponding eigenvalue $A_1|\alpha_1\alpha_2) = a_1|\alpha_1\alpha_2)$
- Similarly, the corresponding operator acting on particle 2 yields

$$A_2|\alpha_1\alpha_2) = a_2|\alpha_1\alpha_2)$$

- Note $P_{12}A_1|\alpha_1\alpha_2) = a_1 P_{12}|\alpha_1\alpha_2) = a_1|\alpha_2\alpha_1) = A_2|\alpha_2\alpha_1)$
- and $P_{12}A_1|\alpha_1\alpha_2) = P_{12}A_1P_{12}^{-1}P_{12}|\alpha_1\alpha_2) = P_{12}A_1P_{12}^{-1}|\alpha_2\alpha_1)$
- Holds for any state; therefore $P_{12}A_1P_{12}^{-1} = A_2$
- It follows that $P_{12}HP_{12}^{-1} = H$ or $[P_{12}, H] = 0$

Symmetric and antisymmetric two-particle states

- So $$[P_{12}, H] = 0$$
- Common eigenkets either
$$|\alpha_1\alpha_2\rangle_+ = \frac{1}{\sqrt{2}}\{|\alpha_1\alpha_2) + |\alpha_2\alpha_1)\}$$
or
$$|\alpha_1\alpha_2\rangle_- = \frac{1}{\sqrt{2}}\{|\alpha_1\alpha_2) - |\alpha_2\alpha_1)\}$$
- Eigenstates of the Hamiltonian either symmetric $\Rightarrow$ bosons

or antisymmetric $\Rightarrow$ fermions

Fermions

- Antisymmetry: $|\alpha_2\alpha_1\rangle = -|\alpha_1\alpha_2\rangle$
- Both kets represent the same physical state: count only once in completeness relation ⇒ "order" quantum numbers

$$|1\rangle, |2\rangle, |3\rangle, \ldots$$

- Ordered: $\sum_{i<j} |ij\rangle\langle ij| = 1$
- Not ordered: $\frac{1}{2!}\sum_{ij} |ij\rangle\langle ij| = 1$

N-particle states (fermions)

- Product states $|\alpha_1\alpha_2...\alpha_N) = |\alpha_1\rangle\,|\alpha_2\rangle\,...\,|\alpha_N\rangle$
- Normalization

$$\begin{aligned}(\alpha_1\alpha_2...\alpha_N|\alpha'_1\alpha'_2...\alpha'_N) &= \langle\alpha_1|\alpha'_1\rangle\langle\alpha_2|\alpha'_2\rangle...\langle\alpha_N|\alpha'_N\rangle \\ &= \delta_{\alpha_1,\alpha'_1}\delta_{\alpha_2,\alpha'_2}...\delta_{\alpha_N,\alpha'_N}\end{aligned}$$

- Completeness $\sum_{\alpha_1\alpha_2...\alpha_N} |\alpha_1\alpha_2...\alpha_N)(\alpha_1\alpha_2...\alpha_N| = 1$
- Identical particles: symmetric or antisymmetric states
- Fermions: use antisymmetrizer $\mathcal{A} = \frac{1}{N!}\sum_p (-1)^p P$
- Permutation operator product of two-particle permutations
- # of two-particle permutations odd/even $\Rightarrow$ **sign**

Example for 3 particles

- Check odd/even permutation

$$
\begin{aligned}
|\alpha_1\alpha_2\alpha_3\rangle &= \frac{1}{\sqrt{6}}\{|\alpha_1\alpha_2\alpha_3) - |\alpha_2\alpha_1\alpha_3) + |\alpha_2\alpha_3\alpha_1) \\
&- |\alpha_3\alpha_2\alpha_1) + |\alpha_3\alpha_1\alpha_2) - |\alpha_1\alpha_3\alpha_2)\}.
\end{aligned}
$$

- Note normalization (6 states)
- Also note antisymmetry $|\alpha_1\alpha_2\alpha_3\rangle = -|\alpha_2\alpha_1\alpha_3\rangle$
- No two fermions can occupy the same state!!

N fermions

- Completeness with ordered single-particle (sp) quantum numbers

$$\sum_{\alpha_1\alpha_2...\alpha_N}^{ordered} |\alpha_1\alpha_2...\alpha_N\rangle\langle\alpha_1\alpha_2...\alpha_N| = 1$$

- Not ordered

$$\frac{1}{N!}\sum_{\alpha_1\alpha_2...\alpha_N} |\alpha_1\alpha_2...\alpha_N\rangle\langle\alpha_1\alpha_2...\alpha_N| = 1$$

- Normalization with ordered single-particle (sp) quantum numbers

$$\begin{aligned}\langle\alpha_1\alpha_2...\alpha_N|\alpha'_1\alpha'_2...\alpha'_N\rangle &= \langle\alpha_1|\alpha'_1\rangle\langle\alpha_2|\alpha'_2\rangle...\langle\alpha_N|\alpha'_N\rangle \\ &= \delta_{\alpha_1,\alpha'_1}\delta_{\alpha_2,\alpha'_2}...\delta_{\alpha_N,\alpha'_N}\end{aligned}$$

- Not ordered $\Rightarrow$ determinant

$$\langle\alpha_1\alpha_2...\alpha_N|\alpha'_1\alpha'_2...\alpha'_N\rangle = \begin{vmatrix} \langle\alpha_1|\alpha'_1\rangle & \langle\alpha_1|\alpha'_2\rangle & \dots & \langle\alpha_1|\alpha'_N\rangle \\ \langle\alpha_2|\alpha'_1\rangle & \langle\alpha_2|\alpha'_2\rangle & \dots & \langle\alpha_2|\alpha'_N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\alpha_N|\alpha'_1\rangle & \langle\alpha_N|\alpha'_2\rangle & \dots & \langle\alpha_N|\alpha'_N\rangle \end{vmatrix}.$$

Normalized N-particle wave function

- Called a Slater determinant

$$\psi_{\alpha_1\alpha_2\ldots\alpha_N}(x_1x_2\ldots x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \langle x_1|\alpha_1\rangle & \ldots & \langle x_N|\alpha_1\rangle \\ \langle x_1|\alpha_2\rangle & \ldots & \langle x_N|\alpha_2\rangle \\ \vdots & \ddots & \vdots \\ \langle x_1|\alpha_N\rangle & \ldots & \langle x_N|\alpha_N\rangle \end{vmatrix}.$$

- Hard to work with Slater determinants
- Use occupation number representation or second quantization

Second quantization

- Motivation:
  - Slater determinants tedious to work with
  - Relevant operators change only the quantum numbers of one or two particles (and in exceptional cases three)
- Consider states that are labeled by the # of particles occupying sp states $\Rightarrow$ occupation number representation
- Allow states in CVS with different # of particles $\Rightarrow$ Fock space
- Includes new state: the vacuum $|0\rangle$
  - all sp states $\{|\alpha\rangle\}$
  - all antisymmetric two-particle (tp) states $\{|\alpha_1\alpha_2\rangle\}$
  - ..
  - all antisymmetric N-particle states $\{|\alpha_1\alpha_2...\alpha_N\rangle\}$
  - up to infinite number of particles .....

Alternative writing

- Vacuum state $|0\rangle = \underset{\alpha_1\alpha_2...}{|0\ 0...}\ \underset{\alpha_\infty}{0\rangle}$
- Sp state $|\alpha_i\rangle = |0\ 0\ ...0\ \underset{\alpha_i}{1}\ 0...0\rangle$
- Tp state $|\alpha_i\alpha_j\rangle = |0\ 0\ ...0\ \underset{\alpha_i}{1}\ 0...0\ \underset{\alpha_j}{1}\ 0...0\rangle$
- etc.
- Use ordered states $\sum_{N=0}^{\infty} \sum_{\alpha_1\alpha_2..\alpha_N}^{ordered} |\alpha_1\alpha_2...\alpha_N\rangle\langle\alpha_1\alpha_2...\alpha_N| = 1$
- Introduce new operator in Fock space $a^\dagger_\alpha$

Particle addition (creation) operator

- Definition $a^\dagger_\alpha \left|\alpha_1 \alpha_2 ... \alpha_N\right\rangle \equiv \left|\alpha \alpha_1 \alpha_2 ... \alpha_N\right\rangle$
- Takes an antisymmetric N-particle state and turns it into an antisymmetric N+1-particle state with α occupied!!!!
- Note:
  - $\alpha = \alpha_i \Rightarrow$ not a state
  - $\alpha \neq \alpha_i \Rightarrow$ i=1,…,N new state (may require ordering)
- Acts on any state
- Including $a^\dagger_\alpha \left|0\right\rangle = \left|\alpha\right\rangle$
- and $a^\dagger_\alpha \left|\beta\right\rangle = \left|\alpha\beta\right\rangle$
- etc.
- What about the adjoint operator a_α ?

Particle removal (destruction) operator

- Action of adjoint operator?

$$a_\alpha |\alpha_1\alpha_2...\alpha_N\rangle = \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2..\alpha'_M}^{ordered} |\alpha'_1\alpha'_2..\alpha'_M\rangle \langle\alpha'_1\alpha'_2..\alpha'_M| \, a_\alpha \, |\alpha_1\alpha_2..\alpha_N\rangle$$

$$= \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2..\alpha'_M}^{ordered} |\alpha'_1\alpha'_2..\alpha'_M\rangle \langle\alpha_1\alpha_2..\alpha_N| \, a^\dagger_\alpha \, |\alpha'_1\alpha'_2..\alpha'_M\rangle^*$$

$$= \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2..\alpha'_M}^{ordered} |\alpha'_1\alpha'_2..\alpha'_M\rangle \langle\alpha_1\alpha_2..\alpha_N|\alpha\alpha'_1\alpha'_2..\alpha'_M\rangle^*$$

- Consider once α placed in the correct location $\Rightarrow \quad (-1)^{i-1}$

$$\langle\alpha_1\alpha_2...\alpha_N|\alpha'_1\alpha'_2...\alpha\alpha'_i...\alpha'_M\rangle = \delta_{\alpha_1,\alpha'_1}\delta_{\alpha_2,\alpha'_2}...\delta_{\alpha_i,\alpha}\delta_{\alpha_{i+1},\alpha'_i}...\delta_{\alpha_N,\alpha'_{N-1}}$$

- So $\quad a_\alpha |\alpha_1\alpha_2...\alpha_N\rangle = (-1)^{i-1} |\alpha_1\alpha_2...\alpha_{i-1}\alpha_{i+1}...\alpha_N\rangle \qquad \text{if } \alpha = \alpha_i$
- or $\quad a_\alpha |\alpha_1\alpha_2...\alpha_N\rangle = 0 \qquad \text{if } \alpha \neq \alpha_i, i = 1, ..., N$
- Example: $a_\alpha |0\rangle = 0$ Note: again antisymmetric state!

Fermion anticommutation relations

$$\{a_\alpha, a_\beta^\dagger\} = a_\alpha a_\beta^\dagger + a_\beta^\dagger a_\alpha = \delta_{\alpha,\beta}$$

$$\{a_\alpha, a_\beta\} = \{a_\alpha^\dagger, a_\beta^\dagger\} = 0$$

- "Easy" to demonstrate
- Rewrite antisymmetric state

$$\begin{aligned} |\alpha_1\alpha_2\alpha_3...\alpha_N\rangle &= a_{\alpha_1}^\dagger |\alpha_2\alpha_3...\alpha_N\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger |\alpha_3...\alpha_N\rangle = ... \\ &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger |0\rangle = \prod_i a_{\alpha_i}^\dagger |0\rangle \end{aligned}$$

- Ensures Pauli principle

$$\begin{aligned} |\alpha_1\alpha_2...\alpha_N\rangle &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger |0\rangle = -a_{\alpha_2}^\dagger a_{\alpha_1}^\dagger ... a_{\alpha_N}^\dagger |0\rangle \\ &= -|\alpha_2\alpha_1...\alpha_N\rangle \end{aligned}$$

- Occupation numbers

$$|n_{\alpha_1} = 1, n_{\alpha_2} = 0, n_{\alpha_3} = 1, 0, ..., 0, ...\rangle = |\alpha_1\alpha_3\rangle$$

One-body operators in Fock space

- Examples?

- 1 particle in sp space $$F = \sum_\alpha \sum_\beta |\alpha\rangle \langle\alpha| F |\beta\rangle \langle\beta|$$

- Operator completely determined by all $\langle\alpha| F |\beta\rangle$

- N-particle space $$F_N = F(1) + F(2) + ... + F(N) = \sum_{i=1}^{N} F(i)$$
- Action of $F(i)$ on a product state

$$F(i)|\alpha_1\alpha_2\alpha_3...\alpha_N) = |\alpha_1\rangle |\alpha_2\rangle ... |\alpha_{i-1}\rangle \left\{\sum_{\beta_i} |\beta_i\rangle \langle\beta_i| F |\alpha_i\rangle\right\} |\alpha_{i+1}\rangle ... |\alpha_N\rangle$$

$$= \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle |\alpha_1...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N)$$

One-body operators (continued)

- Matrix element $\langle\beta_i|\,F\,|\alpha_i\rangle$ same for any particle (dummy variables)
- Then

$$F_N|\alpha_1\alpha_2\alpha_3...\alpha_N) = F(1)\,|\alpha_1\rangle\,|\alpha_2\rangle\,...\,|\alpha_N\rangle + ... + |\alpha_1\rangle\,|\alpha_2\rangle\,...F(N)\,|\alpha_N\rangle$$

$$= \sum_{\beta_1}\langle\beta_1|\,F\,|\alpha_1\rangle\,|\beta_1\alpha_2...\alpha_N) + ... + \sum_{\beta_N}\langle\beta_N|\,F\,|\alpha_N\rangle\,|\alpha_1\alpha_2...\beta_N)$$

$$= \sum_{i=1}^{N}\sum_{\beta_i}\langle\beta_i|\,F\,|\alpha_i\rangle\,|\alpha_1\alpha_2...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N)$$

- Since F_N is symmetric it commutes with the antisymmetrizer $\mathcal{A}$
- Thus

$$F_N\,|\alpha_1\alpha_2\alpha_3...\alpha_N\rangle = \sum_{i=1}^{N}\sum_{\beta_i}\langle\beta_i|\,F\,|\alpha_i\rangle\,|\alpha_1\alpha_2...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N\rangle$$

Fock-space one-body operator

- Consider Fock-space operator $\hat{F} = \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, a^\dagger_\alpha a_\beta$
- Note the "^" notation
- This operator accomplishes the same as F_N for any N!
- Use

$$\begin{aligned}
[\hat{F}, a^\dagger_{\alpha_i}] &= \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, [a^\dagger_\alpha a_\beta, a^\dagger_{\alpha_i}] = \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, (a^\dagger_\alpha a_\beta a^\dagger_{\alpha_i} - a^\dagger_{\alpha_i} a^\dagger_\alpha a_\beta) \\
&= \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, a^\dagger_\alpha (a_\beta a^\dagger_{\alpha_i} + a^\dagger_{\alpha_i} a_\beta) = \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, a^\dagger_\alpha \delta_{\beta,\alpha_i} \\
&= \sum_{\alpha} \langle\alpha| F |\alpha_i\rangle \, a^\dagger_\alpha = \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle \, a^\dagger_{\beta_i}
\end{aligned}$$

- and apply $\hat{F} |\alpha_1\alpha_2\alpha_3 ... \alpha_N\rangle = \hat{F} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} |0\rangle$

$$\begin{aligned}
&= [\hat{F}, a^\dagger_{\alpha_1}] a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} |0\rangle + a^\dagger_{\alpha_1} \hat{F} a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} |0\rangle \\
&= [\hat{F}, a^\dagger_{\alpha_1}] a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} |0\rangle + a^\dagger_{\alpha_1} [\hat{F}, a^\dagger_{\alpha_2}] ... a^\dagger_{\alpha_N} |0\rangle + ... + a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} ... [\hat{F}, a^\dagger_{\alpha_N}] |0\rangle \\
&= \sum_{i=1}^{N} \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle \, a^\dagger_{\alpha_1} ... a^\dagger_{\alpha_{i-1}} a^\dagger_{\beta_i} a^\dagger_{\alpha_{i+1}} ... a^\dagger_{\alpha_N} |0\rangle \\
&= \sum_{i=1}^{N} \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle \, |\alpha_1 ... \alpha_{i-1} \beta_i \alpha_{i+1} ... \alpha_N\rangle \quad ✔
\end{aligned}$$

Examples

- Density operator for N particles $\rho_N(\boldsymbol{r}) = \sum_{i=1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i)$

- Second-quantized form: choose $\{|\boldsymbol{r}, m_s\rangle\}$ basis
- In Fock space

$$\hat{\rho}(\boldsymbol{r}) = \sum_{m_s, m_{s'}} \int d^3 r_1 \int d^3 r_1' \; \langle \boldsymbol{r}_1 m_s | \, \delta(\boldsymbol{r} - \boldsymbol{r}_{op}) \, | \boldsymbol{r}_1' m_{s'} \rangle \, a^\dagger_{\boldsymbol{r}_1 m_s} a_{\boldsymbol{r}_1' m_{s'}}$$

$$= \sum_{m_s} a^\dagger_{\boldsymbol{r} m_s} a_{\boldsymbol{r} m_s}$$

- Kinetic energy $\hat{T} = \sum_{\alpha\beta} \langle \alpha | \, T \, | \beta \rangle \, a^\dagger_\alpha a_\beta$

$$= \sum_{\boldsymbol{p}_1 m_1 \boldsymbol{p}_2 m_2} \langle \boldsymbol{p}_1 m_1 | \, \frac{\boldsymbol{p}_{op}^2}{2m} \, | \boldsymbol{p}_2 m_2 \rangle \, a^\dagger_{\boldsymbol{p}_1 m_1} a_{\boldsymbol{p}_2 m_2}$$

$$= \sum_{\boldsymbol{p}_1 m_1} \frac{\boldsymbol{p}_1^2}{2m} a^\dagger_{\boldsymbol{p}_1 m_1} a_{\boldsymbol{p}_1 m_1}$$

More examples

- Consider $\hat{N} = \sum_\alpha a_\alpha^\dagger a_\alpha$

- Determine $\left[\hat{N}, a_{\alpha_i}^\dagger\right]$

$$\begin{aligned} \left[\hat{N}, a_{\alpha_i}^\dagger\right] &= \sum_\alpha \left[a_\alpha^\dagger a_\alpha, a_{\alpha_i}^\dagger\right] \\ &= a_{\alpha_i}^\dagger \end{aligned}$$

- Therefore $\hat{N}\,|\alpha_1 ... \alpha_N\rangle = N\,|\alpha_1 ... \alpha_N\rangle$

Change of basis $\quad a_\alpha^\dagger\,|0\rangle = |\alpha\rangle = \sum_\lambda |\lambda\rangle\,\langle\lambda|\alpha\rangle = \sum_\lambda a_\lambda^\dagger\,|0\rangle\,\langle\lambda|\alpha\rangle$

Can be done for any state in Fock space $\Rightarrow \quad a_\alpha^\dagger = \sum_\lambda \langle\lambda|\alpha\rangle a_\lambda^\dagger$

Also $\quad a_\alpha = \sum_\lambda \langle\alpha|\lambda\rangle a_\lambda$

Two-body operators in Fock space

- Similar strategy $$V = \sum_{\alpha\beta}\sum_{\gamma\delta} |\alpha\beta)(\alpha\beta|V|\gamma\delta)(\gamma\delta|$$
- N-particles

$$V_N = \begin{cases} V(1,2)+ & V(1,3)+ & V(1,4)+ & \ldots + & V(1,N)+ \\ & V(2,3)+ & V(2,4)+ & \ldots + & V(2,N)+ \\ & & V(3,4)+ & \ldots + & V(3,N)+ \\ & & & \ddots & \vdots \\ & & & & V(N-1,N) \end{cases}$$

$$= \sum_{i<j}^{N} V(i,j) = \frac{1}{2}\sum_{i \neq j}^{N} V(i,j)$$

- Consider

$$V(i,j)|\alpha_1..\alpha_i..\alpha_j..\alpha_N) = \sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j)|\alpha_1..\alpha_{i-1}\beta_i\alpha_{i+1}..\alpha_{j-1}\beta_j\alpha_{j+1}..\alpha_N)$$

- Matrix elements do not depend on the selected pair
- $(\beta_i\beta_j|V|\alpha_i\alpha_j)$ identical for any pair as long as quantum numbers are the same, so

$$V_N|\alpha_1\alpha_2\alpha_3...\alpha_N) = \sum_{i<j}^{N}\sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j)|\alpha_1...\beta_i...\beta_j...\alpha_N)$$

More on two-body operators

- Note: V_N symmetric and therefore commutes with antisymmetrizer
- As a consequence

$$V_N \left|\alpha_1 \alpha_2 \alpha_3 ... \alpha_N\right\rangle = \sum_{i<j}^{N} \sum_{\beta_i \beta_j} (\beta_i \beta_j | V | \alpha_i \alpha_j) \left|\alpha_1 ... \beta_i ... \beta_j ... \alpha_N\right\rangle$$

- Fock-space operator (proof in Phys 540)

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

- accomplishes the same result for any particle number!
- Note ordering

Hamiltonian

- Most common operator
$$\hat{H} = \hat{T} + \hat{V}$$
$$= \sum_{\alpha\beta} \langle\alpha| T |\beta\rangle a^\dagger_\alpha a_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$
- Notation often used $\psi^\dagger_{m_s}(\boldsymbol{r}) \equiv a^\dagger_{\boldsymbol{r}m_s}$
- Use
$$\begin{aligned}\langle \boldsymbol{r}m_s| T |\boldsymbol{r}'m_s'\rangle &= \langle \boldsymbol{r}m_s| \frac{\boldsymbol{p}^2}{2m} |\boldsymbol{r}'m_s'\rangle \\ &= \frac{-i\hbar}{2m}\nabla \cdot \langle \boldsymbol{r}m_s| \boldsymbol{p} |\boldsymbol{r}'m_s'\rangle \\ &= \frac{-\hbar^2}{2m}\nabla^2 \langle \boldsymbol{r}m_s|\boldsymbol{r}'m_s'\rangle \\ &= \frac{-\hbar^2}{2m}\nabla^2 \delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{m_s,m_s'}\end{aligned}$$
- and
$$\begin{aligned}(\boldsymbol{r}_1 m_{s_1}\ \boldsymbol{r}_2 m_{s_2}|V(\boldsymbol{r},\boldsymbol{r}')|\boldsymbol{r}_3 m_{s_3}\ \boldsymbol{r}_4 m_{s_4}) &= \delta(\boldsymbol{r}_1-\boldsymbol{r}_3)\delta(\boldsymbol{r}_2-\boldsymbol{r}_4) \\ &\times\ \delta_{m_{s_1},m_{s_3}}\delta_{m_{s_2},m_{s_4}} V(|\boldsymbol{r}_3-\boldsymbol{r}_4|)\end{aligned}$$
- In this basis
$$\begin{aligned}\hat{H} &= \sum_{m_s}\int d^3r\ \psi^\dagger_{m_s}(\boldsymbol{r})\{\frac{-\hbar^2}{2m}\nabla^2\}\psi_{m_s}(\boldsymbol{r}) \\ &+ \frac{1}{2}\sum_{m_s m_s'}\int d^3r \int d^3r'\ \psi^\dagger_{m_s}(\boldsymbol{r})\psi^\dagger_{m_s'}(\boldsymbol{r}')V(|\boldsymbol{r}-\boldsymbol{r}'|)\psi_{m_s'}(\boldsymbol{r}')\psi_{m_s}(\boldsymbol{r})\end{aligned}$$
- "second quantization"