Quantum Mechanics II

Lots of Identical Particles

(Anti)Symmetrization; Exchange Consequences; Particle Operators

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Pink Floyd: "Another Brick in the Wall (Pt. II)"

Lots of Identical Particles

(Anti)Symmetrization

- Symmetrization postulate:
  - Bosons (particles with integral spin) must be symmetrized

$$\boldsymbol{\Psi}_B(1,\ldots,i,\ldots,j,\ldots) = +\boldsymbol{\Psi}_B(1,\ldots,j,\ldots,i,\ldots),\quad \forall i,j$$

  - Fermions (particles with half-integral spin) must be antisymmetrized

$$\boldsymbol{\Psi}_F(1,\ldots,i,\ldots,j,\ldots) = -\boldsymbol{\Psi}_F(1,\ldots,j,\ldots,i,\ldots),\quad \forall i,j$$

- This (anti)symmetrization affect the full wave-function

$$\boldsymbol{\Psi}_{B,F}(1,\ldots,i,\ldots,j,\ldots) := \sum_{\mathbf{k}} \underbrace{\Psi_{\mathbf{k}}(\vec{r}_1,\ldots,\vec{r}_j,\ldots,\vec{r}_j,\ldots)}_{\text{positions in “real” space}} \cdot \underbrace{\chi_{\mathbf{k}}(1,\ldots,i,\ldots,j,\ldots)}_{\text{everything else positions in “internal” space}}$$

  - where “**k**” represents (a slew of) separation variables
  - The sum, in general, is *not* a product of two factors
  - The sum is *almost never* a product of two factors

“non-separability”
“entanglement”

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Lots of Identical Particles

(Anti)Symmetrization

- Consider the case of just two particles
  - Define some simplifying notation

positional (in "real" space)

$$\Psi^{\pm}(1,2) := \tfrac{1}{\sqrt{2}}\big[\Psi(\vec{r}_1,\vec{r}_2) \pm \Psi(\vec{r}_2,\vec{r}_1)\big]$$

$$\Psi^{\pm}(\vec{r}_1,\vec{r}_2) \equiv \pm\Psi^{\pm}(\vec{r}_2,\vec{r}_1)$$

$$\Psi(\vec{r}_1,\vec{r}_2) \equiv \tfrac{1}{\sqrt{2}}\big[\Psi^{+}(1,2) + \Psi^{-}(1,2)\big]$$

all else (in "internal" space)

$$\chi^{\pm}(1,2) := \tfrac{1}{\sqrt{2}}\big[\chi(1,2) \pm \chi(2,1)\big]$$

$$\chi^{\pm}(1,2) \equiv \pm\chi^{\pm}(2,1)$$

$$\chi(1,2) \equiv \tfrac{1}{\sqrt{2}}\big[\chi^{+}(1,2) + \chi^{-}(1,2)\big]$$

  - Then:

$$\begin{aligned}
\boldsymbol{\Psi}_B(1,2) &= \tfrac{1}{\sqrt{2}}\big[\,\Psi(\vec{r}_1,\vec{r}_2)\cdot\chi(1,2) + \Psi(\vec{r}_2,\vec{r}_1)\cdot\chi(2,1)\,\big] \\
&= \tfrac{1}{\sqrt{2}}\Big\{\big[\,\tfrac{1}{\sqrt{2}}\big(\Psi^{+}(1,2) + \Psi^{-}(1,2)\big)\cdot\tfrac{1}{\sqrt{2}}\big(\chi^{+}(1,2) + \chi^{-}(1,2)\big)\,\big] \\
&\qquad + \big[\,\tfrac{1}{\sqrt{2}}\big(\Psi^{+}(1,2) - \Psi^{-}(1,2)\big)\cdot\tfrac{1}{\sqrt{2}}\big(\chi^{+}(1,2) - \chi^{-}(1,2)\big)\,\big]\Big\} \\
&= \tfrac{1}{2\sqrt{2}}\Big\{\big[\,\Psi^{+}(1,2)\cdot\chi^{+}(1,2) + \Psi^{-}(1,2)\cdot\chi^{+}(1,2) + \Psi^{+}(1,2)\cdot\chi^{-}(1,2) + \Psi^{-}(1,2)\cdot\chi^{-}(1,2)\,\big] \\
&\qquad + \big[\,\Psi^{+}(1,2)\cdot\chi^{+}(1,2) - \Psi^{-}(1,2)\cdot\chi^{+}(1,2) - \Psi^{+}(1,2)\cdot\chi^{-}(1,2) + \Psi^{-}(1,2)\cdot\chi^{-}(1,2)\,\big]\Big\}
\end{aligned}$$

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Lots of Identical Particles

(Anti)Symmetrization

- Consider the case of just two particles
  - Define some simplifying notation

positional (in "real" space) | all else (in "internal" space)

$$\Psi^{\pm}(1,2) := \tfrac{1}{\sqrt{2}}\big[\Psi(\vec r_1,\vec r_2) \pm \Psi(\vec r_2,\vec r_1)\big] \qquad \chi^{\pm}(1,2) := \tfrac{1}{\sqrt{2}}\big[\chi(1,2) \pm \chi(2,1)\big]$$

$$\Psi^{\pm}(\vec r_1,\vec r_2) \equiv \pm\Psi^{\pm}(\vec r_2,\vec r_1) \qquad \chi^{\pm}(1,2) \equiv \pm\chi^{\pm}(2,1)$$

$$\Psi(\vec r_1,\vec r_2) \equiv \tfrac{1}{\sqrt{2}}\big[\Psi^{+}(1,2) + \Psi^{-}(1,2)\big] \qquad \chi(1,2) \equiv \tfrac{1}{\sqrt{2}}\big[\chi^{+}(1,2) + \chi^{-}(1,2)\big]$$

- Then:

$$\begin{aligned}
\boldsymbol{\Psi}_B(1,2) &= \tfrac{1}{\sqrt{2}}\big[\,\Psi(\vec r_1,\vec r_2)\cdot\chi(1,2) + \Psi(\vec r_2,\vec r_1)\cdot\chi(2,1)\,\big]\\
&= \tfrac{1}{2\sqrt{2}}\Big\{\big[\,\Psi^{+}(1,2)\cdot\chi^{+}(1,2) + \Psi^{-}(1,2)\cdot\chi^{+}(1,2) + \Psi^{+}(1,2)\cdot\chi^{-}(1,2) + \Psi^{-}(1,2)\cdot\chi^{-}(1,2)\,\big]\\
&\qquad + \big[\,\Psi^{+}(1,2)\cdot\chi^{+}(1,2) - \Psi^{-}(1,2)\cdot\chi^{+}(1,2) - \Psi^{+}(1,2)\cdot\chi^{-}(1,2) + \Psi^{-}(1,2)\cdot\chi^{-}(1,2)\,\big]\Big\}\\
&= \tfrac{1}{2\sqrt{2}}\Big\{\,2\,\Psi^{+}(1,2)\cdot\chi^{+}(1,2) + 2\,\Psi^{-}(1,2)\cdot\chi^{-}(1,2)\,\Big\}\\
&= \tfrac{1}{\sqrt{2}}\big[\,\Psi^{+}(1,2)\cdot\chi^{+}(1,2) + \Psi^{-}(1,2)\cdot\chi^{-}(1,2)\,\big]
\end{aligned}$$

Lots of Identical Particles

(Anti)Symmetrization

- In the case of just two particles:
  - Two indistinguishable bosons

$$\mathbf{\Psi}_B(1,2) = \tfrac{1}{\sqrt{2}}\big[\,\Psi(\vec{r}_1,\vec{r}_2)\cdot\chi(1,2) + \Psi(\vec{r}_2,\vec{r}_1)\cdot\chi(2,1)\,\big]$$
$$= \tfrac{1}{\sqrt{2}}\big[\,\Psi^+(1,2)\cdot\chi^+(1,2) + \Psi^-(1,2)\cdot\chi^-(1,2)\,\big]$$

  - Two indistinguishable fermions

$$\mathbf{\Psi}_F(1,2) = \tfrac{1}{\sqrt{2}}\big[\,\Psi(\vec{r}_1,\vec{r}_2)\cdot\chi(1,2) - \Psi(\vec{r}_2,\vec{r}_1)\cdot\chi(2,1)\,\big]$$
$$= \tfrac{1}{\sqrt{2}}\big[\,\Psi^+(1,2)\cdot\chi^-(1,2) + \Psi^-(1,2)\cdot\chi^+(1,2)\,\big]$$

- Either way, for either of the two (only) kinds of particles
  - The (anti)symmetrized wave-function is a linear combination of two terms, not factorizable as a simple product of two factors
  - In space of 3 (& more) dimensions, angular momenta can only be
    - either integral (for bosonic states) or half-integral (for fermionic states)

Lots of Identical Particles

Exchange Consequences

- Considering (still) only two particles

$$\hat{H}\Psi(\vec{r}_1,\vec{r}_2) = E\Psi(\vec{r}_1,\vec{r}_2) \qquad \hat{H} = -\frac{\hbar^2}{2M}[\vec{\nabla}_1^2 + \vec{\nabla}_2^2]$$

$$\Psi(\vec{r}_1,\vec{r}_2) = e^{i\vec{k}\cdot\vec{r}_1}e^{i\vec{k}'\cdot\vec{r}_2} \qquad \chi(1,2) = 1$$

Bosons

$$\Psi_B(1,2) = \frac{1}{\sqrt{2}}[e^{i\vec{k}\cdot\vec{r}_1}e^{i\vec{k}'\cdot\vec{r}_2} + e^{i\vec{k}\cdot\vec{r}_2}e^{i\vec{k}'\cdot\vec{r}_1}]$$

$$= \frac{1}{\sqrt{2}}e^{i(\vec{k}+\vec{k}')\cdot\vec{R}}[e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} + e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}}]$$

$$= \sqrt{2}\,e^{i(\vec{k}+\vec{k}')\cdot\vec{R}}\cos[(\vec{k}-\vec{k}')\cdot\vec{r}]$$

Fermions

$$\Psi_F(1,2) = \frac{1}{\sqrt{2}}[e^{i\vec{k}\cdot\vec{r}_1}e^{i\vec{k}'\cdot\vec{r}_2} - e^{i\vec{k}\cdot\vec{r}_2}e^{i\vec{k}'\cdot\vec{r}_1}]$$

$$= \frac{1}{\sqrt{2}}e^{i(\vec{k}+\vec{k}')\cdot\vec{R}}[e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} - e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}}]$$

$$= \sqrt{2}i\,e^{i(\vec{k}+\vec{k}')\cdot\vec{R}}\sin[(\vec{k}-\vec{k}')\cdot\vec{r}]$$

  - so, the probability densities (spatial probability distributions) are

symmetric (bosons) | **antisymmetric** (fermions)

  - which is an observable particle exchange effect
- Additional dynamics ($\chi \neq 1$) complicates this significantly
  - …but leaves the boson/fermion disctinction just as observable

Lots of Identical Particles

Exchange Consequences

- Considering a (neutral) H_2 molecule w/ fixed nuclei, A and B

$$\widehat{H} = \sum_{j=1}^{2} \Big\{ -\frac{\hbar^2}{2M_j} \vec{\nabla}_j^{\,2} + W(\vec{r}_j - \vec{R}_A) + W(\vec{r}_j - \vec{R}_B) \Big\} + V(\vec{r}_1 - \vec{r}_2) \;\; = \widehat{H}_0 + \widehat{H}'$$

$$\widehat{H}_0 = \underbrace{-\frac{\hbar^2}{2M_1}\vec{\nabla}_1^{\,2} + W(\vec{r}_1 - \vec{R}_A)}_{\widehat{h}_1} \underbrace{-\frac{\hbar^2}{2M_2}\vec{\nabla}_2^{\,2} + W(\vec{r}_2 - \vec{R}_B)}_{\widehat{h}_2} \qquad \widehat{h}_j\,\phi_j(\vec{r}_j) = \epsilon_j\,\phi_j(\vec{r}_j)$$

$$\widehat{H}_0\,\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) = (\epsilon_1 + \epsilon_2)\,\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)$$

$$\widehat{H}' = W(\vec{r}_1 - \vec{R}_B) + W(\vec{r}_2 - \vec{R}_A) + V(\vec{r}_1 - \vec{r}_2)$$

- Because of (anti)symmetrization

$$\psi_\pm(\vec{r}_1, \vec{r}_2) := \big[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) \pm \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\big] \qquad E_\pm := \frac{\langle\psi_\pm|\widehat{H}|\psi_\pm\rangle}{\langle\psi_\pm|\psi_\pm\rangle} \qquad \langle\phi_j|\phi_j\rangle = 1$$

$$\langle\psi_\pm|\psi_\pm\rangle = 2\big(1 \pm |\langle\phi_1|\phi_2\rangle|^2\big)$$

$$E_\pm = \frac{\langle\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)|\widehat{H}|\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\rangle \pm \boxed{\langle\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)|\widehat{H}|\phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\rangle}}{1 \pm |\langle\phi_1|\phi_2\rangle|^2}$$

$$E_+ - E_- \approx 2\mathscr{E} \qquad \text{if } \; |\langle\phi_1|\phi_2\rangle| \ll 1 \qquad \boxed{\mathscr{E} = \langle\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)|V|\phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\rangle}$$

Lots of Identical Particles

Particle Operators

- Remember LHO?

$$|\Psi\rangle_{\text{LHO}} = \sum_{n=0}^{\infty} c_n |n\rangle_{\text{LHO}} = \sum_{n=0}^{\infty} c_n \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle_{\text{LHO}} \qquad \hat{a}|0\rangle_{\text{LHO}} = 0 \qquad [\hat{a}, \hat{a}^\dagger] = 1$$

- Now generalize to 3D, i.e., three independent LHO's

$$\begin{aligned} |\Psi\rangle_{\text{3DHO}} &= \sum_{n_1,n_2,n_3=0}^{\infty} c_{n_1,n_2,n_3} |n_1, n_2, n_3\rangle_{\text{3DHO}} \\ &= \sum_{n_1,n_2,n_3=0}^{\infty} c_{n_1,n_2,n_3} \frac{(\hat{a}_1^\dagger)^{n_1}(\hat{a}_2^\dagger)^{n_2}(\hat{a}_3^\dagger)^{n_3}}{\sqrt{n_1!\,n_2!\,n_3!}} |0,0,0\rangle_{\text{3DHO}} \end{aligned}$$

$$\hat{a}_1 |0,0,0\rangle_{\text{3DHO}} = \hat{a}_2 |0,0,0\rangle_{\text{3DHO}} = \hat{a}_3 |0,0,0\rangle_{\text{3DHO}} = 0$$

$$[\hat{a}_1, \hat{a}_1^\dagger] = [\hat{a}_2, \hat{a}_2^\dagger] = [\hat{a}_3, \hat{a}_3^\dagger] = 1 \qquad \text{(all other commutators vanishing)}$$

- Readily generalized to arbitrarily many LHO's

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Lots of Identical Particles

Particle Operators

- Think of $\hat{a}_j^\dagger$ ($\hat{a}_j$) as creating (annihilating) a particle in the state j

$$|\Psi_B\rangle_{3DHO} = \sum_{n_1,n_2,n_3=0}^{\infty} c_{n_1,n_2,n_3} \underbrace{|n_1,n_2,n_3\rangle_B}_{\text{totally symmetric}}$$

$$|n_1,n_2,n_3\rangle_B := \frac{1}{\sqrt{6}}\big[\,|n_1,n_2,n_3\rangle + |n_3,n_1,n_2\rangle + |n_2,n_3,n_1\rangle + |n_1,n_3,n_2\rangle + |n_3,n_2,n_1\rangle + |n_2,n_1,n_3\rangle\,\big]$$

- Now consider

$$\begin{aligned}
\hat{a}_1^\dagger\,\hat{a}_2^\dagger\,|n_1,n_2,n_3\rangle_B &= \hat{a}_1^\dagger\,\sqrt{n_2+1}\,|n_1,n_2+1,n_3\rangle \\
&= \sqrt{n_2+1}\sqrt{n_1+1}\,|n_1+1,n_2+1,n_3\rangle \\
&= \sqrt{n_1+1}\sqrt{n_2+1}\,|n_1+1,n_2+1,n_3\rangle \\
&= \sqrt{n_1+1}\,\hat{a}_2^\dagger\,|n_1+1,n_2,n_3\rangle \\
&= \hat{a}_2^\dagger\,\hat{a}_1^\dagger\,|n_1,n_2,n_3\rangle
\end{aligned}$$

$$\hat{a}_1^\dagger\,\hat{a}_2^\dagger = \hat{a}_2^\dagger\,\hat{a}_1^\dagger$$

$$\big[\,\hat{a}_i^\dagger,\hat{a}_j^\dagger\,\big] = 0 \qquad \big[\,\hat{a}_i,\hat{a}_j\,\big] = 0 \qquad \big[\,\hat{a}_i,\hat{a}_j^\dagger\,\big] = \delta_{i,j}\,\mathbb{1}$$

- D'oh!

$$\hat{a}_j = \sqrt{\frac{M\omega}{\hbar}}\Big[x_j + i\frac{\hbar}{M\omega}\frac{\partial}{\partial x_j}\Big] \qquad [x_i,x_j] = 0 = \Big[\frac{\partial}{\partial x_i},\frac{\partial}{\partial x_j}\Big] \qquad \Big[\frac{\partial}{\partial x_i},x_j\Big] = \delta_{i,j}$$

commuting coordinates

Lots of Identical Particles

Particle Operators

- Generalize this to bosonic particles
  - The Hilbert space for each single particle need not be a simple "ladder"
  - and may depend on various labels, integral and continuous

$$\hat{a}_\alpha,\ \hat{a}_\beta^\dagger,\quad \alpha,\beta = \text{“1”}, \text{“2”}, \ldots \qquad \hat{N}_\alpha := \hat{a}_\alpha^\dagger \hat{a}_\alpha \qquad [\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha,\beta}\mathbb{1}$$

$$|0,0,\ldots,0,\ldots\rangle\ :\ \hat{a}_\alpha\,|0,0,\ldots,0,\ldots\rangle = 0 \quad \forall\alpha$$

  - The Hilbert (Fock) space consists of linear combinations of

$$|n_1,n_2,\ldots,n_\alpha,\ldots\rangle := \frac{(\hat{a}_1^\dagger)^{n_1}(\hat{a}_2^\dagger)^{n_2}\cdots(\hat{a}_\alpha^\dagger)^{n_\alpha}\cdots}{\sqrt{n_1!\,n_2!\cdots n_\alpha!\cdots}}\,|0,0,\ldots,0,\ldots\rangle \qquad n_1,n_2,\ldots,n_\alpha,\cdots \in \mathbb{N}$$

  - and…

$$\hat{a}_\alpha\,|n_1,n_2,\ldots,n_\alpha,\ldots\rangle = \sqrt{n_\alpha}\,|n_1,n_2,\ldots,(n_\alpha-1),\ldots\rangle \qquad \text{annihilation}$$

$$\hat{a}_\alpha^\dagger\,|n_1,n_2,\ldots,n_\alpha,\ldots\rangle = \sqrt{n_\alpha+1}\,|n_1,n_2,\ldots,(n_\alpha+1),\ldots\rangle \qquad \text{creation}$$

Lots of Identical Particles

Particle Operators

- Now consider the fermionic analogue

$$|0\rangle_F \ : \ \hat{c}\,|0\rangle_F = 0 \qquad \hat{c}^\dagger\,|0\rangle_F = |1\rangle_F \qquad \hat{c}\,|1\rangle_F = |0\rangle_F$$

- Then

$$(\hat{c})^2\,|0\rangle_F = \hat{c}\left(\hat{c}\,|0\rangle_F\right) = 0 \qquad (\hat{c})^2\,|1\rangle_F = \hat{c}\left(\hat{c}\,|1\rangle_F\right) = \hat{c}\,|0\rangle_F = 0 \qquad (\hat{c})^2 = 0$$

- Pauli's exclusion principle: $\nexists\,|2\rangle_F \ : \ \hat{c}^\dagger\,|1\rangle_F = 0$

$$(\hat{c}^\dagger)^2\,|0\rangle_F = \hat{c}^\dagger\left(\hat{c}^\dagger\,|0\rangle_F\right) = \hat{c}^\dagger\,|1\rangle_F = 0 \qquad (\hat{c}^\dagger)^2\,|1\rangle_F = \hat{c}^\dagger\left(\hat{c}^\dagger\,|1\rangle_F\right) = 0 \qquad (\hat{c}^\dagger)^2 = 0$$

Lots of Identical Particles

Particle Operators

- Now consider the fermionic analogue

  $|0\rangle$

- Th

  $(\hat{c}$ $= 0$

- Pa

  $(\hat{c}$ $= 0$

This is just like with the angular momentum operators

$$\hat{J}_\pm\,|j,m\rangle = \sqrt{j(j+1)-m(m\pm1)}\,|j,m\pm1\rangle$$

$$\hat{J}_\pm\,|\tfrac{1}{2},+\tfrac{1}{2}\rangle = \sqrt{\tfrac{3}{4}-\tfrac{1}{2}(\tfrac{1}{2}\pm1)}\,|\tfrac{1}{2},\tfrac{1}{2}\pm1\rangle = \begin{cases}\sqrt{0}\,|\tfrac{1}{2},\tfrac{3}{4}\rangle \equiv 0\\ \tfrac{1}{\sqrt{2}}\,|\tfrac{1}{2},-\tfrac{1}{2}\rangle\end{cases}$$

$$\hat{J}_\pm\,|\tfrac{1}{2},-\tfrac{1}{2}\rangle = \sqrt{\tfrac{3}{4}-(-\tfrac{1}{2})(-\tfrac{1}{2}\pm1)}\,|\tfrac{1}{2},-\tfrac{1}{2}\pm1\rangle = \begin{cases}\tfrac{1}{\sqrt{2}}\,|\tfrac{1}{2},+\tfrac{1}{2}\rangle\\ \sqrt{0}\,|\tfrac{1}{2},-\tfrac{3}{4}\rangle \equiv 0\end{cases}$$

So, you may think in terms of the analogy

$$\hat{c} \sim \hat{J}_- \qquad \hat{c}^\dagger \sim \hat{J}_+ \qquad |0\rangle_F \sim |\tfrac{1}{2},-\tfrac{1}{2}\rangle \qquad |1\rangle_F \sim |\tfrac{1}{2},+\tfrac{1}{2}\rangle$$

...except, nothing is spinning here.

Lots of Identical Particles

Particle Operators

- Now consider the fermionic analogue

$$|0\rangle_F \ : \ \hat{c}\,|0\rangle_F = 0 \qquad \hat{c}^\dagger\,|0\rangle_F = |1\rangle_F \qquad \hat{c}\,|1\rangle_F = |0\rangle_F$$

- Then

$$(\hat{c})^2\,|0\rangle_F = \hat{c}\big(\hat{c}\,|0\rangle_F\big) = 0 \qquad (\hat{c})^2\,|1\rangle_F = \hat{c}\big(\hat{c}\,|1\rangle_F\big) = \hat{c}\,|0\rangle_F = 0 \qquad (\hat{c})^2 = 0$$

- Pauli's exclusion principle: $\nexists\,|2\rangle_F \ : \ \hat{c}^\dagger\,|1\rangle_F = 0$

$$(\hat{c}^\dagger)^2\,|0\rangle_F = \hat{c}^\dagger\big(\hat{c}^\dagger\,|0\rangle_F\big) = \hat{c}^\dagger\,|1\rangle_F = 0 \qquad (\hat{c}^\dagger)^2\,|1\rangle_F = \hat{c}^\dagger\big(\hat{c}^\dagger\,|1\rangle_F\big) = 0 \qquad (\hat{c}^\dagger)^2 = 0$$

- Now calculate:

$$[\hat{c}\,\hat{c}^\dagger \pm \hat{c}^\dagger\,\hat{c}]\,|0\rangle_F = \hat{c}\,\hat{c}^\dagger\,|0\rangle_F \pm \hat{c}^\dagger\,\hat{c}\,|0\rangle_F = \hat{c}\,|1\rangle_F \pm \hat{c}^\dagger\cdot 0 = |0\rangle_F$$

$$[\hat{c}\,\hat{c}^\dagger \pm \hat{c}^\dagger\,\hat{c}]\,|1\rangle_F = \hat{c}\,\hat{c}^\dagger\,|1\rangle_F \pm \hat{c}^\dagger\,\hat{c}\,|1\rangle_F = \hat{c}\cdot 0 \pm \hat{c}^\dagger\,|0\rangle_F = \pm\,|1\rangle_F$$

- So:

$$\{\hat{c},\hat{c}^\dagger\} := \hat{c}\,\hat{c}^\dagger + \hat{c}^\dagger\,\hat{c} = \mathbb{1}$$

canonical *anti* commutation

$$[\hat{c},\hat{c}^\dagger]\,|\nu\rangle_F = (-1)^\nu\,|\nu\rangle_F$$

fermion/boson parity operator

Lots of Identical Particles

Particle Operators

- Generalize this to multiple fermions

$$\hat{c}_\alpha,\ \hat{c}^\dagger_\beta,\ \ \alpha,\beta = \text{“1”}, \text{“2”}, \ldots \qquad \hat{N}_\alpha := \hat{c}^\dagger_\alpha \hat{c}_\alpha \qquad \{\hat{c}_\alpha, \hat{c}^\dagger_\beta\} = \delta_{\alpha,\beta}\mathbb{1}$$

- Every linear combination of two fermionic states is fermionic
  - and must obey Pauli's principle:

$$0 \stackrel{!}{=} (a\hat{c}^\dagger_1 + b\hat{c}^\dagger_2)^2 = a^2\cancel{(\hat{c}^\dagger_1)^2} + ab(\hat{c}^\dagger_1\,\hat{c}^\dagger_2 + \hat{c}^\dagger_2\,\hat{c}^\dagger_1) + b^2\cancel{(\hat{c}^\dagger_2)^2}$$

$$0 \stackrel{!}{=} (a\hat{c}_1 + b\hat{c}_2)^2 = a^2\cancel{(\hat{c}_1)^2} + ab(\hat{c}_1\,\hat{c}_2 + \hat{c}_2\,\hat{c}_1) + b^2\cancel{(\hat{c}_2)^2}$$

  - so that

$$\{\hat{c}_\alpha, \hat{c}_\beta\} = 0 = \{\hat{c}^\dagger_\alpha, \hat{c}^\dagger_\beta\} \qquad \{\hat{c}_\alpha, \hat{c}^\dagger_\beta\} = \delta_{\alpha,\beta}\mathbb{1}$$

$$\hat{c}_\alpha\,\hat{c}_\beta = -\hat{c}_\beta\,\hat{c}_\alpha \qquad \hat{c}^\dagger_\alpha\,\hat{c}^\dagger_\beta = -\hat{c}^\dagger_\beta\,\hat{c}^\dagger_\alpha \qquad \hat{c}_\alpha\,\hat{c}^\dagger_\beta = \delta_{\alpha,\beta}\mathbb{1} - \hat{c}^\dagger_\beta\,\hat{c}_\alpha$$

  - Note: $\hat{c}^\dagger_\alpha$ and $\hat{c}_\alpha$ cannot be represented as linear combinations of ordinary coordinates and derivatives with respect to such coordinates
    - …but *are* linear combinations of *anticommuting coordinates* and derivatives with respect to such, which are then themselves *anticommuting operators*

Lots of Identical Particles

Particle Operators

- Generalize this to multiple fermions

$$\hat{c}_\alpha,\ \hat{c}^\dagger_\beta,\quad \alpha,\beta = \text{“1”},\text{“2”},\ldots \qquad \hat{N}_\alpha := \hat{c}^\dagger_\alpha \hat{c}_\alpha \qquad \{\hat{c}_\alpha, \hat{c}^\dagger_\beta\} = \delta_{\alpha,\beta}\mathbb{1}$$

  - with all other *anticommutators* vanishing
- As before,

$$|0,0,\ldots,0,\ldots\rangle \ :\quad \hat{c}_\alpha\,|0,0,\ldots,0,\ldots\rangle = 0 \quad \forall\alpha$$

  - The Hilbert (Fock) space consists of linear combinations of

$$|\nu_1,\nu_2,\ldots,\nu_\alpha,\ldots\rangle := (\hat{c}^\dagger_1)^{\nu_1}(\hat{c}^\dagger_2)^{\nu_2}\cdots(\hat{c}^\dagger_\alpha)^{\nu_\alpha}\cdots|0,0,\ldots,0,\ldots\rangle$$

$$\nu_1,\nu_2,\ldots,\nu_\alpha,\cdots \in \{0,1\}$$

  - and

$$\hat{c}_\alpha\,|\nu_1,\nu_2,\ldots,\nu_\alpha,\ldots\rangle = |\nu_1,\nu_2,\ldots,(\nu_\alpha - 1),\ldots\rangle \qquad \textbf{annihilation}$$

$$\hat{c}^\dagger_\alpha\,|\nu_1,\nu_2,\ldots,\nu_\alpha,\ldots\rangle = |\nu_1,\nu_2,\ldots,(\nu_\alpha + 1),\ldots\rangle \qquad \textbf{creation}$$

  - This notation is too spacious: on the average, half the labels are “0”

Lots of Identical Particles

Particle Operators

- Modify notation:

$$\hat{c}^\dagger_\alpha\,|\mathbf{0}\rangle = \hat{c}^\dagger_\alpha\,|0,0,\ldots,\underset{\alpha}{0},\ldots\rangle = |0,0,\ldots,\underset{\alpha}{1},\ldots\rangle =: |\alpha\rangle$$

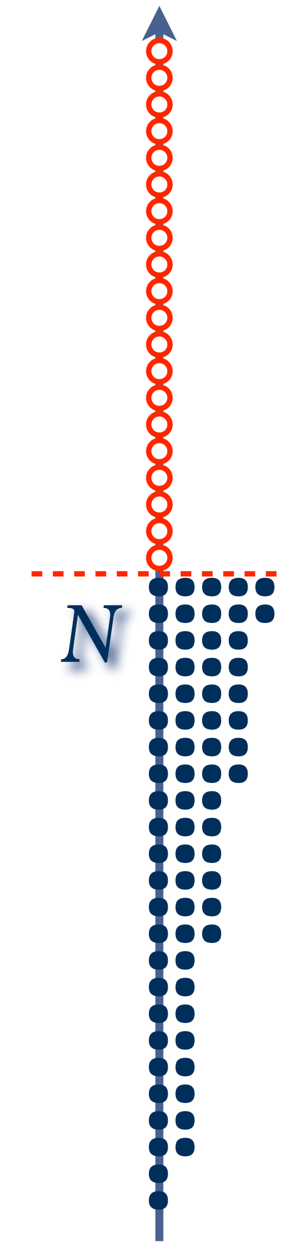
$$\hat{c}^\dagger_\alpha\,\hat{c}^\dagger_\beta\,|\mathbf{0}\rangle = \hat{c}^\dagger_\alpha\,|\beta\rangle = |\alpha\beta\rangle \qquad \alpha\neq\beta$$

$$\hat{c}^\dagger_\beta\,\hat{c}^\dagger_\alpha\,|\mathbf{0}\rangle = |\beta\alpha\rangle = -\,|\alpha\beta\rangle = -\hat{c}^\dagger_\alpha\,\hat{c}^\dagger_\beta\,|\mathbf{0}\rangle \qquad \{\hat{c}^\dagger_\alpha,\hat{c}^\dagger_\beta\} = 0$$

$$|\alpha\alpha\rangle \equiv 0 \quad\Leftrightarrow\quad (\hat{c}^\dagger_\alpha)^2 = 0$$

- The natural ground state of a multi-fermion system is

$$|F\rangle = \prod_{\text{“}\alpha\leqslant N\text{”}} \hat{c}^\dagger_\alpha\,|\mathbf{0}\rangle \qquad \alpha = (a,\sigma) \qquad \langle\vec{r}|\alpha\rangle = \Psi_a(\vec{r})\chi_\sigma$$



$$\boldsymbol{\psi}(\vec{r}) := \sum_\alpha \langle\vec{r}|\alpha\rangle\hat{c}_\alpha = \sum_{(a,\sigma)} \Psi_a(\vec{r})\chi_\sigma\hat{c}_{(a,\sigma)} \qquad \boldsymbol{\psi}_\sigma(\vec{r}) := \sum_a \langle\vec{r}|(a,\sigma)\rangle\hat{c}_{(a,\sigma)} = \chi_\sigma\sum_a \Psi_a(\vec{r})\hat{c}_{(a,\sigma)}$$

$$\boldsymbol{\psi}^\dagger(\vec{r}) = \sum_\alpha \langle\alpha|\vec{r}\rangle\hat{c}^\dagger_\alpha = \sum_{(a,\sigma)} \Psi^*_a(\vec{r})\chi_\sigma\hat{c}^\dagger_{(a,\sigma)} \qquad \boldsymbol{\psi}^\dagger_\sigma(\vec{r}) = \sum_a \langle(a,\sigma)|\vec{r}\rangle\hat{c}^\dagger_{(a,\sigma)} = \chi^*_\sigma\sum_a \Psi^*_a(\vec{r})\hat{c}^\dagger_{(a,\sigma)}$$

$$\hat{N} = \int \mathrm{d}^3\vec{r}\;\underbrace{\boldsymbol{\psi}^\dagger(\vec{r})\,\boldsymbol{\psi}(\vec{r})}_{n(\vec{r})} \qquad \hat{N}_\sigma = \int \mathrm{d}^3\vec{r}\;\underbrace{\boldsymbol{\psi}^\dagger_\sigma(\vec{r})\,\boldsymbol{\psi}_\sigma(\vec{r})}_{n_\sigma(\vec{r})}$$

Lots of Identical Particles

Particle Operators

- Owing to the Pauli exclusion principle

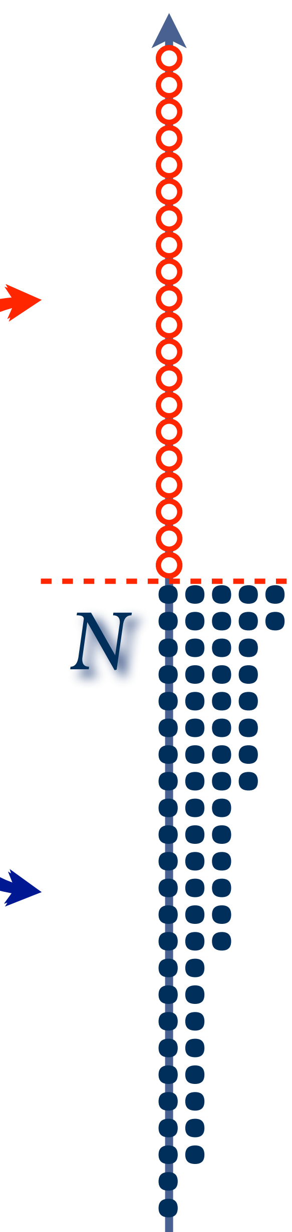
$$\underbrace{\hat{c}^\dagger_\beta\,|F\rangle}_{\text{“}\beta\leqslant N\text{”}} = \hat{c}^\dagger_\beta \prod_{\text{“}\alpha\leqslant N\text{”}} \hat{c}^\dagger_\alpha\,|\mathbf{0}\rangle = \hat{c}^\dagger_\beta \hat{c}^\dagger_1 \hat{c}^\dagger_2 \cdots \hat{c}^\dagger_\beta \cdots |\mathbf{0}\rangle = \pm\,\hat{c}^\dagger_1 \hat{c}^\dagger_2 \cdots (\hat{c}^\dagger_\beta)^2 \cdots |\mathbf{0}\rangle = 0$$

  - a creation operator for a particle that's “already there” acts as if it were an annihilation operator

- Redefine:

$$\hat{b}^\dagger_\alpha = \begin{cases} \hat{c}_\alpha & \text{if } \hat{c}^\dagger_\alpha\,|F\rangle = 0 \quad \text{“}\alpha \leqslant N\text{”} \\ \hat{c}^\dagger_\alpha & \text{if } \hat{c}_\alpha\,|F\rangle = 0 \quad \text{“}\alpha \geqslant N\text{”} \end{cases}$$

$$\hat{b}_\alpha = \begin{cases} \hat{c}^\dagger_\alpha & \text{if } \hat{c}^\dagger_\alpha\,|F\rangle = 0 \quad \text{“}\alpha \leqslant N\text{”} \\ \hat{c}_\alpha & \text{if } \hat{c}_\alpha\,|F\rangle = 0 \quad \text{“}\alpha \geqslant N\text{”} \end{cases}$$



  - This is also convenient for computations

$$\langle \hat{b}_\alpha \hat{b}^\dagger_\alpha \rangle_F = \langle F|\hat{b}_\alpha \hat{b}^\dagger_\alpha|F\rangle = \big|\,\hat{b}^\dagger_\alpha\,|F\rangle\,\big|^2 = 1$$

$$\langle \hat{c}_\alpha \hat{c}^\dagger_\alpha \rangle_F = 1 \quad \text{if “}\alpha \geq N\text{”} \qquad \langle \hat{c}^\dagger_\alpha \hat{c}_\alpha \rangle_F = 1 \quad \text{if “}\alpha \leq N\text{”}$$

$$:\hat{b}_\alpha \hat{b}^\dagger_\alpha: \;\stackrel{\text{def}}{=}\; \hat{b}^\dagger_\alpha \hat{b}_\alpha \;\stackrel{\text{def}}{=}\; :\hat{b}^\dagger_\alpha \hat{b}_\alpha: \longrightarrow \text{“normal ordering”}$$

Quantum Mechanics II

Now, go forth and calculate!!

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