Review single-particle states

- Notation $|...\rangle$
- ... 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

- 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 $P_{12} = P_{21}$ and $P_{12}^2 = 1$

- Hamiltonian for two particles is symmetric for $1 \Leftrightarrow 2$

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 same 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 $\displaystyle\sum_{\alpha_1\alpha_2...\alpha_N} |\alpha_1\alpha_2...\alpha_N)(\alpha_1\alpha_2...\alpha_N| = 1$
- Identical particles: symmetric or antisymmetric states
- Fermions: use antisymmetrizer $\displaystyle\mathcal{A} = \frac{1}{N!}\sum_p (-1)^p P$
- 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

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

- Not ordered

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

- 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

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

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 ⇒ occupation number representation
- Allow states in CVS with different # of particles ⇒ 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 .....