

Error Type	Pauli	Detected by...	Mathematical Logic
Bit Flip	X	Plaquette (Z) Check	$\{X, Z\} = 0$
Phase Flip	Z	Star (X) Check	$\{Z, X\} = 0$
Both	$Y = iXZ$	Both Checks	Anti-commutes with both

11 Class 6: Second Quantization and Many-Body Hamiltonians

11.1 The Complexity of the Many-Body Problem

In first quantization, an N -particle system is described by a wavefunction $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$ in $3N$ dimensions. For identical particles, we must manually enforce symmetry:

- **Bosons:** Ψ is symmetric under exchange.
- **Fermions:** Ψ is anti-symmetric (Pauli Exclusion).

As $N \rightarrow 10^5$, this representation becomes computationally intractable. Second quantization shifts our focus from *tracking individuals* to *tracking occupancy* of states via field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$.

11.2 Field Algebra and Statistics

The fundamental difference between bosons and fermions is encoded in their (anti-)commutation relations:

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}') \quad (\text{Bosons}) \quad (17)$$

$$\{\hat{\psi}_\sigma(\mathbf{r}), \hat{\psi}_{\sigma'}^\dagger(\mathbf{r}')\} = \delta_{\sigma\sigma'} \delta(\mathbf{r} - \mathbf{r}') \quad (\text{Fermions}) \quad (18)$$

where σ denotes the spin state. These relations ensure that the symmetry of the many-body state is automatically satisfied by the operator algebra.

11.3 Explicit Examples: 3-Particle States

11.3.1 3 Bosons in a Single Mode

For three identical bosons in the same spatial mode $\phi(\mathbf{r})$, the state is:

$$|3\rangle_B = \frac{(\hat{b}^\dagger)^3}{\sqrt{3!}} |0\rangle$$

The normalization factor $\sqrt{n!}$ accounts for the fact that there are $n!$ ways to arrange n identical bosons, yet they represent a single physical state.

11.3.2 3 Fermions in 2 Spin States (\uparrow, \downarrow)

Consider three fermions. By the Pauli Exclusion Principle, they cannot all occupy the same state. A typical configuration would be two in the lowest spatial mode $k = 0$ (one \uparrow , one \downarrow) and one in the first excited mode $k = 1$:

$$|\Psi\rangle_F = \hat{c}_{k=0,\uparrow}^\dagger \hat{c}_{k=0,\downarrow}^\dagger \hat{c}_{k=1,\sigma}^\dagger |0\rangle$$

Note that $\hat{c}_\sigma^\dagger \hat{c}_\sigma^\dagger = 0$ due to the anti-commutation $\{\hat{c}_\sigma^\dagger, \hat{c}_\sigma^\dagger\} = 2(\hat{c}_\sigma^\dagger)^2 = 0$. This naturally enforces the exclusion principle without requiring Slater determinants.

11.4 Transition to the Many-Body Hamiltonian

The many-body Hamiltonian is derived by taking the expectation value of the single-particle and two-particle operators over the field operators.

11.4.1 The Field Hamiltonian

In the continuum, the Hamiltonian is:

$$\hat{H} = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$$

11.4.2 Mapping to the Hubbard Model

To transition to a lattice (Classes 7-10), we expand the field operator in a basis of localized Wannier functions $w(\mathbf{r} - \mathbf{R}_i)$ at site i :

$$\hat{\psi}(\mathbf{r}) = \sum_i w(\mathbf{r} - \mathbf{R}_i) \hat{a}_i$$

Substituting this into the Field Hamiltonian and keeping only nearest-neighbor terms ($\langle i, j \rangle$) and on-site interactions ($i = j$) yields the Hubbard models:

1. **Bose-Hubbard:**

$$\hat{H}_{BH} = -t \sum_{\langle i, j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)$$

2. **Fermi-Hubbard (Spin-1/2):**

$$\hat{H}_{FH} = -t \sum_{\langle i, j \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

11.5 Summary of Principles

- **Kinetic Energy** \rightarrow **Hopping** (t): Represents particles tunneling between sites.
- **Interactions** \rightarrow **On-site Energy** (U): Represents the energy cost of two particles occupying the same localized Wannier state.