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 $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ 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 $N \to 10^5$, 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:

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

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

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 Deriving Algebra from Symmetrization

Consider two identical particles and two available states, $|\phi_1\rangle$ and $|\phi_2\rangle$. We define the many-body state by the order of creation: $|\Psi_{12}\rangle = \hat{a}_1^\dagger \hat{a}_2^\dagger |0\rangle$.

11.3.1 Exchange Symmetry

The physical requirement that the particles are identical implies:

$$\hat{a}_1^\dagger \hat{a}_2^\dagger |0\rangle = \zeta \hat{a}_2^\dagger \hat{a}_1^\dagger |0\rangle$$

where $\zeta = +1$ for Bosons and $\zeta = -1$ for Fermions. This leads directly to the fundamental relations:

$$[\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0 \quad \text{(Bosons)}$$

$$\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0 \quad \text{(Fermions)}$$

11.3.2 The Pauli Principle as Algebra

For Fermions, the case where $i = j$ yields:

$$\hat{a}_i^\dagger \hat{a}_i^\dagger + \hat{a}_i^\dagger \hat{a}_i^\dagger = 2(\hat{a}_i^\dagger)^2 = 0 \implies (\hat{a}_i^\dagger)^2 = 0$$

This operator identity ensures that no two fermions can occupy the same quantum state, as the probability amplitude for such a state is identically zero.

11.4 Derivation of the Bosonic Commutator

We can derive $[\hat{a}, \hat{a}^\dagger] = 1$ by requiring that second quantization remains consistent with the normalization of the first-quantized wavefunction $\Psi(x_1, x_2) = \phi(x_1)\phi(x_2)$.

11.4.1 The Action on Fock States

Let $|2\rangle = C(\hat{a}^\dagger)^2 |0\rangle$. To satisfy the requirement that the number operator $\hat{n} = \hat{a}^\dagger \hat{a}$ yields the number of particles as an eigenvalue:

$$\hat{n} |2\rangle = \hat{a}^\dagger \hat{a} |2\rangle = 2 |2\rangle$$

By substituting the ansatz $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger \hat{a} + k$, we find:

$$\hat{a}^\dagger \hat{a}(\hat{a}^\dagger \hat{a}^\dagger |0\rangle) = \hat{a}^\dagger(\hat{a}^\dagger \hat{a} + k)\hat{a}^\dagger |0\rangle + \hat{a}^\dagger k \hat{a}^\dagger |0\rangle = 2k(\hat{a}^\dagger)^2 |0\rangle$$

For the eigenvalue to be 2, we must have $k = 1$, which defines the fundamental commutator:

$$[\hat{a}, \hat{a}^\dagger] = 1$$

11.4.2 Normalization Constants

This algebra dictates the normalization of n-boson states. For a state $|n\rangle = C_n(\hat{a}^\dagger)^n |0\rangle$ to be normalized ($\langle n|n\rangle = 1$), the constant must be:

$$C_n = \frac{1}{\sqrt{n!}}$$

This $n!$ factor is the same one found in the symmetrization of n identical particles in first quantization.

11.5 Explicit Examples: 3-Particle States

11.5.1 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.

11.5.2 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 $k = 1$:

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

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

11.6 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.

11.6.1 The Field Hamiltonian

In the continuum, the Hamiltonian is:

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

11.6.2 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:**
$$\hat{H}_{BH} = -t\sum_{\langle i,j\rangle}\hat{b}^\dagger_i\hat{b}_j + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)$$

2. **Fermi-Hubbard (Spin-1/2):**
$$\hat{H}_{FH} = -t\sum_{\langle i,j\rangle,\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

11.7 Summary of Principles

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

12 Class 7: Solving the Bose-Hubbard Model

12.1 Physical Picture and the Ground State

The Bose-Hubbard model describes the competition between delocalization (kinetic energy) and localization (interaction energy).

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

- **Superfluid (SF) Limit ($U/t \to 0$):** The ground state is a product of single-particle coherent states. Particles are delocalized across all sites, characterized by long-range phase coherence. For N particles over M sites, the state is:

$$|\Psi_{SF}\rangle \propto \left(\sum_{i=1}^{M} \hat{b}_i^\dagger\right)^N |0\rangle$$

- **Mott Insulator (MI) Limit ($U/t \to \infty$):** At integer filling ($N/M = g$), the ground state is a Fock state $|g, g, \ldots, g\rangle$. Large U penalizes number fluctuations, "freezing" the atoms into a rigid lattice:

$$|\Psi_{MI}\rangle = \prod_{i=1}^{M} \frac{(\hat{b}_i^\dagger)^g}{\sqrt{g!}} |0\rangle = |g, g, \ldots, g\rangle$$

12.2 Hilbert Space Dimensionality

For N bosons in M sites, the size of the Hilbert space D is given by:

$$D(N, M) = \frac{(N + M - 1)!}{N!(M-1)!}$$

As N and M increase, D grows combinatorially:

- $N = 2, M = 2 \implies D = 3$
- $N = 3, M = 3 \implies D = 10$
- $N = 4, M = 4 \implies D = 35$
- $N = 5, M = 5 \implies D = 126$

12.3 Example for $N = 2, M = 2$

Choosing the occupancy basis $\mathcal{B} = \{|2,0\rangle, |1,1\rangle, |0,2\rangle\}$, we construct the Hamiltonian matrix. Note the bosonic enhancement factor $\sqrt{n+1}$ during hopping:

$$H = \begin{pmatrix} U & -\sqrt{2}t & 0 \\ -\sqrt{2}t & 0 & -\sqrt{2}t \\ 0 & -\sqrt{2}t & U \end{pmatrix}$$

12.4 Eigenvalues and the Energy Gap

For the $N = 2, M = 2$ system, the three eigenenergies of the Hamiltonian are:

$$\begin{aligned} E_g &= \frac{U - \sqrt{U^2 + 16t^2}}{2} \qquad \text{(Ground State)} \\ E_1 &= U \\ E_2 &= \frac{U + \sqrt{U^2 + 16t^2}}{2} \end{aligned}$$

The ground state $|\Psi_g\rangle$ reveals the transition from delocalized to localized behavior:

- **Superfluid Limit ($U \ll t$):** $|\Psi_g\rangle \approx \frac{1}{2}|2,0\rangle + \frac{1}{\sqrt{2}}|1,1\rangle + \frac{1}{2}|0,2\rangle$. This is a coherent state where each particle occupies the $\frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ orbital.
- **Mott Limit ($U \gg t$):** $|\Psi_g\rangle \to |1,1\rangle$. The system minimizes energy by ensuring exactly one boson per site, effectively "freezing" the atoms.

The energy gap Δ is the difference between the ground state and the first excited state that allows for particle transport.

$$\Delta = E_1 - E_g = U - \frac{U - \sqrt{U^2 + 16t^2}}{2}$$

In the Mott limit ($U/t \to \infty$), the gap $\Delta \to U$. This gap represents the energy cost to create a particle-hole excitation (moving an atom to an already occupied site). The existence of this gap is the hallmark of the Mott Insulating phase and explains the system's incompressibility.

12.5 Thermal Equilibrium

Solving for the complete set of eigenvalues E_n and eigenstates $|n\rangle$ allows us to describe the system's behavior under both equilibrium and non-equilibrium conditions.

At a finite temperature T, the system is not in a single pure state but is described by a density matrix $\hat{\rho}$. In the canonical ensemble, this is the thermal Gibbs state:

$$\hat{\rho}(T) = \frac{1}{Z} e^{-\hat{H}/k_B T} = \frac{1}{Z} \sum_n e^{-E_n/k_B T} |n\rangle \langle n|$$

where $Z = \sum_n e^{-E_n/k_B T}$ is the partition function.

The expectation value of any observable $\hat{O}$ (such as local occupancy or phase coherence) at temperature T is the weighted average over all eigenstates:

$$\langle \hat{O} \rangle_T = \mathrm{Tr}(\hat{\rho}\hat{O}) = \frac{1}{Z} \sum_n e^{-E_n/k_B T} \langle n| \hat{O} |n\rangle$$

As $T \to 0$, only the ground state E_g contributes, and we recover the zero-temperature properties discussed earlier. As T increases, higher-energy excitations (particle-hole pairs) blur the distinction between the SF and MI phases.

12.6 Quantum Dynamics: Unitary Time Evolution

If the system is prepared in an initial pure state $|\Psi(0)\rangle$ that is *not* an eigenstate (e.g., a quench experiment where U/t is suddenly changed), we use the eigenstates to evolve the wavefunction.

First, we project the initial state onto the eigenbasis:

$$|\Psi(0)\rangle = \sum_n c_n |n\rangle, \quad \text{where } c_n = \langle n|\Psi(0)\rangle$$

The state at any later time t is then given by:

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi(0)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |n\rangle$$

The time-dependent expectation value $\langle \hat{O} \rangle(t) = \langle \Psi(t)| \hat{O} |\Psi(t)\rangle$ will exhibit oscillations at frequencies corresponding to the energy differences (Bohr frequencies) $(E_n - E_m)/\hbar$. In our 2-site example, a sudden quench from $U \to \infty$ to $U = 0$ would result in the periodic "sloshing" of atoms between sites, known as Bloch oscillations or Josephson-like dynamics.

13 Class 8: Superfluid-Mott insulator Quantum Phase Transition

To quantify the phase transition and the change in the system's many-body "texture," we evaluate the following four observables.

1. On-site Number Fluctuations This local probe measures the variance of the occupancy at a single site:

$$\sigma_n^2 = \langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2$$

- **SF Phase:** High fluctuations. For $N = M = 2$, $\sigma_n^2 = 0.5$ at $U = 0$. Particles move freely, so the occupancy is uncertain.
- **MI Phase:** Fluctuations are suppressed ($\sigma_n^2 \to 0$ as $U/t \to \infty$). The interaction U "pins" exactly g atoms to each site.

2. One-Body Density Matrix (Phase Coherence) We define the spatial correlation function as $g_{ij} = \langle \hat{b}_i^\dagger \hat{b}_j \rangle$.

- **SF Phase:** Exhibits off-diagonal long-range order (ODLRO). g_{ij} remains constant even for large $|i - j|$, signaling global phase coherence.
- **MI Phase:** Correlations decay exponentially, $g_{ij} \sim e^{-|i-j|/\xi}$. Since particles are localized, the phase relationship between distant sites is lost.

3. Momentum Distribution (Time-of-Flight) This is the Fourier transform of the one-body density matrix, representing what is typically measured in the lab after releasing the atoms from the trap:

$$n(\mathbf{k}) = \frac{1}{M} \sum_{i,j} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \langle \hat{b}_i^\dagger \hat{b}_j \rangle$$

- **SF Phase:** Sharp, high-contrast interference (Bragg) peaks at $\mathbf{k} = 0$ and reciprocal lattice vectors.

- **MI Phase:** The interference pattern washes out, leaving a broad, incoherent background.

4. Compressibility Compressibility $\kappa = \partial n / \partial \mu$ describes how the density n responds to a change in chemical potential μ.

- **SF Phase:** $\kappa > 0$. The system is "soft" and can easily adjust its density.
- **MI Phase:** $\kappa = 0$. The system is "incompressible." Due to the energy gap Δ, adding or removing a particle requires a discrete jump in energy, creating the characteristic "Mott plateaus."

13.1 Determining the Critical Point

While true phase transitions only occur in the thermodynamic limit ($N, M \to \infty$), we can estimate the critical point $(U/t)_c$ by finding where the fluctuations drop significantly or where the energy gap opens. For the 1D Bose-Hubbard model at unit filling, the Berezinskii-Kosterlitz-Thouless (BKT) transition occurs at:

$$(U/t)_c \approx 3.29$$

In our 2-site model, the "crossover" happens when the diagonal and off-diagonal terms are of the same order, roughly $U \approx 2\sqrt{2}t$.

14 Class 9: From Hubbard Model to Gross-Pitaevskii equation

In previous lectures, we described bosons on discrete lattice sites using the site operators $\hat{a}_i$ and $\hat{a}_i^\dagger$. To bridge the gap to a continuous fluid description, we define the **Field Operator** $\hat{\psi}(\mathbf{r})$ as a superposition of these localized modes:

$$\hat{\psi}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})\hat{a}_i, \quad \hat{\psi}^\dagger(\mathbf{r}) = \sum_j \phi_j^*(\mathbf{r})\hat{a}_j^\dagger \tag{19}$$

where $\phi_i(\mathbf{r})$ are orthonormal localized basis functions (e.g., Wannier functions) centered at site i.

We can derive the commutation relation for the continuous field using the discrete bosonic rule $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$:

$$\begin{aligned}
[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] &= \left[\sum_i \phi_i(\mathbf{r})\hat{a}_i, \sum_j \phi_j^*(\mathbf{r}')\hat{a}_j^\dagger\right] && (20)\\
&= \sum_{i,j} \phi_i(\mathbf{r})\phi_j^*(\mathbf{r}')[\hat{a}_i, \hat{a}_j^\dagger] && (21)\\
&= \sum_{i,j} \phi_i(\mathbf{r})\phi_j^*(\mathbf{r}')\delta_{ij} && (22)\\
&= \sum_i \phi_i(\mathbf{r})\phi_i^*(\mathbf{r}') && (23)
\end{aligned}$$

By the **completeness relation** of an orthonormal basis, $\sum_i \phi_i(\mathbf{r})\phi_i^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$. Thus, the discrete granularity vanishes into a point-like continuous relation:

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}') \tag{24}$$

14.1 The Field Hamiltonian

In the continuum limit, the Bose-Hubbard summations $\sum_i$ become volume integrals $\int d\mathbf{r}$. The kinetic hopping maps to the gradient operator, and the on-site repulsion becomes a contact interaction strength g:

$$\hat{H} = \int d\mathbf{r} \left(\hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{g}{2}\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \right) \tag{25}$$

where $g = \frac{4\pi\hbar^2 a_s}{m}$ is determined by the s-wave scattering length a_s.

14.2 The Heisenberg Equation and the "Sifting" Effect

The dynamics of the field are governed by the Heisenberg equation. Because of the commutation relation derived in Section 1, the spatial integration in the Hamiltonian is removed:

$$i\hbar\frac{\partial\hat{\psi}(\mathbf{r})}{\partial t} = [\hat{\psi}(\mathbf{r}), \hat{H}] \tag{26}$$

When computing the commutator with the interaction term:

$$\left[\hat{\psi}(\mathbf{r}), \int \frac{g}{2}\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}')\, d\mathbf{r}' \right] = g\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \tag{27}$$

The delta function $\delta(\mathbf{r} - \mathbf{r}')$ acts as a "sifter," selecting only the operator value at point $\mathbf{r}$ and collapsing the integral. The resulting equation of motion is local:

$$i\hbar\frac{\partial\hat{\psi}(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}) \right) \hat{\psi}(\mathbf{r}) \tag{28}$$

14.3 The Mean-Field Approximation (Gross-Pitaevskii)

For a Bose-Einstein Condensate where $N \gg 1$, we replace the operator with a classical complex order parameter $\Psi(\mathbf{r}, t)$, the macroscopic wavefunction:

$$\hat{\psi}(\mathbf{r}, t) \approx \Psi(\mathbf{r}, t), \qquad \int |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = N \tag{29}$$

This yields the **Time-Dependent Gross-Pitaevskii Equation**:

$$i\hbar\frac{\partial\Psi(\mathbf{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g|\Psi(\mathbf{r}, t)|^2 \right] \Psi(\mathbf{r}, t) \tag{30}$$

Assuming the phase evolves as $\Psi(\mathbf{r}, t) = \Psi(\mathbf{r})e^{-i\mu t/\hbar}$, where μ is the **chemical potential**, we obtain the **Time-Independent GPE**:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g|\Psi(\mathbf{r})|^2 \right] \Psi(\mathbf{r}) = \mu\Psi(\mathbf{r}) \tag{31}$$

14.4 Thomas-Fermi Approximation

If $gN \gg \hbar\omega$, we neglect the kinetic energy term $\nabla^2\Psi$.

$$V(\mathbf{r}) + g|\Psi(\mathbf{r})|^2 = \mu \implies n(\mathbf{r}) = \max\left(0, \frac{\mu - V(\mathbf{r})}{g}\right) \tag{32}$$

For a harmonic trap $V(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$, the density profile $n(\mathbf{r})$ is an **inverted parabola**:

$$n(\mathbf{r}) = n_0\left(1 - \frac{r^2}{R_{TF}^2}\right), \quad R_{TF} = \sqrt{\frac{2\mu}{m\omega^2}} \tag{33}$$

where R_{TF} is the Thomas-Fermi radius where the density vanishes.