Physics 452:
Assignment 2: Lattice Models and Second Quantization

Instructor: Prof. Cheng Chin

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Part 1: Identical Particles and Second Quantization

1. **Density Distributions and Quantum Statistics:** Consider two particles occupying two spatial modes, $\phi_a(x)$ and $\phi_b(x)$. Assume the particles are at positions x_1 and x_2.

   (a) Write the two-particle density distribution function $P(x_1, x_2) = |\Psi(x_1, x_2)|^2$ for the following three cases:

   - Distinguishable Particles: The state is a simple product $\Psi = \phi_a(x_1)\phi_b(x_2)$.
   - Identical Bosons: The state is the normalized symmetric superposition.
   - Identical Fermions: The state is the normalized anti-symmetric superposition.

   Simplify the expressions for $P(x_1, x_2)$ using the interference term:

   $$I(x_1, x_2) = \phi_a(x_1)\phi_b(x_2)\phi_a^*(x_2)\phi_b^*(x_1) + \text{c.c.}$$

   (b) **Non-orthonormal modes:** What is the one-body density distribution $n(x)$ of the bosonic and fermionic particles if the two modes ϕ_a and ϕ_b are not orthonormal? Define your result in terms of the overlap $S = \int \phi_a^*(x)\phi_b(x)dx$.

   (c) **Algebraic derivation:** Based on the requirements for (anti-)symmetrization, derive the commutation relations $[\hat{a}, \hat{a}^\dagger] = 1$ and $\{\hat{c}, \hat{c}^\dagger\} = 1$.

2. **State Representations:** Consider a system of particles in the orthonormal spatial modes $\{\phi_a, \phi_b, \phi_c\}$.

   (a) **Bosonic Configuration:** Write the normalized 1st-quantization wavefunction $\Psi(r_1, r_2, r_3)$ for a system of 3 bosons where 2 particles occupy mode ϕ_a and 1 particle occupies mode ϕ_b. Then, write the equivalent state $|\Psi\rangle_B$ in 2nd-quantization Fock space using creation operators.

   (b) **Fermionic Configuration:** Write the normalized 1st-quantization wavefunction (Slater determinant) for 3 fermions occupying three different spatial modes $\{\phi_a, \phi_b, \phi_c\}$, assuming all have the same spin $\uparrow$. Write the equivalent state $|\Psi\rangle_F$ in 2nd-quantization.

   (c) **Operator Transitions:** Define the state $|\Phi\rangle$, representing 3 bosons all in state a. Determine the specific combination of creation and annihilation operators ($\hat{a}_a, \hat{a}_b, \hat{a}_a^\dagger, \hat{a}_b^\dagger$) required to transition from state $|\Phi\rangle$ to the bosonic state described in part (a). Explain the origin of the $\sqrt{3}$ factor in the 1st quantization picture.

3. **Unitary Mapping:** The transition between representations is governed by the field operator $\hat{\psi}^\dagger(r) = \sum_i \phi_i^*(r)\hat{a}_i^\dagger$.

(a) Show that the 1st-quantized N-particle state $\Psi(r_1, \ldots, r_N) = \frac{1}{\sqrt{N!}} \langle 0| \hat{\psi}(r_N) \ldots \hat{\psi}(r_1) |\Psi\rangle$ is equivalent to the projection of the Fock state onto the position basis.

(b) Prove that the total number operator $\hat{N} = \int \hat{\psi}^\dagger(r)\hat{\psi}(r)dr$ is invariant under a unitary transformation of the basis modes ϕ_i.

4. **Fermionic Anti-commutation:** Using the requirement that a 2-fermion wavefunction must be anti-symmetric under particle exchange, $\Psi(r_1, r_2) = -\Psi(r_2, r_1)$, prove that the corresponding creation operators must satisfy the anti-commutation relation $\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0$. What is the physical implication of the case $i = j$?

Part 2: The Bose-Hubbard Model

The Bose-Hubbard model is the standard theoretical framework for describing interacting bosons in a periodic potential, such as cold atoms in an optical lattice. The Hamiltonian is defined as:

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

where t represents the **hopping amplitude** (kinetic energy) and U represents the **on-site repulsion** (potential energy). This model captures the quantum phase transition between a **Superfluid (SF)** phase, where atoms are delocalized and phase-coherent, and a **Mott Insulator (MI)** phase, where atoms are localized due to strong interactions.

Setup: In class, we solved the $N = 2$ atoms, $M = 2$ sites case. In this part, you will extend the analysis to $N = 3$ bosons on $M = 3$ sites. Assume a 1D chain with **periodic boundary conditions**, meaning the sites form a ring where site 3 is adjacent to site 1.

5. **Hilbert Space Construction:** Determine the dimension D of the Hilbert space for $N = 3, M = 3$. List all basis states in the occupancy format $|n_1, n_2, n_3\rangle$.

6. **Hamiltonian Matrix:** Write down the $D \times D$ Hamiltonian matrix for the Bose-Hubbard model:

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

   Identify which matrix elements are enhanced by the bosonic factor $\sqrt{n+1}$.

7. **Ground State Limits:** Using a numerical solver or analytic arguments:

   (a) Find the ground state energy E_g and state vector $|\Psi_g\rangle$ for $U/t = 0$ and $U/t \to \infty$.

   (b) Calculate the on-site number fluctuation σ_n^2 for both limits. Compare these results with the $N = 2$ case. Does the fluctuation increase or decrease as N increases?

8. **Finite Size Scaling:** Plot the energy gap $\Delta = E_1 - E_g$ as a function of U/t. Discuss how one might use the scaling of this gap for $N = 2, 3, 4$ to estimate the critical point $(U/t)_c$ in the thermodynamic limit.

Part 3: From Fermi-Hubbard to Heisenberg model

Consider the Fermi-Hubbard model at **half-filling**. This corresponds to a system where the number of electrons equals the number of lattice sites ($N_e = M$), specifically with $N_\uparrow = M/2$ and $N_\downarrow = M/2$ electrons. The Hamiltonian is:

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

where t is the hopping amplitude, U is the on-site repulsion, $\hat{c}_{i\sigma}$ is the annihilation operator for an electron at site i with spin $\sigma \in \{\uparrow, \downarrow\}$, and $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ is the number operator.

9. **The Strong Coupling Limit and Scaling:** Assume $U \gg t$ and exactly one electron per site.

   (a) Show that second-order perturbation theory maps the model to the Heisenberg Hamiltonian $\hat{H}_{eff} = J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - 1/4)$ with $J = 4t^2/U$. Here, the spin vector is $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha,\beta} \hat{c}_{i\alpha}^\dagger \sigma_{\alpha\beta} \hat{c}_{i\beta}$, where σ are the Pauli matrices.

   (b) Determine the Hilbert space dimensions for the $S_z^{total} = 0$ sector (half-filling) for $N = 2, 4$, and 6 electrons in $M = N$ sites.

   (c) For $N = 2, M = 2$, write the Hamiltonian in matrix form using the basis states $\{|\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle\}$.

10. **Geometric Frustration in a Triangular Hubbard Cluster**

    In magnetic systems, "frustration" occurs when the geometric arrangement of sites prevents the simultaneous minimization of all local interaction energies. A classic example is the antiferromagnetic Heisenberg model on an equilateral triangle. If two spins align anti-parallel to satisfy their mutual bond, the third spin cannot be anti-parallel to both neighbors simultaneously. This leads to a highly correlated ground state with unique topological properties.

    Setup: Consider a system of $N = 3$ fermions on $M = 3$ sites arranged in an equilateral triangle. Assume each site couples to the other two equally with a hopping amplitude t and on-site repulsion U.

    (a) Determine the dimension of the Hilbert space for the $S_z^{total} = +1/2$ sector. (Hint: Consider the total number of ways to arrange two $\uparrow$ spins and one $\downarrow$ spin across the three sites).

    (b) Write the Hamiltonian in matrix form for the strong-coupling regime ($U \gg t$). Assume exactly one fermion per site (Mott limit) and use the effective exchange J. The effective Hamiltonian is given by:

    $$\hat{H}_{eff} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

    where the sum runs over all unique pairs $(1, 2), (2, 3)$, and $(3, 1)$.

    (c) Determine J and solve for the ground state energy and the state vector. By evaluating the spin-spin correlator $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ for any pair, justify whether the system exhibits ferromagnetic or anti-ferromagnetic tendencies. Discuss how the resulting value differs from a non-frustrated dimer and how it reflects the "frustrated" nature of the triangular geometry.