P452 Project 2: Simulation of Many-Body System

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Introduction

In this project, the goal is to develop a full-stack simulation tool to solve many-body systems. Examples are bosons, fermions and spins. You will perform diagonalization of systems with N-particles by hand for small number of particles $N = 2, 3...$ and by exact diagonalization package for $N \gg 4$. AI-assisted programming is encouraged.

Phase 1: Exact Diagonalization of the Heisenberg Model

The Heisenberg model is a cornerstone of condensed matter physics, providing a microscopic description of magnetism in localized electron systems. Unlike the Ising model, which only considers longitudinal spin components, the Heisenberg model accounts for the full $SU(2)$ symmetry of spin interactions. It describes how exchange coupling—originating from the Pauli exclusion principle and Coulomb repulsion—leads to collective phenomena such as ferromagnetism, anti-ferromagnetism, and quantum spin liquids. In this project, we focus on the $S = 1/2$ case, where quantum fluctuations are most pronounced. you will investigate how exchange interactions (J) and external magnetic fields (H) compete to define the ground state.

Theoretical Framework

The Hamiltonian for N spins (with $S = 1/2$) is:

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + H \sum_{i=1}^{N} \hat{S}_i^z \tag{1}$$

where $J > 0$ (anti-ferromagnetic) and H is the external magnetic field.

Operators: Spin operators relate to Pauli matrices $\hat{\sigma}$ via $\hat{S}^\alpha = \frac{\hbar}{2}\hat{\sigma}^\alpha$. In numerical units ($\hbar = 1$):

$$\hat{S}^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{S}^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{S}^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{2}$$

The interaction term expands to: $\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j = \hat{S}_i^z \hat{S}_j^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+)$.

Checkpoint 1.1: The 2-Site Dimer and Spin Frustration (Pen and Paper)

Solve a system of $N = 2$ spins ($S = 1/2$) in $N = 2$ sites with finite anti-ferromagnetic coupling $J > 0$ and external field H.

1. **Hilbert Space:** List the basis states using the z-projection notation $\{|\uparrow\rangle, |\downarrow\rangle\}$. What is the dimension of the Hilbert space?
2. **Hamiltonian Matrix:** Construct $\hat{H}$ in the matrix form. *Step-by-step: First, compute the diagonal elements using $\hat{S}^z$ and H, then use the ladder operators to find the off-diagonal "spin-flip" terms between $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$.*

3. **Ground State Transition:** Plot the eigen-energies vs H. Discuss the spin configuration of the ground state: Identify the critical field H_c where the energy of the fully polarized state $|\uparrow\uparrow\rangle$ drops below the singlet $|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

4. **Spin Frustration:** Consider 3 Heisenberg spins on a ring (triangular lattice) with $J > 0$ and $H = 0$. We will explore why such system is spin frustrated.

   - **Symmetry Reduction:** Show and explain how the 8 dimensional Hilbert space can be blocked into smaller matrices. (Hint: H commutes with the total spin projection S^z_{total}, which takes the values of $\pm 1/2$ and $\pm 3/2$.)
   - **Calculation:** Determine the Hamiltonian in the matrix form in each spin sector $S_z = \pm 3/2$ and $\pm 1/2$. Which spin sector(s) contains the ground state?
   - **Analysis:** Plot the eigenvalues vs H. Determine the ground state degeneracy at low $H = 0$ and high $H \gg J$ fields. Discuss how this relates to the physical concept of *frustration*, the inability to satisfy all anti-ferromagnetic bonds simultaneously in the ground state.

Checkpoint 1.2: From 2×2 to 6×6 Square Lattices

In this section, you will bridge the gap between manual calculation and numerical simulation by analyzing the square lattice Heisenberg model.

Analytical Foundation: The 2×2 Lattice

Consider $N = 4$ sites arranged in a 2×2 square lattice.

1. **Hilbert Space and Dimension:**

   - Calculate the total dimension of the Hilbert space for $N = 4$.
   - In particular, consider the subspace where we have equal number of spins up and spins down. Restrict your analysis to the $S^z_{total} = 0$ sector. List all basis states in this subspace and determine its dimension D.

2. **The Role of the External Field:** Show mathematically that for any state $|\phi\rangle$ within the $S^z_{total} = 0$ sector, the Zeeman term $H \sum \hat{S}^z_i |\phi\rangle = 0$. Explain why this means the external field H does not shift or split the energy levels within this specific block.

3. **Hamiltonian Construction:** Build the $D \times D$ Hamiltonian matrix for this sector.

4. **Eigenenergies and Limiting Regimes:** Discuss in which sector $S^z_{total} = 0, \pm 1, \pm 2$ would you expect to find the ground state?

   - **Limiting case $H = 0$ or $J = 0$:** Identify the ground state and its energy. Compare its energy to the classical anti-ferromagnetic configuration.
   - **General case $H, J > 0$:** Note that the external field H does not influence the S^z_{total} block, and does not mix the blocks, it does shifts other sectors ($S^z_{total} = \pm 1, \pm 2$). Determine the ground state at finite field H and determine the critical values H_c when the S^z_{total} transitions from 0 to 1 and then to 2, which is called the magnetization staircase.

Numerical Scaling: 4×4 and 6×6

Using a numerical ED library (e.g., `QuSpin` or `NetKet`), implement the square lattice with periodic boundary conditions.

1. **Validation:** Run your code for $N = 2 \times 2$ and verify that the eigenenergies match your analytical results from above.

2. **Energy Spectrum Scaling:** Scale your calculation to 4×4 ($N = 16$) and 6×6 ($N = 36$).

- Plot the lowest few energy eigenvalues as a function of $0 \leq H/J \leq 10$.
- **Computational Note:** For $N = 36$, if the full Hilbert space is too large to handle, consider the $S^z_{total} = 0$ symmetry sector.

3. **Magnetization and Phase Transition:**
   - Plot the average magnetization $\langle M_z \rangle = \frac{1}{N}\langle \sum \hat{S}^z_i \rangle$ versus H/J.
   - Identify the "magnetization plateaus." (Hint: When field increases, S_z jumps from 0 to 1... to $N^2/2$, and then magnetization is fully saturated.)
   - Discuss in the thermodynamic limit $N \to \infty$ how does the system undergo a transition from the AFM phase to the fully polarized Ferromagnetic (FM) phase. How would you assign the critical value $(H/J)_c$ in such limit?

Numerical Implementation Guide

To solve these systems efficiently:

- **Subspace Symmetry:** Use the fact that $[\hat{H}, \hat{S}^z_{total}] = 0$. Solve $\hat{H}$ within blocks of fixed S^z to reduce matrix size.
- **Sparse Matrices:** For $N > 20$, the Hamiltonian is too large for dense storage. Use `scipy.sparse.linalg.eigsh` or `QuSpin`'s `basis` and `hamiltonian` objects to find only the lowest eigenvalues.
- **Online Resources:** Documentation for `QuSpin` can be found at `https://weinbe58.github.io/QuSpin/`.

Phase 2: Hydrodynamics of Bose-Fermi Mixtures

In this problem, you will analyze the coupled equations governing a co-trapped mixture of bosons and fermions. While bosons tend to condense into a single quantum state, fermions are governed by the Pauli Exclusion Principle, creating a "Fermi pressure" that resists compression. You will explore how the inter-species interaction g_{BF} modifies these fundamental behaviors.

Theoretical Framework

The dynamics of a Bose-Fermi mixture are described by a set of coupled non-linear equations. We treat the bosons within the Gross-Pitaevskii framework and the fermions using a hydrodynamic approach. Neglecting higher-order corrections (such as Lee-Huang-Yang terms), the equations for the bosonic order parameter Ψ_B and the effective fermionic amplitude* Ψ_F are:

$$\begin{aligned} i\hbar\partial_t \Psi_B &= \left(-\frac{\hbar^2\nabla^2}{2m_B} + V_B(r) + g_B|\Psi_B|^2 + g_{BF}|\Psi_F|^2\right)\Psi_B = \mu_B \Psi_B \\ i\hbar\partial_t \Psi_F &= \left(K_F(n_F) + V_F(r) + g_{BF}|\Psi_B|^2\right)\Psi_F = \mu_F \Psi_F \end{aligned} \tag{3}$$

(* What is a Fermionic Density Amplitude? The field Ψ_F is a hydrodynamic construction rather than a single-particle wavefunction. Because fermions cannot occupy a single quantum state, we define Ψ_F such that $n_F(r) = |\Psi_F(r)|^2$. In this formulation, the kinetic term $K_F(n_F)$ represents the **Fermi pressure**, the kinetic energy cost of squeezing fermions together due to the Pauli Exclusion Principle. This allows us to treat the fermionic cloud as a fluid governed by an effective non-linear equation, analogous to the Gross-Pitaevskii equation used for the bosons.)

- **Couplings:** $g_B = \frac{4\pi\hbar^2 a_B}{m_B}$ is the boson-boson coupling; $g_{BF} = \frac{2\pi\hbar^2 a_{BF}}{\mu}$ is the boson-fermion coupling with reduced mass $\mu = m_B m_F/(m_B + m_F)$.
- **Fermionic Term:** Unlike the bosonic cubic term, the term $K_F(n_F)$ arises from the **Fermi Energy** of a degenerate Fermi gas, acting as an effective "self-interaction" driven by statistics rather than collisions.

Checkpoint 2.1: Uniform Gas in the ground state

Consider $N_B \gg 1$ bosons and $N_F \gg 1$ fermions in a volume V ($V_{B,F} = 0$) with uniform densities $n_B = N_B/V$ and $n_F = N_F/V$. Assume $V_B = V_F = 0$ inside the box.

1. **Bosonic Chemical Potential:** Without interspecies interaction $a_{BF} = 0$, use the Thomas-Fermi approximation (neglecting kinetic energy) to determine the chemical potential μ_B in terms of n_B and g_B. Show that positive compressibility $\partial\mu/\partial n > 0$ indicates stability of the gas against collapse of the BEC.

2. **Fermionic "Interaction":** For a non-interacting Fermi gas with $a_{BF} = 0$, the chemical potential of a uniform gas is given by the Fermi energy:

$$E_F = \frac{\hbar^2}{2m_F}(6\pi^2 n_F)^{2/3} \tag{4}$$

   Derive the kinetic term $K_F(n_F)$ in the hydrodynamic equation that yields this $\mu = E_F$. How does the power-law scaling with n differ between the bosonic and fermionic cases?

3. **Interspecies Coupling:** Now consider finite a_{BF}.

   - Solve for the chemical potentials μ_B and μ_F in terms of n_F and n_B.
   - Comparing with $\mu_B(n_B)$ and $\mu_F(n_F)$ you obtained for independent Bose and Fermi gases, could you derive an effective $g_{B,eff}$ and "$g_{F,eff}$" for the bosons and fermions by eliminating the explicit dependence on the other species? (Hint: For Fermions, you may introduce $g_F|\Psi_F|^2$ in the hydrodynamic equation to capture the fermionic interactions mediated by bosons.)
   - **Stability Analysis:** Under what conditions (g_B, g_{BF}, n_F) does the uniform mixture become unstable toward **phase separation** or **mean-field collapse***?

   *Technical Insight: Stability of the Mixture

   For a single-component gas, stability is simply defined by compressibility $\frac{\partial\mu}{\partial n} > 0$. In a two-component mixture, we must ensure the system is stable against both **collapse** and **phase separation**. This is determined by the positivity of the 2×2 stability matrix:

$$\mathbf{M} = \begin{pmatrix} \frac{\partial\mu_B}{\partial n_B} & \frac{\partial\mu_B}{\partial n_F} \\ \frac{\partial\mu_F}{\partial n_B} & \frac{\partial\mu_F}{\partial n_F} \end{pmatrix} \tag{5}$$

   The mixture is stable only if $\det(\mathbf{M}) > 0$, which yields the condition:

$$g_B \cdot \frac{\partial E_F}{\partial n_F} > g_{BF}^2 \tag{6}$$

   - If $g_{BF} > 0$ and this condition is violated, the species become **immiscible** and will spontaneously phase-separate to minimize their overlap.
   - If $g_{BF} < 0$ and this condition is violated, the mutual attraction overcomes the internal pressures, leading to a **mean-field collapse** (implosion) of the mixture.

Checkpoint 2.2: Mixtures in a Trap

Consider the mixture in spherical harmonic potentials $V_i(r) = \frac{1}{2}m_i\omega_i^2 r^2$.

1. **Thomas-Fermi (TF) Limit for Bosons:** In the limit of large N_B, the kinetic energy (quantum pressure) is negligible. Derive the bosonic density profile $n_B(r)$ as a function of the local fermionic density $n_F(r)$ and the trap potential. Note that density $n \geq 0$.

2. **Local Density Approximation (LDA) for Fermions:** We assume the fermions reach a local equilibrium $\mu_F = V_F(r) + E_F[n_F(r)] + g_{BF}n_B(r)$. Determine the fermionic density profile $n_F(r)$ as a function of the local bosonic density $n_B(r)$.

3. **The Coupled Density Profiles:**
   - Derive the set of algebraic equations that must be solved self-consistently for $n_B(r)$ and $n_F(r)$.
   - **Physical Intuition:** Describe qualitatively how the clouds interact:
     - **Attractive ($g_{BF} < 0$):** Do the clouds pull each other toward the center (forming a dense core)?
     - **Repulsive ($g_{BF} > 0$):** Does the BEC act as a "plunger," pushing the fermions out to the edges of the trap?
4. **Numerical Validation:** Develop a calculator to input your parameters ($g_B, g_{BF}, \omega_B, \omega_F, m_B, m_F$) and generate density profiles of the mixtures. Plot and compare representative density profiles in the non-interacting, weak-interacting and phase separation regimes for negative, zero and positive interspecies interactions g_{BF}. Comment on the change of the sample size (Thomas-Fermi radii) and the atomic density at the trap center as a_{BF} deviates from zero toward larger values. For the plots, specify your choices of atomic masses, trap frequencies, numbers, and a_B in dimensional or dimensionless unit. Clarify your assumptions in the code and plots.