Computational Methods: Final Project: Thermal Stability of Bose-Einstein Condensates

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Homework is due during Final Exam Period.

I. THE SCIENCE PROBLEM : ROTATING BOSE-EINSTEIN CONDENSATES

The study of vortices in dilute atomic Bose-Einsetein condensates constitutes our final project in this class. The scientific problem is detailed in the paper: D.J. Dean and T. Papenbrock, Phys. Rev. A 65, 043603 (2002). You will have an opportunity to investigate the methods discussed in this paper during the course of the project.

We are working with bosons here. Boson wave functions exhibit symmetry under interchange of any two particles, so that

$$a_i^\dagger a_j^\dagger \mid --\rangle = \mid n_i\rangle \mid n_j\rangle = \mid n_j\rangle \mid n_i\rangle = a_j^\dagger a_i^\dagger \mid --\rangle \ . \tag{1}$$

Therefore, boson creation and annihilation operators obey the following relationships.

$$\begin{aligned} a_i^\dagger a_j^\dagger - a_j^\dagger a_i^\dagger &= 0 \\ a_i a_j - a_j a_i &= 0 \\ a_i^\dagger a_j - a_j a_i^\dagger &= \delta_{ij} \end{aligned} \tag{2}$$

We can place more than one boson in a given state. Let n_j be the number of bosons with angular momentum j in a system. The wave function in Fock space will then be represented as

$$\mid n_0 n_1 n_2 n_3 \cdots\rangle \ . \tag{3}$$

Operators for the number of particles, N, and the angular momentum L are given by

$$\begin{aligned} \hat{N} &= \sum_j \hat{n}_j = \sum_j a_j^\dagger a^j \\ \hat{L} &= \sum_j j\hat{n}_j = \sum_j j a_j^\dagger a^j \ . \end{aligned} \tag{4}$$

The paper asks about the stability of the one-vortex state (where $L/N = 1$) against thermal fluctuations. Small systems do not exhibit phase transitions. Nevertheless, finite systems may display precursors of phase transitions. By finding the distribution of zeros of the partition function in the complex plane, we should be able to deduce the order of the phase transition in an infinite system based on calculations performed in a finite system.

Basis states of the system can be constructed for $N = L$. As an example, consider the system with $N = 6$ particles. Several of the basis states are

$$\begin{aligned} &\mid 5000001\rangle \\ &\mid 4100010\rangle \\ &\mid 3200100\rangle \\ &\mid 2301000\rangle \end{aligned} \tag{5}$$

The Hamiltonian of an N-boson system with contact interaction reads

$$\hat{H} = v_0 \sum_{i,j,k,l} \frac{(k+l)!\delta_{k+l}^{i+j}}{2^{k+l}(i!j!k!l!)^{1/2}} a_i^\dagger a_j^\dagger a_k a_l \tag{6}$$

Zeros of the partition function (or poles of the specific heat) may be found by looking at the partition function in the complex plane. We accomplish this by transforming variables. $\mathcal{B} = \beta + i\tau$. The partition function then becomes

$$Z(\mathcal{B}) = \sum_i \exp\left(-\mathcal{B}E_i\right) \ . \tag{7}$$

Zeros of the partition function are determined conveniently by locating the poles of the specific heat which is given by

$$C_v(\mathcal{B}) = \frac{\partial^2 \ln Z(\mathcal{B})}{\partial \mathcal{B}} =< E >^2 - < E**2 > \tag{8}$$

One can characterize the phase transitions of the system through constructing some simple quantities. The density of zeros in the vicinity of a given τ_k is given by

$$\phi(\tau_k) = \frac{1}{2}\left(\frac{1}{\mid \mathcal{B}_k - \mathcal{B}_{k-1} \mid} + \frac{1}{\mid \mathcal{B}_{k+1} - \mathcal{B}_k \mid}\right) , \tag{9}$$

with $k = 2, 3, 4, ...A$. A simple power law describes the density of zeros for small τ, namely $\phi(\tau) \sim \tau^{\alpha}$. Using only the first three zeros yields

$$\alpha = \frac{\ln \phi(\tau_3) - \ln \phi(\tau_2)}{\ln \tau_3 - \ln \tau_2} . \tag{10}$$

Finally, the derivative near the real axis is given by

$$\gamma = \tan \nu = \tan \frac{\beta_2 - \beta_1}{\tau_2 - \tau_1} . \tag{11}$$

II. WHAT YOU NEED TO DO

This problem involves two major parts. The first part is to construct an algorithm that generates the Hamiltonian matrix for the system of bosons.

- You need to construct the Hamiltonian matrix H_{IJ} where I represents a particular basis state of the problem.
- Once you have the Hamiltonian matrix, you can move to a calculation of eigenvalues of the matrix. You can use the Lanzcos algorithm for that purpose. You will need to calculate at least 200 states for larger systems that we will be working with.
- Once you have the eigenvalues, you can then find the zeros of the partition function. For a system of $N = 30$ and $N = 40$ particles, you should be able to reproduce the Fig. 1c and Fig. 2a of the paper.
- For the N=40 system, can you extract the τ_1, γ and α as shown in Table I of the paper?
- Based on your calculations and figures, can you give a physical interpretation of the two different phases that the system would find itself in? Does the system 'remember' in which state it exists for a very long or very short time? (Recall that the τ direction is a direction in time.)