Summary of Research at HKUST

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Introduction

This research project investigated ultracold ^{166}Er atoms confined in a two-dimensional box trap. The main goal was to use time-of-flight (ToF) measurements to obtain the particle distribution, calculate the theoretical distribution under specific chemical potentials and temperatures, and perform fitting to determine the sample's temperature and chemical potential.

This study is part of a broader project on two-dimensional ultracold atomic gases. In our experiment, a strong harmonic potential was applied along the z-direction to achieve quasi-two-dimensional confinement. The quasi-2D condition requires that both the chemical potential and temperature are smaller than the energy gap between the ground state and the first excited state of the harmonic potential. To determine the sample's temperature and chemical potential, time-of-flight (ToF) imaging and Equation of State (EoS) methods are commonly used [1]. However, due to the attractive red-detuned optical dipole trap used in our setup, the EoS method is inapplicable, making it necessary to use ToF measurements.

Methods and Procedures

1. Theoretical Calculations

1.1 Numerical Methods in Hartree-Fock Calculations

The Hartree-Fock (HF) method was employed to obtain the eigenstates and eigenenergies of the interacting particle system [2, 4]. We discretized the spatial domain along the z-axis using a finite difference method, with a discretization step size Δz and a grid spanning from $-L$ to L, where L is the dimensionless length parameter.

The single-particle wavefunctions $\phi_j(z)$ are determined by solving the discretized Hartree-Fock equation:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V_{\text{trap}}(z) + 2gn(z)\right]\phi_j(z) = \varepsilon_j\phi_j(z), \tag{1}$$

where $V_{\text{trap}}(z) = \frac{1}{2}m\omega_z^2 z^2$ is the harmonic trap potential. The second derivative was approximated using a central difference scheme, resulting in a tridiagonal matrix for efficient computation. We employed the 'eigh_tridiagonal' function from the SciPy library in Python to solve for the eigenvalues and eigenvectors.

To improve numerical stability and accuracy, we nondimensionalized the equations by introducing scaled units:

$$\tilde{z} = \frac{z}{\ell_z},$$
$$\tilde{\varepsilon}_j = \frac{\varepsilon_j}{\hbar\omega_z}.$$

Here, $\ell_z = \sqrt{\hbar/(m\omega_z)}$ is the harmonic oscillator length. The particle number density $n(z)$ was calculated iteratively using the self-consistent equations:

$$n(z) = -\frac{1}{\lambda^2}\sum_j \ln\left[1 - e^{(\mu-\varepsilon_j)/(k_BT)}\right]|\phi_j(z)|^2, \tag{2}$$

where $\lambda = \sqrt{2\pi\hbar^2/(mk_BT)}$ is the thermal de Broglie wavelength, μ is the chemical potential, and T is the temperature. The iteration continued until convergence was achieved.

1.2 Computational Efficiency in ToF Calculations

To calculate the particle distribution after time-of-flight, we needed to perform convolutions of the initial density distribution with a free-space propagation kernel. The integral for the ToF distribution is given by [1]:

$$n_i(r,t) = \frac{m^2}{(2\pi\hbar t)^2} \int_{L_x,L_y} d^2r'\, g_0\left(Z_i e^{-a|r-r'|^2}\right), \tag{3}$$

where $a = m/(2t^2 k_B T)$. To improve computational efficiency, we transformed the convolution into the frequency domain using Fast Fourier Transforms (FFT). This significantly reduced the computation time compared to direct numerical integration.

2. Experimental Data Processing

2.1 Data Reading and Averaging

Experimental data in HDF5 format were read using the 'h5py' library. The optical density (OD) images were extracted and transposed to match the coordinate system used in our analysis. We identified the region of interest by thresholding the OD images and locating the brightest area using the 'scipy.ndimage.label' function.

The OD is related to the particle number density n by:

$$n = \frac{\mathrm{OD}}{\sigma_0}, \tag{4}$$

where σ_0 is the resonant cross-section:

$$\sigma_0 = \frac{3\lambda^2}{2\pi}. \tag{5}$$

We cropped the region containing the highest signal to focus on the atoms in the trap and averaged over 30 measurements to improve reliability.

2.2 Data Correction and Alignment

The experimental data contained background noise and slight misalignments. We subtracted a linear background from the integrated density profiles to correct for any residual background signal. To align the density profiles, we interpolated the data and shifted the peak position to $x = 0$ by finding the maximum of the interpolated function using the 'minimize scalar' function from SciPy.

3. Parameter Fitting

3.1 Definition of Loss Function

We defined a custom loss function that focuses on the thermal wings of the density profile, ignoring the central region where a condensate may be present [3]. The loss function is given by:

$$\mathrm{Loss}(T,\mu) = \sum_{|x|>x_0} \left[n_{\mathrm{exp}}(x) - n_{\mathrm{theory}}(x;T,\mu)\right]^2, \tag{6}$$

where x_0 is a cutoff position defining the wings, $n_{\mathrm{exp}}(x)$ is the experimental density, and $n_{\mathrm{theory}}(x;T,\mu)$ is the theoretical density computed using the methods described above.

3.2 Optimization Algorithms

We performed a two-parameter fitting using the L-BFGS-B optimization algorithm implemented in SciPy's 'minimize' function. The initial guesses and bounds for the temperature T and chemical potential μ were set based on expected physical values. Constraints were applied to ensure that the optimized parameters remained within physically meaningful ranges.

Results

1. Theoretical Calculations

Using the Hartree-Fock method with the numerical techniques described, we obtained the eigenstates and eigenenergies of the interacting ^{166}Er system under various chemical potentials and temperatures. The nondimensionalization improved the stability and convergence of the numerical solutions.

Figure 1 shows theoretical predictions of the ToF particle density at various times, illustrating that the box trap shape is preserved during expansion.

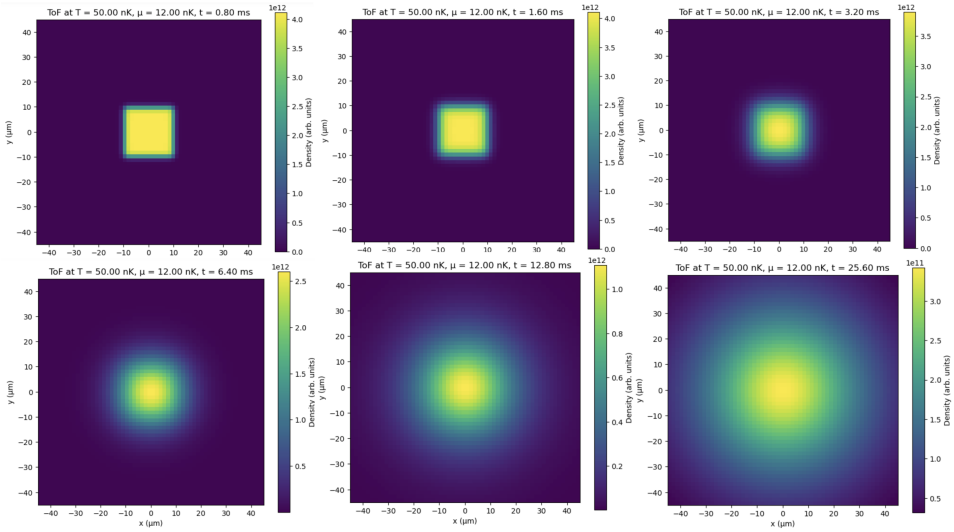

Figure 1: Theoretical ToF predictions at various times.

2. Comparison between Hartree-Fock Methods

We compared the Hartree-Fock method under different approaches—considering interactions versus neglecting interactions—to understand their impact on energy levels and occupations. Figure 2 shows the difference in particle densities for lower modes, highlighting the importance of interactions.

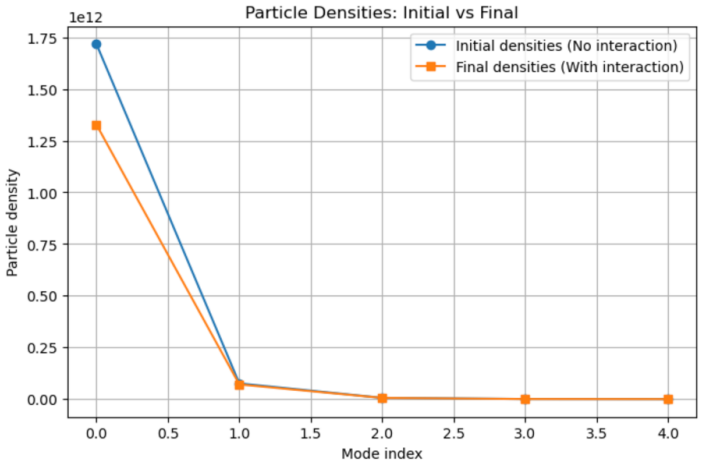

Figure 2: Particle density of different modes, comparing interacting case with non-interacting case.

3. Experimental Data Analysis

Experimental data from 30 ToF images were processed to obtain the average particle density distribution (Figure 3). The two-dimensional particle density was integrated along the z-axis to obtain a

one-dimensional profile along the x-axis (Figure 4).

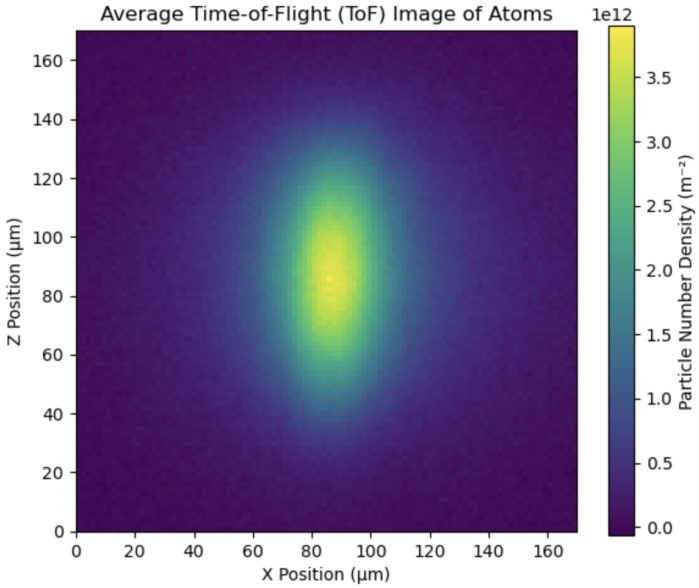

Figure 3: Average ToF data.

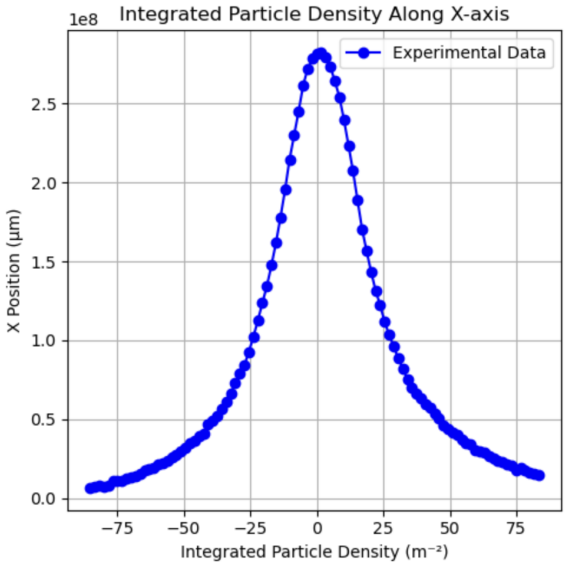

Figure 4: Density distribution along the x-axis.

4. Parameter Fitting

The optimal fitting was performed on the thermal wings of the experimental data, yielding a temperature of $T = 5.9 \times 10^{-8}$ K and a chemical potential of $\mu = 3.04 \times 10^{-31}$ J. Figure 5 shows the comparison between the experimental and theoretical density profiles.

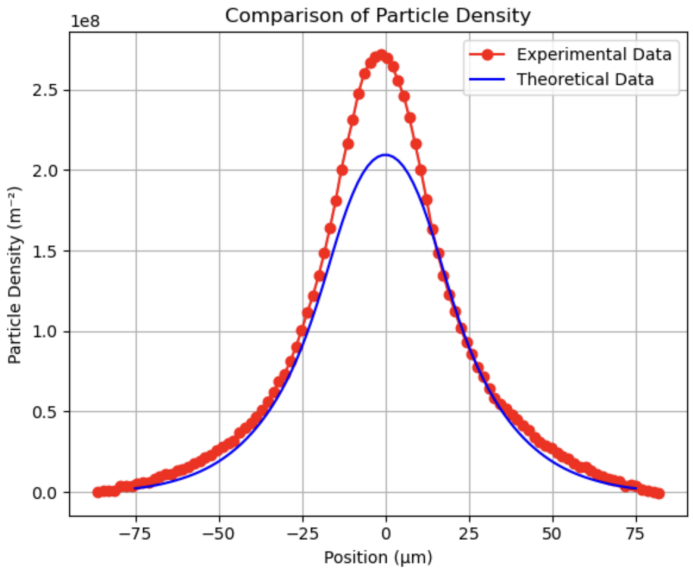

Figure 5: Fitting of the density distribution along the x-axis.

Challenges Overcome

1. Numerical Issues in Hartree-Fock Calculations

During the numerical solution of the Hartree-Fock equations, I encountered issues with incorrect results that were strongly dependent on the discretization step size. By nondimensionalizing the equations and carefully choosing the discretization parameters, I improved the numerical stability and accuracy. Utilizing efficient tridiagonal matrix solvers further enhanced computational performance.

2. Computational Efficiency in ToF Calculations

The original integration method for ToF distributions was inefficient. By implementing Fast Fourier Transforms (FFT) to perform convolutions in the frequency domain, I significantly improved computational speed, reducing computation time from hours to minutes.

3. Experimental Data Preprocessing

The experimental data contained significant background noise and off-center peak positions. I designed a preprocessing procedure that included thresholding to identify the region of interest, background subtraction to remove noise, and alignment of the density profiles by shifting the peak positions. This ensured the data were suitable for reliable fitting.

Skills and Knowledge Gained

1. Hartree-Fock Method and Numerical Solutions

Mastered the application of the Hartree-Fock method to interacting particle systems, particularly in calculating energy eigenstates and particle density distributions. Learned to improve numerical precision by nondimensionalizing differential equations and utilizing efficient numerical solvers.

2. Computational Efficiency Optimization

Enhanced my understanding of numerical efficiency by transforming integration problems into the frequency domain using FFTs, significantly improving calculation speed.

3. Experimental Data Processing and Fitting

Gained experience in preprocessing experimental data, including thresholding, background subtraction, and peak alignment. Learned to define effective loss functions for parameter fitting and utilized optimization algorithms to extract physical parameters.

4. Literature Review and Theoretical Insights

Conducted a literature review on ultracold atoms, understanding topics such as the two-dimensional Berezinskii-Kosterlitz-Thouless (BKT) transition, superfluidity, and the Gross-Pitaevskii equation (GPE).

5. Overall Research Competency

Improved understanding of the theory-experiment interplay, developed independent problem-solving skills, and gained confidence in tackling research questions.

Conclusion

This study investigated the particle number density distribution of ultracold ^{166}Er atoms in a two-dimensional box trap. Using time-of-flight measurements, data preprocessing, and parameter fitting, we extracted key physical parameters such as the temperature and chemical potential of the sample.

Challenges such as numerical stability, computational efficiency, and experimental data preprocessing were successfully addressed, resulting in reliable theoretical and experimental comparisons. The project allowed me to master key methods in ultracold atomic physics, gain practical experience in numerical and experimental techniques, and deepen my understanding of two-dimensional superfluidity and the BKT transition.

Future Work

Future research could focus on exploring the effects of varying interaction strengths and trap geometries on particle distribution. Implementing more advanced many-body techniques, such as Quantum Monte Carlo simulations, could provide deeper insights into the system's behavior beyond the Hartree-Fock approximation.

Acknowledgments

I would like to express my sincere gratitude to Prof. Gyu-Boong Jo for his guidance throughout this research project. I am also grateful to Dr. Haoting Zhen, Dr. Yifei He, and Dr. Mithilesh K. Parit for their invaluable support and assistance. Their expertise and insights were instrumental in the success of this work.

References

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