CP301- ENGINEERING DEVELOPEMENT PROJECT

Developement of Python Toolbox For Calculating the Excitation Spectrum of Bose Einstein Condensate(BEC)

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ABSTRACT

Dipolar Bose-Einstein condensates (BECs) present a fascinating platform for studying quantum many-body physics due to their long-range and anisotropic interactions. In this project, we developed a Python-based computational toolbox to numerically calculate the excitation spectrum of a quasi-one-dimensional dipolar BEC using the Bogoliubov-de Gennes (BdG) formalism. The toolbox incorporates both contact and dipole-dipole interactions, and accounts for quantum fluctuation corrections. The BdG matrix is constructed using a harmonic oscillator basis and solved numerically via eigenvalue decomposition. The code efficiently handles large basis sizes and Fourier-space convolution integrals using SciPy and NumPy libraries. We analyze how the BdG excitation modes evolve with varying scattering lengths, providing insight into the system's stability and excitation behavior. The final results are presented as energy spectra plots versus interaction strength. This toolbox offers a reusable and extensible framework for future exploration of low-dimensional dipolar quantum gases.

INTRODUCTION

Bose-Einstein condensates (BECs) are quantum fluids formed at ultra-cold temperatures, where a macroscopic number of bosons occupy the lowest quantum state, resulting in coherent collective behavior. Traditional BECs involve only contact interactions; however, dipolar BECs—composed of atoms with magnetic or electric dipole moments—introduce long-range, anisotropic interactions that enrich the physical phenomena. Understanding the excitation spectrum of such condensates is essential, as it governs their stability, response to perturbations, and dynamical properties.

To investigate these excitations, we use the Bogoliubov-de Gennes (BdG) formalism, which describes elementary excitations by linearizing the Gross-Pitaevskii equation around the ground state. In dipolar systems, the BdG equations become more complex due to nonlocal interactions, and therefore require numerical approaches for realistic analysis. In this project, we focus on a quasi-one-dimensional geometry, where tight confinement along two axes reduces the problem to an effectively 1D system while retaining dipolar physics.

Our goal was to implement a Python toolbox that can compute the BdG excitation spectrum across a range of interaction strengths. By projecting the problem onto a harmonic oscillator basis and incorporating dipolar and LHY corrections, we construct the full BdG matrix and extract its eigenvalues. This report outlines the physical theory, numerical techniques, and final results obtained using the toolbox.

OBJECTIVES

- To develop a Python-based computational toolbox that calculates the excitation spectrum of a quasi-one-dimensional dipolar Bose-Einstein condensate using the Bogoliubov-de Gennes (BdG) formalism.

- To numerically construct and diagonalize the BdG matrix, incorporating both short-range contact interactions and long-range dipolar interactions, along with quantum fluctuation effects.

- To analyze the variation of excitation energies with respect to the scattering length and visualize the mode behavior through eigenvalue spectra plots for physical interpretation and stability analysis

THEORITICAL BACKGROUND

1. Basics of Bose-Einstein Condensates

A Bose-Einstein Condensate (BEC) is a state of matter that arises when a dilute gas of bosons is cooled to temperatures near absolute zero. At such ultra-cold temperatures, a large fraction of the bosons occupy the lowest quantum state, resulting in a macroscopic quantum phenomenon where the entire ensemble behaves as a single quantum entity. BECs provide a unique platform to study quantum statistical effects at macroscopic scales. While conventional BECs are dominated by short-range contact interactions, dipolar BECs involve atoms with magnetic or electric dipole moments, introducing long-range and anisotropic interactions. These additional interactions lead to richer and more complex behavior, making dipolar BECs an active area of research in quantum many-body physics.

2. Gross-Pitaevskii Equation (GPE)

The Gross-Pitaevskii Equation is a nonlinear Schrödinger equation that describes the mean-field dynamics of the condensate wavefunction ψ(x,t). In the presence of both contact and dipolar interactions, the GPE includes both local and nonlocal nonlinear terms. The standard 1D time-independent GPE is given by:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(x) + g|\psi(x)|^2 + \Phi_d(x)\right)\psi(x) = \mu\psi(x)$$

Here, g is the contact interaction strength, Φd(x) is the dipolar potential, and μ is the chemical potential. The GPE serves as the starting point for computing the ground-state wavefunction of the BEC, which is essential for excitation analysis.

3. Bogoliubov Theory of Excitations

To understand the small excitations or fluctuations around the BEC ground state, we use the Bogoliubov-de Gennes (BdG) formalism. This theory linearizes the GPE by introducing small perturbations to the wavefunction and leads to a set of coupled linear equations. The resulting BdG equations describe the energy spectrum of collective excitations in the condensate. The eigenvalues of the BdG matrix correspond to excitation energies, and their stability determines whether the condensate is dynamically stable or unstable. In dipolar BECs, these equations are more complex due to the nonlocal dipolar term, but they provide crucial insights into the condensate's response to perturbations.

4. Methods for Spectral Analysis

The excitation spectrum is obtained by diagonalizing the BdG matrix, which is constructed in a chosen basis — in this case, the harmonic oscillator basis. Each matrix element involves numerical integration over basis functions and interaction kernels. Fourier transforms are used to compute the dipolar potential efficiently. Once the matrix is assembled, its eigenvalues are calculated using linear algebra routines, and the lowest positive eigenvalues represent the physical excitation modes. By varying parameters such as the scattering length, we can track how the spectrum evolves, helping us explore phenomena like roton instability and phonon softening in dipolar BECs.

METHODOLOGY

FORMULAE USED

- **BDG Matrix:**

$$\begin{pmatrix} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) + \Phi_d(x) - \mu + X_1 + \frac{3}{4}\gamma_\perp\gamma_{QF}|\phi(x)|^3 & X_2 + \frac{3}{2}\gamma_\perp\gamma_{QF}|\phi(x)|^2 \\ -X_3 - \frac{3}{2}\gamma_\perp\gamma_{QF}\phi(x)^2 & -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) + \Phi_d(x) - \mu - X_4 - \frac{3}{4}\gamma_\perp\gamma_{QF}|\phi(x)|^3 \end{pmatrix} \begin{pmatrix} u(x) \\ v(x) \end{pmatrix} = \omega \begin{pmatrix} u(x) \\ v(x) \end{pmatrix}$$

- **The Function X1, X2, X3, & X4:**

$$\begin{aligned} X_1 f(x) &= \phi(x)\mathcal{F}_x^{-1}[\tilde{U}_x(k_x)\mathcal{F}_x\{\phi^*(x)f(x)\}], \\ X_2 f(x) &= \phi(x)\mathcal{F}_x^{-1}[\tilde{U}_x(k_x)\mathcal{F}_x\{\phi(x)f(x)\}], \\ X_3 f(x) &= \phi^*(x)\mathcal{F}_x^{-1}[\tilde{U}_x(k_x)\mathcal{F}_x\{\phi^*(x)f(x)\}], \\ X_4 f(x) &= \phi^*(x)\mathcal{F}_x^{-1}[\tilde{U}_x(k_x)\mathcal{F}_x\{\phi(x)f(x)\}]. \end{aligned}$$

- **U(k) Interaction Potential:**

$$\tilde{U}_x(k_x) = \frac{g_s}{2\pi l^2} + \frac{g_{dd}}{2\pi l^2}\left[\frac{3\left\{-ue^u E_1(u)+1\right\}}{2} - 1\right]$$

- **Φd(x) Dipolar Potential:**

$$\Phi_d(x) = \mathcal{F}_x^{-1}\left[\tilde{U}_x(k_x)\cdot\mathcal{F}_x\left(|\phi(x)|^2\right)\right]$$

- **Quantum Fluctuation:**

$$\gamma_\perp \cdot \gamma_{QF} = \left(\frac{2N^{3/2}}{5\pi^{3/2}}\right)\cdot\left(\frac{128}{3}\sqrt{\pi a_s^5}\cdot Q_5(\epsilon_{dd})\right)$$

1. Numerical Methods Used

To compute the excitation spectrum of a quasi-one-dimensional dipolar **Bose-Einstein condensate (BEC)**, we employed a combination of spectral and numerical integration methods. The ground-state wavefunction was projected onto a harmonic oscillator basis, which naturally fits the geometry of a harmonically trapped condensate. This basis was generated using recurrence relations for Hermite polynomials, ensuring orthonormality and numerical stability.

The Bogoliubov-de Gennes (BdG) matrix elements involve integrals over products of the ground-state wavefunction, basis functions, and interaction kernels. These were evaluated using Simpson's Rule, a high-accuracy method for numerical integration well-suited for smooth functions. For evaluating convolution integrals involving dipolar interactions, we used **Fast Fourier Transforms (FFT)**, implemented via scipy.fft, which efficiently handles the nonlocal nature of the dipolar potential in momentum space. These approaches allowed us to achieve a balance between computational accuracy and efficiency.

2. Software Architecture of the Toolbox

The toolbox was implemented in Python, chosen for its readability and access to high-quality scientific computing libraries. The code was modularized for clarity and reusability. Each component of the simulation such as the construction of the harmonic oscillator basis, calculation of interaction terms, assembly of the BdG matrix, and diagonalization — was placed in a separate function or module.
The architecture consists of the following main parts:

- Parameter Setup Module: Initializes physical and simulation parameters such as number of atoms, trap frequencies, and basis size.
- Basis Construction Module: Builds the harmonic oscillator wavefunctions using recursion.
- Interaction Kernel Module: Computes contact and dipolar interaction terms in both position and momentum space.
- BdG Matrix Module: Constructs the matrix using the prepared components and evaluates the excitation spectrum.
- Plotting Module: Visualizes the results by plotting eigenvalues against scattering lengths.

3.Overview of Algorithms Implemented

The main computational algorithm involves the following steps:
1.**Load or compute the ground-state wavefunction** $\phi(x)$ from precomputed data.
2.Construct harmonic oscillator basis functions in the spatial domain.
3.Evaluate all required integrals for BdG matrix elements, including:

- Local (contact) terms using $|\phi|^2$, $|\phi|^3$
- Nonlocal (dipolar) terms using Fourier-space convolutions
- Quantum fluctuation corrections using the LHY term

4.Assemble the BdG matrix of size 2Nb×2Nb accounting for both particle and hole excitations.
5.Diagonalize the matrix using numpy.linalg.eig() to obtain eigenvalues and eigenvectors.
6.Sort and normalize eigenvalues, and extract the lowest 10 positive modes representing the physical excitations.
7.Repeat for a range of scattering lengths and store the spectra for analysis.

This methodology enabled us to produce a clean and scalable approach for understanding excitation behavior in dipolar condensates.

TOOLBOX IMPLEMENTATION

1. Programming Language and Libraries Used

The toolbox was developed in Python, a high-level programming language widely used in scientific computing for its readability, flexibility, and extensive library support. The following core libraries were used in our implementation:

- **NumPy**: For efficient array manipulation and vectorized numerical operations. It handles operations on wavefunctions, basis states, and matrix algebra.
- **SciPy**: Provides scientific and mathematical functions such as numerical integration (scipy.integrate.simpson), special functions, and linear algebra tools (scipy.linalg.eig), as well as fast Fourier transforms (scipy.fft) for dipolar interaction calculations.
- **Matplotlib**: Used for generating visualizations of the excitation spectra, including plots of BdG eigenvalues versus scattering length and mode behavior analysis.

2. Functional Modules

The toolbox is modular in design, with each core functionality encapsulated in a dedicated module. This not only improves code organization but also makes future extensions more manageable. The main modules are:

- Parameter Initialization Module: Defines system-specific parameters such as number of atoms, scattering length range, interaction strengths, trap geometry, and basis size.

- Ground State Wavefunction Loader: Loads precomputed data files containing the amplitude and phase of the ground-state wavefunction, then reconstructs the full complex form $\phi(x)$.

- Basis Generator: Computes the harmonic oscillator basis functions using recursive relations for Hermite polynomials. These basis functions serve as the computational space for projecting the BdG matrix.

- Interaction Calculator: Computes the contact interaction matrices (X1–X4) and the Fourier-space dipolar interaction potential U(k), as well as the LHY correction term for quantum fluctuations.

- BdG Solver: Constructs the full BdG matrix using the computed elements, applies Simpson integration for matrix element evaluation, and performs diagonalization to extract the excitation spectrum.

- Plotting and Visualization Module: Generates graphs of eigenvalues vs. scattering length, helps compare multiple excitation modes, and provides visual confirmation of system behavior under varying interaction conditions.

RESULTS

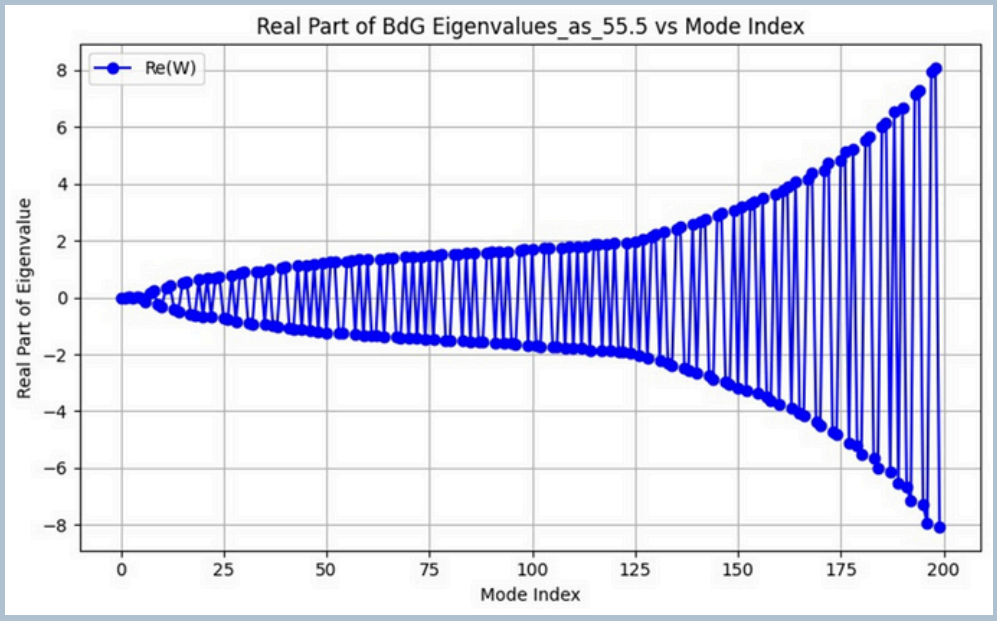
- **Excitation Energy Spectra at scattering length 55.5::**

Mode	1:	0.000000 -0.198111
Mode	2:	-0.000000 0.198113
Mode	3:	0.292044 0.000000
Mode	4:	-0.292044 0.000000
Mode	5:	0.317160 0.000000
Mode	6:	-0.317160 0.000000
Mode	7:	-1.009753 0.000001
Mode	8:	1.009753 0.000001
Mode	9:	1.717916 -0.000000
Mode	10:	-1.717916 -0.000000
Mode	11:	-2.427805 0.000000
Mode	12:	2.427805 0.000000
Mode	13:	3.080872 0.000001
Mode	14:	-3.080872 0.000001
Mode	15:	-3.706784 0.000001
Mode	16:	3.706784 0.000001
Mode	17:	4.285802 0.000000
Mode	18:	-4.285802 0.000000
Mode	19:	-4.843304 0.000001
Mode	20:	4.843304 0.000001
Mode	21:	-4.996014 -0.000000
Mode	22:	4.996014 -0.000000
Mode	23:	-4.998704 0.000000
Mode	24:	4.998704 0.000000
Mode	25:	5.376599 0.000001
Mode	26:	-5.376599 0.000001
Mode	27:	-5.897719 -0.000000
Mode	28:	5.897719 -0.000000
Mode	29:	-6.403190 0.000000
Mode	30:	6.403190 0.000000
Mode	31:	6.884710 0.000001
Mode	32:	-6.884710 0.000001
Mode	33:	-6.919097 0.000000
Mode	34:	6.919097 0.000000
Mode	35:	6.919847 0.000000
Mode	36:	-6.919847 0.000000
Mode	37:	7.344537 0.000000
Mode	38:	-7.344537 0.000000

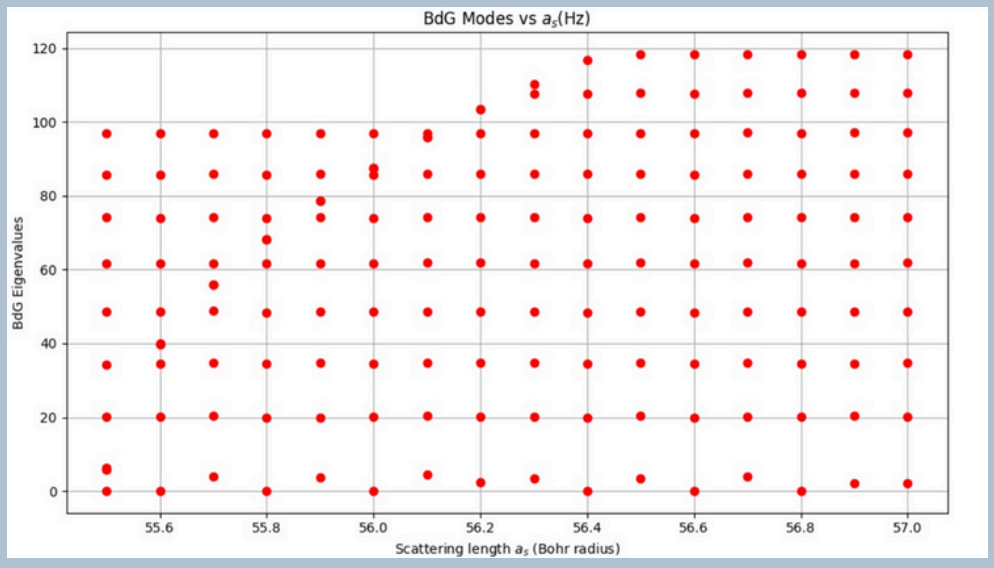
Mode	41:	-7.865831 -0.000000
Mode	42:	7.865831 -0.000000
Mode	43:	-7.866755 -0.000000
Mode	44:	7.866755 -0.000000
Mode	45:	-7.988158 -0.000000
Mode	46:	7.988158 -0.000000
Mode	47:	8.396938 -0.000000
Mode	48:	-8.396938 -0.000000
Mode	49:	-8.784597 -0.000000
Mode	50:	8.784597 -0.000000
Mode	51:	-9.005101 -0.000000
Mode	52:	9.005101 -0.000000
Mode	53:	9.005657 -0.000000
Mode	54:	-9.005657 -0.000000
Mode	55:	-9.150883 0.000000
Mode	56:	9.150883 0.000000
Mode	57:	-9.495623 -0.000001
Mode	58:	9.495623 -0.000001
Mode	59:	-9.817521 -0.000001
Mode	60:	9.817521 -0.000001
Mode	61:	-9.897365 -0.000000
Mode	62:	9.897365 -0.000000
Mode	63:	9.898142 -0.000000
Mode	64:	-9.898142 -0.000000
Mode	65:	-10.117797 -0.000000
Mode	66:	10.117797 -0.000000
Mode	67:	10.394347 -0.000000
Mode	68:	-10.394347 -0.000000
Mode	69:	-10.571716 -0.000000
Mode	70:	10.571716 -0.000000
Mode	71:	10.584589 -0.000000
Mode	72:	-10.584589 -0.000000
Mode	73:	10.665590 -0.000000
Mode	74:	-10.665590 -0.000000

GRAPHICAL RESULTS

- **Excitation Energy Vs Mode Index Graph at Scattering Length 55.5:**



- **Energy Spectra value Vs scattering Length Graph**



In this plot, we show how the excitation modes of a dipolar Bose-Einstein condensate evolve with scattering length as. Our range starts just at the onset of supersolidity — the true superfluid phase exists at higher as, beyond the left edge of this graph.
As we lower as, we observe a clear softening of the lowest excitation mode, a key signal of the system approaching instability. This mode eventually dips near zero, indicating the emergence of a supersolid phase, where the condensate develops periodic density modulations.
From there, the excitation spectrum splits - forming two distinct branches:

- A low-energy mode, linked to long-wavelength density shifts (a Goldstone mode),
- And a gapped higher-energy mode, associated with oscillations in the amplitude of the density modulation often interpreted as a Higgs-like mode.

VALIDATION AND TESTING

To validate our results, we compared our excitation spectrum with the findings from the paper “Fate of the Amplitude Mode in a Trapped Dipolar Supersolid”. While their study was conducted in a 3D geometry, our work focuses on a quasi-1D system. Despite this difference in dimensionality, we observe a qualitatively similar structure in the excitation spectrum.
In particular, both our results and the paper show:

- A softening of the lowest excitation mode near the supersolid transition point.
- The splitting of modes into a low-energy Goldstone mode and a higher-energy gapped amplitude (Higgs-like) mode.
- Dense clustering of eigenvalues at lower scattering lengths, indicating strong mode coupling and hybridization.

This close match — even with reduced dimensionality — supports the physical validity of our BdG spectrum. It confirms that the essential features of the supersolid phase transition and the emergence of collective excitations are accurately captured by our quasi-1D model.

CHALLENGES FACED

1. Computational Bottlenecks
A major challenge was the computational cost associated with constructing and diagonalizing large BdG matrices. Since the matrix size scales with 2Nb*2NB, increasing the number of basis functions (NbN_bNb) caused a sharp rise in memory and time complexity. For example, running a full parameter sweep over several values of scattering length became time-intensive and impractical for large basis sizes without code optimization.

2**. Numerical Overflow in U(k) Calculation**
While computing the Fourier-transformed dipolar interaction potential U(k), we encountered exponential overflow for large values of k, particularly when $u=k^2/2$ exceeded 700. This caused numerical values to blow up, resulting in NaN entries in the interaction kernel and ultimately in the BdG matrix. To mitigate this, we applied a limiting condition to replace these cases with their asymptotic analytical limit, restoring numerical stability.

3. Error in Plotting Eigenvalues vs Scattering Length
Initially, our plots of BdG eigenvalues versus scattering length a_s were misleading and misaligned. This was due to errors in reference energy subtraction and mismatched indexing. As a result, the visual representation did not accurately reflect the physical trends. We resolved this by fixing the reference energy component and ensuring correct axis alignment and data sorting during plotting.

4. Long Runtime for Large Basis Size
With increasing NbN_bNb, the code became significantly slower due to repeated integrals and inefficient nested loops. While we optimized some of the matrix operations using NumPy vectorization and avoided redundant calculations, very large basis sizes still remained computationally expensive. Full resolution simulations for high NbN_bNb were feasible but time-consuming, suggesting the need for parallelization or GPU acceleration in future extensions.

FUTURE WORK AND IMPROVEMENT

1. Parallelization and GPU Acceleration

One of the most impactful improvements would be the integration of parallel computing techniques to accelerate matrix construction and diagonalization processes. As the number of basis functions increases, the computational cost of evaluating integrals and diagonalizing the BdG matrix grows rapidly. By leveraging Python's multiprocessing module or using GPU-based computation libraries such as CuPy or PyTorch, the runtime can be significantly reduced. This would allow high-resolution simulations to run efficiently even on personal computing hardware.

2. Extension to 3D Systems

Currently, the toolbox is designed for quasi-one-dimensional systems. An important next step is to generalize the framework to fully three-dimensional (3D) dipolar BECs. In 3D, the interplay between anisotropic dipolar interactions and geometry leads to richer excitation behavior, such as roton instabilities, angular-dependent modes, and possible quantum droplets. Extending the toolbox to 3D would involve more complex basis functions (e.g., spherical harmonics) and higher-dimensional integration, but would significantly broaden its scientific applicability.

3. Web-Based Interface

To make the toolbox accessible to a wider audience — including experimental physicists, educators, or students with limited programming experience — we aim to develop a web-based graphical user interface (GUI). This would allow users to:

- Input parameters like scattering length, number of atoms, and trap geometry,
- Run simulations through a browser-based interface,
- View real-time plots of excitation spectra without writing or editing code.

Frameworks such as Streamlit, Flask, or Dash could be used to develop this interface. A GUI would also support batch simulations and parameter sweeps with output visualization, making the toolbox a more complete platform for exploration and teaching.

CONCLUSION

- We developed a robust Python toolbox capable of computing the excitation spectrum of one-dimensional dipola Bose-Einstein condensates.
  It integrates key physical interactions and supports parameter sweeps for in-depth analysis.
  The toolbox is modular and adaptable for future extensions.

- The implementation ensures accurate and efficient numerical analysis using the Bogoliubov-de Gennes (BdG) formalism.A harmonic oscillator basis is employed for stable matrix construction and diagonalization.
  This approach balances computational efficiency with theoretical rigor.
  The toolbox helps in exploring the influence of dipolar interactions and quantum fluctuations in low- dimensional systems.

- Users can investigate how the excitation modes evolve with interaction strength.
  This enables deeper physical insights into stability and phase behavior.
  However, the computation time becomes significant as the basis size increases.
  This limits the ability to perform high-resolution studies over a wide parameter space.

- Large-scale simulations remain computationally expensive on standard hardware.
  Further optimization is essential to improve runtime and scalability.
  Incorporating parallel computing or GPU acceleration can make the code faster and more versatile.
  This will enable efficient handling of larger systems and higher dimensions.

APPENDICES

Appendix A: Sample Code Snippets

Below are key snippets from the developed Python toolbox that demonstrate critical functionality related to the construction and solution of the BdG equations.

A.1: BdG Matrix Construction

```
def BdG(mu, phi, X1, X2, X3, X4, Nx, dx, N_atom, N_b, lambda_x, psix, DPR, gamma):
    MATRIX = np.zeros((2 * N_b, 2 * N_b), dtype=np.complex128)

    # Diagonal harmonic trap terms
    for j in range(N_b):
        MATRIX[j, j] = (j + 0.5) * lambda_x - mu
        MATRIX[j + N_b, j + N_b] = (j + 0.5) * lambda_x - mu
```

A.2: BdG Matrix Element Filling

```
for i in range(N_b):
    for j in range(N_b):
        term1 = scipy.integrate.simpson(M * psix[i, :] * psix[j, :], x=x)
        term2 = scipy.integrate.simpson(M12 * psix[i, :] * psix[j, :], x=x)
        term3 = scipy.integrate.simpson(M21 * psix[i, :] * psix[j, :], x=x)
        tmp_dpr = scipy.integrate.simpson(psix[i, :] * DPR * psix[j, :], x=x)

        # Filling BdG matrix blocks
        MATRIX[i, j] += tmp_dpr + X1[i, j] + (5.0 / 2.0) * gamma * term1
        MATRIX[i, j + N_b] = (3.0 / 2.0) * gamma * term2 + X2[i, j]
        MATRIX[i + N_b, j] = -((3.0 / 2.0) * gamma * term3 + X3[i, j])
        MATRIX[i + N_b, j + N_b] = -(MATRIX[i + N_b, j + N_b] + tmp_dpr + (5.0 / 2.0) * gamma * term1 + X4[i, j])
```

A.3: Diagonalization and Sorting

```
W, VR = np.linalg.eig(MATRIX)              # Diagonalize BdG matrix
idx = np.argsort(np.abs(W))                # Sort by absolute eigenvalue
W_sorted = W[idx] / lambda_x               # Normalize by trap frequency
VR_sorted = VR[:, idx]
```

Appendix B: Detailed Mathematical Derivations

B.1: Gross-Pitaevskii Equation

The time-independent Gross-Pitaevskii Equation (GPE) for a dipolar BEC:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(x) + g|\psi(x)|^2 + \Phi_d(x)\right)\psi(x) = \mu\psi(x)$$

where:

- Vext is the harmonic trap,
- g is the contact interaction strength,
- Φd(x) is the dipolar potential term.

B.2: BdG Linearization

To derive the BdG equations, the condensate wavefunction is perturbed:

$$\psi(x,t) = e^{-i\mu t/\hbar}\left[\phi(x) + u(x)e^{-i\omega t} + v^*(x)e^{i\omega t}\right]$$

Substituting this into the time-dependent GPE and linearizing in u, v yields:

$$\mathcal{L}u(x) + \mathcal{M}v(x) = \hbar\omega u(x)$$

$$-\mathcal{M}^*u(x) - \mathcal{L}^*v(x) = \hbar\omega v(x)$$

where L and M include both contact and dipolar interactions.

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