Computations in Quantum Mechanics Python Implementation

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IISc

April 23, 2025

Computational Methods

This presentation covers the following computational techniques for quantum mechanical problems:

- **Matrix Representations**: Construction of quantum operators using ladder operators and tensor products.
- **Eigenvalue/Eigenvector Calculations**: Numerical diagonalization for energy spectra and eigenstates.
- **Time Evolution Simulations**: Solving the time-dependent Schrödinger equation using matrix exponentiation.
- **Open Quantum Systems**: Modeling particle loss and decoherence using Lindblad master equations.
- **Many-Particle Systems**: Analysis of Bose-Hubbard models for interacting bosons.

Introduction

- Quantum mechanics can be numerically simulated using matrix representations of Hilbert space operators.
- This project explores various quantum systems, including one-dimensional potentials, angular momentum operators, and many-particle systems.
- Numerical methods include finite difference techniques, spectral analysis, and time evolution simulations.
- The implementation is done in Python using libraries like NumPy, SciPy, and Matplotlib, translating concepts from MATLAB-based quantum computations.
- Visualization of quantum dynamics and energy spectra provides insights into physical phenomena.

Paper Reference

arXiv:1603.04167v1 [quant-ph] 14 Mar 2016

Computations in quantum mechanics made easy

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Abstract. Convenient and simple numerical techniques for performing quantum computations based on matrix representations of Hilbert space operators are presented and illustrated by various examples. The applications include the calculations of spectral and dynamical properties for one-dimensional and two-dimensional single-particle systems as well as bosonic many-particle and open quantum systems. Due to their technical simplicity these methods are well suited as a tool for teaching quantum mechanics to undergraduates and graduates. Explicit implementations of the presented numerical methods in MATLAB are given.

Submitted to: *Eur. J. Phys.*

1. Introduction

In [1] it was shown how to calculate the spectra of one-dimensional quantum systems in a simple, convenient and effective way by means of matrix representations of Hilbert space operators. Here we extend these techniques in various ways including the computation of dynamical properties as well applications to higher dimensional systems, bosonic many-particle and open quantum systems.

As discussed in [1] the basic building blocks for the discrete matrix representation of operators used in the following programs are the operators $\hat{a}$ and $\hat{a}^\dagger$, well known from the harmonic oscillator, where they act as ladder operators on the harmonic oscillator eigenstates $|n\rangle$, $n = 0, 1, 2, \ldots$:

$$\hat{a}\,|n+1\rangle = \sqrt{n+1}\,|n\rangle\,, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle\,, \quad \hat{a}^\dagger\hat{a}\,|n\rangle = n\,|n\rangle\,. \tag{1}$$

Motivated, e.g., by the application to the radiation field described by harmonic oscillators with frequency ω_0 these operators create or annihilate a photon of this frequency or, more generally, a bosonic particle in second quantization. Therefore these

Python Code Example

```
1 Parameters N = 1000 xmin, xmax = -10, 10 dx = (xmax - xmin) / N x =
  np.linspace(xmin, xmax, N)
2 Potential (harmonic oscillator) V = 0.5 * x**2
3 Kinetic energy matrix (using finite difference) diagonals = [np.ones(N-1),
  -2*np.ones(N), np.ones(N-1)] offsets = [-1, 0, 1] T = sp.diags(diagonals, offsets)
  * (-0.5/(dx**2))
4 Hamiltonian H = T + sp.diags(V, 0)
5 Solve eigenvalue problem eigenvalues, eigenvectors = spla.eigsh(H, k=6,
  which='SM')
```

MATLAB Code Example

```
; xmin = -10; xmax = 10; dx = (xmax-xmin)/N; x = linspace(xmin, xmax, N);
V = 0.5 * x.^2;
e = ones(N,1); T = spdiags([e -2*e e], -1:1, N, N) * (-0.5/(dx^2));
H = T + spdiags(V(:), 0, N, N);
[psi, E] = eigs(H, 6, 'sm'); E = diag(E);
```

Advantages of Each Implementation

MATLAB Advantages

- Intuitive matrix syntax
- Integrated visualization
- Strong documentation
- Built-in eigenvalue solvers
- Academic community support

Python Advantages

- Open-source and free
- Better scalability
- Integrates with ML frameworks
- Growing quantum packages
- Modern development practices

Methodology

- **Matrix Representation of Operators:**
  - Ladder operators a and $a^\dagger$ are used to build position and momentum operators:

$$\hat{x} = \sqrt{\frac{1}{2}}(a^\dagger + a), \quad \hat{p} = i\sqrt{\frac{1}{2}}(a^\dagger - a)$$

- **Eigenvalue Computation:**
  - Spectral analysis via `numpy.linalg.eig()` or `scipy.linalg.eigh()`.
- **Time Evolution:**
  - Time-dependent wavefunction evolution using matrix exponentiation e^{-iHt}.
- **Many-Particle Systems:**
  - Modeled using the Bose-Hubbard Hamiltonian with tensor products of creation/annihilation operators.
- **Open Quantum Systems:**
  - Lindblad master equation models particle loss due to environment interaction.

Analytical vs Computational Comparison

System	Analytical Approach	Computational Approach
1D Quantum System	- Exact solutions for simple potentials (e.g., harmonic oscillator).	- Matrix representation of $\hat{x}$, $\hat{p}$, and $\hat{H}$. - Diagonalize to get eigenvalues and wavefunctions.
Bloch Oscillation	- Bloch theorem predicts periodic motion. - Energy spectrum: $E_n = \varepsilon + dFn$.	- Time evolution using tight-binding Hamiltonian. - Simulate wave packet dynamics with $\hat{U} = e^{-i\hat{H}\Delta t}$.
Angular Momentum	- Commutation relations & ladder operators used to derive energy levels.	- Construct $\hat{J}_x, \hat{J}_y, \hat{J}_z$ matrices numerically. - Apply to spin systems and rigid bodies.
Asymmetric Top	- No general closed-form solution for energy levels. - Only special cases (symmetric tops).	- Full numerical diagonalization of the asymmetric rotor Hamiltonian. - Histogram reveals classical-like features.
Many-Particle System	- Analytical treatment possible only for few particles or simplified limits.	- Use tensor products to build many-body operators. - Diagonalize Bose-Hubbard Hamiltonian for energy spectrum.
Open Quantum System	- Master equations (Lindblad form) can be written but are rarely solvable.	- Use density matrix formalism and time integration (e.g., predictor-corrector) to simulate dissipation and dynamics.

Table: Comparison of Analytical and Computational Approaches

One-Dimensional Quantum Systems – Theory

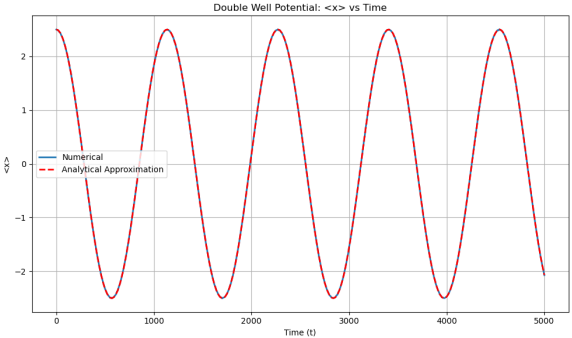
- **Hamiltonian Form:**

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

Describes a single particle in a one-dimensional potential.

- **Matrix Representation:** Position $\hat{x}$ and momentum $\hat{p}$ operators are constructed using ladder operators a, $a^\dagger$:

$$\hat{x} = \frac{1}{\sqrt{2}}(a^\dagger + a), \quad \hat{p} = \frac{i}{\sqrt{2}}(a^\dagger - a)$$



Visualization of potential $V(x)$

Bound State and Time Evolution

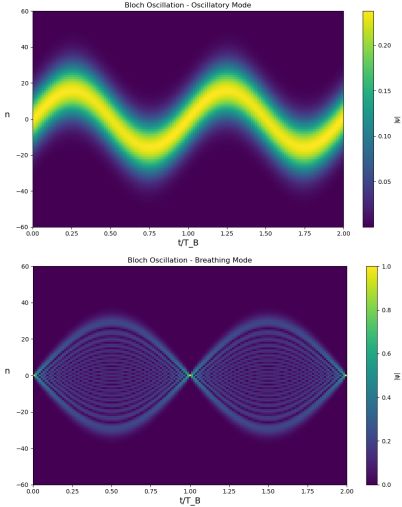
- **Bound State Calculation:**
  - Potential example: **Double well**

$$V(x) = \frac{1}{2}(|x| - x_0)^2$$

  - Numerical diagonalization yields energy eigenvalues and eigenstates.
- **Time Evolution:**
  - Time evolution via operator:

$$\hat{U} = e^{-i\hat{H}\Delta t}$$

  - Expectation value $\langle \hat{x} \rangle$ tracked over time to observe quantum dynamics.



Wave packet dynamics visualization

Bloch Oscillations – Theory

- **System Setup:**
  - Particle in a periodic potential subjected to a constant external force F.
  - Total potential:
$$V(x) = V_0(x) + Fx$$
- **Tight-Binding Approximation:**
  - Hamiltonian expressed in Wannier basis $|n\rangle$ as:
$$\hat{H} = \sum_n (\epsilon + dFn) |n\rangle \langle n| - \frac{\Delta}{4}(|n+1\rangle \langle n| + |n\rangle \langle n+1|)$$
  - d: lattice spacing, Δ: bandwidth, ϵ: on-site energy.
- **Bloch Oscillations:**
  - Despite applied force, the particle doesn't accelerate indefinitely.
  - Instead, it undergoes periodic motion with Bloch period:
$$T_B = \frac{2\pi\hbar}{dF}$$

Wave Packet Dynamics and Directed Transport

- **Wave Packet Dynamics:**
  - Narrow initial wave packet $\rightarrow$ Breathing mode.
  - Broad initial packet (Gaussian) $\rightarrow$ Oscillatory motion across lattice sites.
- **Directed Transport via Field Flipping:**
  - Alternating the force direction every half Bloch period cancels backward motion.
  - Results in net transport across lattice.
  - Velocity of transport is independent of F:

$$v = \frac{\Delta d}{\pi \hbar}$$

- **Visualization:**
  - Simulation shows wave packet spreading and oscillating.

Wave packet dynamics visualization

Angular Momentum Operators – Theory

- **Angular Momentum Basis:**
  - Quantum states labeled as $|j, m\rangle$ with:
    - j: total angular momentum (integer or half-integer),
    - m: magnetic quantum number (from $-j$ to $+j$).
- **Ladder Operators:**
  - Defined as:

$$\hat{J}_+|j, m\rangle = \sqrt{j(j+1) - m(m+1)}|j, m+1\rangle$$

$$\hat{J}_- = \hat{J}_+^\dagger$$

- **Cartesian Components:**

$$\hat{J}_x = \frac{1}{2}(\hat{J}_- + \hat{J}_+), \quad \hat{J}_y = \frac{i}{2}(\hat{J}_- - \hat{J}_+), \quad \hat{J}_z = \frac{1}{2}[\hat{J}_+, \hat{J}_-]$$

Rigid Body Hamiltonian

- **Hamiltonian:**

$$\hat{H} = \frac{\hat{J}_x^2}{2I_x} + \frac{\hat{J}_y^2}{2I_y} + \frac{\hat{J}_z^2}{2I_z}$$

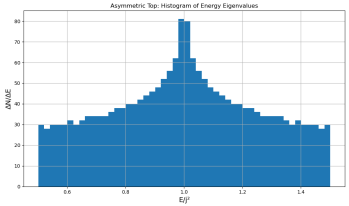
  - Models asymmetric top with different moments of inertia.
  - For symmetric tops (e.g., $I_x = I_y$), analytical solutions exist.
- **Quantum-Classical Connection:**
  - For large j, energy levels approximate classical behavior on a sphere:
    - Energy surface has **minima**, **maxima**, and **saddle points**.
  - Energy histogram (for large j) shows peak near saddle point due to infinite classical orbit period.
- **Density of States Insight:**
  - Eigenvalue density peaks at classical saddle energy.
  - Demonstrates correspondence principle — quantum mirrors classical phase space structure.

Asymmetric Top: Histogram of Energy Eigenvalues

- The plot shows the distribution of energy levels for a quantum asymmetric top with angular momentum $j = 1000$.
- The x-axis is normalized energy E/j^2, and the y-axis shows the number of states per energy bin $\Delta N/\Delta E$.
- The system models a rigid rotating body (e.g., a molecule) with three unequal moments of inertia: $I_x \neq I_y \neq I_z$.
- The energy levels are obtained by diagonalizing the Hamiltonian:

$$\hat{H} = \frac{\hat{J}_x^2}{2I_x} + \frac{\hat{J}_y^2}{2I_y} + \frac{\hat{J}_z^2}{2I_z}$$

- The sharp peak at $E/j^2 = 1$ corresponds to the classical saddle point energy, where classical orbits are unstable, causing quantum states to cluster.



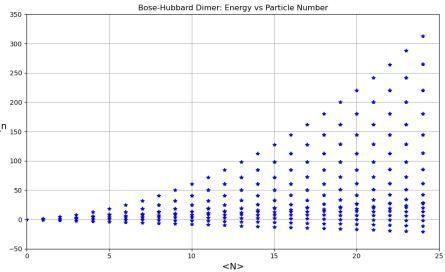
Histogram of energy eigenvalues for an asymmetric top

Many-Particle System – Bose-Hubbard Dimer (1/2)

- **System Description:**
  - Two-site system for interacting bosons, also known as a Bose-Hubbard dimer.
  - Hamiltonian:

$$\hat{H} = \epsilon(\hat{n}^1 - \hat{n}^2) + v(\hat{a}^{1\dagger}\hat{a}^2 + \hat{a}^{2\dagger}\hat{a}^1) + c(\hat{n}^1 - \hat{n}^2)^2$$

  - Operators:
    - $\hat{a}^i, \hat{a}^{i\dagger}$: annihilation/creation operators at site i,
    - $\hat{n}^i = \hat{a}^{i\dagger}\hat{a}^i$: particle number operator.
- **Key Parameters:**
  - ϵ: site energy difference,
  - v: hopping strength,
  - c: interaction strength.



Visualization of Bose-Hubbard dimer dynamics

Many-Particle System – Bose-Hubbard Dimer (2/2)

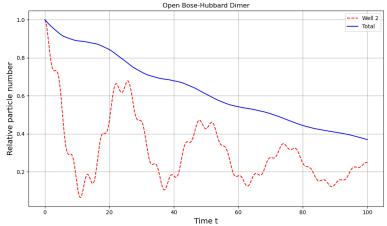
- **Numerical Setup:**
  - System modeled in a truncated Fock basis with total particle number N.
  - Full Hamiltonian built using tensor products of single-site operators.
- **Graph Description:**
  - **x-axis:** Expected total particle number $\langle N \rangle$,
  - **y-axis:** Corresponding energy eigenvalues E_n.
  - Shows distribution of converged energy levels as a function of particle number.
- **Physical Insight:**
  - Hopping promotes delocalization of particles.
  - Interaction causes level splitting and nonlinear energy structure.
  - Energy levels grouped by fixed N, with degeneracy and structure reflecting quantum correlations.

Open Quantum System – Particle Decay Dynamics

- **System Setup:**
  - Bose-Hubbard dimer with 2 particles.
  - Tunneling strength $v = 0.3$.
  - Interaction $c = 0.6$.
  - Decay rate $\gamma = 0.02$ from site 2.
- **Model:**
  - Lindblad Master Equation governs evolution:

$$\dot{\rho} = -i[\hat{H}, \rho] - \frac{\gamma}{2}(\hat{a}_2^\dagger \hat{a}_2 \rho + \rho \hat{a}_2^\dagger \hat{a}_2 - 2\hat{a}_2 \rho \hat{a}_2^\dagger)$$

  - Includes coherent evolution and dissipative decay.
- **Key Insights:**
  - Particles oscillate between wells due to tunneling.
  - Overall particle number decreases over time due to decay.
  - Interaction causes deviation from simple Rabi oscillations.



Red Dashed Line: $\langle n_2(t) \rangle / N$ (particles in decaying site).
Blue Line: $(\langle n_1(t) \rangle + \langle n_2(t) \rangle)/N$ (total particle number).

Thank you!

Questions?