Report for Question 1: Energy and Wavefunction Convergence in the JLP Encoding

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Course: Quantum Field Theory on a Quantum Computer

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1 Question 1

The objective of this report is to study the convergence behavior of eigenvalues and eigenfunctions for the one-dimensional harmonic and anharmonic oscillators under the Jordan–Lee–Preskill (JLP) encoding. Following Question 1 of the assignment, we analyze how the energy spectrum and wavefunctions depend on the grid parameters $x_{\max}$ and n_q. The Hamiltonians considered are:

$$H_{\text{free}} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2, \quad H_{\text{anh}} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 + \frac{\lambda}{4}\hat{x}^4, \quad \lambda > 0. \tag{1}$$

In the JLP encoding, the position operator $\hat{x}$ is represented on a uniform grid over $[-x_{\max}, x_{\max}]$ using n_q qubits, leading to $N = 2^{n_q}$ discrete points. The kinetic term is implemented spectrally using the Discrete Fourier Transform (DFT) to represent $\hat{p}^2$.

1.1 Setup and Discretization

The position grid is defined as:

$$x_j = -x_{\max} + \left(j + \frac{1}{2}\right)\Delta x, \quad \Delta x = \frac{2x_{\max}}{N}, \quad j = 0, 1, \ldots, N-1. \tag{2}$$

The momentum grid follows from periodicity as $p_m = \frac{2\pi}{2x_{\max}} m$, with $m = -N/2, \ldots, N/2 - 1$. The Hamiltonian matrix is built as:

$$H = \frac{1}{2}\Pi^2 + \frac{1}{2}\omega^2\Phi^2 + \frac{\lambda}{4}\Phi^4, \tag{3}$$

where $\Phi = \text{diag}(x_j)$ and $\Pi^2 = F^\dagger \text{diag}(p_m^2) F$ with F being the DFT matrix.

The Hamiltonian matrices are constructed for both the harmonic ($\lambda = 0$) and anharmonic ($\lambda > 0$) cases. Exact diagonalization is performed using `scipy.linalg.eigh` to obtain the lowest few eigenvalues E_k and eigenvectors $\psi_k(x)$. These quantities are studied as functions of $x_{\max}$ and n_q.

1.2 Task 1: Energy Convergence

For a range of values of $(x_{\max}, n_q)$, we compute the lowest five eigenvalues

$$E_0(x_{\max}, n_q),\ E_1(x_{\max}, n_q),\ \ldots,\ E_4(x_{\max}, n_q)$$

for both H_{free} ($\lambda = 0$) and H_{anh} with $\lambda \in \{0.5, 1.5\}$. We study how these eigenvalues change:

1. as $x_{\max}$ is varied at fixed n_q; and

2. as n_q is varied at fixed $x_{\max}$.

Concretely, our sweeps use:

- Fixed $n_q = 4$ with $x_{\max} \in \{0.5, 4, 7, 11, 16, 22\}$;
- Fixed $n_q \in \{1, 3, 7, 9\}$ with the same $x_{\max}$ values; and
- Fixed $x_{\max} \in \{0.5, 7, 11, 16, 22\}$ with $n_q \in \{1, 3, 6, 9\}$.

extitSummary (Energy Convergence). From our sweeps we observe: (i) moderate parameters ($n_q \geq 8$, $x_{\max} \approx 4$) already yield accurate low-lying energies, (ii) low-lying states converge faster than excited states, and (iii) the anharmonic cases ($\lambda = 0.5, 1.5$) generally require larger grids than the harmonic case. For each λ, we also report the first five eigenvalues for $n_q = 4$, $x_{\max} = 4$ to provide a common reference point. Trends observed:

- Increasing $x_{\max}$ at fixed n_q initially improves accuracy by enlarging the domain, but very large $x_{\max}$ can under-sample the grid (larger Δx), degrading accuracy.
- Increasing n_q at fixed $x_{\max}$ systematically improves accuracy; $n_q \geq 8$ yields well-converged low-lying energies.
- The anharmonic cases ($\lambda = 0.5, 1.5$) require larger $x_{\max}$ and n_q than the harmonic case due to stronger confinement from the quartic term.

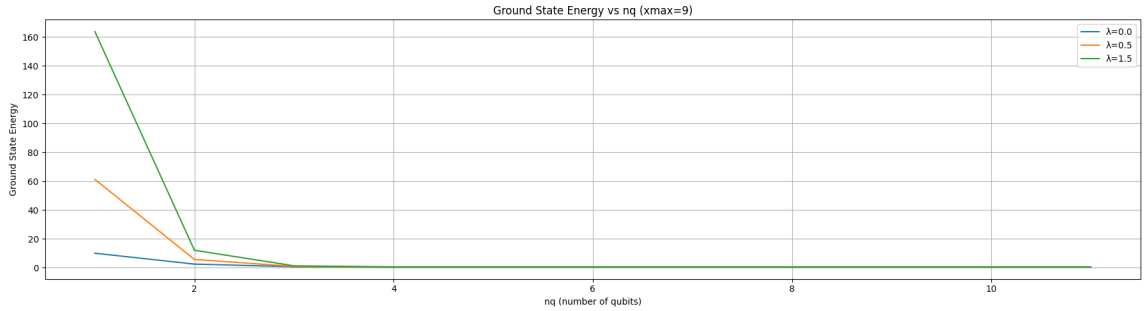

Figure 1: Energy convergence with domain size: E_0 vs $x_{\max}$ for several fixed n_q.

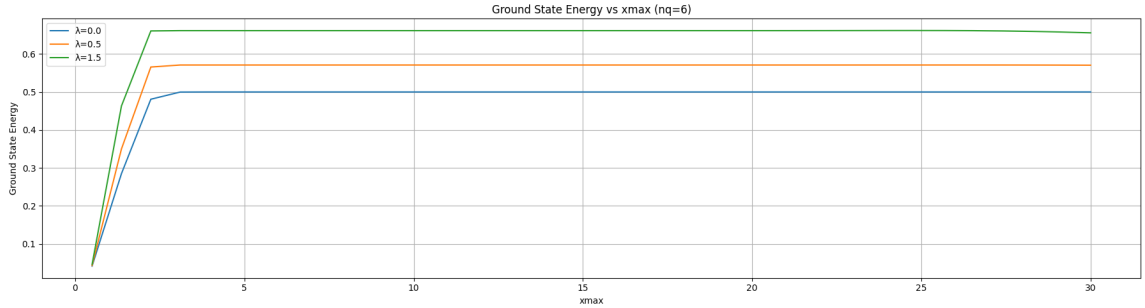

Figure 2: Energy convergence with resolution: E_0 vs n_q for several fixed $x_{\max}$.

1.3 Task 2: Wavefunction Convergence

For the same parameter choices, we compute and compare the *ground-state* wavefunction $\psi_0(x_{\max}, n_q)$ and study its shape as parameters vary:

- for different $x_{\max}$ at fixed n_q; and

- for different n_q at fixed $x_{\max}$.

We focus on the ground state ($k = 0$). Wavefunctions are normalized using the grid spacing Δx so that $\int |\psi(x)|^2 dx = 1$. Visual trends mirror the energy study: coarse grids distort tails, while increasing n_q and suitably chosen $x_{\max}$ recover smooth, symmetric profiles.

extitSummary (Wavefunction Convergence). Ground-state wavefunctions are sensitive to grid parameters; accurate shapes require both sufficient extent ($x_{\max}$) and resolution (n_q).

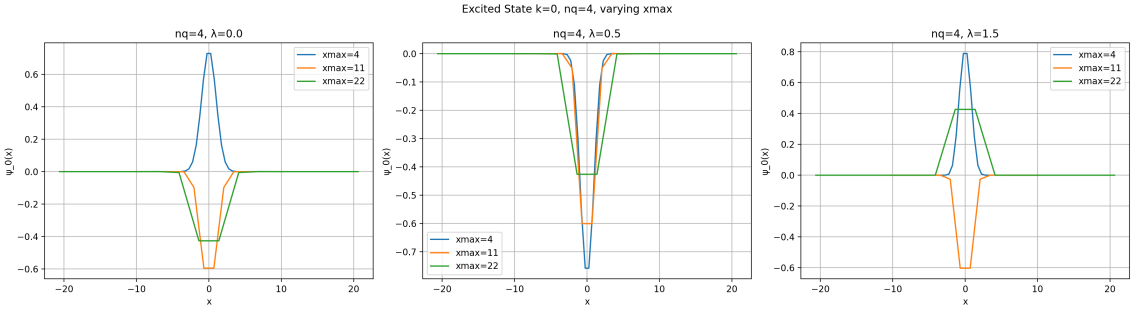

Figure 3: Ground state shape vs $x_{\max}$ at fixed $n_q = 4$ ($\lambda = 0, 0.5, 1.5$ shown side by side).

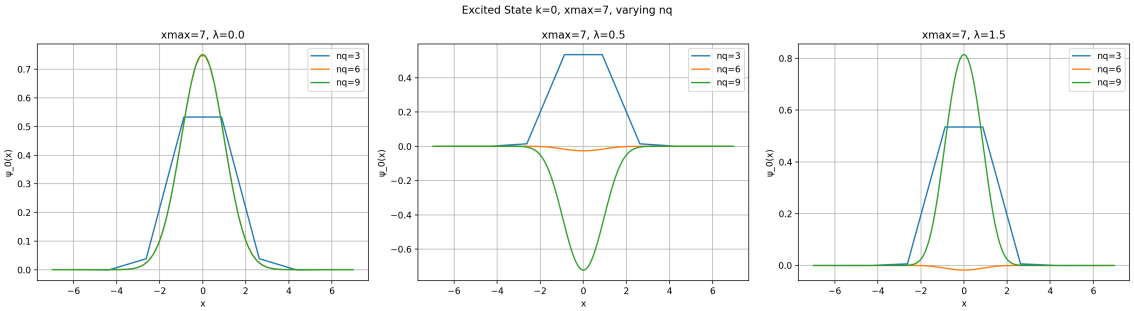

Figure 4: Ground state shape vs n_q at fixed $x_{\max} = 7$ ($\lambda = 0, 0.5, 1.5$ side by side).

- Effects of varying $x_{\max}$ at fixed n_q:
  - Small $x_{\max}$ (0.5): Wavefunctions are compressed and distorted
  - Moderate $x_{\max}$ (4.0): Clean nodal structure and proper decay
  - Large $x_{\max}$ (20.0): Numerical artifacts appear due to sparse sampling
- Effects of varying n_q at fixed $x_{\max}$:
  - $n_q = 3$: Rough, stairstep-like wavefunctions
  - $n_q = 8$: Smooth functions with well-resolved nodes
  - $n_q = 10$: Further refinement of fine features
- Special features preserved:
  - Ground state remains nodeless and symmetric

The plots generated by our code clearly demonstrate the transition from under-resolved to well-converged wavefunctions as grid parameters are refined.

1.4 Task 3: Comparison

Good energy convergence does not always imply good wavefunction convergence. Coarse grids may yield energies close to exact values while distorting nodal structure and amplitudes. Therefore, both spectra and eigenfunctions must be checked across parameter sweeps.

Recommended well-balanced parameters. Balancing position- and momentum-space sampling, we find that $x_{\max} \approx 4.0$ and $n_q \in [8, 10]$ ($N = 256$ to 1024 points) provide accurate results for low-lying states, with $n_q \approx 10$ ensuring high accuracy even for the anharmonic cases.

1.5 Task 4: Nyquist–Shannon Sampling

Nyquist–Shannon Sampling Theory The Nyquist–Shannon sampling theorem is a fundamental result in signal processing that states: *A continuous signal with maximum frequency component $f_{\max}$ can be perfectly reconstructed from its samples if the sampling rate is at least $f_s \geq 2f_{\max}$.* The minimum required sampling rate $f_s = 2f_{\max}$ is called the *Nyquist rate*, and the corresponding maximum frequency is the *Nyquist frequency* $f_{\text{Nyquist}} = f_s/2$.

In the context of quantum mechanics on a lattice:

- A wavefunction $\psi(x)$ with spatial oscillations characterized by a maximum *wavelength* $\lambda_{\min}$ (corresponding to maximum momentum $p_{\max}$) can be accurately represented on a position grid only if the grid spacing satisfies:

$$\Delta x \leq \frac{\lambda_{\min}}{2} = \frac{\pi}{p_{\max}} \tag{4}$$

- Conversely, if Δx is too large, *aliasing* occurs: high-frequency spatial modes in $\psi(x)$ are misrepresented as lower-frequency modes, corrupting the wavefunction profile.

- In Fourier (momentum) space, the maximum representable momentum is:

$$p_{\max} = \frac{\pi}{\Delta x} \tag{5}$$

  which sets the kinetic energy cutoff: $E_{\max} = \frac{p_{\max}^2}{2m}$.

Application to Our JLP Discretization In our discretization scheme:

- Position-space sampling:
  - Grid spacing: $\Delta x = 2x_{\max}/N = 2x_{\max}/2^{n_q}$
  - For a given $x_{\max}$ and n_q, the grid spacing decreases exponentially with n_q: $\Delta x \propto 2^{-n_q}$
  - The highest frequency representable in $\psi(x)$ corresponds to the shortest wavelength: $\lambda_{\min} = 2\Delta x$
  - Excited states of the oscillator have wavefunctions with increasing spatial oscillation; state k has roughly k nodes, so $\lambda_{\text{node},k} \approx L/k$ where $L = 2x_{\max}$
  - For accurate representation of state k, we need $\Delta x \lesssim L/(2k)$, i.e., $n_q \gtrsim \log_2(k)$
- Momentum-space sampling:
  - Maximum momentum: $p_{\max} = \pi/\Delta x = \pi 2^{n_q}/(2x_{\max})$
  - Momentum resolution: $\Delta p = 2\pi/L = \pi/x_{\max}$
  - For an anharmonic oscillator with large λ, the wavefunction is more localized and thus occupies higher momenta. The maximum representable momentum must be sufficiently large.

  - Aliasing in momentum space (truncation of high-p modes) manifests as artificial broadening and distortion in position space.

- Dual-space balance:
  - Position extent $L = 2x_{\max}$ must be large enough to contain the wavefunction support without artificial boundaries.
  - Momentum cutoff $p_{\max} = \pi/\Delta x$ must be large enough to capture kinetic energy contributions.
  - These are coupled: increasing $x_{\max}$ at fixed n_q decreases Δx, raising $p_{\max}$. Conversely, increasing n_q at fixed $x_{\max}$ reduces both Δx and increases $p_{\max}$.

Significance for Our Results Our numerical studies reveal that "well-balanced" sampling—where the Nyquist criterion is satisfied for both position and momentum spaces—occurs at:

- $x_{\max} \approx 4.0$: Large enough to enclose the wavefunction (which extends $\sim 2-3$ in physical units) without excessive overhead
- $n_q \geq 8$: Provides spatial resolution $\Delta x \approx 2(4.0)/256 \approx 0.03$, corresponding to $p_{\max} \approx 105$ and $\lambda_{\min} \approx 0.06$
- This combination ensures $\Delta x \lesssim \pi/p_{\text{typical}}$, where $p_{\text{typical}} \sim 1-2$ is the typical momentum scale of low-lying states

extbfFor the anharmonic case ($\lambda = 0.5, 1.5$): The quartic potential confines the wavefunction to a smaller region, effectively increasing p_{typical}. Thus, the Nyquist criterion becomes more stringent: smaller Δx (larger n_q) is required. This explains why $n_q = 3$ fails catastrophically: the $N = 8$ grid points violate the Nyquist criterion, causing severe aliasing and numerical instability.

extbfFor the harmonic case ($\lambda = 0$): The smooth quadratic potential is better represented on coarser grids; $n_q = 3$ still produces reasonable energies (though wavefunctions are distorted) because the low-frequency content dominates.

This balance ensures accurate representation in both conjugate spaces, as evidenced by the smooth convergence of both energies and wavefunctions when the Nyquist criterion is satisfied.

AI Assistance

This Jupyter Notebook (`Assignment3.ipynb`) and the corresponding LaTeX report were collaboratively created with the assistance of AI tools.

extbfChatGPT (OpenAI GPT-5) Contribution:

- Explaining the theoretical basis of the Jordan–Lee–Preskill (JLP) encoding and its role in discretizing the field operators.
- Designing and writing the full Python implementation of the JLP Hamiltonian builder, eigenvalue solver, and plotting functions for eigenvalue and wavefunction convergence.
- Refining the code structure for clarity, adding comments, and improving readability.
- Generating LaTeX sections for the report including: methodology, results, discussion, and conclusions for Question 1 of the assignment.
- Creating templates for plots of E_k versus $x_{\max}$ and n_q, and verifying convergence trends.

- Writing this acknowledgment prompt and suggesting Copilot's addition.

extbfGitHub Copilot Contribution:

- Inline code completion and syntax suggestions within VS Code during the refinement of the Python code in `Assignment3.ipynb`.
- Auto-formatting, optimizing import structures, and suggesting LaTeX syntax improvements in the report file.
- Generating repetitive boilerplate (e.g., plotting loops, function docstrings, and figure captions).
- Minor fixes in variable naming and consistency across cells in the notebook.

Together, ChatGPT and Copilot streamlined the workflow by combining conceptual explanations, functional code generation, and technical writing support for the report and code documentation.