Workshop “High Energy Physics in the Quantum Era”

Improved quantum algorithm for calculating eigenvalues of differential operators and its application to estimating the decay rate of the perturbation distribution tail in stochastic inflation

(arXiv:2410.02276)

Dec 03, 2024

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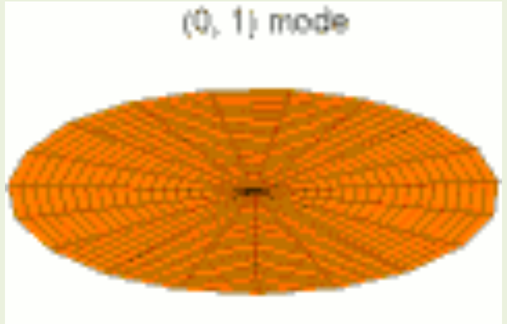
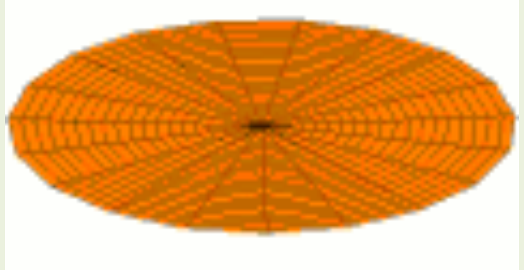
1. **Improved quantum algorithm for calculating eigenvalues of differential operators**

Eigenvalues of differential operators

- **<u>Solving partial differential equations</u>** is a major target of quantum computing
  - e.g.) Heat equation: $\frac{\partial}{\partial t} f(t, \mathbf{x}) = \Delta f(t, \mathbf{x}),\ \Delta \coloneqq \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$
  - Quantum algorithms to "solve" a PDE†, which output a quantum state encoding the solution in amplitudes: $|f\rangle = \sum_i f(x_i)|i\rangle^{\ddagger}$ (x_i: ith grid point)
  - Extracting the entire function from $|f\rangle$ takes a large complexity. We often try to extract a few quantities characterizing f.
- How about targeting such quantities from the beginning?
  - Focus on **<u>the eigenvalues of the differential operator</u>** $\mathcal{L}$
    - ✓ e.g.) $\mathcal{L}f = \lambda f, \lambda \in \mathbb{R}$
    - ✓ Important quantities that characterize the behavior of the solution



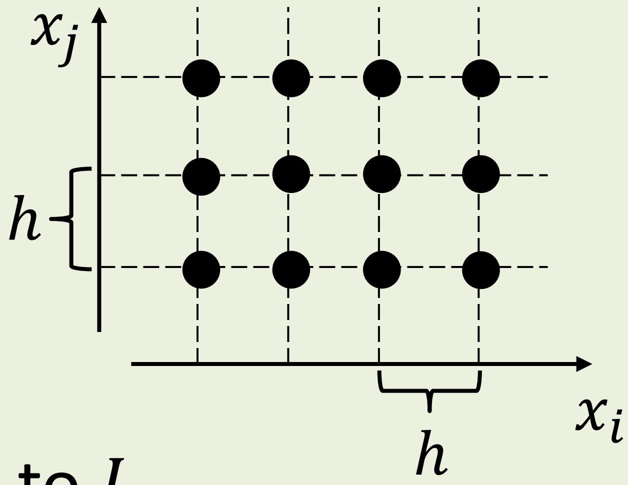
https://commons.wikimedia.org/wiki/Category:Drum_vibration_animations



† Cao+, New J. Phys. 15 013021 (2013); Linden+, Commun. Math. Phys. 395, 601 (2022); Jin+, PRA 108, 032603 (2023) ...etc ‡ The normalization factor is omitted.

A common way: finite difference method

- Set grid points in the space and approximate derivatives by the **finite difference method** (FDM)



  - e.g., central diff. $\frac{\partial}{\partial x_i} f(\mathbf{x}) \simeq \frac{1}{2h}\left(f(\mathbf{x}+h\mathbf{e}_i) - f(\mathbf{x}-h\mathbf{e}_i)\right)$ †
- This converts the differential op. $\mathcal{L}$ into a matrix L, then we apply some method for matrix eigenvalue problem to L

$$\text{e.g., } \mathcal{L} = \frac{\partial^2}{\partial x^2} \to L = \begin{pmatrix} -2/h^2 & 1/h^2 & & & \\ 1/h^2 & -2/h^2 & 1/h^2 & & \\ & \ddots & \ddots & \ddots & \\ & & 1/h^2 & -2/h^2 & 1/h^2 \\ & & & 1/h^2 & -2/h^2 \end{pmatrix}$$

- But FDM suffers from **the curse of dimensionality**
  - In d-dim cases, if we set n_{gr} grid points in each direction, L is $n_{\mathrm{gr}}^d \times n_{\mathrm{gr}}^d$
    $\to$ for large d, intractable in classical computing!

† $\mathbf{e}_i$: the unit vector in the ith direction

Previous works

- Quantum algorithms can perform exponentially large matrix calculations
  - e.g., HHL for matrix inversion: $O(\mathrm{poly}\log N)$ complexity for $N\times N$ matrices
- In fact, some works in the 2000s† proposed quantum algorithms for calculating differential op. eigenvalues, based on that for matrix eigenvalues‡
  - But, not consider multi-dimensional cases or rigorously evaluate the dependence of complexity on d
  - No paper since then, so recent progress in quantum algorithms has not been incorporated
- Let's improve the quantum algorithm using state-of-the-art techniques such as **block encoding** & **quantum singular value transformation**!

† Szkopek et al., PRA 72, 062318 (2005); Papageorgiou et al., Quantum Inf. Process. 4, 87 (2005); Bessen, J. Complex. 22, 660 (2006)
‡ Abrams & Lloyd, PRL 83, 5162 (1999)

Block encoding & Quantum singular value transformation

- Block encoding: embed a general matrix into the upper-left block of a unitary

$$U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix}$$

  - If A is sparse and we have a quantum circuit to access A's entries $O_A^{\mathrm{ent}}|i\rangle|j\rangle|0\rangle = |i\rangle|j\rangle|A_{ij}\rangle$, we can construct a block-encoding of A efficiently†

- Quantum singular value transformation (QSVT)†

  - Technique to construct a block-encoding $U_{g_{\mathrm{SV}}(A)} = \begin{pmatrix} g_{\mathrm{SV}}(A) & * \\ * & * \end{pmatrix}$ of $g_{\mathrm{SV}}(A)$, which is given by transforming A's singular values σ_i by a function g:

$$A = V \begin{pmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \ddots \end{pmatrix} W^\dagger \to g_{\mathrm{SV}}(A) = V \begin{pmatrix} g(\sigma_1) & & \\ & g(\sigma_2) & \\ & & \ddots \end{pmatrix} W^\dagger$$

(V, W: unitary)

  - enables various operations related to A

† Gilyén et al., STOC 2019 pp. 193-204; strictly, we need a few other oracles.

Our quantum algorithm: problem setting

- Consider operators of the Sturm–Liouville type

  $\mathcal{L} = -\sum_{i=1}^{d} \frac{\partial}{\partial x_i}\left(a_i \frac{\partial}{\partial x_i}\right) + a_0 \ \ (a_0, a_1, \dots, a_d : \overline{\mathcal{D}} \to \mathbb{R}_+)$

  on $\mathcal{D} \coloneqq (U, L) \times \cdots (U, L) \subset \mathbb{R}^d$

  - includes Laplacian Δ, (a part of) Fokker-Planck,
    the problem in stochastic inflation considered later, and so on
  - We impose the Dirichlet boundary condition ($f = 0$ on $\partial\mathcal{D}$)
  - All the eigenvalues are positive

Our quantum algorithm: finite-difference approx.

- Set n_{gr} points at equal intervals of h in each direction and approximate $\mathcal{L}$ as†

$$\mathcal{L}f(\mathbf{x}_{\mathbf{j}}^{\text{gr}}) \approx \sum_{i=1}^{d}\frac{-1}{h^2}\Big[a_i(\mathbf{x}_{\mathbf{j}}^{\text{gr}}+\tfrac{h}{2}\mathbf{e}_i)f(\mathbf{x}_{\mathbf{j}}^{\text{gr}}+h\boldsymbol{e}_i)-\Big(a_i(\mathbf{x}_{\mathbf{j}}^{\text{gr}}+\tfrac{h}{2}\boldsymbol{e}_i)+a_i(\mathbf{x}_{\mathbf{j}}^{\text{gr}}-\tfrac{h}{2}\boldsymbol{e}_i)\Big)f(\mathbf{x}_{\mathbf{j}}^{\text{gr}}) + a_i(\mathbf{x}_{\mathbf{j}}^{\text{gr}}-\tfrac{h}{2}\boldsymbol{e}_i)f(\mathbf{x}_{\mathbf{j}}^{\text{gr}}-h\boldsymbol{e}_i)\Big]+a_0(\mathbf{x}_{\mathbf{j}}^{\text{gr}})$$

($\mathbf{x}_{\mathbf{j}}^{\text{gr}}$: grid point in $\mathcal{D}$ labeled by $\mathbf{j}=(j_1,\dots,j_d)\in\{1,\dots,n_{\text{gr}}\}^{\times d}$)

- By this, $\mathcal{L}$ is converted into Hermitian $L\in\mathbb{R}^{N_{\text{gr}}\times N_{\text{gr}}}$
  ($N_{\text{gr}}=n_{\text{gr}}^d$: total # of grid points)

- When $n_{\text{gr}}\to\infty$, L's eigenvalues λ_k^L converge to $\mathcal{L}$'s eigenvalues λ_k‡

$$\left|\lambda_k^L-\lambda_k\right|=O\left(\frac{1}{n_{\text{gr}}^2}\right)$$

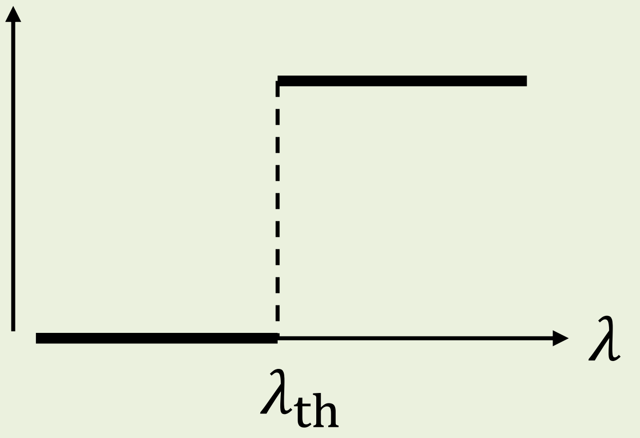
† Larsson and Thomée, "Partial differential equations with numerical method" (2003) ‡ Kuttler, SIAM J. Numer. Anal., 7, 206 (1970)

Our quantum algorithm: find the first singular value

- Now, L is Hermitian and positive-definite, so L's eigenvalue = L's singular value

- We are often interested in the first (=smallest) eigenvalue of $\mathcal{L}$

- We use a QSVT-based algorithm to find the first eigenvalue of a matrix†
  - (informal) Given a block-encoding U_H of a Hermitian H and a vector $|v\rangle$‡ that overlaps the first eigenvector $|\psi_1\rangle$ of H well (i.e., $|\langle\psi_1|v\rangle|$ is large), we find an ϵ-approx. of H's first eigenvalue λ_1 with $\tilde{O}(\|H\|/\epsilon)$ queries to U_H
  - **<u>Not dependent on *H*'s size</u>**
  - Outline : ・Using QSVT with a step-function, we can divide eigenvalues smaller/larger than threshold λ_{th}
    ・Binary search finds λ_1



† Lin and Tong, Quantum 4, 372 (2020) ‡ Strictly, suppose that we are given a quantum circuit to generate a quantum state with such a state vector.

Our quantum algorithm: complexity

- Main theorem (informal)
  - Given quantum circuits O_{a_i} to compute the coefficient functions a_i
    $O_{a_i}|\mathbf{x}\rangle|0\rangle = |\mathbf{x}\rangle|a_i(\mathbf{x})\rangle$
    and a trial function† $\tilde{f}_1: \mathcal{D} \to \mathbb{R}$ that overlaps the first eigenfunction f_1 well
    $\left|\int_{\mathcal{D}} f_1(\mathbf{x})\tilde{f}_1(\mathbf{x})\mathrm{d}\mathbf{x}\right| \geq \gamma,$
    we find an ϵ-approx. of $\mathcal{L}$'s first eigenvalue λ_1 with
    $\tilde{O}(d^3/\gamma\epsilon^2)$ queries to O_{a_i}'s.

- Polynomial complexity with respect to d

- Regarding the dependency on ϵ, compared to Szkopek et al. (2005) ($\tilde{O}(1/\epsilon^3)$), our algorithm makes an improvement.

† Strictly, suppose that we are given a quantum circuit to generate a quantum state that encodes $\tilde{f}_1$ in the amplitudes.

2. Application to estimating the decay rate of the perturbation distribution tail in stochastic inflation

Stochastic inflation

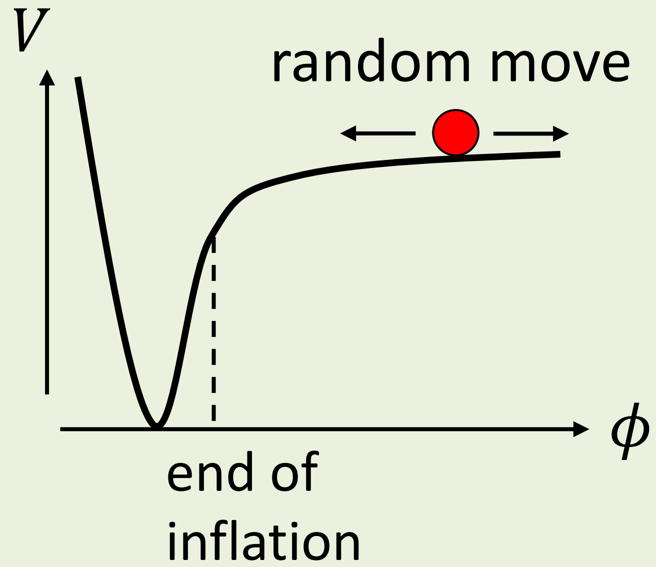
- Probabilistic framework to analyze inflationary perturbations†
  - dynamics of inflatons $\boldsymbol{\phi} = (\phi_1, \dots, \phi_d)$ (coarse-grained on a large scale‡)

$$\mathrm{d}\phi_i = -\frac{1}{v(\boldsymbol{\phi})}\partial_{\phi_i} v(\boldsymbol{\phi})\mathrm{d}N + \sqrt{2v(\boldsymbol{\phi})}\mathrm{d}W_i$$

  ($v = V/24\pi^2$, V: inflatons' potential, W_i: Wiener process, M_{Pl} is set to 1)

  - e-fold N: time variable (indicating how much the Universe has expanded)

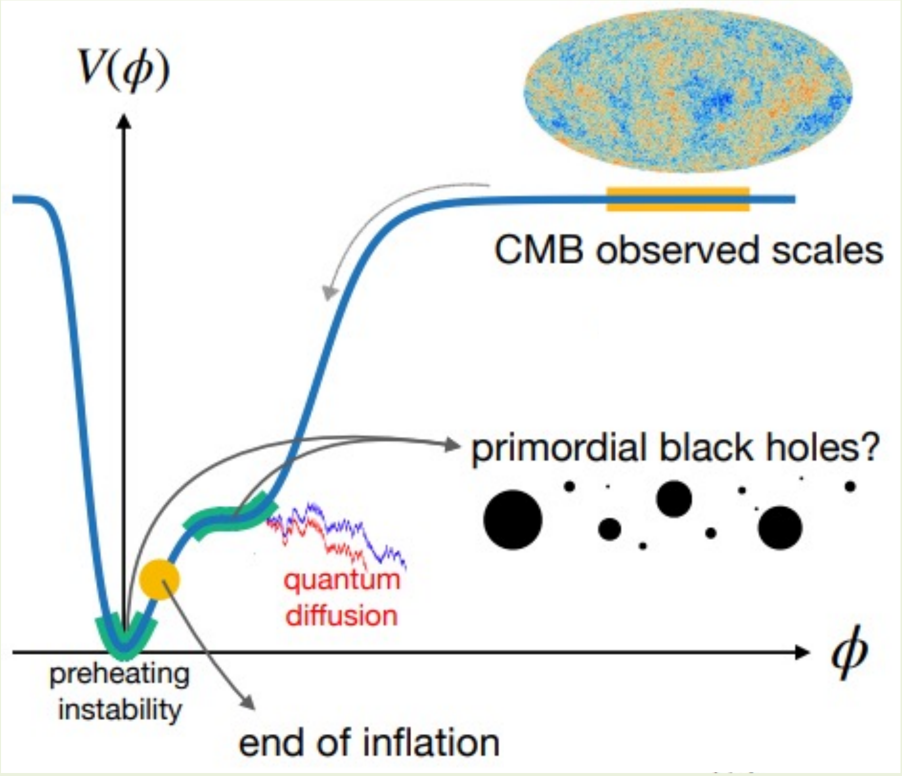
- Density perturbation = δN (roughly speaking)
  - Inflation occurs while $\boldsymbol{\phi}$ is rolling in a flat region of V, then ends when $\boldsymbol{\phi}$ reaches a steep region
  - δN: spatial fluctuation of the duration of inflation
  - long/short duration → large/small expansion → low/high density



† For a review, see Cruces, Universe 8, 334 (2022) ‡ Supper Hubble scale

Eigenvalue problem in stochastic inflation

- If inflatons go through a very flat region (e.g., inflection point), random movement dominates slow-roll
  → **Fat tail** in the probability distribution of density perturbations
  → primordial black holes



Vennin, arXiv:2009.08715

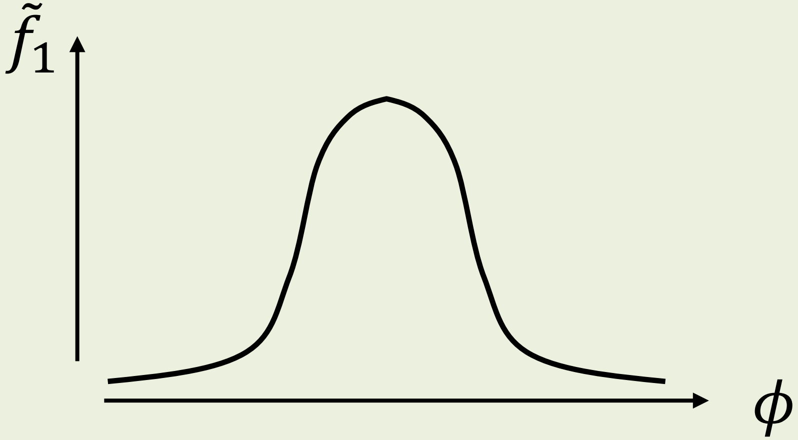
- Conditioned that inflatons are at $\boldsymbol{\phi}$ at some time, the probability density of $\mathcal{N}$, e-fold to the end of inflation, obeys the adjoint Fokker-Plack eq.

$$\partial_{\mathcal{N}} P(\mathcal{N}|\boldsymbol{\phi}) = \mathcal{L}_{\mathrm{FP}}^{\dagger} P(\mathcal{N}|\boldsymbol{\phi}),\ \mathcal{L}_{\mathrm{FP}}^{\dagger} = \sum_{i=1}^{d} \left(-\frac{\partial_{\phi_i} v}{v} \partial_{\phi_i} + v \partial_{\phi_i}^2 \right)$$

- Eigenvalues of $\mathcal{L}_{\mathrm{FP}}^{\dagger}$ = decay rate of $P(\mathcal{N}|\boldsymbol{\phi})$ w.r.t. $\mathcal{N}$
  ⇒ If $\mathcal{L}_{\mathrm{FP}}^{\dagger}$ has small eigenvalues, $P(\mathcal{N}|\boldsymbol{\phi})$ may have a fat tail!

Applying our quantum algo to find the eigenvalue of $\mathcal{L}_{\rm FP}^\dagger$

- d may be large (multifield inflation) → classically intractable
- Our quantum algorithm can be applied
  - $\mathcal{L}_{\rm FP}^\dagger$ is not of the Strum-Liouville type, but can be transformed to $\widetilde{\mathcal{L}_{\rm FP}^\dagger}$ of that type with the same eigenvalues
- Issue: Can we choose a trial function $\tilde{f}_1$ overlapping the first eigenfunc f_1 well?
  - $\left|\int_{\mathcal{D}} f_1(\mathbf{x})\tilde{f}_1(\mathbf{x})\mathrm{d}\mathbf{x}\right|$ should be as large as possible
  - But we do not know f_1...
- Idea: f_1 is expected to have a simple shape (no node, single bump,...) → **How about a Gaussian?**
  - Let's confirm through a test case!



Test case: Hybrid inflation with an inflection point

- 2-field model with the following potential

$$V(\phi,\psi) = V_\phi(\phi) + V_0\left[\left(1-\left(\frac{\psi}{M}\right)^2\right)^2 + 2\left(\frac{\phi\psi}{\phi_c M}\right)^2\right]$$

- For ϕ's potential, we take an inflection-type one

$$V_\phi(\phi) = V_0\beta(\phi-\phi_c)^3$$

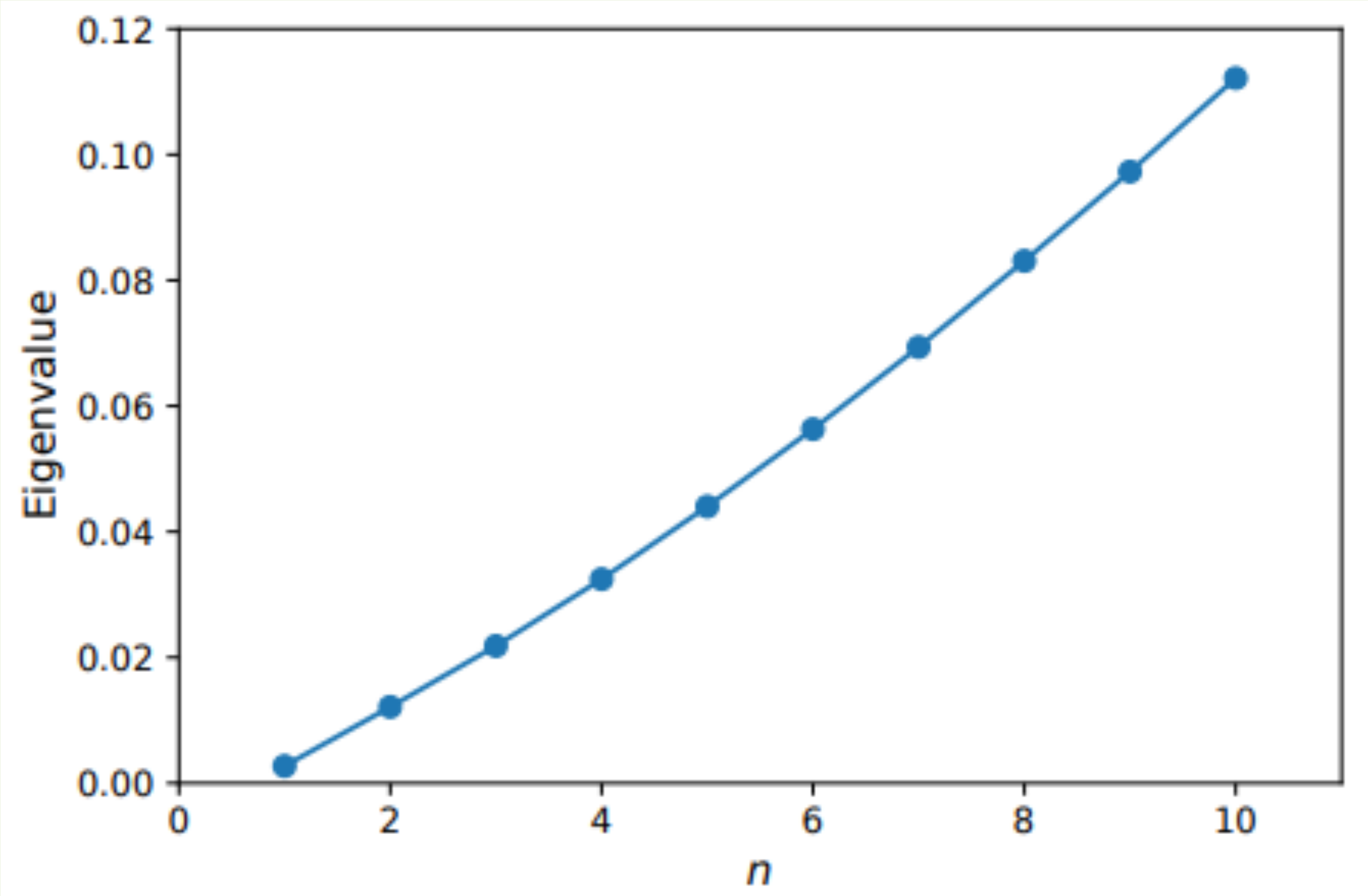
- In 2-dim cases, calculating eigenvalues by FDM can be tractable by classical computers, so we have performed it and seen the overlap between f_1 and the Gaussian trial function $\tilde{f}_1$.

- Tested parameters:

$$V_0 = 10^{-15}, M = 10^{16}\mathrm{GeV}, \phi_c = \sqrt{2}M, \beta = 10^4$$

Test case: Hybrid inflation with an inflection point

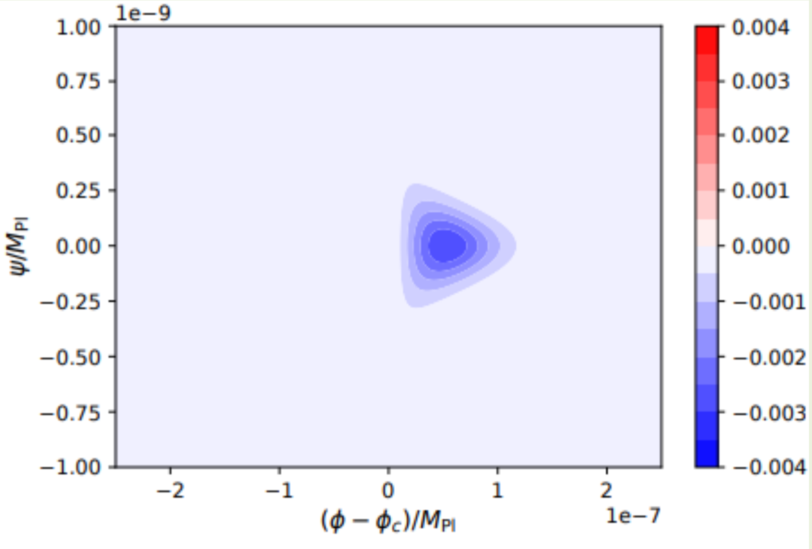
- Lowest eigenvalues



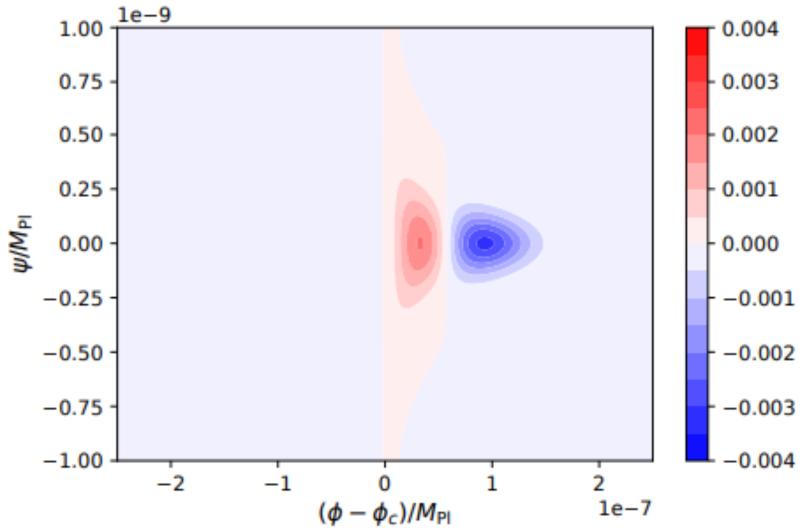
- ➢There are small eigenvalues

Test case: Hybrid inflation with an inflection point

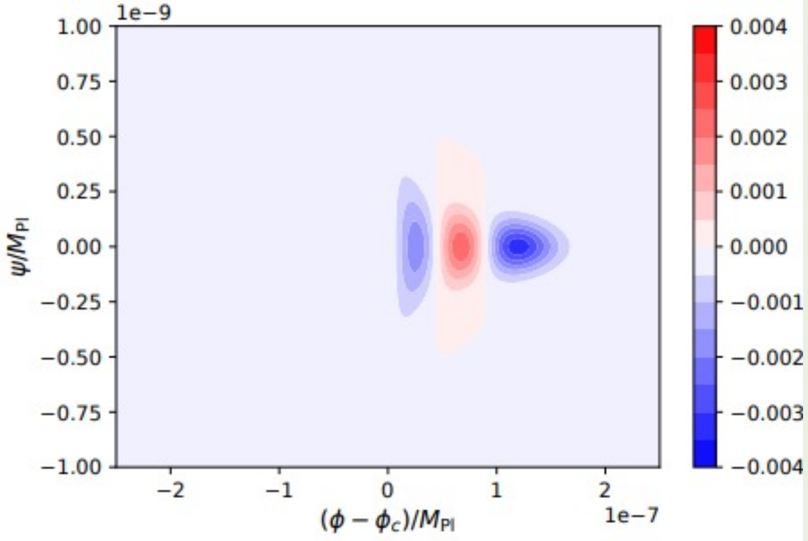
- Lowest eigenfunctions



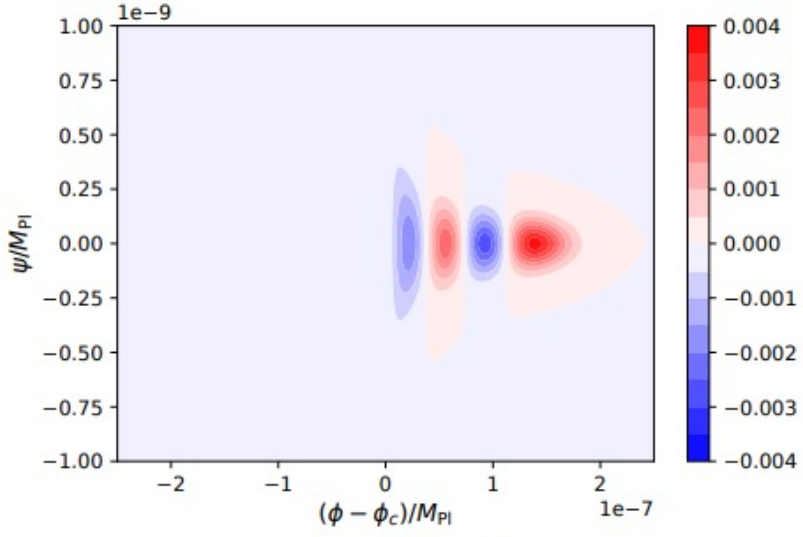
(a) $n = 1$



(b) $n = 2$



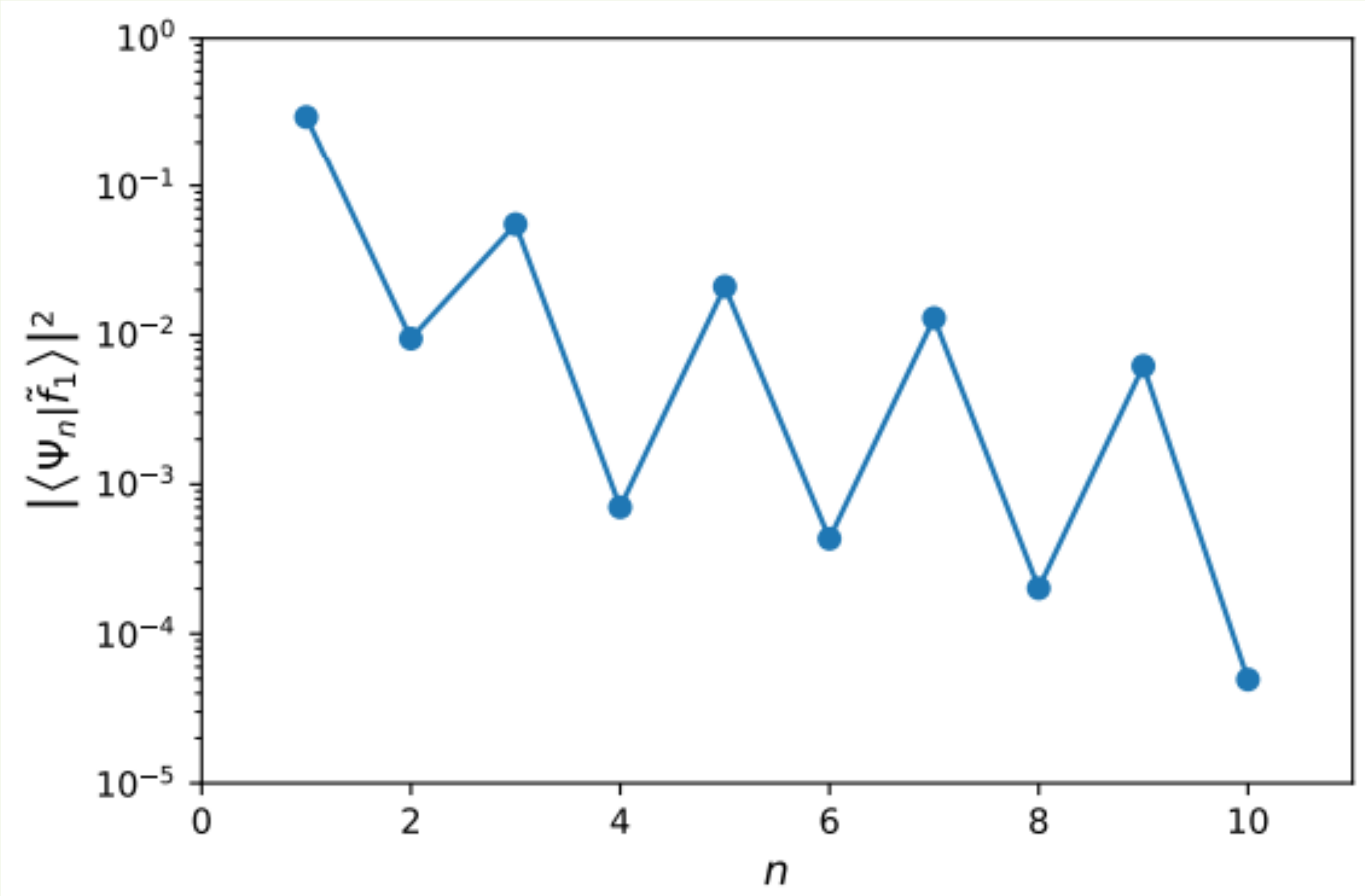
(c) $n = 3$



(d) $n = 4$

Test case: Hybrid inflation with an inflection point

- Overlap between the trial function and the lowest eigenfunctions



➢Overlap with the first eigenfuction is about 0.3

→ Our quantum algorithm is expected to work!

3. Summary

Summary

- Calculating eigenvalues of differential operators is an important task for understanding the behavior of solutions of PDEs, but the FDM approach suffers from the curse of dimensionality.

- We proposed an improved quantum algorithm for this task based on QSVT
  - query complexity: $\tilde{O}(d^3/\gamma\epsilon^2)$
    (d: dimension, ϵ: accuracy, γ: overlap b/w trial function & eigenfunction)

- HEP use-case: stochastic inflation
  - small eigenvalues of the adjoint Fokker-Planck op.
    → fat tail in the probability distribution of the density perturbation
    → PBH
  - Demonstrated the FDM for hybrid inflation with an inflection-type potential
    → Gaussian trial function works