A VARIATIONAL APPROACH TO QUANTUM FIELD THEORY

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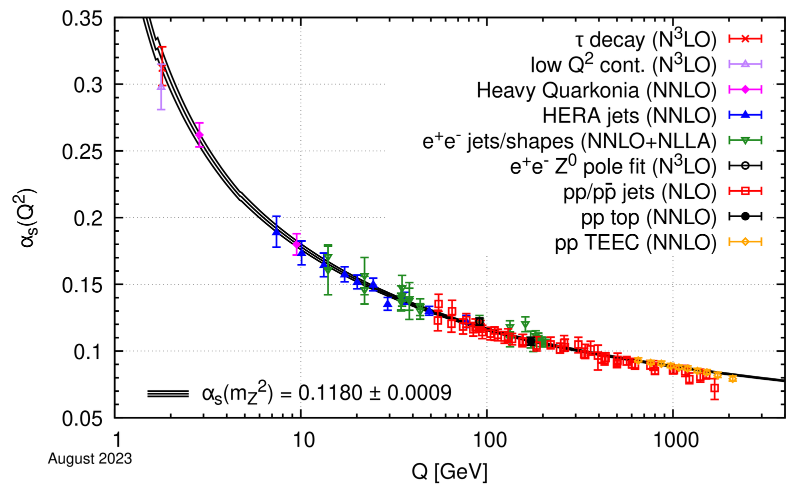
1 INTRODUCTION

- Perturbation theory cannot always be applied to compute observables in QCD.
- Coupling constant becomes large in the low-energy regime (quark confinement).
- We employ the variational method, a rigorous, non-perturbative approach which provides variational upper bounds on the ground state energy.
- We study the viability of employing a neural network as our variational ansatz.
- We study scalar field theories, which serve as a toy model for Yang-Mills theories.

[1] S. Navas et al. (Particle Data Group). Review of Particle Physics. Phys. Rev. D, 110(03001), 2024.



[2] C.N. Yang and R. L. Mills. Conservation of isotopic spin and isotopic gauge invariance. Phys. Rev., 96(1):191–195, 1954.

2 METHODS

- Monte Carlo integration with importance sampling is used to compute the energy

$$E[\Psi_\alpha] = \frac{\langle\Psi_\alpha|\hat{H}|\Psi_\alpha\rangle}{\langle\Psi_\alpha|\Psi_\alpha\rangle} \geq E_0$$

$$\Psi_\alpha = \Psi_0^{\text{free}} \cdot \text{NN}_\alpha$$

- Gradient descent optimizes the variational parameters $\boldsymbol{\alpha}$.

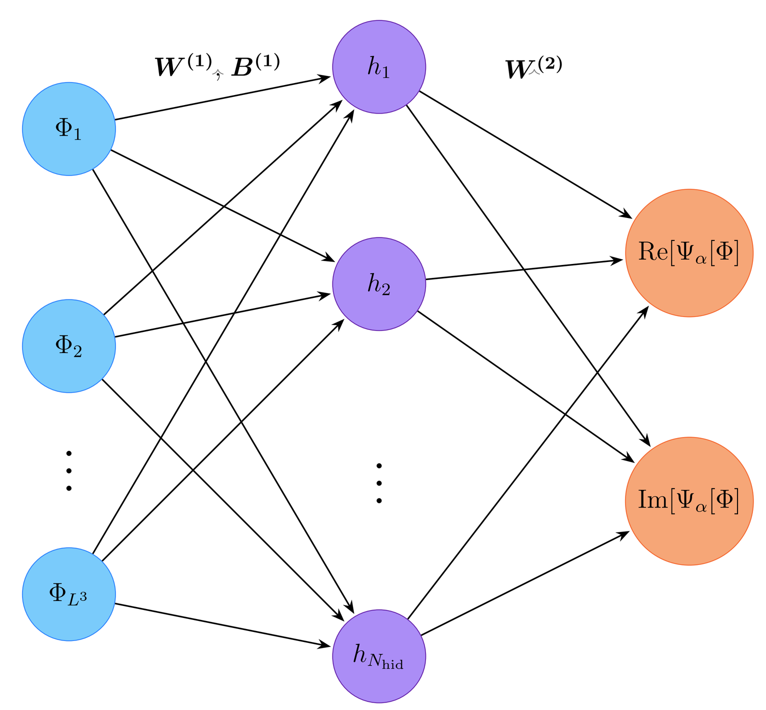


Fig. 1. Neural Network (NN) architecture serving as the ansatz for a quantum field theory, where the wavefunction is complex.

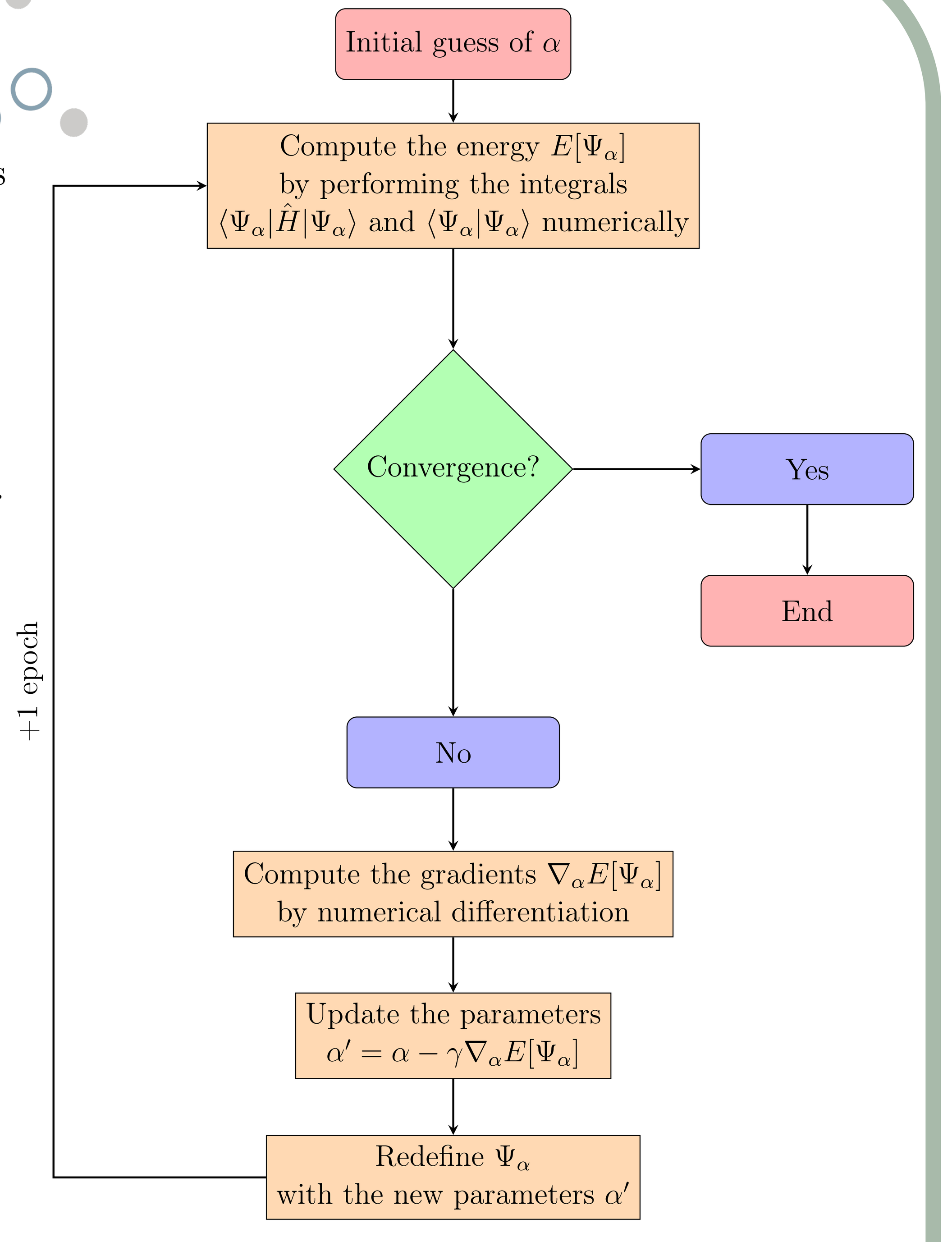


Fig. 2. Flowchart of the gradient descent algorithm.

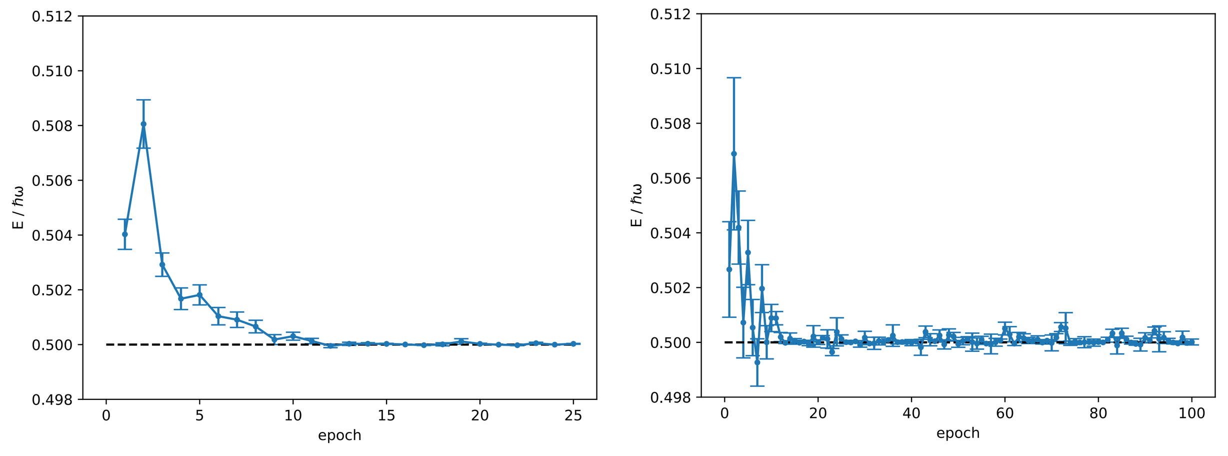
[3] Javier Rozalén Sarmiento. Machine learning tools for quantum mechanics. https: //github.com/javier-rozalen/ml-tools-for-qm, 2023.

[4] C. Gattringer and C. B. Lang. Quantum Chromodynamics on the Lattice: An Introductory Presentation, volume 788 of Lecture Notes in Physics. Springer, 2010.

Download the poster by scanning the QR code.

3 QUANTUM MECHANICS

- Harmonic oscillator and anharmonic oscillators (with different values of λ) are studied.
- Variational upper bounds saturated for the harmonic oscillator.
- Variational result for the anharmonic oscillator are compared with the ones of perturbation theory.



(a) $N_{cf} = 10^4$, epochs = 25 (b) $N_{cf} = 10^3$, epochs = 100

Fig. 3. Evolution of the energy for the gradient descent algorithm as a function of the epoch. The exact ground state energy $E = 1/2\ \hbar\omega$ is also plotted.

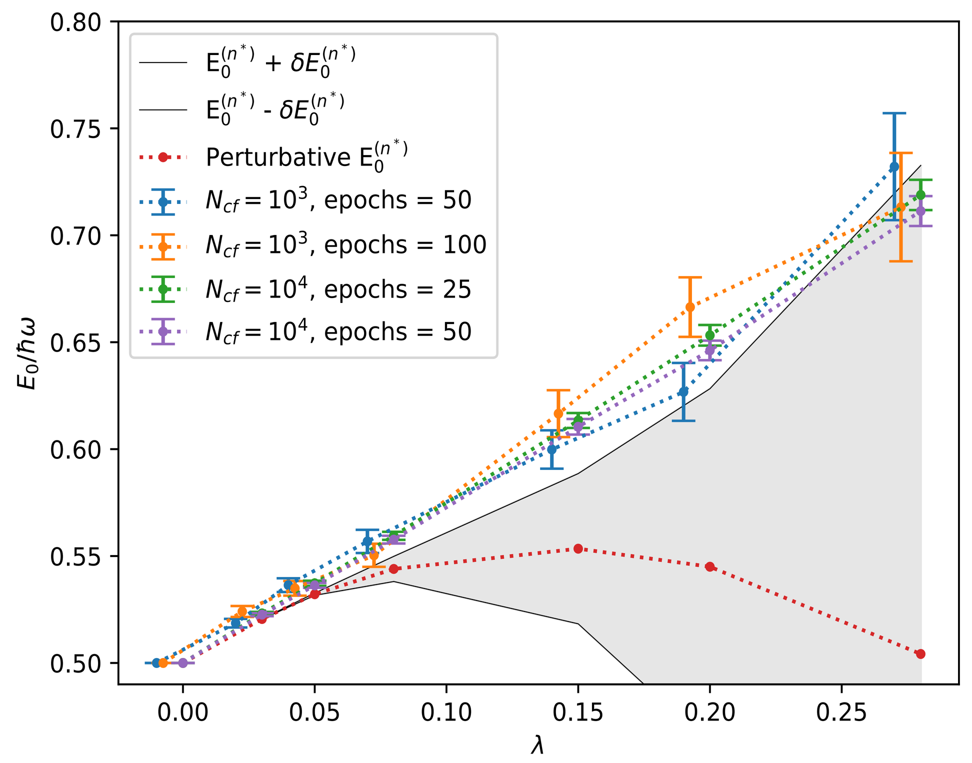


Fig. 4. Variational estimate of the energy as a function of λ. $N_{cf} = 10^3$ values are offset. Results from perturbation theory, along with its error are also shown.

[5] Carl M. Bender and Tai Tsun Wu. Anharmonic oscillator. Physical Review, 184(5):1231– 1260, 1969.

4 ϕ^4 FIELD THEORY

- We are now studying the variational **wavefunctional**.
- The lattice regularized Hamiltonian is:

$$\hat{H} = \hat{T} + \hat{U},$$

$$\hat{T} = a^3 \sum_{\boldsymbol{n}\in\Lambda} \frac{1}{2}\hat{\Pi}(\boldsymbol{n})^2 = a^3 \sum_{\boldsymbol{n}\in\Lambda} \frac{1}{2}\left(-\frac{i}{a^3}\frac{\partial}{\partial\Phi(\boldsymbol{n})}\right)^2 = -\frac{1}{2a^3}\sum_{\boldsymbol{n}\in\Lambda}\frac{\partial^2}{\partial\Phi(\boldsymbol{n})^2},$$

$$\hat{U} = a^3 \sum_{\boldsymbol{n}\in\Lambda}\left[\frac{1}{2}\sum_{j=1}^{3}\left(\frac{\hat{\Phi}(\boldsymbol{n}+\hat{j}) - \hat{\Phi}(\boldsymbol{n}-\hat{j})}{2a}\right)^2 + \frac{1}{2}m^2\hat{\Phi}(\boldsymbol{n})^2 + V(\hat{\Phi}(\boldsymbol{n}))\right].$$

[6] M. E. Peskin and D. V. Schroeder. An Introduction to Quantum Field Theory. Westview Press, 1995.

[7] Martí Rovira. Neural networks for variational quantum field theory. https://github.com/martirovira/nn_for_variational_qft, 2024.

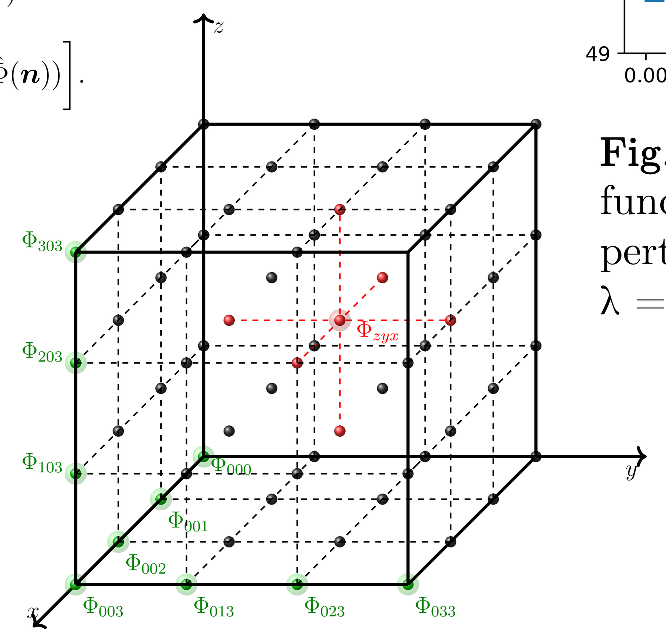


Fig. 6. Representation of a 4^3 lattice.

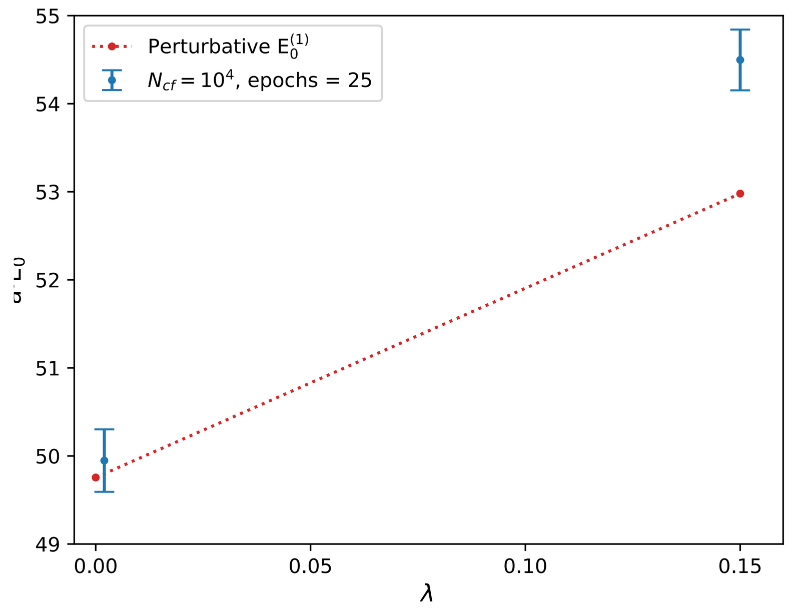


Fig. 7. Variational estimate energies as function of λ. The results from perturbation theory are also shown. The $\lambda = 0$ value is slightly offset.

5 CONCLUSIONS

- ✓ The algorithm seems to achieve convergence and reproduce well the harmonic and anharmonic oscillators in one dimension when a neural network is used as ansatz. It also gives satisfactory upper bounds to the ground energy of these systems. That is also the case for the free field and the interacting field in three dimensions.
- ✓ For the anharmonic oscillator, different values of λ are explored. Its variational results are compared with those obtained in perturbation theory. An agreement between both is observed.
- ✓ In all cases, the ansatz succeeds in reproducing the true ground state, with the optimal settings. It takes around 10-15 iterations to achieve convergence.
- ✓ For the field theories, round states are computed analytically in a 4^3 lattice. The values are:
  - aE0($\lambda = 0$) = 49.75 for a free field,
  - aE0($\lambda = 0.15$) = 52.98 for a ϕ^4 theory.

6 FUTURE RESEARCH

Focus on the optimization of the algorithm. As it takes ≈ 80 min/iteration for the field theory, in comparison with the 43 s/iteration of HO.

Different values of λ for the interacting field theory could be explored and compared with perturbation theory.

In both, quantum mechanics and quantum field systems, projector operators could be presented, in order to compute excited states.

Going beyond scalar field theory, like QCD. This would require improving the code and changing the Φ^4 Lagrangian for the QCD one.