On the mapping of a vibrational Hamiltonian model on a quantum computer.

KNAPIK Joachim[a,b]; **LASORNE Benjamin**[b]; **SENJEAN Bruno**[b]; **SCRIBANO Yohann**[a]

a) Laboratoire Univers et Particules de Montpellier, Université de Montpellier, UMR-CNRS 5299, 34095 Montpellier Cedex, France
b) ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, France

joachim.knapik@umontpellier.fr

As a relatively new topic, simulation of the vibrational structure problem with qubit-based quantum computers raises several questions [1,2]. Unlike the fermionic particules in electronic structure, bosons do not follow the Pauli exclusion principle. For the simulation of fermions one can map directly the occupation of a spin orbital or the parity on the state of a qubit. Mapping a bosonic system, wich is a more than two-level system, on a qubit basis is not straightforward and encodings that overcomes this issue have been developed [3,4]. Here we present some of these encodings with their advantages and drawbacks. To do so, we focus on a one mode tunnelling system, with a double-well potential using an harmonic oscillator basis set. We highlight the importance of ordering operators in the second quantized formulation of the Hamiltonian, due to the truncation of the supposed infinite basis. Our study point out that significant errors occur, in the eigenvalues computation, if the second quantized Hamiltonian is not properly ordered.

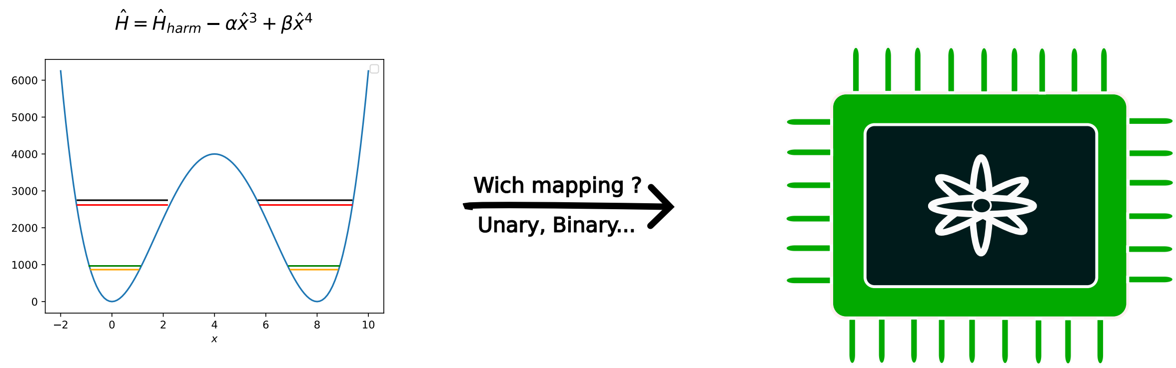

Figure 1. Illustration of the aim of the study i.e. to map a model Hamiltonian with a one mode double-well potential on a quantum computer.

Keywords: Quantum Computing, Vibrational eigenproblem, Unary Encoding, Binary Encoding

[1] N. P. D. Sawaya, T. Menke, T. H. Kyaw, S. Johri, A. Aspuru-Guzik, and G. G. Guerreschi, npj Quantum Information, 6 (2020) 1-13
[2] C Lyu, Z. Zou, X.Xu, M. Yung, A. Bayat, arXiv, quant-ph,(2024)
[3] R. D. Somma, G. Ortiz, E. H. Knill, and J. Gubernatis, Quantum Information and Computation (E. Donkor, A. R. Pirich, and H. E. Brandt, eds.), (2003)
[4] X-Y. Huang et al, arXiv, quant-ph, (2022)