Simulating Quantum Drude Oscillators on a photonic quantum computer

Matthieu Sarkis*
Department of Physics and Materials Science
University of Luxembourg, L-1511,
Luxembourg City, Luxembourg.

Adel Sohbi†
ORCA
(Dated: December 11, 2022)

I. INTRODUCTION

II. DEFINITION OF THE MODEL

$$\begin{aligned} H &= \frac{1}{2}\sum_{i=1}^{N}\left(x_i^2+p_i^2\right)+\sum_{i<j}\gamma_{ij}x_ix_j \\ &= \sum_{i=1}^{N}a_i^\dagger a_i+\sum_{i<j}\gamma_{ij}x_ix_j+\frac{N}{2} \end{aligned} \tag{1}$$

with

$$a_i=\frac{x_i+ip_i}{\sqrt{2}}\,,\qquad a_i^\dagger=\frac{x_i-ip_i}{\sqrt{2}} \tag{2}$$

III. PHOTONIC CIRCUIT

The circuit implements a unitary $U(\theta)$ acting on an input state that we simply take to be the vacuum state $|0\rangle$. The state prepared by the circuit is therefore given by

$$|\psi(\theta)\rangle=U(\theta)|0\rangle\,. \tag{3}$$

IV. VARIATIONAL ALGORITHM

We define the following loss function:

$$\mathcal{C}(\theta):=\langle\psi(\theta)|H|\psi(\theta)\rangle \tag{4}$$

with the Hamiltonian defined in eq. (1). In order to compute this loss, one therefore has to measure both the photon number operator on each channel, as well as the position quadrature operator on each channel.

V. CONCLUSION

ACKNOWLEDGMENTS

DATA AVAILABILITY

CODE AVAILABILITY

The reader will find an open source python code accompanying this paper following this github repository.

---

[1] O. Kiss, F. Tacchino, S. Vallecorsa, and I. Tavernelli, "Quantum neural networks force fields generation," *Machine Learning: Science and Technology*, vol. 3, no. 3, p. 035004, jul 2022. [Online]. Available: https://doi.org/10.1088/2632-2153/ac7d3c

[2] A. W. Harrow, A. Hassidim, and S. Lloyd, "Quantum algorithm for linear systems of equations," *Physical Review Letters*, vol. 103, no. 15, p. 150502, 2009.

[3] M. Schuld, I. Sinayskiy, and F. Petruccione, "The quest for a quantum neural network," *Quantum Information Processing*, vol. 13, no. 11, pp. 2567–2586, Nov 2014.

[4] J. Romero, J. P. Olson, and A. Aspuru-Guzik, "Quantum autoencoders for efficient compression of quantum data," *Quantum Science and Technology*, vol. 2, no. 4, p. 045001, aug 2017.

[5] C. Ciliberto, M. Herbster, A. D. Ialongo, M. Pontil, A. Rocchetto, S. Severini, and L. Wossnig, "Quantum machine learning: a classical perspective," *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 474, no. 2209, p. 20170551, 2018.

[6] V. Dunjko and H. J. Briegel, "Machine learning & artificial intelligence in the quantum domain: a review of recent progress," *Reports on Progress in Physics*, vol. 81, no. 7, p. 074001, jun 2018.

[7] C. Zoufal, A. Lucchi, and S. Woerner, "Quantum generative adversarial networks for learning and loading random distributions," *npj Quantum Information*, vol. 5, no. 1, p. 103, Nov 2019.

[8] N. Killoran, T. R. Bromley, J. M. Arrazola, M. Schuld, N. Quesada, and S. Lloyd, "Continuous-variable quan-

* matthieu.sarkis@uni.lu
† sohbi@kias.re.kr

tum neural networks," *Phys. Rev. Research*, vol. 1, p. 033063, Oct 2019.
[9] E. Farhi and H. Neven, "Classification with quantum neural networks on near term processors," 2018.
[10] K. Beer, D. Bondarenko, T. Farrelly, T. J. Osborne, R. Salzmann, D. Scheiermann, and R. Wolf, "Training deep quantum neural networks," *Nature Communications*, vol. 11, no. 1, p. 808, Feb 2020.
[11] A. Abbas, D. Sutter, C. Zoufal, A. Lucchi, A. Figalli, and S. Woerner, "The power of quantum neural networks," 2020.
[12] M. Cerezo, A. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio, and P. J. Coles, "Variational quantum algorithms," 2020.
[13] M. Schuld, K. Brádler, R. Israel, D. Su, and B. Gupt, "Measuring the similarity of graphs with a gaussian boson sampler," *Physical Review A*, vol. 101, no. 3, p. 032314, 2020.
[14] C. Blank, D. K. Park, J.-K. K. Rhee, and F. Petruccione, "Quantum classifier with tailored quantum kernel," *npj Quantum Information*, vol. 6, no. 1, p. 41, May 2020.
[15] K. Bartkiewicz, C. Gneiting, A. Černoch, K. Jiráková, K. Lemr, and F. Nori, "Experimental kernel-based quantum machine learning in finite feature space," *Scientific Reports*, vol. 10, no. 1, p. 12356, Jul 2020.
[16] Y. Liu, S. Arunachalam, and K. Temme, "A rigorous and robust quantum speed-up in supervised machine learning," 2020.
[17] H.-Y. Huang, M. Broughton, M. Mohseni, R. Babbush, S. Boixo, H. Neven, and J. R. McClean, "Power of data in quantum machine learning," 2020.
[18] J. Preskill, "Quantum Computing in the NISQ era and beyond," *Quantum*, vol. 2, p. 79, Aug. 2018. [Online]. Available: https://doi.org/10.22331/q-2018-08-06-79
[19] A. W. Harrow, A. Hassidim, and S. Lloyd, "Quantum algorithm for linear systems of equations," *Phys. Rev. Lett.*, vol. 103, p. 150502, Oct 2009. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.103.150502
[20] L. K. Grover, "A fast quantum mechanical algorithm for database search," 1996. [Online]. Available: https://arxiv.org/abs/quant-ph/9605043
[21] D. S. Abrams and S. Lloyd, "Simulation of many-body fermi systems on a universal quantum computer," *Phys. Rev. Lett.*, vol. 79, pp. 2586–2589, Sep 1997. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.79.2586
[22] ——, "Quantum algorithm providing exponential speed increase for finding eigenvalues and eigenvectors," *Phys. Rev. Lett.*, vol. 83, pp. 5162–5165, Dec 1999. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.83.5162
[23] A. Y. Kitaev, "Quantum measurements and the abelian stabilizer problem," 1995. [Online]. Available: https://arxiv.org/abs/quant-ph/9511026
[24] R. P. Feynman, "Simulating physics with computers," *International Journal of Theoretical Physics*, vol. 21, no. 6, pp. 467–488, Jun 1982. [Online]. Available: https://doi.org/10.1007/BF02650179
[25] L. Ruddigkeit, R. van Deursen, L. C. Blum, and J.-L. Reymond, "Enumeration of 166 billion organic small molecules in the chemical universe database gdb-17," *Journal of Chemical Information and Modeling*, vol. 52, no. 11, pp. 2864–2875, Nov 2012. [Online]. Available: https://doi.org/10.1021/ci300415d
[26] R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld, "Quantum chemistry structures and properties of 134 kilo molecules," *Scientific Data*, vol. 1, 2014.
[27] M. Born and W. Heisenberg, *Zur Quantentheorie der Molekeln*. Berlin, Heidelberg: Springer Berlin Heidelberg, 1985, pp. 216–246. [Online]. Available: https://doi.org/10.1007/978-3-642-61659-4_16
[28] G. E. Crooks, "Gradients of parameterized quantum gates using the parameter-shift rule and gate decomposition," 2019.
[29] J. Hoja, L. M. Sandonas, B. Ernst, A. Vazquez-Mayagoitia, R. A. D. Jr., and A. Tkatchenko, "Qm7-x: A comprehensive dataset of quantum-mechanical properties spanning the chemical space of small organic molecules," nov 2020. [Online]. Available: https://doi.org/10.5281/zenodo.4288677
[30] J. Hoja, L. Medrano Sandonas, B. G. Ernst, A. Vazquez-Mayagoitia, R. A. DiStasio, and A. Tkatchenko, "Qm7-x, a comprehensive dataset of quantum-mechanical properties spanning the chemical space of small organic molecules," *Scientific Data*, vol. 8, no. 1, Feb 2021. [Online]. Available: http://dx.doi.org/10.1038/s41597-021-00812-2
[31] V. Havlíček, A. D. Córcoles, K. Temme, A. W. Harrow, A. Kandala, J. M. Chow, and J. M. Gambetta, "Supervised learning with quantum-enhanced feature spaces," *Nature*, vol. 567, no. 7747, p. 209–212, Mar 2019. [Online]. Available: http://dx.doi.org/10.1038/s41586-019-0980-2
[32] D. Fedorov, B. Peng, N. Govind, and Y. Alexeev, "Vqe method: A short survey and recent developments," 03 2021.
[33] K. Schütt, P.-J. Kindermans, H. E. Sauceda Felix, S. Chmiela, A. Tkatchenko, and K.-R. Müller, "Schnet: A continuous-filter convolutional neural network for modeling quantum interactions," in *Advances in Neural Information Processing Systems*, I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, Eds., vol. 30. Curran Associates, Inc., 2017. [Online]. Available: https://proceedings.neurips.cc/paper/2017/file/303ed4c69846ab36c2904d3ba8573050-Paper.pdf
[34] K. T. Schütt, F. Arbabzadah, S. Chmiela, K. R. Müller, and A. Tkatchenko, "Quantum-chemical insights from deep tensor neural networks," *Nature Communications*, vol. 8, no. 1, Jan 2017. [Online]. Available: http://dx.doi.org/10.1038/ncomms13890
[35] M. Rupp, A. Tkatchenko, K.-R. Müller, and O. A. von Lilienfeld, "Fast and accurate modeling of molecular atomization energies with machine learning," *Physical Review Letters*, vol. 108, no. 5, Jan 2012. [Online]. Available: http://dx.doi.org/10.1103/PhysRevLett.108.058301
[36] M. Schuld, "Supervised quantum machine learning models are kernel methods," *arXiv e-prints*, p. arXiv:2101.11020, Jan. 2021.
[37] J. Dai and R. V. Krems, "Quantum gaussian process model of potential energy surface for a polyatomic molecule," 2022. [Online]. Available: https://arxiv.org/abs/2202.10601
[38] J. Preskill, "Quantum computing in the NISQ era and beyond," *Quantum*, vol. 2, p. 79, aug 2018. [Online]. Available: https://doi.org/10.22331%2Fq-2018-08-06-79

[39] T. Haug, C. N. Self, and M. S. Kim, “Large-scale quantum machine learning,” 2021. [Online]. Available: https://arxiv.org/abs/2108.01039

[40] K. Temme, S. Bravyi, and J. M. Gambetta, “Error mitigation for short-depth quantum circuits,” *Physical Review Letters*, vol. 119, no. 18, nov 2017. [Online]. Available: https://doi.org/10.1103%2Fphysrevlett.119.180509

[41] J. Rogers, G. Bhattacharyya, M. S. Frank, T. Jiang, O. Christiansen, Y.-X. Yao, and N. Lanatà, “Error mitigation in variational quantum eigensolvers using probabilistic machine learning,” 2021. [Online]. Available: https://arxiv.org/abs/2111.08814

[42] A. Strikis, D. Qin, Y. Chen, S. C. Benjamin, and Y. Li, “Learning-based quantum error mitigation,” *PRX Quantum*, vol. 2, no. 4, nov 2021. [Online]. Available: https://doi.org/10.1103%2Fprxquantum.2.040330

[43] A. Seif, Z.-P. Cian, S. Zhou, S. Chen, and L. Jiang, “Shadow distillation: Quantum error mitigation with classical shadows for near-term quantum processors,” 2022. [Online]. Available: https://arxiv.org/abs/2203.07309

[44] R. LaRose, A. Mari, V. Russo, D. Strano, and W. J. Zeng, “Error mitigation increases the effective quantum volume of quantum computers,” 2022. [Online]. Available: https://arxiv.org/abs/2203.05489

[45] A. Greene, M. Kjaergaard, M. E. Schwartz, G. O. Samach, A. Bengtsson, M. O’Keeffe, D. K. Kim, M. Marvian, A. Melville, B. M. Niedzielski, A. Vepsalainen, R. Winik, J. Yoder, D. Rosenberg, S. Lloyd, T. P. Orlando, I. Marvian, S. Gustavsson, and W. D. Oliver, “Error mitigation via stabilizer measurement emulation,” 2021. [Online]. Available: https://arxiv.org/abs/2102.05767

[46] E. R. Bennewitz, F. Hopfmueller, B. Kulchytskyy, J. Carrasquilla, and P. Ronagh, “Neural error mitigation of near-term quantum simulations,” 2021. [Online]. Available: https://arxiv.org/abs/2105.08086

[47] P. Suchsland, F. Tacchino, M. H. Fischer, T. Neupert, P. K. Barkoutsos, and I. Tavernelli, “Algorithmic error mitigation scheme for current quantum processors,” *Quantum*, vol. 5, p. 492, jul 2021. [Online]. Available: https://doi.org/10.22331%2Fq-2021-07-01-492

[48] N. Cao, J. Lin, D. Kribs, Y.-T. Poon, B. Zeng, and R. Laflamme, “Nisq: Error correction, mitigation, and noise simulation,” 2021. [Online]. Available: https://arxiv.org/abs/2111.02345

[49] K. Wang, Y.-A. Chen, and X. Wang, “Measurement error mitigation via truncated neumann series,” 2021. [Online]. Available: https://arxiv.org/abs/2103.13856

[50] S. Ferracin, A. Hashim, J.-L. Ville, R. Naik, A. Carignan-Dugas, H. Qassim, A. Morvan, D. I. Santiago, I. Siddiqi, and J. J. Wallman, “Efficiently improving the performance of noisy quantum computers,” 2022. [Online]. Available: https://arxiv.org/abs/2201.10672

[51] Y. Li and S. C. Benjamin, “Efficient variational quantum simulator incorporating active error minimization,” *Physical Review X*, vol. 7, no. 2, jun 2017. [Online]. Available: https://doi.org/10.1103%2Fphysrevx.7.021050

[52] K. Hansen, F. Biegler, R. Ramakrishnan, W. Pronobis, O. A. von Lilienfeld, K.-R. Müller, and A. Tkatchenko, “Machine learning predictions of molecular properties: Accurate many-body potentials and nonlocality in chemical space,” *The Journal of Physical Chemistry Letters*, vol. 6, no. 12, pp. 2326–2331, 2015, pMID: 26113956. [Online]. Available: https://doi.org/10.1021/acs.jpclett.5b00831

[53] I. Kerenidis and A. Prakash, “Quantum machine learning with subspace states,” 2022. [Online]. Available: https://arxiv.org/abs/2202.00054

[54] I. Kerenidis, J. Landman, A. Luongo, and A. Prakash, “q-means: A quantum algorithm for unsupervised machine learning,” 2018. [Online]. Available: https://arxiv.org/abs/1812.03584

[55] I. Kerenidis and A. Prakash, “A quantum interior point method for lps and sdps,” 2018. [Online]. Available: https://arxiv.org/abs/1808.09266

[56] V. Havlíček, A. D. Córcoles, K. Temme, A. W. Harrow, A. Kandala, J. M. Chow, and J. M. Gambetta, “Supervised learning with quantum-enhanced feature spaces,” *Nature*, vol. 567, no. 7747, p. 209, 2019.

[57] K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii, “Quantum circuit learning,” *Phys. Rev. A*, vol. 98, p. 032309, Sep 2018.

[58] M. Schuld and N. Killoran, “Quantum machine learning in feature hilbert spaces,” *Physical Review Letters*, vol. 122, no. 4, feb 2019. [Online]. Available: https://doi.org/10.1103%2Fphysrevlett.122.040504

[59] U. Chabaud, D. Markham, and A. Sohbi, “Quantum machine learning with adaptive linear optics,” *Quantum*, vol. 5, p. 496, jul 2021. [Online]. Available: https://doi.org/10.22331%2Fq-2021-07-05-496

[60] H.-Y. Huang, M. Broughton, M. Mohseni, R. Babbush, S. Boixo, H. Neven, and J. R. McClean, “Power of data in quantum machine learning,” *Nature Communications*, vol. 12, no. 1, may 2021. [Online]. Available: https://doi.org/10.1038%2Fs41467-021-22539-9

[61] A. Tkatchenko, R. A. DiStasio, R. Car, and M. Scheffler, “Accurate and efficient method for many-body van der waals interactions,” *Phys. Rev. Lett.*, vol. 108, p. 236402, Jun 2012. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.108.236402

[62] C. Adamo and V. Barone, “Toward reliable density functional methods without adjustable parameters: The pbe0 model,” *The Journal of Chemical Physics*, vol. 110, no. 13, pp. 6158–6170, 1999. [Online]. Available: https://doi.org/10.1063/1.478522

[63] M. Seeger, “Gaussian processes for machine learning,” *International journal of neural systems*, vol. 14, no. 02, pp. 69–106, 2004.

[64] M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, and G. Seifert, “Self-consistent-charge density-functional tight-binding method for simulations of complex materials properties,” *Phys. Rev. B*, vol. 58, pp. 7260–7268, Sep 1998. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevB.58.7260

[65] M. Gaus, Q. Cui, and M. Elstner, “Dftb3: extension of the self-consistent-charge density-functional tight-binding method (scc-dftb),” *Journal of chemical theory and computation*, vol. 7, no. 4, pp. 931–948, 2011.

[66] A. Ambrosetti, A. M. Reilly, R. A. DiStasio, and A. Tkatchenko, “Long-range correlation energy calculated from coupled atomic response functions,” *The Journal of Chemical Physics*, vol. 140, no. 18, p. 18A508, 2014. [Online]. Available: https://doi.org/10.1063/1.4865104

[67] M. Rupp, “Machine learning for quantum mechanics in a nutshell,” *International Journal of Quantum Chemistry*,

vol. 115, no. 16, pp. 1058–1073, 2015.

[68] M. Rupp, A. Tkatchenko, K.-R. Müller, and O. A. Von Lilienfeld, “Fast and accurate modeling of molecular atomization energies with machine learning,” *Physical review letters*, vol. 108, no. 5, p. 058301, 2012.

[69] D. Weininger, “Smiles, a chemical language and information system. 1. introduction to methodology and encoding rules,” *Journal of chemical information and computer sciences*, vol. 28, no. 1, pp. 31–36, 1988.

[70] E. J. Bjerrum and R. Threlfall, “Molecular generation with recurrent neural networks (rnns),” *arXiv preprint arXiv:1705.04612*, 2017.

[71] E. J. Bjerrum, “Smiles enumeration as data augmentation for neural network modeling of molecules,” *arXiv preprint arXiv:1703.07076*, 2017.