Plenary Talk PV II Mon 9:45 E415

Quantum Chemistry on Quantum Computers: Challenges and New Directions — •Sabrina Maniscalco — Algorithmiq Ltd, Kanavakatu 3C, 00160 Helsinki, Finland — QTF Centre of Excellence, Department of Physics, Faculty of Science, University of Helsinki, Finland

Simulating electronic structure problems is one of the most attractive applications of quantum computers. Current devices, however, are limited: they are still operating with small number of qubits and high level of noise. Moreover, they are affected by a large number of both technical and fundamental problems. In my talk I will focus on one of the most studied applications of quantum computers, namely quantum chemistry simulations, and I will highlight both the current major roadblocks and a new framework to overcome them. As an example I will focus on three key steps, namely how to map optimally fermionic systems to qubits [1], how to initialise the quantum computers [3], and how to measure them in the most efficient manner [4,5].

References: [1] A. Miller, Z. Zimborás, S. Knecht, S. Maniscalco, G. García-Pérez, arXiv:2212.09731. [2] A. Nykänen, M. A. C. Rossi, E. Borrelli, S. Maniscalco, G. García-Pérez, arXiv:2212.09719. [3] A. Fitzpatrick, A. Nykänen, N. Talarico, A. Lunghi, S. Maniscalco, G. García-Pérez, S. Knecht, arXiv:2212.11405. [4] G. García-Pérez, M.A. C. Rossi, B. Sokolov, F. Tacchino, P. Kl. Barkoutsos, G. Mazzola, I. Tavernelli, S. Maniscalco, PRX Quantum 2, 040342 (2021). [5] A. Glos, A. Nykänen, E. Borrelli, S. Maniscalco, M. A. C. Rossi, Z. Zimborás, G. García-Pérez, arXiv:2208.07817.