Diagrammatic Monte Carlo simulation of quantum impurity models

Philipp Werner¹

¹Columbia University, 538 West, 120th Street, New York, NY 10027, USA

Quantum impurity models play an important role as representations of molecular conductors and in the "dynamical mean field" method, currently one of the most promising tools for studying the physics of fermionic lattice models. Despite their zero-dimensional nature, the numerical simulation of impurity models remains a challenging task. Progress has been achieved with the recent development of diagrammatic Monte Carlo techniques [1–4]. This simulation approach relies on a diagrammatic expansion of the partition function and the stochastic sampling of collections of diagrams. I will explain the key ideas behind this diagrammatic method for fermionic systems, and illustrate its power and flexibility with dynamical mean field results for multi-orbital models [5].

- [1] A. N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein, Phys. Rev. B 72, 035122 (2005).
- [2] P. Werner, A. Comanac, L. de' Medici, M. Troyer and A. J. Millis, Phys. Rev. Lett. 97, 076405 (2006).
- [3] P. Werner and A. J. Millis, Phys. Rev. B 74, 155107 (2006).
- [4] E. Gull, P. Werner, O. Parcollet and M. Troyer, arXiv:0802.3222.
- [5] P. Werner and A. J. Millis, Phys. Rev. Lett. 99, 126405 (2007).