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Stuttgarter Physikalisches Kolloquium

Max-Planck-Institut für Festkörperforschung
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Fachbereich Physik, Universität Stuttgart

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Login data will be announced by e-mail and on the colloquium webpage.

Dienstag, 4. Mai 2021 | **16.15 Uhr** | **Online-Vortrag**

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Past and recent progress of the variational approach by quantum Monte Carlo

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Abstract

I review the most simple, but in my opinion most powerful, technique to describe the electron correlation in realistic materials, the nowadays standard Variational Monte Carlo method. I report several progress in this field [1], that cover two main achievements, developed in the last decades: i) the possibility to optimize stochastically the energy of a highly accurate many-body wave function, described by several variational parameters, ii) the development of the so called Jastrow Mean-Field ansatz that will be shown to be extremely accurate and nevertheless computationally feasible even for large scale electronic structure applications, especially in recent high-performance supercomputers. Moreover we discuss also a recent technique VAFQMC (Variational Auxiliary Field Quantum Monte Carlo) [2] that combines the power and simplicity of Variational Monte Carlo, with a path integral approach based on the auxiliary field technique. It will be shown that this new method has the potential to achieve unbiased results in the thermodynamic limit for the celebrated Hubbard model, probably the most important and still unsolved model in condensed matter theory.

[1] 7045 K. Nakano et al. "TurboRVB: A many-body toolkit for ab initio electronic simulations by quantum Monte Carlo", J. Chem. Phys. 152, 204121 (2020); https://doi.org/10.1063/5.0005037
[2] S. Sorella, "The phase diagram of the Hubbard model by Variational Auxiliary Field quantum Monte Carlo" arXiv:2101.0