Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Tuesday, June 13th , 2017 – 2:00 p.m.
CFEL Seminar room IV (Bldg. 99)

Michael Lubasch

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Density Functional and Tensor Network Theory

In my talk I will discuss this question: How can density functional and tensor network theory be combined in such a way that they benefit from each other. In particular I will present our publication [1] in which we developed a systematic procedure for the approximation of density functionals in density functional theory that consists of two parts. In the first part, for the efficient approximation of a general density functional, we introduced an efficient ansatz whose non-locality can be increased systematically. In the second part, we presented a fitting strategy that is based on systematically increasing a reasonably chosen set of training densities. I will present our results from reference [1] for strongly correlated fermions on a one-dimensional lattice. In this context we focused on the exchange-correlation energy and demonstrated how an efficient approximation can be found that includes and systematically improves beyond the local density approximation. Remarkably, we could show this systematic improvement for target densities that are quite different from the training densities.

[1] M. Lubasch, J. I. Fuks, H. Appel, A. Rubio, J. I. Cirac, and M.-C. Banuls, New Journal of Physics 18, 083039 (2016)."

Host: Angel Rubio

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