Project A6: Multi-flavour Mott transitions and magnetism of ultracold quantum gases on optical lattices

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Multiflavour mixtures of ultracold fermionic atoms on optical lattices provide unique opportunities for studying a wide range of correlation effects with direct access to the relevant control parameters. This has already been demonstrated for the paramagnetic Mott metal-insulator transition; it is expected that also the generic low-temperature antiferromagnetism (or at least precursors thereof) will soon be seen in 2-flavour experiments. Once this milestone is accomplished, cold-atom systems may serve as quantum simulators of strongly correlated materials and, thereby, help solve both fundamental and technically relevant open questions in this field. The central goal of this project is to develop appropriate theoretical tools for cold-atom specific aspects of correlation physics and to explore both the analogies and fundamental differences between correlated cold-atom systems and materials, with a specific focus on genuine multi-flavour effects.

Research Highlights

Discriminating antiferromagnetic signatures in ultracold fermions by tunable geometric frustration

Recently, it has become possible to tune optical lattices continuously between square and triangular geometries [1]. We compute thermodynamics and spin correlations in the corresponding Hubbard model using a determinant quantum Monte Carlo technique and show that the frustration effects induced by the variable hopping terms can be clearly separated from concomitant bandwidth changes by a proper rescaling of the interaction [2]. An enhancement of the double occupancy by geometric frustration signals the destruction of nontrivial antiferromagnetic correlations at weak coupling and entropy $s \lesssim \ln(2)$ (and restores Pomeranchuk cooling at strong frustration), paving the way to the long-sought experimental detection of antiferromagnetism in ultracold fermions on optical lattices.

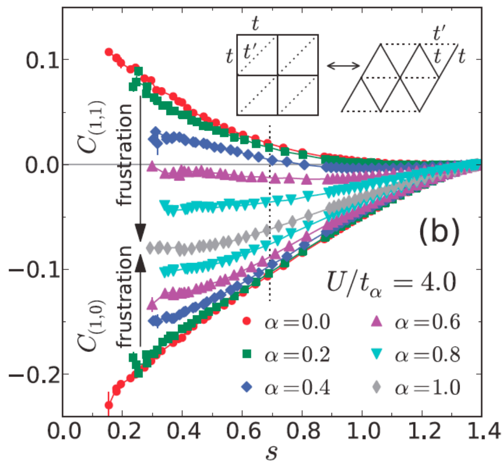

Figure 1. Short-range spin-correlation functions $C_{(1,0)}$ and $C_{(1,1)}$ (equivalent in triangular limit α=1) at $U=4t_\alpha$.

[1] L. Tarruell, D. Greif, T. Uehlinger, G. Jotzu, and T. Esslinger, Nature **483**, 302 (2012); D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, and T. Esslinger, Science **340**, 1307 (2013).
[2] C.-C. Chang, R. T. Scalettar, E. V. Gorelik, and N. Blümer, Phys. Rev. B **88**, 195121 (2013).

Role of dimensionality: Universal probes for AF correlations and entropy in cold fermions on optical lattices

We determine AF signatures in the half-filled Hubbard model at strong coupling on a cubic lattice and in lower dimensions [3]. Upon cooling, the transition from the charge-excitation regime to the AF Heisenberg regime is signaled by a universal minimum of the double occupancy at entropy $s \equiv S/(Nk_B)=s^{*}\approx \ln(2)$ per particle and a linear increase of the next-nearest-neighbor (NNN) spin correlation function for $s<s^{*}$. This crossover, driven by a gain in kinetic exchange energy, appears as the essential AF physics relevant for current cold-atom experiments. The onset of long-range AF order (at low s on cubic lattices) is hardly visible in nearest-neighbor spin correlations versus s, but could be detected in spin correlations at or beyond NNN distances.

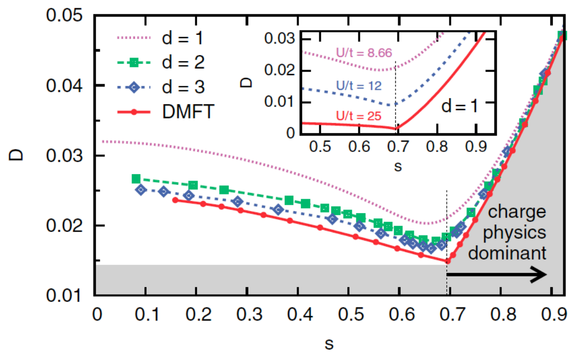

Figure 1. Hypercubic lattice at strong coupling: Double occupancy vs entropy.

[3] E. V. Gorelik, D. Rost, T. Paiva, R. Scalettar, A. Klümper, N. Blümer, Phys. Rev. A **85**, 061602(R) (2012).

Full-scale calculations for anisotropically trapped cold atoms

We have revisited computational approaches to inhomogeneous correlated systems, with special emphasis on the reliability for ordered phases. Proximity effects, washing out the domain boundary between a central core with (local) antiferromagnetic (AF) order and a surrounding metallic shell, appear significant even for realistically weak confinement. Thus, the use of LDA for a posteriori reconstructing the properties of the trapped system provides rather poor estimates for observables sensitive to AF correlations. This is also true even if elaborate methods beyond the mean-field approximation are employed in the homogeneous calculations.

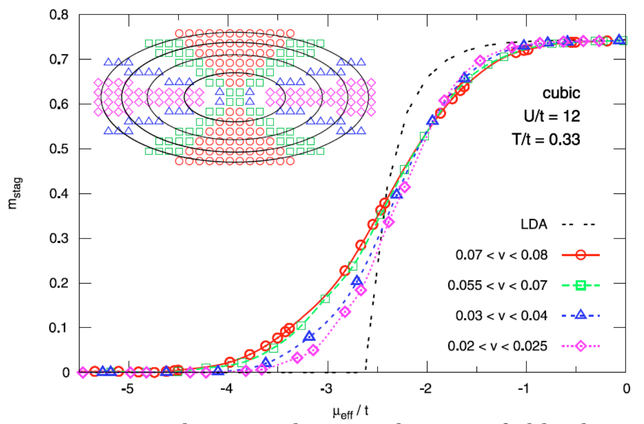

Figure 3. Real-space dynamical mean-field theory estimates of order parameter for cubic lattice with anisotropic confinement

We present an accurate and computationally effective strategy towards simulations of three-dimensional trapped fermionic systems of the experimentally relevant sizes, connecting the properties of the full confined system with those of its central slab [4].

[4] E. V. Gorelik, N. Blümer, Journal of Low Temperature Physics **165** (2011) 195-212.

Publications

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in *The LDA+DMFT approach to strongly correlated materials*
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Forschungszentrum Jülich GmbH, Institute for Advanced Simulations, ISBN 978-3-89336-734-4 (2011)

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Phys. Rev. A **80**, 051602(R) (2009)