Correlations in the anisotropic Hubbard model

Jakub Imriška,[1] Emanuel Gull,[2] and Matthias Troyer[1]
[1] Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
[2] University of Michigan, Ann Arbor, MI 48109, USA

We study the anisotropic 3D Hubbard model with anisotropic hopping amplitudes using the dynamical cluster approximation and compare the results to a quantum simulation experiment of ultracold fermions in an optical lattice. We find significant enhancement of the short-range spin correlations in the direction of stronger hoppings for moderate temperatures. Our results agree with the experimental observations and allow for quantification of the excess heat in the experiment. We furthermore investigate the dependence of the critical entropy at the Néel transition on anisotropy.

I. INTRODUCTION

We investigate the Hubbard model on these lattice structures:

- coupled 1D chains: cubic lattice with larger hopping t in 1 direction and weaker (t') in the perpendicular directions;[5]
- layered square lattice: cubic lattice with larger in-layer hopping t and weaker interlayer hopping t';
- layered honeycomb lattice: with larger in-layer hopping t and weaker interlayer hopping t'.

Note that the dominant hopping is always denoted by t. The coupled 1D chains and layered square lattice coincide at $t = t'$ ($\rightarrow$ isotropic cubic lattice).

The interest on the anisotropic lattices was drawn by the cold gas optical lattice experiment[1] which succeeded to measure short-range magnetic correlations C on neighboring sites i and j,

$$C = -\left\langle \hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y \right\rangle . \quad (1)$$

The authors utilized the coupled 1D chains lattice. That raised questions about the reached temperature, the effect of the anisotropy, the amount of excess heat and possible optimizations of the experiment by tuning parameters.

II. METHOD

We investigate the Hubbard model by the dynamical cluster approximation (DCA)[2], a cluster extension of the dynamical mean field approximation/theory (DMFA/DMFT)[3]. The fermionic problem, which is within the method described by an effective action, was solved by the numerically exact quantum Monte Carlo continuous-time auxiliary-field solver[4]. By an extrapolation in cluster size we get quantities for the homogeneous system at different temperatures and fillings in the thermodynamic limit. The confining (harmonic) potential present in the experiment was treated by the local density approximation.

III. DISORDERED PHASE

In the disordered phase at $T \approx t$ and for anisotropy t/t' greater than 4 we found that the spin correlation C is enhanced on the lattices with smaller strong hopping coordination number Z_t.[8] The enhancement at half filling and at fixed entropy is roughly proportional to the inverse Z_t ratio. That makes the coupled 1D chains to a suitable system for the measurement of spin correlations. We checked that the correlations remain of short-range nature. At the same time the transverse spin correlations are suppressed, as expected. In a simple picture we may understand this behavior by ignoring the weak hopping terms t', which are in high-temperature regime. In the strong hopping directions the (short-range) correlations are built up and singlets are formed. The strong hopping coordination number Z_t counts the number of singlets in which each site is involved.

Our numerical simulation performed according to the experimental parameters (without any free parameters) in combination with the experimental datapoints delivers an access to the quantification of the excess heat during the lattice loading, see in Fig. 1. The main plot shows small heating down to (initial) entropy 1.4 per particle, with increasing excess heat below that threshold. As may be seen on the upper temperature axis, elimination of the heating would allow for temperatures 2-times lower than current limit. Therefore it is essential to be able to quantitavely estimate the heating and find space for improvements in the lattice loading.

IV. ANTIFERROMAGNETIC PHASE

One of the goals for the future experiments is to reach the ordered phase – for the mentioned lattices we mean the antiferromagnetic ordering. To achieve that in the experiment the temperature has to be lowered further. A quest for the numerics is to look for the most suitable systems, with highest entropy per particle at the transition. In order to follow the query, we restricted ourselves to the half-filled system, at which the transition temperature is the highest.

The presence of enhanced short-range correlations within the disordered phase does not necessarily mean en-

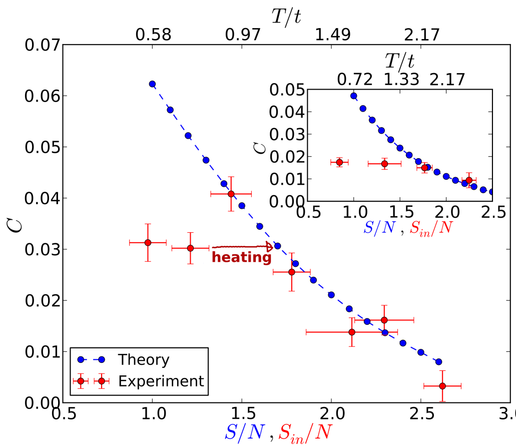

FIG. 1: N.n. spin correlation in direction of strong hopping (C) plotted as a function of entropy per particle, coupled 1D chains for $t/t' = 7.36$ and $U = 1.4375t$. The experimental data is plotted as a function of the initial S/N before loading into the lattice; the blue curve comes from the numerics. Notice the excess heat (entropy) for the lowest initial entropies in the experiment. Inset: same plot for coupled 1D chains at $t/t' = 4.21$, $U = 2.98t$. Adapted figure from[5].

larged transition temperature to the ordered system. The expectations shall be clear when regarding the limit of decoupled 1D chains or 2D layers – the Mermin–Wagner–Hohenberg theorem[6,7] states that these cannot order at any finite temperature. Thus the critical temperature (and entropy) shall vanish at large anisotropy. This we could verify for the coupled 1D chains, see Fig. 2. For the cubic lattice ($t = t'$) the optimal U in terms of largest critical temperature (entropy) is around $U = 8t$. The non-monotonicity of the S_{crit} for $U = 4t$ in Fig. 2 may be accounted to the tuning of the interaction strength U relative to the bandwidth $W = 4(t + 2t')$ by change of the anisotropy towards the optimal value.

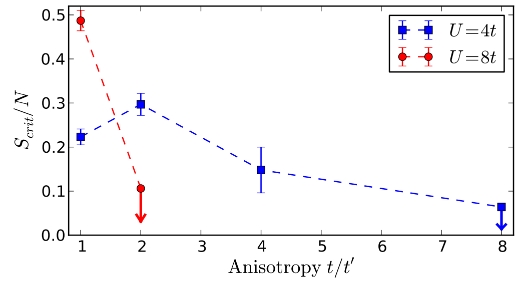

FIG. 2: Critical entropy per particle S_{crit}/N at the Néel transition vs. anisotropy for the coupled 1D chains at half-filling. The data points shown with an arrow are upper bounds. Adapted figure from[5].

The layered square lattice shows at $t = 2t'$ almost same optimal S_{crit}/N as the isotropic cubic lattice. For larger anisotropies we expect slower suppresion compared to the coupled 1D chains. The layered honeycomb lattice shows a reduced critical entropy per particle already for $t = t'$ with respect to the cubic lattice. Our results suggest that the optimal value of critical entropy per particle $0.487(23)$[5] for the isotropic cubic lattice around $U = 8t$ remains unbeaten.

Acknowledgments

We greatly appreciate the collaboration with the quantum optics group of Prof. Esslinger (ETH Zürich). We would like to thank to L. Wang, M. Iazzi, J. Gukelberger and P. Staar.

---

[1] D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, and T. Esslinger, *Short-Range Quantum Magnetism of Ultracold Fermions in an Optical Lattice*, Science **340**, 1307 (2013).

[2] T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, *Quantum cluster theories*, Rev. Mod. Phys. **77**, 1027 (2005).

[3] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions*, Rev. Mod. Phys. **68**, 13 (1996).

[4] E. Gull, P. Werner, O. Parcollet, and M. Troyer, *Continuous-time auxiliary-field Monte Carlo for quantum impurity models*, EPL **82**, 57003 (2008).

[5] J. Imriška, M. Iazzi, L. Wang, E. Gull, D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, T. Esslinger, and M. Troyer, *Thermodynamics and magnetic properties of the anisotropic 3d hubbard model*, Phys. Rev. Lett. **112**, 115301 (2014).

[6] N. D. Mermin and H. Wagner, *Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic heisenberg models*, Phys. Rev. Lett. **17**, 1133 (1966).

[7] P. C. Hohenberg, *Existence of long-range order in one and two dimensions*, Phys. Rev. **158**, 383 (1967).

[8] $Z_t = 6$ for the isotropic cubic lattice, $Z_t = 4$ for the layered square lattice, $Z_t = 3$ for the layered honeycomb lattice, $Z_t = 2$ for the coupled 1D chains.