

## Quantum simulation of Hubbard model

*Experimental realization of a long-range antiferromagnet in the Hubbard model with ultracold atoms*

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**Recommended with a Commentary by Dung-Hai Lee, U.C. Berkeley, USA**

The Hubbard model, a lattice model for spin 1/2 fermions with nearest neighbor “hopping” and an on-site repulsion, plays a special role in condensed matter physics. It is the simplest theoretical model describing correlated electronic systems. Originally introduced to describe the effects of screened Coulomb interaction in narrow band materials, the Hubbard model defined on square lattice gains a different level of interest when it was proposed by Anderson[1] that it is the model for the copper-oxide (cuprate) high temperature superconductors[2].

Regardless of the spatial dimension and the geometry of the lattice the properties of the Hubbard model are determined by two dimensionless parameters: (1)  $U/t$ : which is proportional to the ratio between the local repulsion energy and the kinetic energy bandwidth, and (2)  $n$ : the average number of fermion per lattice site.

Despite its simplicity the Hubbard model has escaped solution except in one space dimension[3]. Very recently, in Ref.[4], a nice quantum simulation of a 15 site doped one dimensional Hubbard model (with  $U/t = 7.25$ ,  $n \lesssim 1$ ) using trapped  ${}^6\text{Li}$  atoms is achieved. Among other things it is demonstrated that the finite temperature spin correlation of the doped system is the same as that of the Heisenberg model on a squeezed lattice, i.e. the lattice obtained by omitting the holes[5]. However unlike the original theory, which addresses the  $U/t \rightarrow \infty$  and  $T = 0$  limit, the experiment is done for finite  $U/t$  and  $T$ .

In the following I focus on the recommended paper by Mazurenko *et al.* Here an approximately 80 site square lattice of  ${}^6\text{Li}$  atoms with Hubbard interaction (with  $U/t \approx 7.2$  and  $0 \leq 1 - n \lesssim 0.25$ ) was simulated. (To model the cuprate superconductors  $n$  should be close to 1 and  $U/t$  should be significantly larger than 1, e.g.  $\sim 8$ .)

Although the 2D Hubbard model has not been solved it is well understood when  $n = 1$ . In that case the ground state is an insulator with checkerboard,  $(\pi, \pi)$ , antiferromagnetic long range order, and the low energy excitations are spin waves. The question is how about away from  $n = 1$  (especially for large  $U/t$ ), does the ground state exhibit superconducting order?

It turns out that studying the large  $U/t$  2D Hubbard  $n = 1$  is a very challenging theoretical problem. The only “small parameter” we can identify is  $|n - 1|$ . However numerical evidence suggests that as  $n$  deviates from 1 the nature of ground state changes rather quickly. For example numerical density matrix renormalization group calculation done on a small  $(6 \times 7)$  square

lattice suggests that once doped the extra carriers distribute non-uniformly in the form of “stripes”, and across each stripe the antiferromagnetic correlation undergoes a  $\pi$  phase shift[6]. In addition, there is numerical evidence that for large  $U/t$  and small  $|n - 1|$  there are many metastable states with close by energies which makes approximation-free theoretical methods in high demand. Unfortunately all known such methods are either limited by the size and/or the shape (quasi one dimensional) of the lattices they can study. For quantum Monte Carlo method, which can treat substantial size square lattices, the fermion sign problem forbids the calculation to reach low a temperatures when  $n \neq 1$ .

Mazurenko *et al.* cool their Hubbard lattice to temperature  $((T/t)_{\min} \approx 0.25$ . This allows them to observe the antiferromagnetic correlation with significant correlation length (the longest correlation length is comparable with their system size). At the coldest temperature they find the commensurate  $(\pi, \pi)$  antiferromagnetic order up to 15% doping. It is interesting that this agrees qualitatively with the experimental findings for electron doped cuprates. However there is no evidence of the stripe seen in Ref.[6]! Mazurenko *et al.* suggest that this might be due to their lattice size being too small to detect the incommensurate magnetic order. But the lattice size studied in Ref.[6] is about a factor of two smaller, and for  $U/t \sim 8$  (with 4 holes) a sharp stripe was observed[6]. If stripes exist it should not be difficult to observe – there should be charge density modulation which could be imaged directly. Of course it is entirely possible that the lowest temperature reached by Mazurenko *et al.* is not low enough. However even the high temperature regime of Hubbard model could be very interesting. In fact two of the most interesting properties of the cuprates, namely the pseudogap and the “strange metal” behaviors both set in at high temperatures. The prospect that in not too distant future large cold atom Hubbard lattices can be cooled down sufficiently to reveal the true ground state is truly exciting.

While we wait for such result it is important to bear in mind that the nearest-neighbor-hopping Hubbard model is most likely not an adequate description of the cuprate superconductors. While the Hubbard model is particle-hole symmetric, it is known that the electron doped ( $n > 1$ ) and hole doped ( $n < 1$ ) cuprates behave very differently. This is even reflected in the phase diagram by, e.g., the robustness of the antiferromagnetic order on the electron doped but not on the hole doped side. In addition there are experimental evidence of broken symmetries that only occur on the hole doped side[7].

On a more microscopic level, when holes are doped into cuprates they mainly go into the oxygen orbitals. In the literature an effective model, namely the t-J model [8], is used to describe the hole doped cuprates. In contrast upon electron doping the extra carriers enter the copper orbitals. For the Hubbard model electrons or holes are of course accommodated by the same orbitals.

Finally whether or not it describes the cuprates the phase diagram and the low energy properties of the Hubbard model is definitely worth understanding. It can serve as a benchmark for future studies of strongly correlated materials. As to the mechanism of Cooper pairing, for the cuprates it is widely believed

that the antiferromagnetic correlation plays an important role. It is less clear whether it is assisted by other important players to yield high  $T_c$ .

## References

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