Achieving the Néel state in an optical lattice

Arnaud Koetsier,[1] R.A. Duine,[1] Immanuel Bloch,[2] and H. T. C. Stoof [1]

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Universiteit Utrecht

[1] Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands
[2] Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Germany

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Motivation

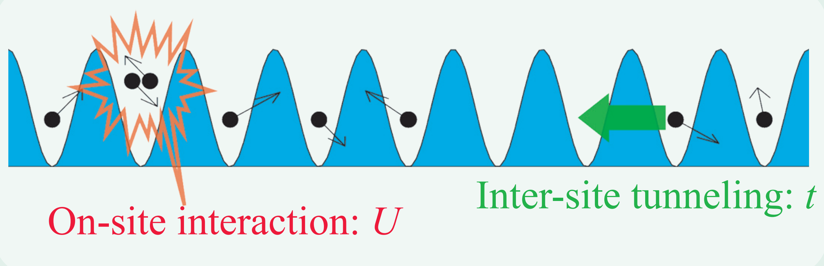
We can use ultracold neutral atoms in a regular periodic potential called an optical lattice to map out the **Fermi-Hubbard model**, which consists of interacting fermions in the tight-binding limit. At half-filling, corresponding to one fermion per lattice site, the ground state of this model is antiferromagnetic, i.e., a Néel-ordered state, for strong enough on-site interactions. As the filling factor is reduced by doping, the system is conjectured to undergo a quantum phase transition to a d-wave superconducting state. Understanding this transition would be a major step towards understanding high-temperature superconductivity of the cuperates.

An experimental exploration of this issue using ultracold atoms is now within reach. In view of this, a significant problem is determining how to reach the Néel state with untracold atoms?

The Fermi-Hubbard Model

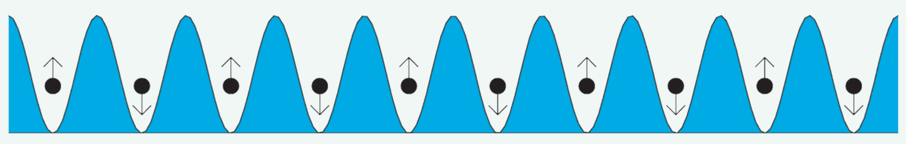
Our starting point is the Fermi-Hubbard model describing fermions in a periodic potential

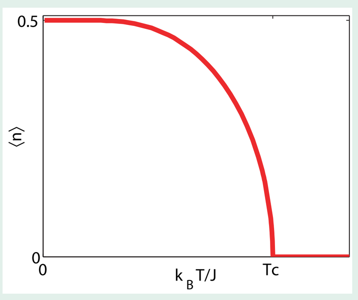
$$H = -t\sum_{\sigma}\sum_{\langle jj'\rangle} c^{\dagger}_{j,\sigma}c_{j',\sigma} + U\sum_{j} c^{\dagger}_{j,\uparrow}c^{\dagger}_{j,\downarrow}c_{j,\downarrow}c_{j,\uparrow}$$



- Sums depend on dimension (d=3) and number of occupied sites N;
- Sum $\langle jj'\rangle$ over nearest-neighbours only;
- Consider positive-U (=repulsive) Hubbard model, relevant to high-temperature superconductivity.

The **Néel state** is the antiferromagnetic ground state of the Hubbard model at half filling, in the limit $U \gg t$:





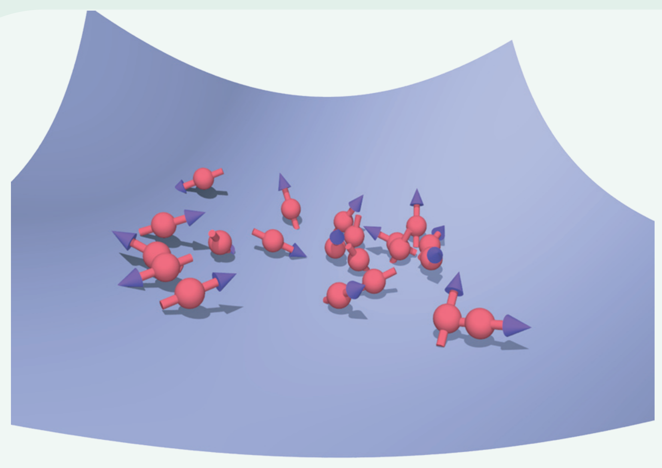
Néel order parameter $0 \le \langle|\mathbf{n}|\rangle \le 0.5$ measures amount of "anti-alignment":

$$\mathbf{n}_j = (-1)^j\langle\mathbf{S}_j\rangle$$

Below some critical temperature T_c, $\langle|\mathbf{n}|\rangle$ becomes non-zero and we enter the Néel phase.

Cooling into the Néel state

1. We start with a gas of ultracold fermionic atoms in a harmonic trap at temperature T_{ini}.



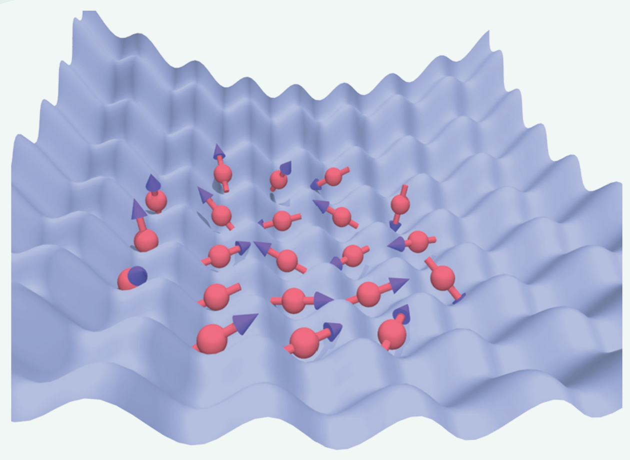
Entropy in the harmonic trap:

$$S_{FG} = Nk_B\pi^2\frac{T}{T_F}$$

The number of particles is N and the **Fermi temperature in the trap** is:

$$k_BT_F = (3N)^{1/3}\hbar\omega$$

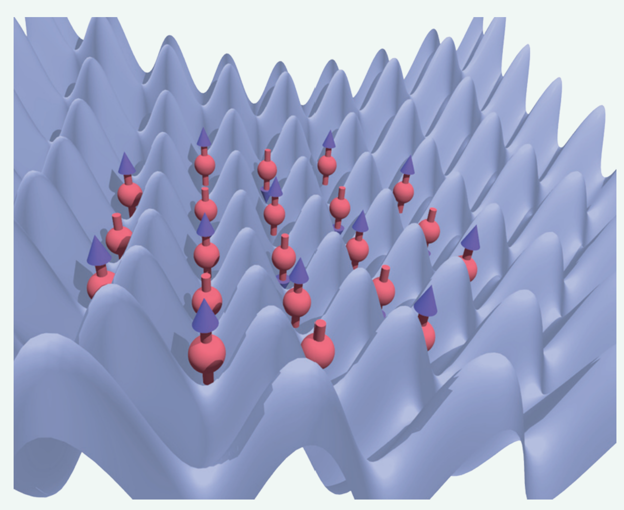
2. Next, ***adiabatically*** turn on the optical lattice. The entropy remains constant.



Since we consider balenced gases with $U \gg t$ here, we now enter the Mott insulator phase with one particle per site.

The physics is now understood in terms of the **Heisenberg model!**

3. The temperature of the atoms changes as their entropy does not. Eventually, we cross the critical temperature T_c and they begin to antialign:



The initial entropy in the trap at temperature T_{ini} equals the final entropy in the lattice below T_c

$$S_{FG}(T_{ini}) = S_{Lat}(T \le T_c)$$

Thus, we **need to know the entropy in the lattice**.

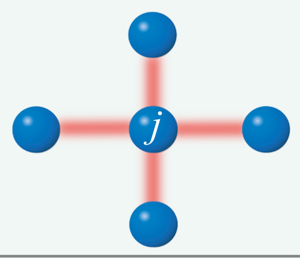
Heisenberg Model - Mean Field Theory

At half filling, for lattice depths such that $U \gg t$, and temperatures $k_BT \ll U$, the dynamics are descibed by an the effective Hamiltonian for the spins alone - the Heisenberg model:

$$H = \frac{J}{2}\sum_{\langle jk\rangle}\mathbf{S}_j\cdot\mathbf{S}_k$$

where $\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$ is the spin operator and $J = \frac{4t^2}{U}$ is superexchange constant describing virtual hops to neighbouring lattice sites.

Usual mean-field analysis: Treat the interaction of site j with its nearest neighbours within mean-field theory,



$$H \simeq \frac{J}{2}\sum_{\langle jk\rangle}\left\{\langle\mathbf{S}_j\rangle\mathbf{S}_k + \mathbf{S}_j\langle\mathbf{S}_k\rangle - J\langle\mathbf{S}_j\rangle\langle\mathbf{S}_k\rangle\right\}$$

Diagonalize the resulting 4×4 problem to obtain the Landau free energy f_L, then we obtain the entropy thus:

(1) Solve self-consistency condition for $\langle\mathbf{n}\rangle$:

$$\left.\frac{\partial f_L(\mathbf{n})}{\partial\mathbf{n}}\right|_{\mathbf{n}=\langle\mathbf{n}\rangle} = 0$$

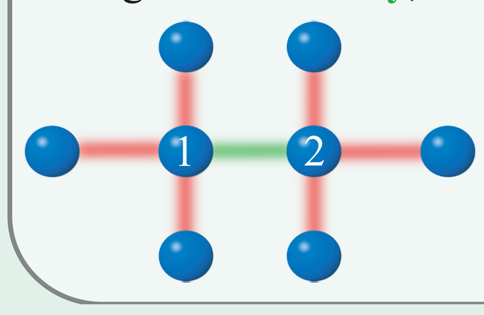
(2) Calculate the entropy with this $\langle\mathbf{n}\rangle$:

$$S = -N\frac{\partial f_L(\langle\mathbf{n}\rangle)}{\partial T}$$

The entropy and Néel order parameter obtained in this way are plotted as the black curves in Fig. 1 below. Although this theory has the correct $T=0$ and $T=\infty$ limits, is does not include spin waves present near $T=0$ nor critical fluctuations:

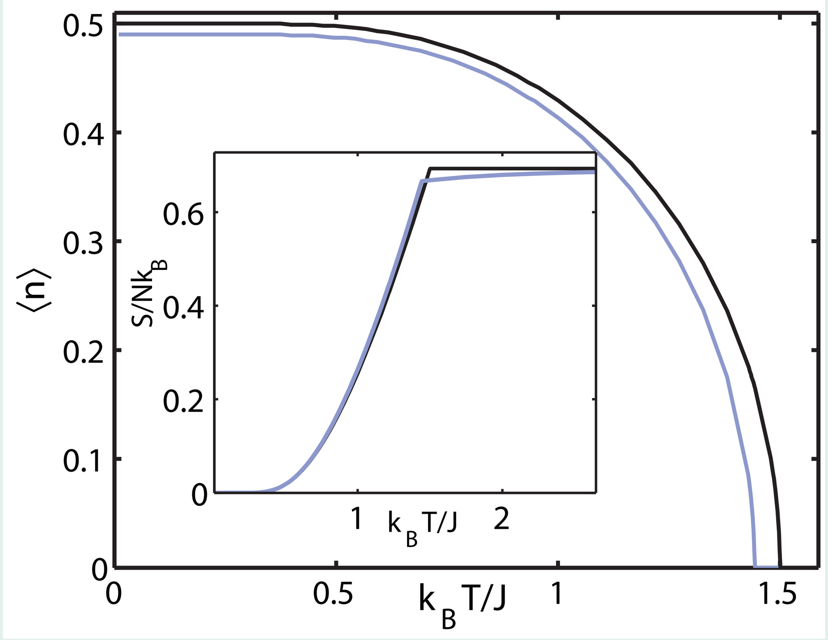
- ✘ No temperature dependence above T_c: $S = Nk_B\ln(2)$.
- ✘ Incorrect low temperature behaviour
- ✘ Incorrect critical temperature behaviour

Improved mean-field analysis: Attempt to improve on standard mean-field approach by the including interaction between a site and one of its nearest neighbours **exactly**, treating the rest of the neigbours within **mean-field** theory.



$$H \simeq J\mathbf{S}_1\cdot\mathbf{S}_2 + J(z-1)|\mathbf{n}|(\mathbf{S}^z_1 - \mathbf{S}^z_2) + J(z-1)\mathbf{n}^2$$

Néel order parameter and entropy obtained as above. Results plotted in Fig. 1. Now, there is a **2% depletion** of $\langle\mathbf{n}\rangle$ at $T=0$ due to quantum fluctuations, and the entropy has temperature dependence above Tc:



- ✔ Temperature dependence above T_c.
- ✘ Incorrect low temperature behaviour
- ✘ Incorrect critical temperature behaviour

Fig. 1. Results from 1-site (black) and 2-site (blue) mean-field theory. The inset shows the entropy per particle. (Results plotted in a lattice of depth $V_0 = 6.5E_R$, where E_R is the recoil energy).

Fluctuations

Using the critical temperature $T_c = 0.957\,k_B/J$ found from numerical simulations [Staudt], the correct entropy curve interpolates between three regiemes:

(1) Low temperature entropy, dominated by magnons:

$$S(T \ll T_c) = Nk_B\frac{4\pi^2}{45}\left(\frac{k_BT}{2\sqrt{3}J\langle\mathbf{n}\rangle}\right)^3$$

(2) Critical behaviour:

$$S(T=T_c) = S(T_c) \pm A^{\pm}|t|^{d\nu-1}, \quad t = \frac{T-T_c}{T_c} \to 0^{\pm}$$

[Zinn-Justin]: $d=3$, $\nu = 0.63$, $A^+/A^- \simeq 0.54$

(3) High temperature entropy, from 2-site mean-field theory:

$$S(T \gg T_c) = Nk_B\left[\ln(2) - \frac{3J^2}{64k_B^2T^2}\right]$$

Result: **Initial temperature in the trap required to reach Tc in the lattice is significantly lowered by fluctuations compared to mean-field theory**, see Fig. 2.

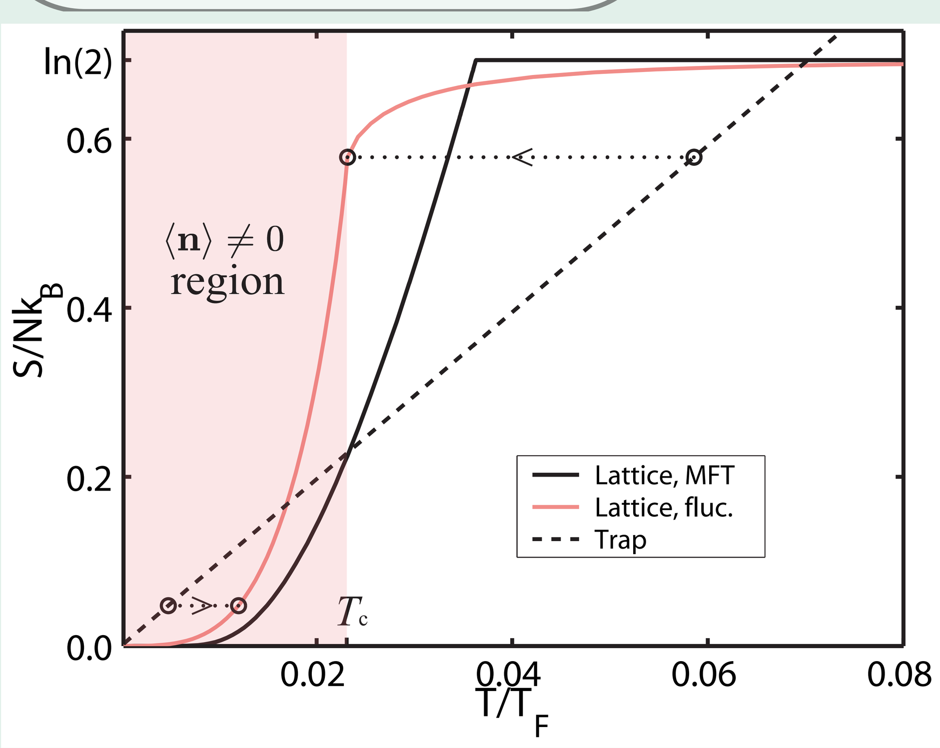


Fig. 2. The entropy per particle in the harmonic trapping potential (dashed line), and in the lattice from usual mean field theory (solid curve) and including fluctuations (red curve). The horizontal lines illustrate cooling and heating which may occur in going from the harmonic trap to the lattice adiabatically.

(Results plotted in a lattice of depth $V_0 = 6.5E_R$, where E_R is the recoil energy).

Conclusion

- We find, for all lattice depths such that $U \gg t$, the Néel state is reached by adiabatically ramping up an optical lattice if the initial temperature is at or below $0.059T_F$
- Initial temperature close to limit of what is experimentally viable, accurate determination of the critical temperature is therefore crucial; **fluctuations play an important role and must be included.**

Future research:

- ***d* = 2 case:** start with $d=3$ Néel state then decrease tunneling in one direction
- **Doping:** introduce an imbalence in the population of atomic spin states
- Quantum magnetism: frustration by non-cubic lattice, impurity scattering, etc.

Insight into High-T_c SC

References:

[Staudt] R. Staudt, M. Dzierzawa, and A. Muramatsu, *Phase diagram of the three-dimensional Hubbard model at half filling,* Eur. Phys. J. B {\bf 17}, 411 (2000);

[Zinn-Justin] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, 4th Edition (Oxford, 2002).