# A6

# Flavour-selective Mott transitions of ultracold quantum gases on optical lattices

**Nils Blümer** (Mainz)

## Project Overview

**Goals:** Prediction and analysis of flavour-selective Mott transitions and phases in mixtures of ultracold fermions on optical lattices

**Flavours:**
- Atomic species: $^6$Li, $^{40}$K (also $^{173}$Yb?)
- Hyperfine states
- Vibrational levels

**Methods:**
- Generalised multi-band Hubbard models
- Dynamical mean-field theory (DMFT)
- Quantum Monte Carlo (QMC) method and other DMFT solvers (e.g.: SFT)

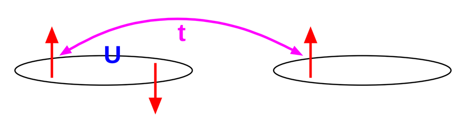
**Strongest connections:** A1 A2 A3

## Introduction

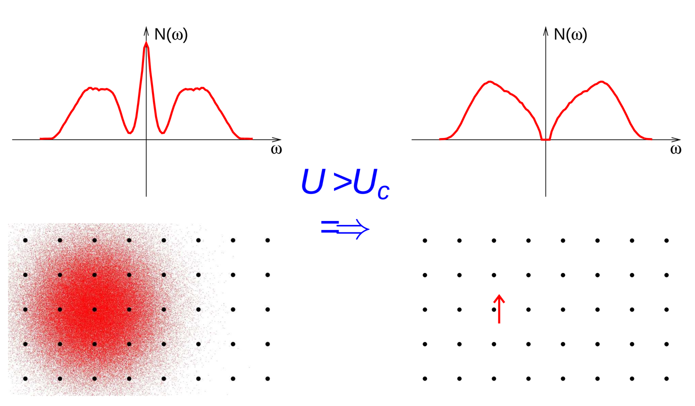
### Classical Mott transition

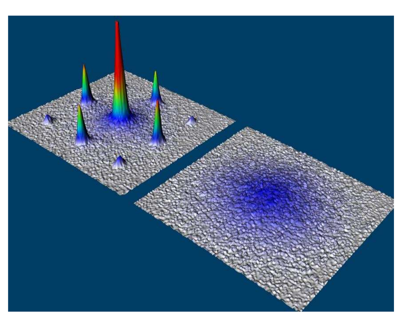
Consider 1-band Hubbard model (within DMFT)

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

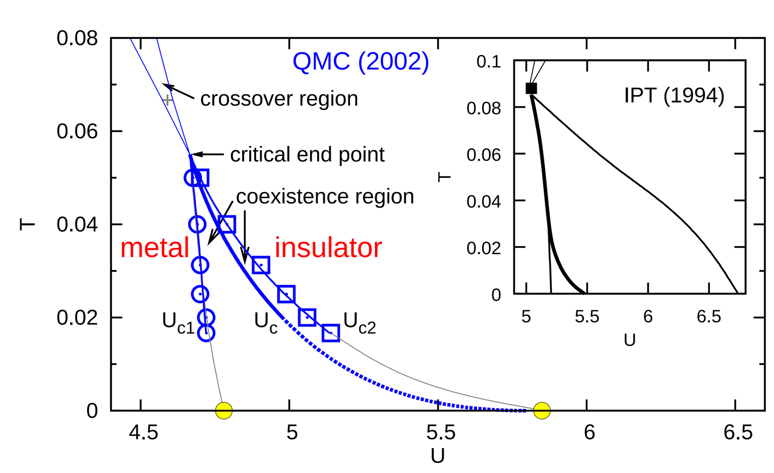



localization by interactions



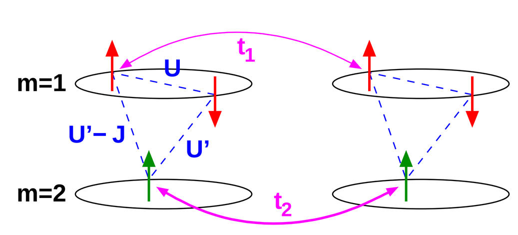
Localization (= decoherence) of ultracold bosons on optical lattice (Bloch group, 2002)



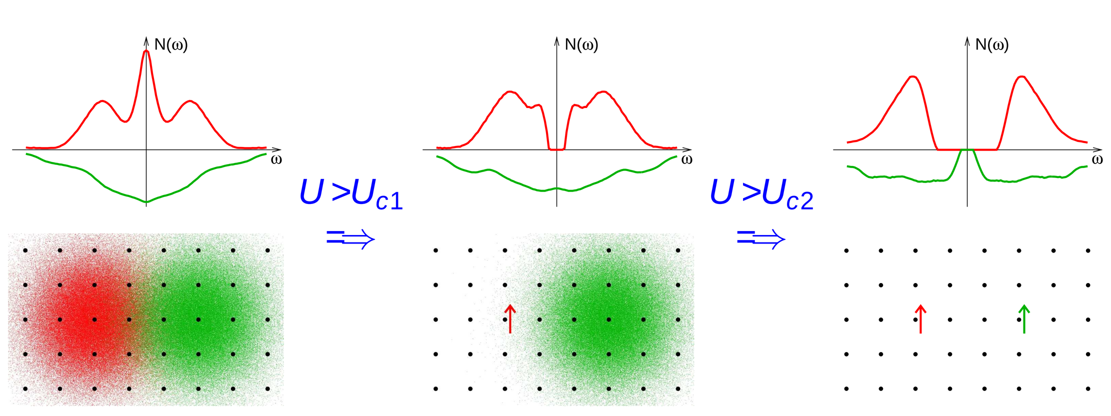

Phase diagram of the 1-band Hubbard model within DMFT as obtained using QMC [1]; inset: earlier results from Iterative Perturbation Theory (IPT) [2].

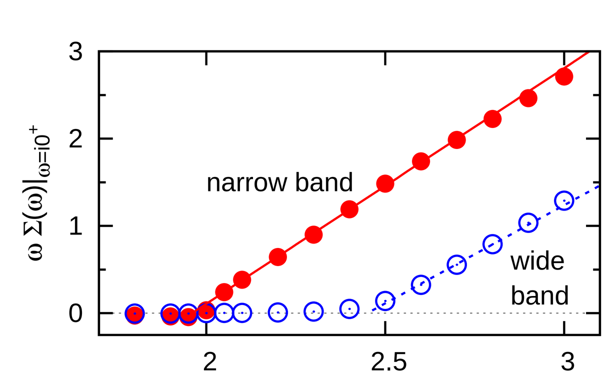
### Orbital-selective Mott transitions

2-band Hubbard model with orbital-dependent hopping and Ising-type Hund rule couplings ($U = 2U' = 4J_z$)




$$H = \sum_{m=1}^{2} \Big[ -\sum_{\langle ij\rangle\sigma} t_m c^\dagger_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big] + \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z)\, n_{i1\sigma} n_{i2\sigma'} \qquad (1)$$

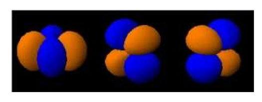


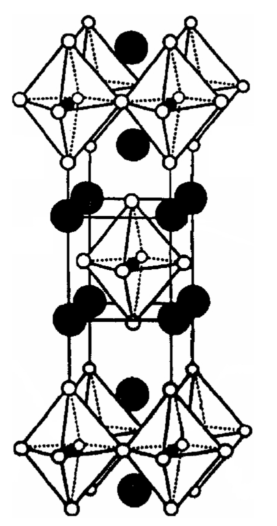




Weights of singularities in QMC self-energies (at $\omega = 0$) indicate **sequence of 2 orbital-selective Mott transitions (OSMTs)** [3]; same conclusion from analytic methods [de' Medici et al. (PRB 2005), Rüegg et al. (EPJB 2005).]

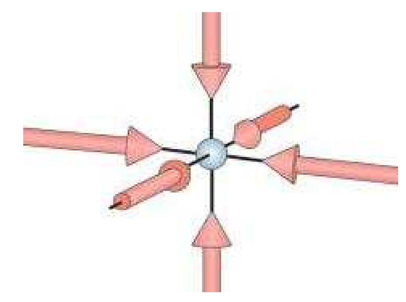
## Experimental References

### Systems with inequivalent orbitals/flavors

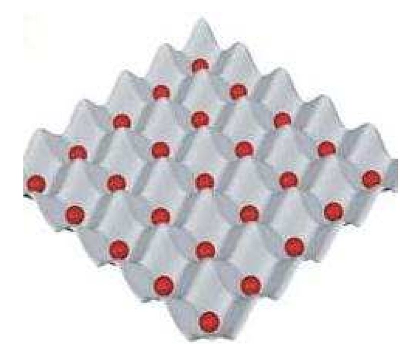




1) $t_{2g}$ electrons in layered perovskites [Nakatsuji, Maeno (2000)]



2) Flavour mixtures of ultracold fermions on optical lattices: hopping amplitudes generically flavour dependent!



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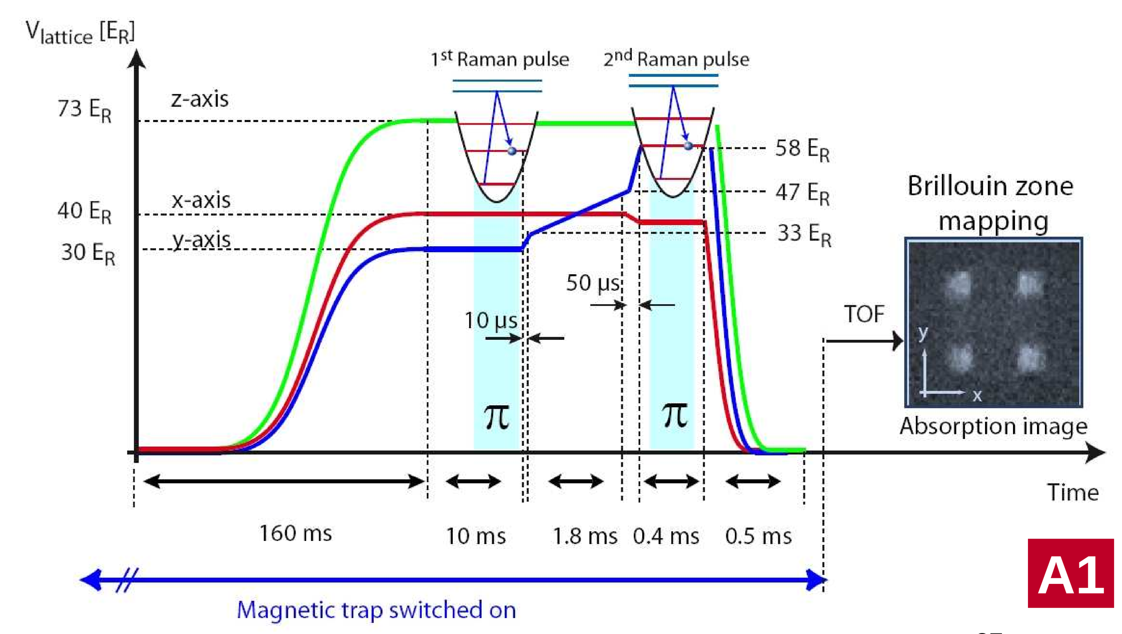
Related: 5f electrons in $UPt_3$ [Zwicknagl et al., PRB (2002)]

### Raman excitation of higher Bloch bands

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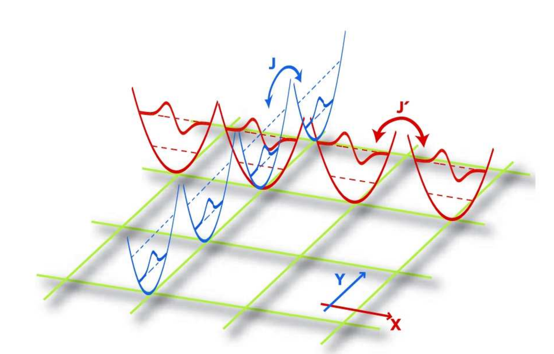
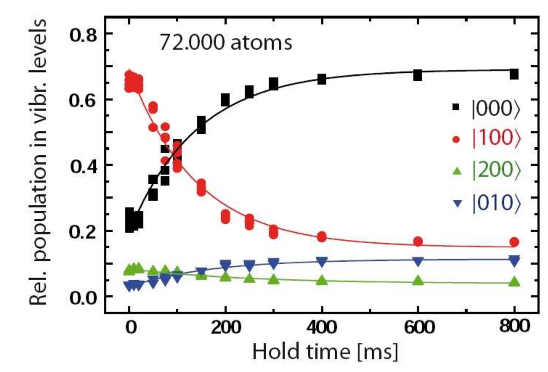
Preparation of states excited both in $x$ and in $y$ direction (for $^{87}$Rb) [4]



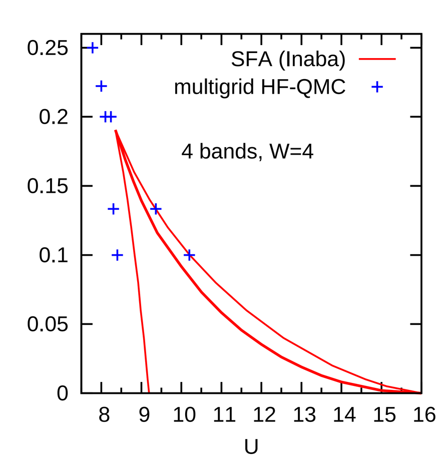
2D illustration of hopping amplitudes of ultracold atoms excited along the $x$ direction [4]

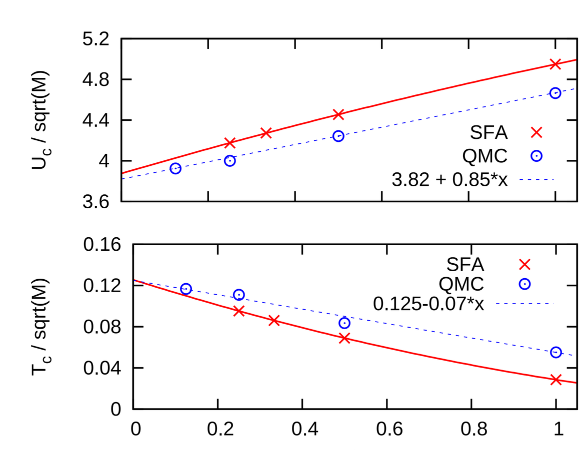



Population of different Bloch bands after excitation of $^{87}$Rb atoms to the $|100\rangle$ state [4]

## First Results

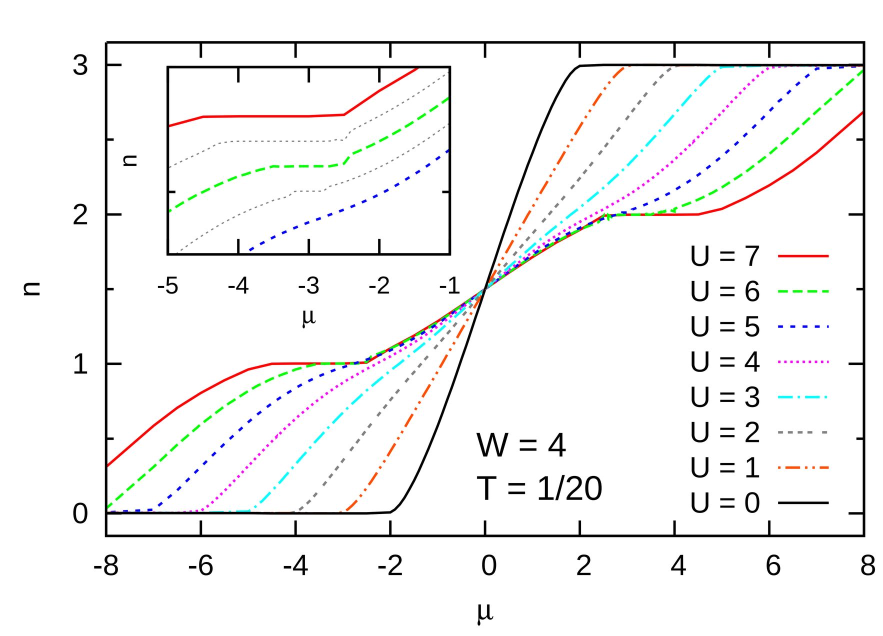
### Mott transition at variable degeneracy $SU(2M)$




**Left:** Phase diagram from multigrid HF-QMC in the 4-band case in comparison with SFA esimates [9]. **Right:** Scaling of critical parameters $T_c$ and $U_c$ with the number of bands.

### Beyond electronic systems: 3 spins/flavors




Density vs. filling for the 3-spin/flavor system in paramagnetic phase
Plateaus: incompressible Mott phase (for $U \gtrsim 6$).

## Project Description

### Generalised multi-band Hubbard model

$$H = -\sum_{\langle ij\rangle} \sum_{m=1}^{M} \sum_{\alpha=1}^{K_m} t_m c^\dagger_{im\alpha} c_{jm\alpha} + \frac{1}{2} \sum_{im} \left[ U_m n_{im}(n_{im} - 1) + \varepsilon_m n_{im} \right] + \sum_i \sum_{m \neq m'} \sum_{\alpha=1}^{K_m} \sum_{\alpha'=1}^{K_{m'}} V^{\alpha\alpha'}_{m,m'} n_{im\alpha} n_{im'\alpha'} \qquad (2)$$

$M$ classes of flavours with multiplicity $K_m$ each

Limiting cases:

| $M$ | $K_1$ | $K_2$ | $t_1$ | $t_2$ | model |
|---|---|---|---|---|---|
| 1 | 1 | - | $t$ | - | spinless fermions |
| 1 | 2 | - | $t$ | - | 1-band Hubbard model (HM) |
| 1 | 3 | - | $t$ | - | SU(3) symmetric HM A3 |
| >1 | 2 | 2 | $t$ | $t$ | multi-band HM (for $V^{\alpha\alpha'}_{m,m'} = V - \delta_{\alpha,\alpha'} J$) |
| 2 | 1 | 1 | $t$ | 0 | Falicov-Kimball model |
| 2 | 2 | 2 | 0.5 | 1 | OSMT model (1) (for $U_1 = U_2$) |

Focus on multi-band cases with inequivalent orbitals / flavours ($M > 1$, $t_i \neq t_j$ for some $i, j$)

### Work program

- Flavour-selective Mott transitions for various multiplicities of flavours (e.g.: 1+1, 1+2, 1+3 flavours)
- Flavour-selective Mott transitions for 2+2 flavours (away from electronic parameter ranges)
- Characterisation of phases A1
- Computation of experimentally accessible observables: momentum distributions, correlation functions, magnetic order parameters, excitation spectra . . .
- Effects of elevated temperatures
- Frustration, disorder and superlattices A2
- Bosons and boson-fermion mixtures
- (Partially) attractive interactions A3

## References


[1] N. Blümer, Thesis, University of Augsburg (2002).
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[3] C. Knecht, N. Blümer and P.G.J. van Dongen, Phys. Rev. B **72**, 081103(R) (2005).
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[9] K. Inaba, A. Koga, S. Suga and N. Kawakami, Phys. Rev. B **72**, 085112 (2005).


## Staff

### Principal investigator


**Juniorprofessor Dr. Nils Blümer**
Project head, novel types of calculations, methodological development

**Dr. Elena Gorelik**
Postdoc (since 7/2008)