Energy barriers between metastable states in first order quantum phase transitions

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Bose Hubbard Model (BHM)

Gersch, Knollman 1963

$$H_{\mathrm{BH}} = \mathcal{T} + \sum_{i=1}^{K} \frac{U_s}{2} n_i(n_i - 1) - \mu \sum_{i=1}^{K} n_i$$

$\mathcal{T} = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i)$
nearest neighbor hopping

on site repulsion

chemical potential

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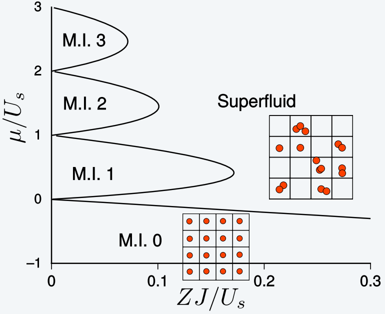
mean-field phase diagram Sachdev



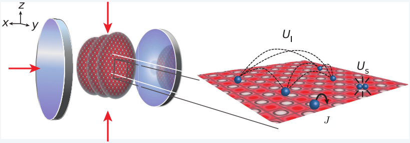
applications

- solvable in MF (↔ Fermi-HM)
- captures MI - SF transition
- ultra-cold atoms in optical lattices
- next step after BEC towards
  macroscopic quantum phenomena
- connect to many-body quantum
  properties

Long range BHM

experimental setup

Landig *et al* '16



- BEC: $4.2(4) \cdot 10^4$ ^{87}Ru atoms
- $2D$ optical lattice:
- ultrahigh-finesse optical cavity
- ~ 2.8 atoms per lattice site

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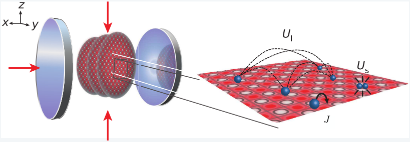

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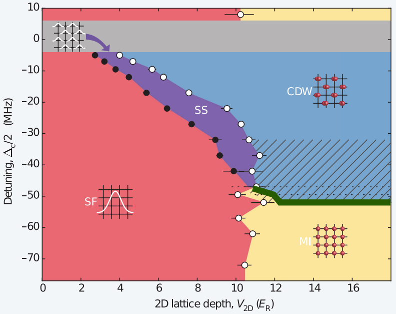
theoretical description (canonical)

$$H = H_{\mathrm{BH}} - \frac{U_\ell}{K}\Big(\underbrace{\sum_{i\in e} n_i - \sum_{i\in o} n_i}_{\Theta}\Big)^2$$

experimental results

Landig *et al*, Nature'16



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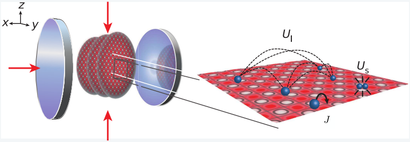

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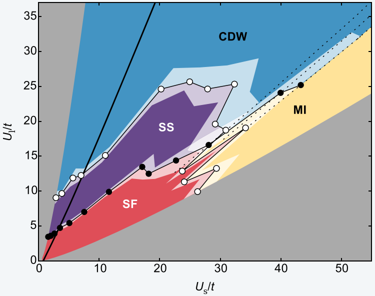

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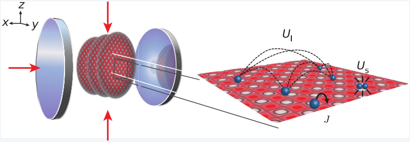

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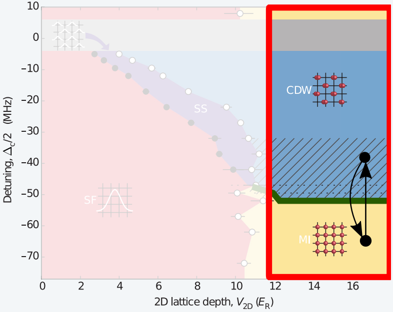

Hysteresis

Phase Diagram

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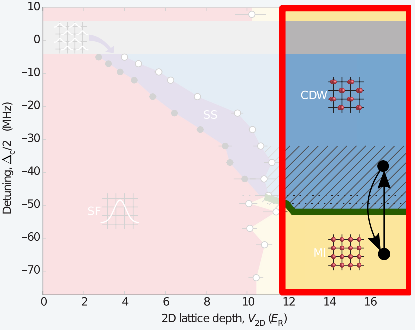
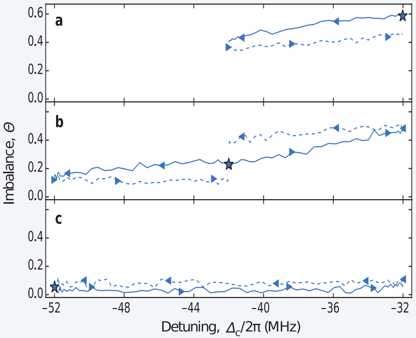


Hysteresis curves



Overview

1. Exact Landau theory in the zero hopping limit
   - Energy landscape and hysteresis loops for $\rho = 1$
   - Different fillings: $\rho \neq 1$
2. Variational Ansatz: $J \neq 0$
   - Physical requirements for reduced Hilbert space
   - Construction of variational states
3. Numerical Analysis
   - Physical observables and phase diagram
4. Discrete WKB method
   - Energy barriers between meta-stable quantum phases
5. Conclusion
6. Outlook

The Zero Hopping Limit

Landau free energy

- CDW & MI: $J/U_s \ll 1$

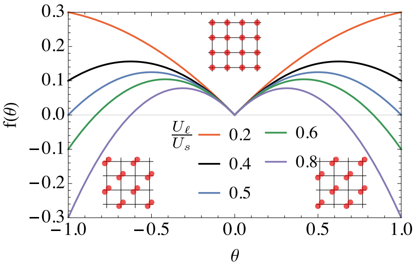
$$H_{J\to 0} = \sum_{i=1}^{K} \frac{U_s}{2}\hat{n}_i(\hat{n}_i - 1) - \frac{U_\ell}{K}\Theta^2$$

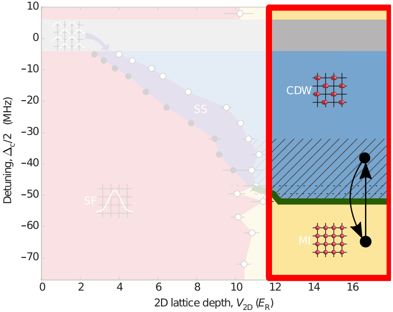
- Fock basis: H diagonal
- free energy:

$$f(\theta) = -U_\ell\theta^2 + \frac{\phi(\rho+\theta)+\phi(\rho-\theta)}{2}$$

$$\phi(\rho_x) = \frac{U_s}{K}\min_{N_x}\left\{\sum_i n_i(n_i-1)\right\}$$

- $\rho = 1 \Rightarrow f(\theta) = -U_\ell\theta^2 + \frac{U_s}{2}|\theta|$





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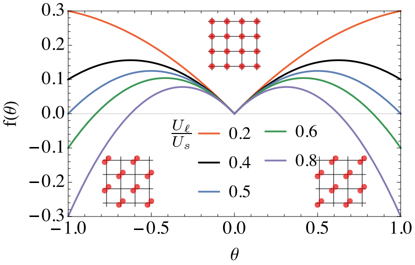

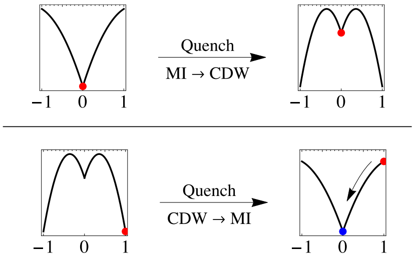

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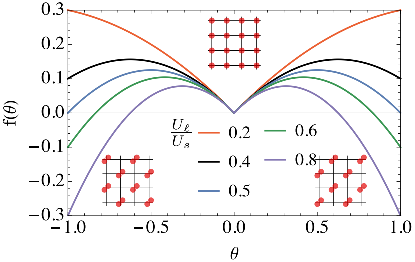

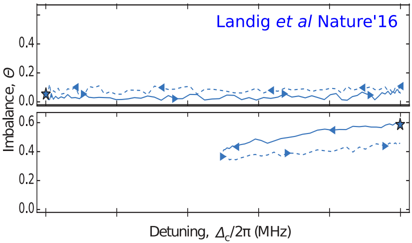

Different fillings: $\rho \neq 1$

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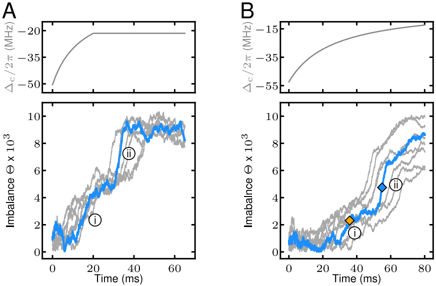

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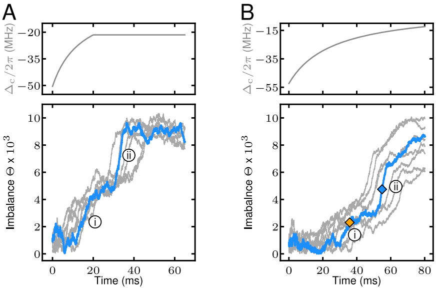
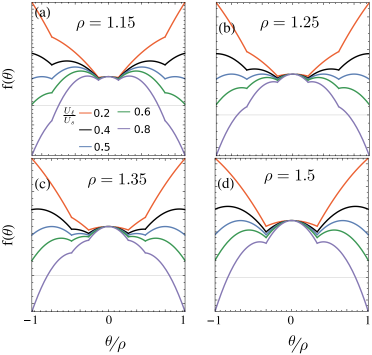




- several meta-stable minima appear
- qualitative explanation for plateaus in experiments

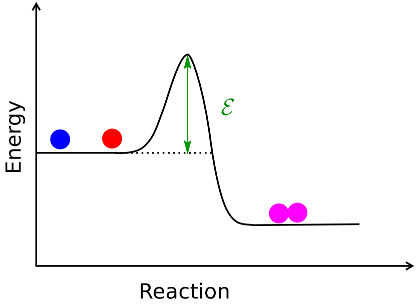
core message

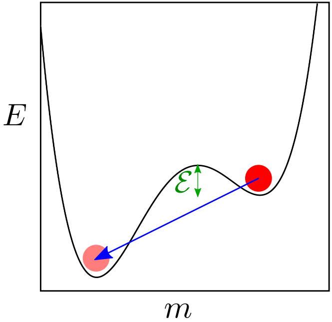
energy landscape explains many experimentally relevant findings

Energy barriers and landscapes

Goal

- describe idea of an energy barrier between the MI & CDW
- how to overcome barrier ?
- Arrhenius theory, Ginzburg-Landau theory: thermally assisted
- $T = 0$? quantum fluctuations ?





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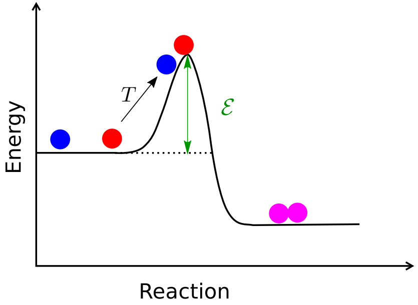

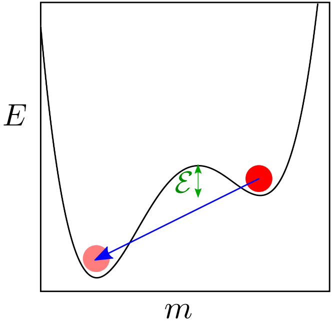

Variational Ansatz: $J \neq 0$

Requests

- CDW & MI: $J/U_s \ll 1$
- focus on $\rho = 1$
- $|\text{MI}\rangle = |1...1;1...1\rangle$
  $|\text{CDW}\rangle = |2...2;0...0\rangle$
- choose intermediate states:
  - restrict to $n_i = 0, 1, 2 \ \forall i$
  - $\Theta|Q,\nu\rangle = Q|Q,\nu\rangle$ with
    $\Theta = \left(\sum_{i\in e} n_i - \sum_{i\in o} n_i\right)^2$
- $|1,2,1,2;0,1,0,1\rangle$; $|1,2,1,2;0,0,0,2\rangle$
  - additional U_s without U_ℓ gain
  - distribute atoms in sublattices

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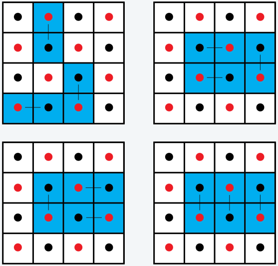
Choice of variational states

- $\mathcal{T} = -\sqrt{2}J(\mathcal{T}_e + \mathcal{T}_o)$, with
  - (i) $\mathcal{T}_o = \mathcal{T}_e^\dagger$
  - (ii) $[\Theta, \mathcal{T}_e] = 2\mathcal{T}_e$
  - (iii) $[\Theta, \mathcal{T}_o] = -2\mathcal{T}_o$
- $\mathcal{T}_{e/o}$: creation/annihilation operator of imbalance
- tight-binding:
  $\langle\psi|H|\psi\rangle = \sum_Q \epsilon_Q \psi_Q^* \psi_Q + \gamma_Q^+ \psi_{Q+2}^* \psi_Q + \gamma_Q^- \psi_{Q-2}^* \psi_Q$
- nucleation of CDW $0-2$ pairs
- $|Q\rangle = \frac{1}{\sqrt{A(Q)}} (\tilde{\mathcal{T}}_e)^{Q/2} |MI\rangle$

Variational Ansatz - Mean Field

Normalisation constants

- $\gamma_Q^+ := \langle Q+2|\mathcal{T}|Q\rangle \propto \sqrt{\frac{A(Q+2)}{A(Q)}}$
- normalisation constants?
- maps to matching problem



- no analytical solution
- # P-hard $\leftrightarrow Z_{3D-Ising}$

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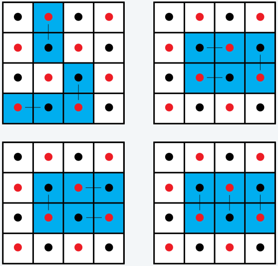


  - no analytical solution
  - $\#$ P-hard $\leftrightarrow Z_{3D-Ising}$

Lattice deformation

- deform CDW generator
  - **eliminate lattice structure**
  - ∞-range hopping $e \leftrightarrow o$
  - emergence of **non-local** CDW
- for Q-states only !
- $A(Q) = \binom{K/2}{Q/2}^2$

$$\gamma_Q^+ = -\frac{\alpha}{4K}\begin{cases}(K-Q)(Q+2) & Q \geq 0\\ (K-|Q|+2)|Q| & Q < 0\end{cases}$$

- **no predictions** for lattice dependent properties (e.g. CDW-SF)

Numerical Analysis

Numerical details

- analyse GS properties
- $K = 2000$ lattice sites
- different hopping: $\alpha = 8\sqrt{2}J$

Physical quantities

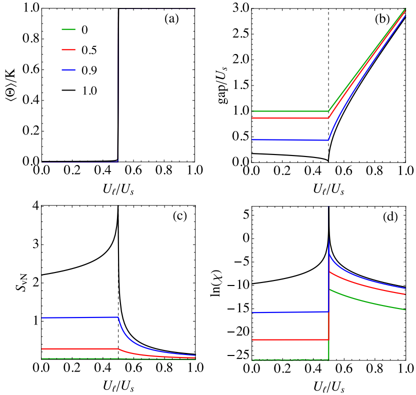
a) $\langle\Theta\rangle/K = \pm 1$: CDW or MI ?

b) $\Delta E_{k\to 0}$: compressible phase ?

c) $S_{\mathrm{vN}} = -\operatorname{tr}\rho_e \ln \rho_e$

d) $\chi = -\partial_\delta^2 \ln |\langle\psi(U_\ell)|\psi(U_\ell+\delta)\rangle||_{\delta=0}$

pinpoints all transitions for $K = 10$!



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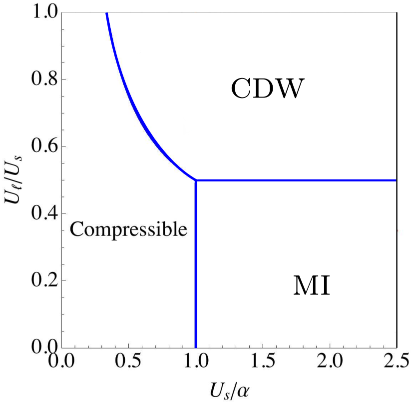

- $\exists$ compressible phase
  - no distinction: SS & SF
  - MI - SF: off by factor 2
- MI - CDW: accurate
- similar to Gutzwiller and QMC

Batrouni et al '17

Discrete WKB method

Procedure

- effective Hamiltonian

$$\langle\psi|H|\psi\rangle = \sum_Q \epsilon_Q \psi_Q^* \psi_Q + \gamma_Q^+ \psi_{Q+2}^* \psi_Q + \gamma_Q^- \psi_{Q-2}^* \psi_Q$$

- define momenta:

$$\cos p(Q) = \frac{E - \epsilon_Q}{2\gamma_Q}$$

- with $\gamma_Q := \frac{\gamma_Q^+ + \gamma_Q^-}{2}$
- effective tight-binding model
- **classically allowed regions**:

$$p(Q) \in \mathbb{R}$$
$$\Rightarrow \epsilon_Q + 2\gamma_Q \leq E \leq \epsilon_Q - 2\gamma_Q$$

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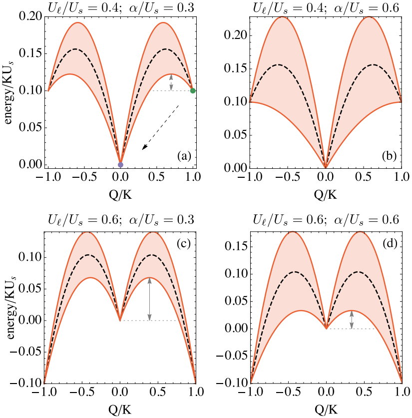
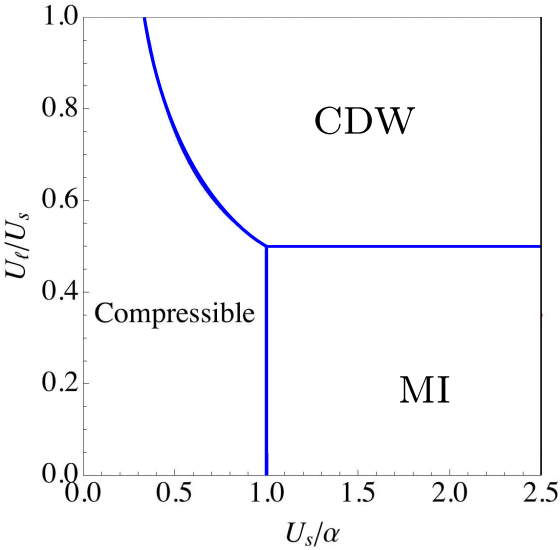


- hopping: simplifies transition

$$\Delta\mathcal{E} = \frac{K/8}{2U_\ell - \alpha} \begin{cases} (U_s - \alpha)^2, & \text{CDW} \\ (\alpha + U_s - 4U_l)^2, & \text{MI} \end{cases}$$

Augmented phase diagram



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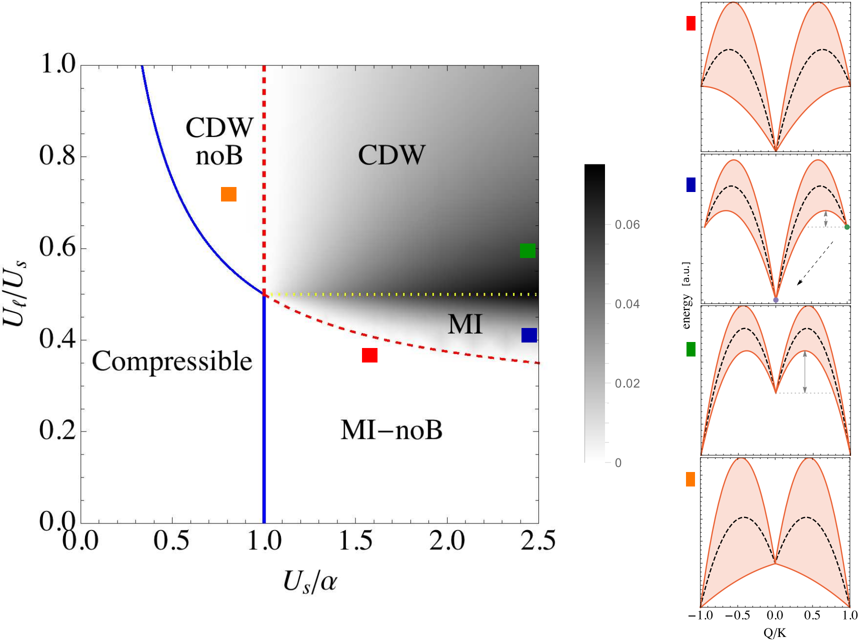

Conclusion

- role of quantum fluctuations in phase reconfig. of 1^{st} order transition
- long-range Bose-Hubbard model: MI - CDW transition
  - ultra-cold Ru atoms in optical lattice + cavity
  - full control on many-body properties
- exact Landau theory at zero hopping: hysteresis experiments
  - MI phase: meta stable + protected by barrier
  - explain: asymmetric hysteresis + plateaus
- variational description: render problem tractable
  - truncated Hilbert space
  - neglect lattice structure (mean-field like)
  - generate states $\left|Q\right\rangle$ by ∞ range hopping
  - numerical study: Θ, ΔE, S_{vN}, $\chi \Rightarrow$ phase diagram
- discrete WKB
  - construct phase diagram analytically
  - augment phase diagram by energy barrier
  - observe: tunneling lowers energy barrier

Outlook

- study dynamics in reduced Hilbert space: $\mathcal{L} = \langle\psi|(i\partial_t - H)|\psi\rangle$
  - different quench protocols
  - hysteresis loops

- construct a mean-field Hamiltonian
  - exact descriptions possible ?
  - ∞ range interaction $\Rightarrow$ mean-fiel reliable guide ? CDW - MI

- extend or modify variational $|Q\rangle$ states
  - $\exists$ extension that covers more details of the phase diagram ?
  - distinguish between SS and SF

- describe model as open quantum system: Lindblad, Q-Langevin ?
  - cavity loss
  - incoherent scattering for long-range interaction