Energy barriers between metastable states in first order quantum phase transitions


S Wald, A Timpanaro, C Cormick and GT Landi

Queens, Feb. 15, 2018
Bose Hubbard Model (BHM)

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

\[ \mathcal{T} = -J \sum_{\langle i,j \rangle} (b^\dagger_i b_j + b^\dagger_j b_i) \]

nearest neighbor hopping

on site repulsion

chemical potential

Gersch, Knollman 1963
Bose Hubbard Model (BHM)

Gersch, Knollman 1963

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

\[ \mathcal{T} = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) \]

nearest neighbor hopping

on site repulsion

chemical potential

mean-field phase diagram

Sachdev

\[ \mu / U_s \]

\[ Z J / U_s \]

M.I. 3

M.I. 2

Superfluid

M.I. 1

M.I. 0

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

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

**experimental setup**

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

**theoretical description** (canonical)

$$H = H_{BH} - \frac{U_l}{K} \left( \sum_{i \in e} n_i - \sum_{i \in o} n_i \right)^2$$

**experimental results**
Long range BHM

**Experimental setup**

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

**Theoretical description (canonical)**

$$H = H_{BH} - \frac{U_\ell}{K} \left( \sum_{i \in e} n_i - \sum_{i \in o} n_i \right)^2$$

**Experimental results**

![Graph showing experimental results](image-url)
Long range BHM

**experimental setup**

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

---

**theoretical description (canonical)**

$$H = H_{BH} - \frac{U_\ell}{K} \left( \sum_{i \in e} n_i - \sum_{i \in o} n_i \right)^2$$

---

**experimental results**
Hysteresis curves

Phase Diagram

Landig et al. '16

Hysteresis

Detuning, $\Delta / 2\pi$ (MHz)

2D lattice depth, $V_{2D} (E_R)$

CDW

MI

SS

SF

Imbalance, $\theta$

Detuning, $\Delta / 2\pi$ (MHz)
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: $J/U_s \ll 1$

$$H_{J\to0} = \sum_{i=1}^{K} \frac{U_s}{2} \hat{n}_i(\hat{n}_i - 1) - \frac{U_\ell}{K} \Theta^2$$

- Fock basis: $H$ diagonal
- free energy:

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

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

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

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

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

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

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

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

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

[Graph showing $f(\theta)$ vs $\theta$ with different values of $U_\ell/U_s$.]

[Graph showing Imbalance, $\Theta$, vs Detuning, $\Delta/2\pi$ (MHz).]
Different fillings: $\rho \neq 1$

Dogra et al '17
Different fillings: $\rho \neq 1$

- 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?
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?
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
    \[ \Theta = (\sum_{i \in e} n_i - \sum_{i \in o} n_i)^2 \]
  - \( |1, 2, 1, 2; 0, 1, 0, 1\rangle; |1, 2, 1, 2; 0, 0, 0, 2\rangle \)
    - additional \( U_s \) without \( U_\ell \) gain
    - distribute atoms in sublattices
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 $U_\ell$ gain
  - distribute atoms in sublattices

**Choice of variational states**

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

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

- no analytical solution
- \# P-hard \( \leftrightarrow Z_{3D-Ising} \)
Variational Ansatz - Mean Field

**Normalisation constants**

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

![Diagram](image)

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

**Lattice deformation**

- deform CDW generator
- eliminate lattice structure
- $\infty$-range hopping $e \leftrightarrow o$
- emergence of **non-local** CDW
- for $Q$-states only!

- $A(Q) = \left(\frac{K}{Q/2}\right)^2$

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

- **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) $S_{\nu N} = - \text{tr} \rho_e \ln \rho_e$

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

pinpoints all transitions for $K = 10$!
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) $\Delta E_{k \rightarrow 0}$: Compressible phase?

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

d) $\chi = -\partial^2_{\delta} \ln |\langle \psi(U_\ell) | \psi(U_\ell + \delta) \rangle|_{\delta=0}$
   
   - Pinpoints all transitions for $K = 10$!

- $\exists$ 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:

\[ p(Q) \in \mathbb{R} \]

\[ \Rightarrow \epsilon_Q + 2\gamma_Q \leq E \leq \epsilon_Q - 2\gamma_Q \]
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:**

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

- **hopping:** simplifies transition

\[
\Delta \mathcal{E} = \frac{K/8}{2U_l - \alpha} \begin{cases} (U_s - \alpha)^2, & \text{CDW} \\ (\alpha + U_s - 4U_l)^2, & \text{MI} \end{cases}
\]
Augmented phase diagram

\[ \frac{U_e}{U_s} \times \frac{U_s}{\alpha} \]

- CDW
- Compressible
- MI
Augmented phase diagram
Conclusion

- **role of quantum fluctuations** in phase reconfig. of 1st 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 $|Q\rangle$ by $\infty$ range hopping
  - numerical study: $\Theta, \Delta E, S_{vN}, \chi \Rightarrow$ 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?
  - \( \infty \) range interaction \( \Rightarrow \) mean-field 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