Energy barriers between metastable states in first order quantum phase transitions

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S Wald, A Timpanaro, C Cormick and GT Landi

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

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

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

- nearest neighbor hopping
- on site repulsion
- chemical potential

Gersch, Knollman 1963
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- on site repulsion
- chemical potential

mean-field phase diagram

- 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

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**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 phase transitions and other data points]
Long range BHM

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\]

Experimental results

\[
\begin{array}{c}
\text{CDW} \\
\text{SS} \\
\text{SF} \\
\text{MI}
\end{array}
\]

\[
\begin{array}{c}
u/t \\
35 \\
30 \\
25 \\
20 \\
15 \\
10 \\
5 \\
0
\end{array}
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$$H = H_{BH} - \frac{U_L}{K} \left( \sum_{i \in e} n_i - \sum_{i \in o} n_i \right)^2$$

**Experimental Results**

Landig et al, Nature'16
Hysteresis

Phase Diagram

Hysteresis curves

Landig et al '16
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|$$
The Zero Hopping Limit

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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
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- $T = 0$? quantum fluctuations?
Variational Ansatz: $J \neq 0$

### Requests

- **CDW & MI**: $J/U_s \ll 1$
- **Focus on** $\rho = 1$
- $|\text{MI}\rangle = |1\ldots1;1\ldots1\rangle$
  $|\text{CDW}\rangle = |2\ldots2;0\ldots0\rangle$
- **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 $\rho = 1$ |
| $|MI\rangle = |1...1; 1...1\rangle$ |
| $|CDW\rangle = |2...2; 0...0\rangle$ |
| 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 |

| 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 |
| $|Q\rangle = \frac{1}{\sqrt{A(Q)}}(\tilde{T}_e)^Q/2|MI\rangle$ |
**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

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

\begin{align*}
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}
\end{align*}

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

Lattice deformation

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

\begin{align*}
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(K - Q)(Q + 2) & Q \geq 0 \\
(K - |Q| + 2)|Q| & Q < 0
\end{cases}
\end{align*}

- 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) $S_{vN} = - \text{tr} \rho_e \ln \rho_e$
d) $\chi = - \partial^2_\delta \ln |\langle \psi(U_1) | \psi(U_1 + \delta) \rangle|_{\delta = 0}$

pinpoints all transitions for $K = 10$!
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Physical quantities

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

[Graph showing phase diagram]

- $\exists$ 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**

\[
\langle \psi | H | \psi \rangle = \sum_Q \epsilon_Q \psi_Q^{\ast} \psi_Q + \gamma^+_Q \psi_{Q+2}^{\ast} \psi_Q + \gamma^-_Q \psi_{Q-2}^{\ast} \psi_Q
\]

- **define momenta:**

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- **effective tight-binding model**

- **classically allowed regions:**

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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

$U_i/U_s$ vs $U_s/\alpha$

- CDW
- Compressible
- MI
Augmented phase diagram

- CDW
- CDW
- MI
- MI-noB
- Compressible

- $U_e/U_s$
- $U_s/\alpha$
- $Q/K$
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