Dynamic melting and condensation of topological dislocation modes

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arXiv link of the work

Objectives

1. Does the signature of topological dislocation modes survive in translationally inert insulators, reached from a translationally active topological insulator(TATI) via a real time ramp?
2. Can topological dislocation modes be dynamically generated via a ramp, taking the system into a TATI phase from translationally inert insulators?

Introduction

- *Bulk dislocation lattice defects:* To identify translationally active topological insulators (TATIs), featuring band inversion at a finite momentum (K_{inv}).
- Characterization and $\boldsymbol{K}\cdot\boldsymbol{b}$ rule: Burgers vector (b). $\Phi_{dis} = K_{inv}\cdot b$
- $\Phi_{dis} = 0$ in the Γ phase, as $K_{inv} = 0$.
- M-phase: b and K_{inv} are such that $\Phi_{dis} = \pi$ (modulo 2π).

M-phase dislocation mode and ramping scheme

- $$H = t_1 \sum_{j=x,y} \sin(k_j a)\tau_j + \left(t_0 \sum_{j=x,y} \cos(k_j a) - m_0\right)\tau_z. \quad (1)$$

  τ: orbital degrees of freedom

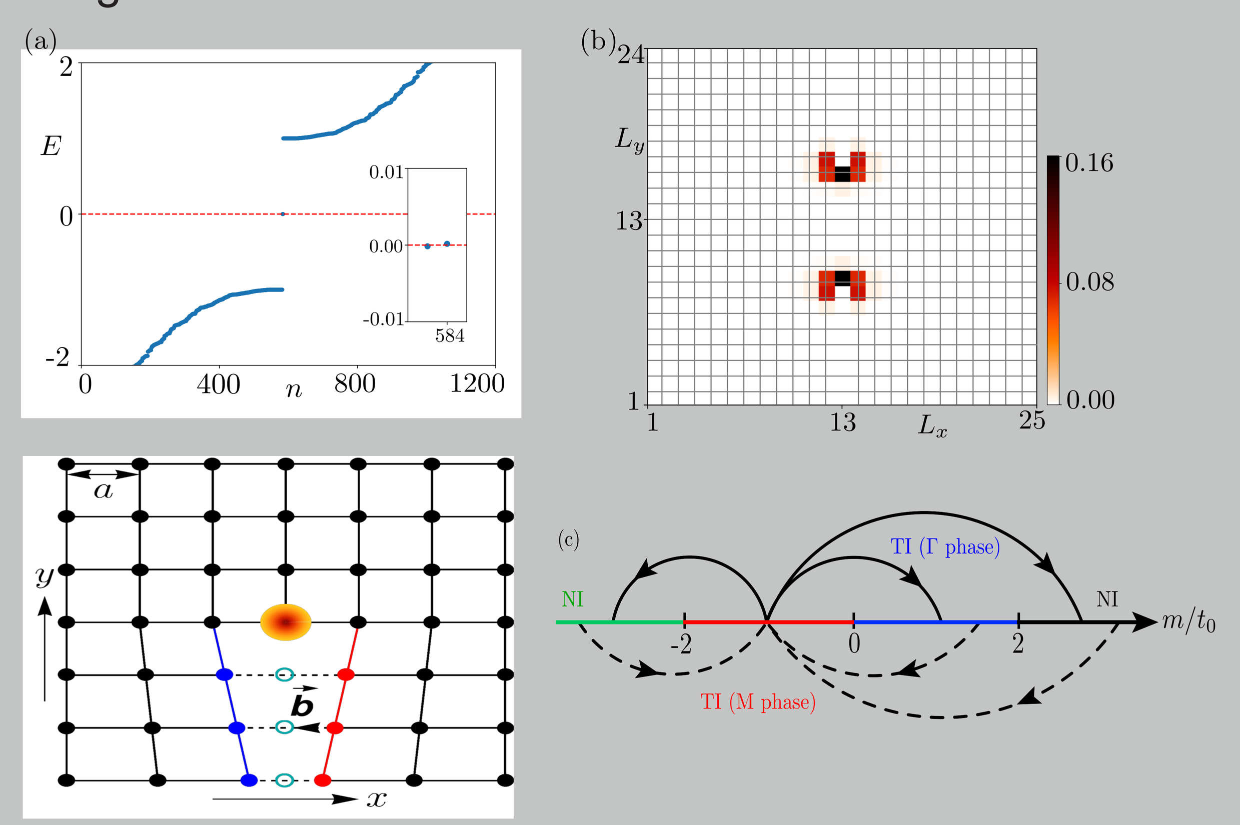

Figure: (a) Energy spectra of the static Hamiltonian [Eq. (1)] for $t = t_0 = -m_0 = 1$, yielding a TATI with the band inversion at the M point (M phase). (b) The local density of states (LDOS) of these two modes are highly localized near the defect cores. (c) Phase diagram of the static Hamiltonian. Ramps out of (into) the M phase to (from) translationally inert insulators are shown by solid (dashed) arrows.

Mathematical toolbox: von Neumann equation

- Time evolution of density matrix:
$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}\,[H(t), \rho(t)]\,. \quad (2)$$
- Time ramp profile:
$$m(t) = m_i + (m_f - m_i)\ [1 - \exp(-\alpha t)]\,. \quad (3)$$
  - ramp speed is given by α. Time is measured in units of α^{-1}.
- Probability of finding the dislocation mode
$$P(t) = \langle\Psi|\rho(t)|\Psi\rangle\,, \quad (4)$$
- Site resolved LDOS:
$$D_i(t) = \sum_{\tau=1,2} \langle i,\tau|\rho(t)|i,\tau\rangle\,. \quad (5)$$
  - i (τ) is the site (orbital) index, and $|i,\tau\rangle$ is the single particle state vector at site i with orbital τ.

Results: Limit (I) → Ramping out of TATI

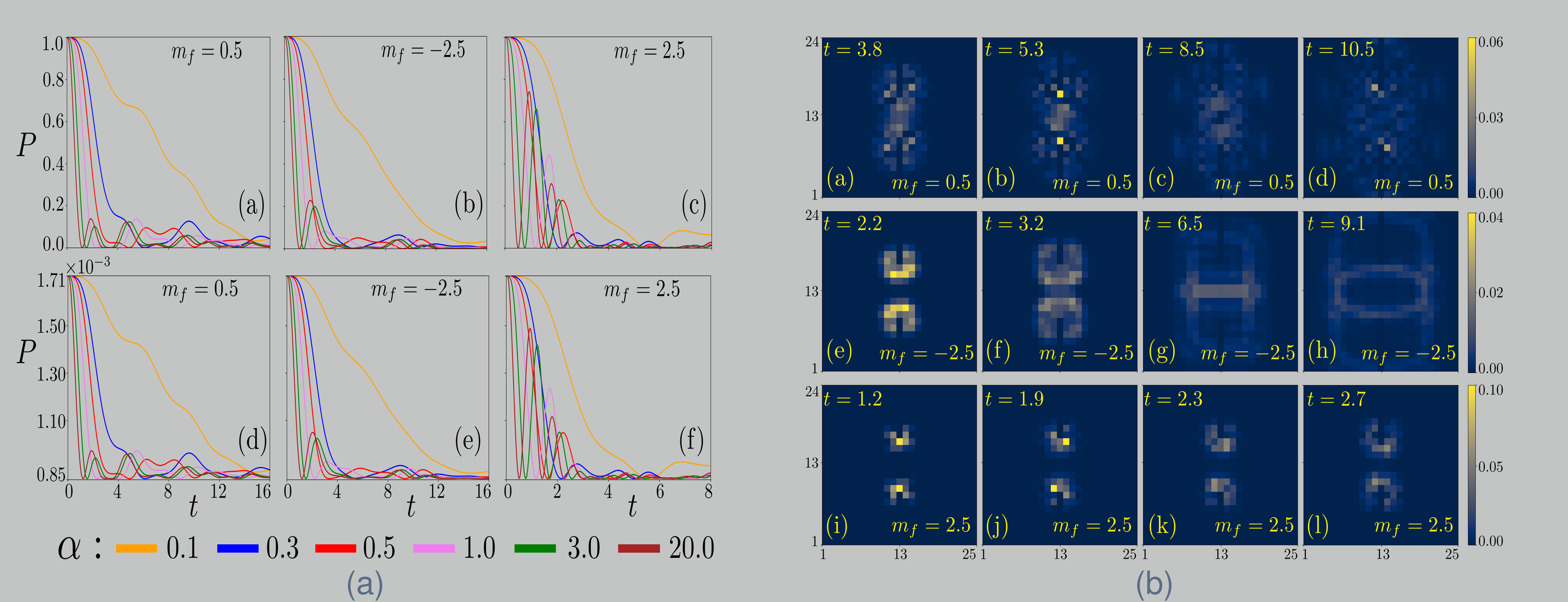

Figure: $P(t)$ for various ramp speed, and site resolved LDOS.

Results: Limit (II) → Ramping into TATI

- In quantum materials midgap dislocation modes can only be occupied upon filling all the negative energy bulk states.
- **Particle-hole symmetry**: a half-filled system displays a uniform average electronic density equal to one always.
- Mixed density matrix:
$$\rho(0) = \frac{1}{N+1}\sum_{i=1}^{N+1} |\Psi_i\rangle\langle\Psi_i|\,. \quad (6)$$
  $|\Psi\rangle = \left(|\Psi_1^{dis}\rangle + |\Psi_2^{dis}\rangle\right)/\sqrt{2}$, and $P(0) = (N+1)^{-1}$.

Results: Limit (II) density matrix with pure state : ✗

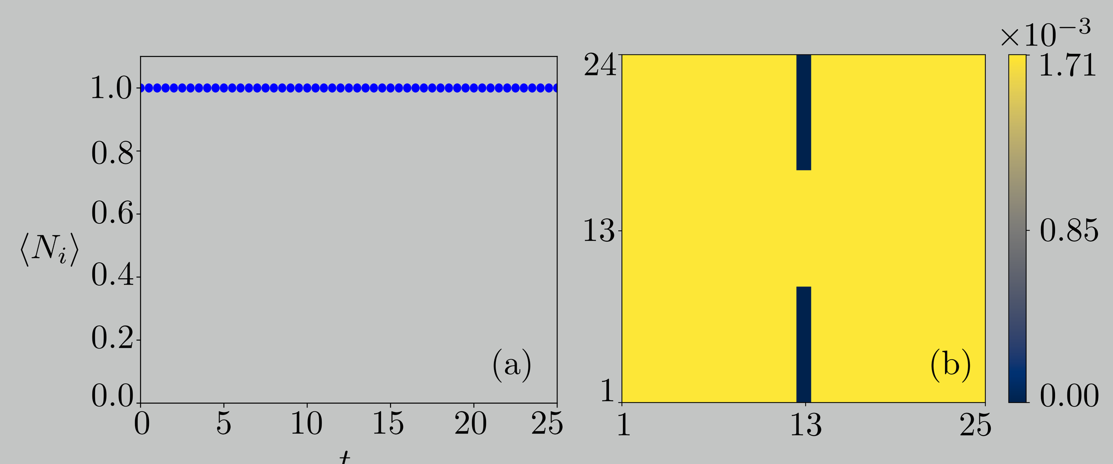

Figure: (a) Time dependence of the average electronic density $\langle N_i(t)\rangle$ in a half-filled system for any value of i (site index) for any values of α, m_i and m_f. (b) Correspondingly, the site resolved LDOS $D_i(t)$ shows constant value for all the sites in the entire system.

Results: Limit (II) → Figure

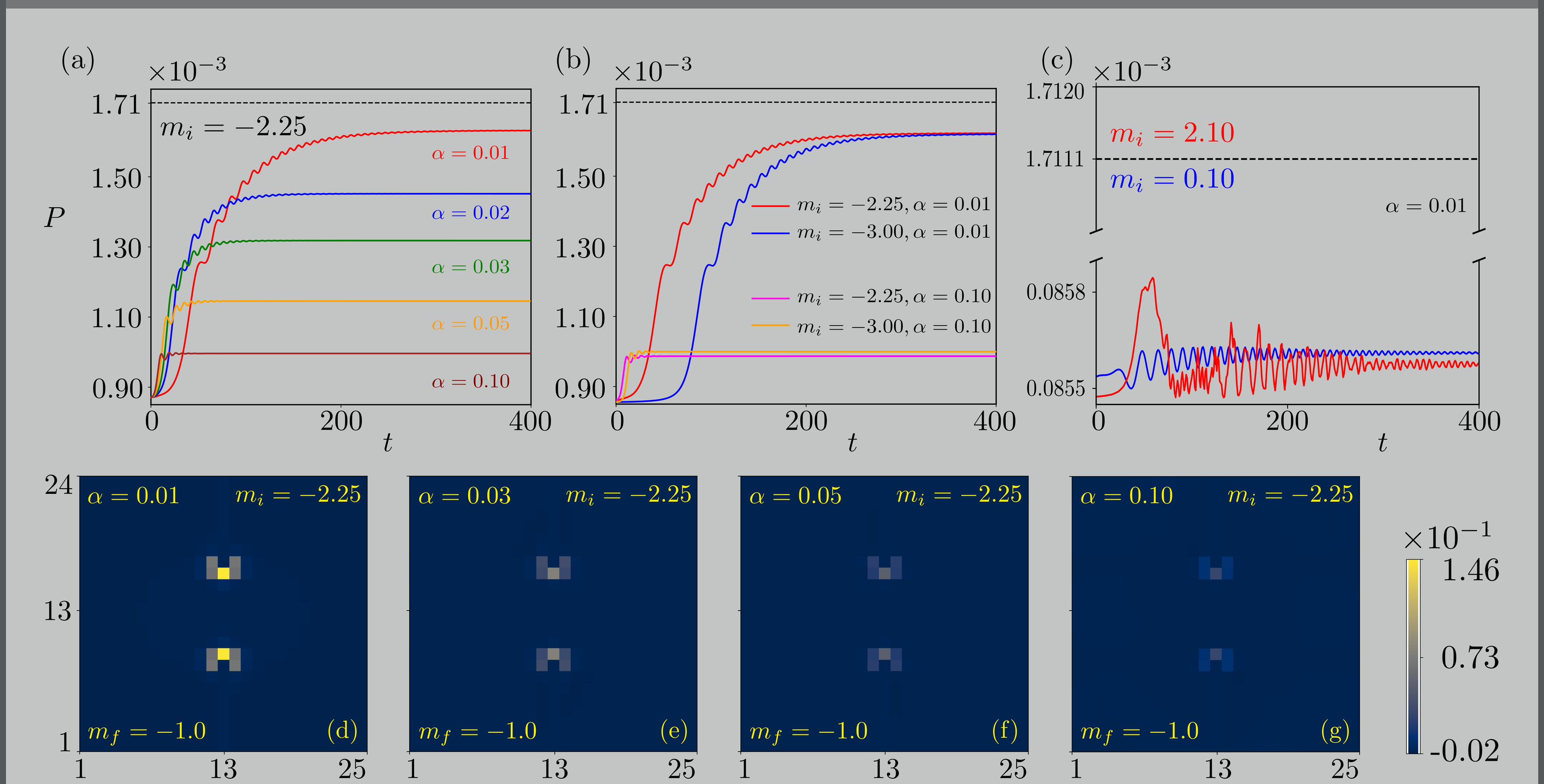

Figure: Top: Probability $P(t)$ of dynamic condensation of dislocation modes. Bottom: (d)-(g) Difference between the initial and final site resolved LDOS for various α, confirming prominent dynamic generation of the dislocation modes, comparable to those in the M phase in the static system, for sufficiently slow ramp.

Conclusions

1. Melting: Ramping out of the TATI phase: dislocation modes survive for sometime and shows periodic revive irrespective of the nature of the final phase.
2. Site resolved LDOS displays periodic peaks and deeps at the dislocation core.
3. Condensation: Dynamic condensation of dislocation modes is most prominent when the initial state is a normal insulator, residing close to the M phase, with the noninverted band minima near the M point.
4. **Slower ramp speed → better probability of dynamic generation of dislocation modes → *Adiabatic principle*.**

References

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