Equilibrium Phases in the 1-D Hubbard Model

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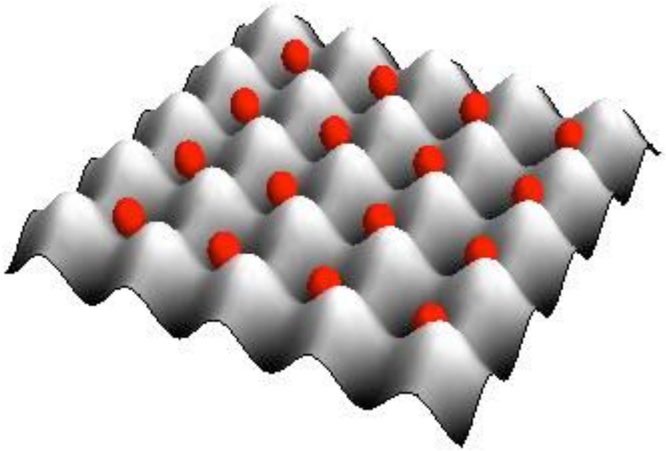
Background

- John Hubbard (1963)
- Fermions + interactions
  - "Strongly correlated behavior"
- High-temperature superconductivity in cuprates
- Ultracold atoms

"Levitating superconductor"

Challenges

- Many-body quantum system
  - # of states: 4^n
  - Hard to simulate directly
- Mutual interactions
  - Hard to analyze



Hubbard Model in 1-D

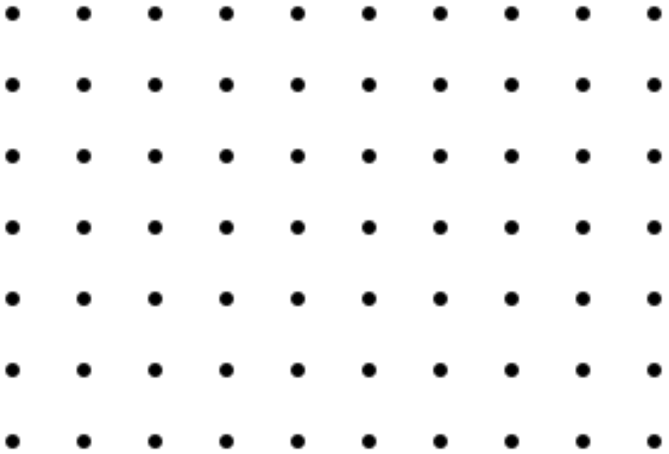
$$\hat{H} = -t \sum_{i\sigma} \left(\hat{c}^\dagger_{i\sigma} \hat{c}_{(i+1)\sigma} + \hat{c}^\dagger_{(i+1)\sigma} \hat{c}_{i\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})$$

- t: kinetic energy -- “hopping term”
- U: on-site interaction
- μ: external chemical potential

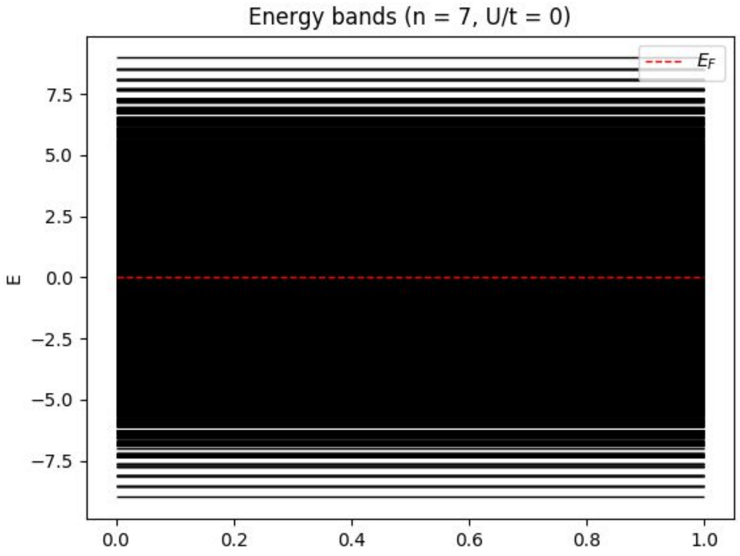
Exact Diagonalization (ED)

$$\hat{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

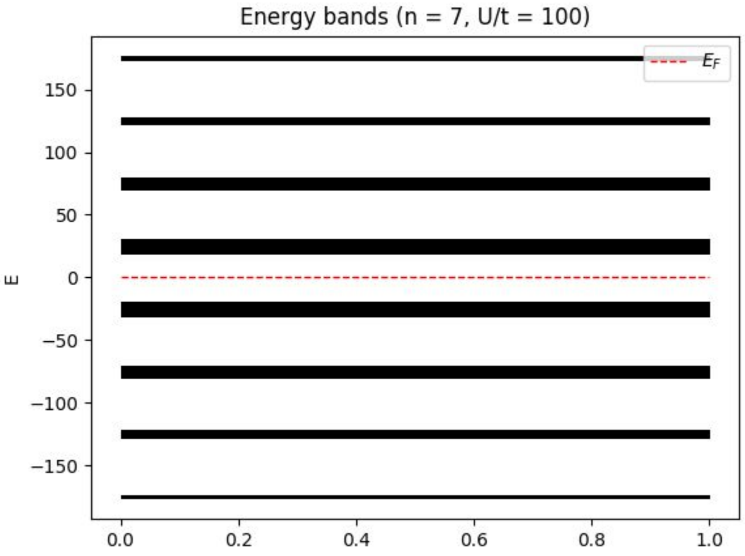
- Encode Hamiltonian and solve TISE directly
- Small systems only…
- For Fermi-Hubbard:
    - Enumerate in number basis
    - Periodic boundary conditions
    - Particle number conserved -- block diagonalize



N=7: Band Gap



Energy bands (n = 7, U/t = 0)
E_F
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
E
0.0
0.2
0.4
0.6
0.8
1.0



Energy bands (n = 7, U/t = 100)
E_F
150
100
50
0
−50
−100
−150
E
0.0
0.2
0.4
0.6
0.8
1.0

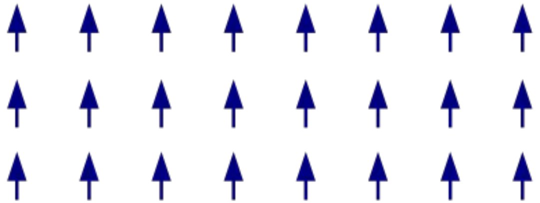
Mean Field Theory

- Interactions are hard, fields are easy

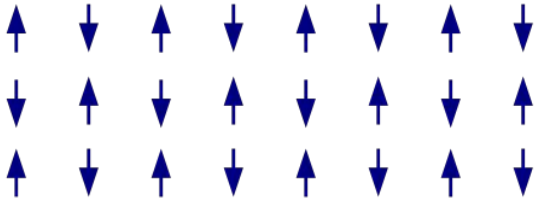
$$\cancel{\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}} \longrightarrow \hat{n}_{i\uparrow}\left\langle \hat{n}_{i\downarrow} \right\rangle$$

What is the mean field?

- Depends on our guess…
- Can solve energies analytically in both
- For Fermi-Hubbard:
    - Iterate over densities and interactions
    - Compute energy under FM and AFM
    - Pick the phase with lower energy

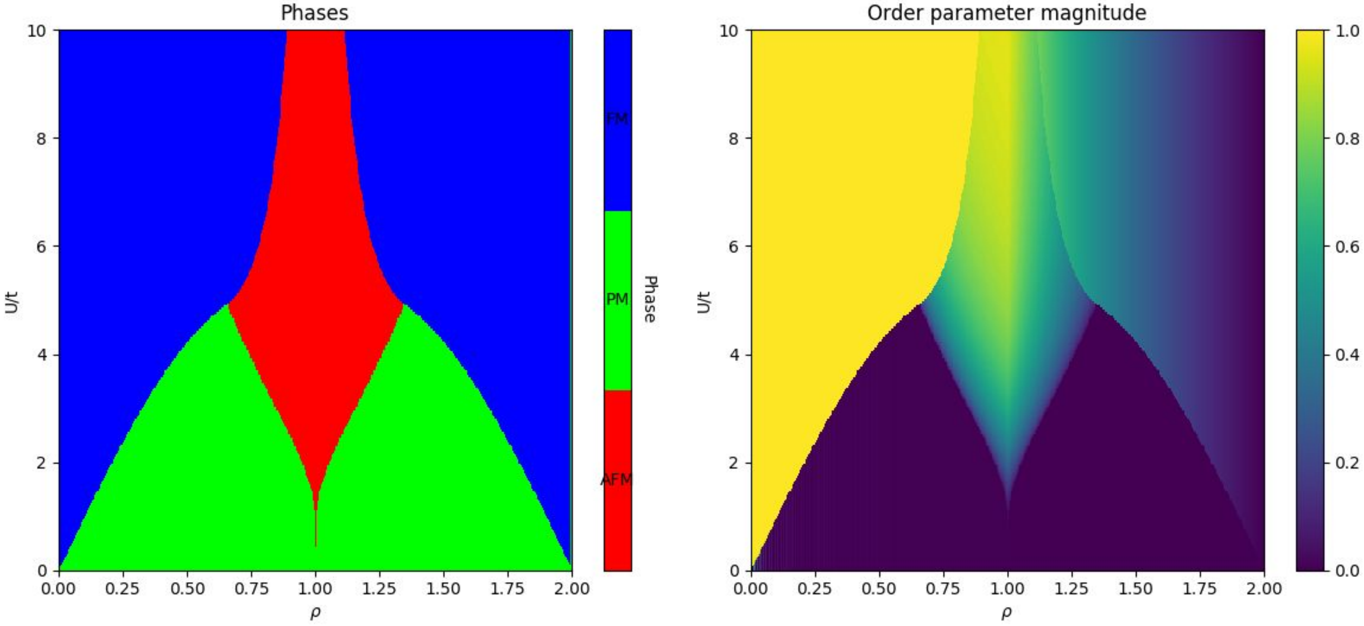


“Ferromagnetic ordering”



“Antiferromagnetic ordering”

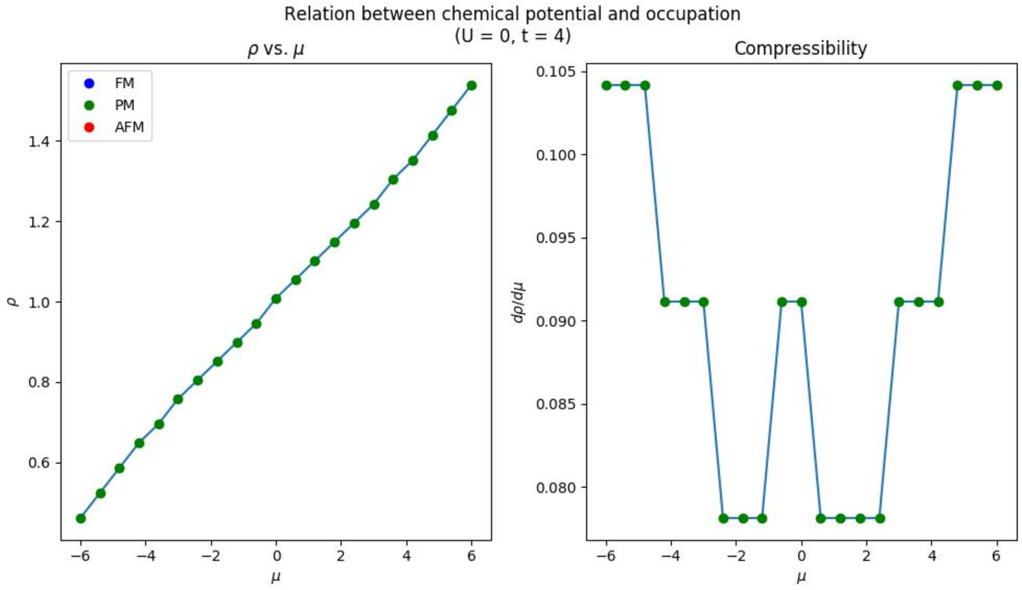
Equilibrium Phase Diagram



Compressibility (dρ/dμ)

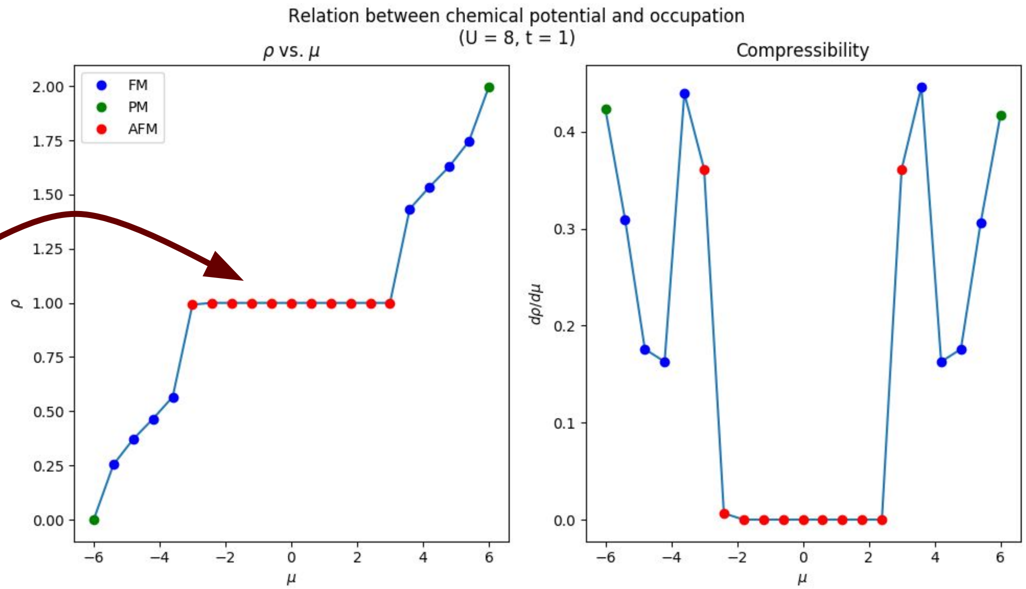
- Raise the external chemical potential μ. How much does density change?
- An easy-to-calculate "surrogate" for conductivity
  - How readily electrons can be "forced" through the system?
- For Fermi-Hubbard: more annoying to calculate
  - Don't know what density is for given μ, but need density to compute mean field
  - Guess-update iteration until self-consistent
  - Initial-guess dependent... randomize and do a bunch of trials

Compressibility (U/t = 0)



Compressibility (U/t = 8)

“Mott Plateau”



Conclusions

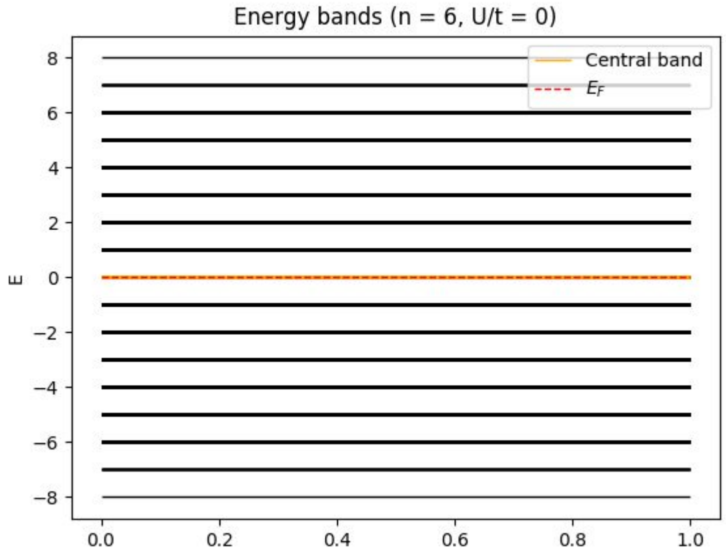
- Having interactions between fermions greatly changes behavior
- System can become ordered where it wasn't without interactions

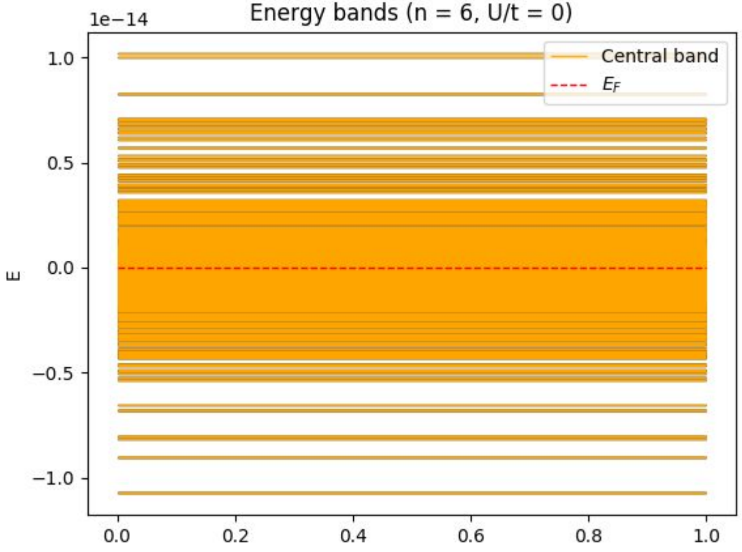
Sources

- “Levitating superconductor” by Julian Litzel is licensed under CC BY-SA 3.0: https://upload.wikimedia.org/wikipedia/commons/1/15/Levitating_superconductor.jpg
- “Lattice mott” by Sakurai2: https://upload.wikimedia.org/wikipedia/commons/b/b8/Lattice_mott.JPG
- “Square lattice” by Jim.belk: https://commons.wikimedia.org/wiki/File:SquareLattice.svg
- “Ferromagnetic ordering” and “Antiferromagnetic ordering” by Michael Schmid is licensed under CC BY-SA 3.0: https://commons.wikimedia.org/wiki/File:Ferromagnetic_ordering.svg, https://commons.wikimedia.org/wiki/File:Antiferromagnetic_ordering.svg

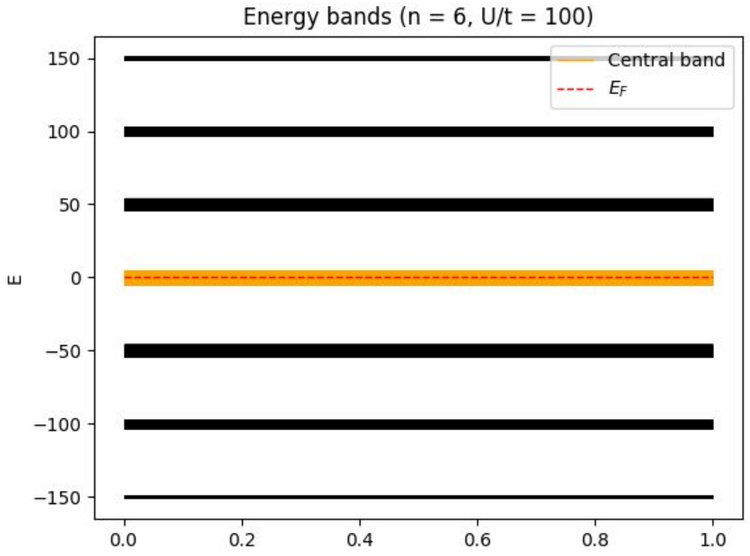
Backup

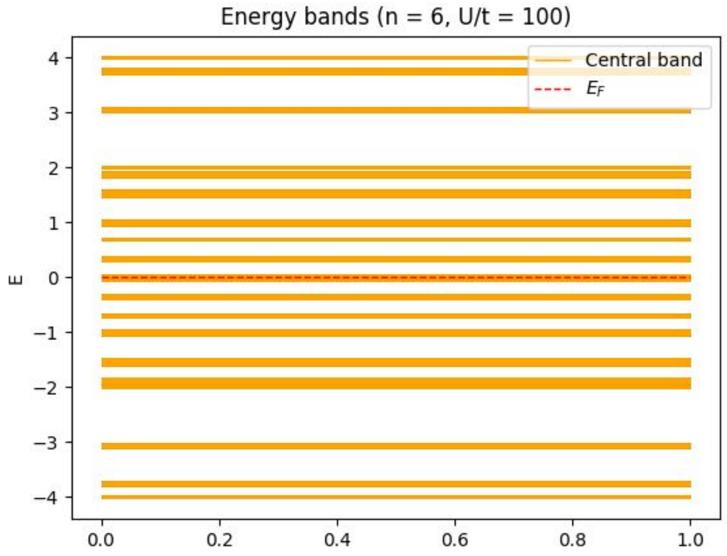
Spectrum: N = 6, U/t = 0





Spectrum: N = 6, U/t = 100: Band Gap





Compressibility (U/t = 1)