In Le Bellac’s lectures: **Caldeira Leggett Model**
* Simple enough to be exactly soluble
* Insight into Brownian Motion, Fluctuation-Dissipation, ...
* But,... spring forces between particles far apart?!

Likewise Batrouni/Hebert: **XY Model**:
* Simple
* Insight into superfluidity
* But,... pretty distant from $^4$He!

**Ising, Heisenberg Models**
* Magnetism arising from local spins.

This Seminar: **Hubbard Model**
* Itinerant Magnetism (spins sit on electrons which can move)
* Metal-Insulator transitions arising from electron-electron interactions
* High Temperature superconductivity
* But,... Simplicity $\rightarrow$ significant approximations (for solids)

Are there systems (AMO) for which it might be more realistic?
Forty Years of the Hubbard Model
From the Solid State to Cold Atoms on Optical Lattices

- Transition Metal Oxides
- The Fermion Hubbard Model
- Transition Metal Oxides - The Whole Story
- High Temperature Superconductors
- Monte Carlo and Quantum Monte Carlo
- Disordered Superconductors
- The Boson Hubbard Model
- Conclusions
Purpose

Brief introduction to the rich history of the Hubbard Model in condensed matter physics

Successes!! and Limitations!!

Make connections to new field of cold atom physics.

Recent suggestion: Cold atom systems will give us insight into physics of solids.

Collaborators

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From Atoms to Solids

Individual atoms: discrete energy levels
Atoms far apart: electrons are localized on single atom
Atoms brought together (solid): degenerate level couple and broaden into a band. Eigenvectors are delocalized (plane/“Bloch” waves)

\[
\begin{pmatrix}
E_n & t \\
t & E_n
\end{pmatrix}
\]

Eigenvalues \( \lambda = E_n \pm t \)

Eigenvectors \( \psi = \frac{1}{\sqrt{2}} \left( \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \right) \)

\[
x \ e^{-r/a_0} \quad -13.6 / n^2
\]

s p d
Band Insulators

Energy band completely filled: Insulator
Finite energy gap to next unoccupied level
Simple counting arguments predict whether many solids are metallic or insulating!!
k eigenstate can be occupied by two electrons (spin $\uparrow, \downarrow$).
Solids with an odd number of electrons per unit cell must be metallic.
Alkalis (Li, Na, K): one valence $e^-$ ($2s^1, 3s^1, 4s^1$) per unit cell: Good metal.
Diamond, silicon, and germanium (C, Si, Ge): eight valence electrons per unit cell ($2s^22p^2, 3s^23p^2, 4s^24p^2$): insulators.
Transition Metal Monoxides (MnO, FeO, CoO)

Simplest band structure picture

Mn$^{2+}$ has 3d$^5$ configuration
half-filled band → metal

Experimentally
* insulating
* antiferromagnetic ($T_{\text{Neel}} = 122^\circ$ K)
Can however make MnO have the expected metallic behavior...

**Diamond Anvil Cell**

Apply pressure (and lots of it!) to push atoms closer.

- **Direct measurement of resistance**
- **Probe magnetic moments with synchotron radiation (APS at Argonne)**
Resistance drops to typical metallic values at $P \approx 100$ GPa.

Temperature dependence changes:

- **Insulating (gapped)**
  - $R$ increases as $T$ lowered

- **Metallic**
  - $R$ decreases as $T$ lowered
**RIXS:** Energy of x-rays emitted when core (1s) hole created, and 3p $e^-$ decays to fill it. Magnetic moment on 3d, if present, splits 3p level and induces secondary $K\beta'$ peak

**RESULTS:** $K\beta'$ intensity exhibits step-like structure.

- $0 < P < 30 \text{ GPa}$: $I(K\beta')/I(K\beta) \approx 0.10$
- $60 < P < 105 \text{ GPa}$: $I(K\beta')/I(K\beta) \approx 0.05$
- $105 < P < 130 \text{ GPa}$: $I(K\beta')/I(K\beta) \approx 0.00$ → Moment destroyed

![Graph showing $K\beta'$ intensity](image-url)
Temperature-Pressure phase diagram (Yoo etal., PRL, 2005)

[1] $P \approx 30$ GPa  
Structural phase transition

[2] $P \approx 90$ GPa  
Antiferromagnetic to paramagnetic transition (moments disordered)

[3] $P \approx 105$ GPa  
moments destroyed  
Insulator to metal phase transition  
Isostructural Volume Collapse ($\Delta V \approx 6.6\%$)
The Hubbard Hamiltonian

$$H = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Operators $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) create (destroy) an electron of spin $\sigma$ on site $i$. Includes electron kinetic energy ($t$) and interaction energy ($U$).

Momentum space

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + U \sum_{k,p,q} c_{k+q\uparrow}^\dagger c_{p-q\downarrow}^\dagger c_{k\uparrow} c_{p\downarrow}$$

$$\epsilon_k = -2t (\cos k_x + \cos k_y)$$

In two dimensions, bandwidth $W = 8t \approx 2 \text{ eV}$.

on site repulsion $U \approx 2 - 10 \text{ eV}$

$t = 1 \approx 0.25 \text{ eV} = 300^\circ K$ is usual choice to set energy scale.

$\beta = t/T = 1/T = 10$ means $T \approx 300^\circ K$. 
Mott Insulator

$U/t$ large and $\langle n \rangle = 1$.

All sites occupied by exactly one $e^-$. Hopping causes double occupancy, costs $U$.

Chemical potential $\mu$

* Cost to add particle
* Jumps at $\rho = 1$

---

U=4.0 N=8x8

---

N=8x8 U=4t $\mu=0.25t$
Mott Insulator

$U/t$ large and $\langle n \rangle = 1$.
All sites occupied by exactly one $e^{-}$.
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Chemical potential $\mu$
* Cost to add particle
* Jumps at $\rho = 1$

$U=4.0 \ N=8\times8$

$N=8\times8 \ U=4t \ \mu=0.25t$
Mott Insulator

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* Cost to add particle
* Jumps at $\rho = 1$

$U=4.0$  $N=8x8$

$N=8x8$  $U=4t$  $\mu=0.25t$
$U/t$ large and $\langle n \rangle = 1$.
All sites occupied by exactly one $e^-$. Hopping causes double occupancy, costs $U$.
Chemical potential $\mu$
* Cost to add particle
* Jumps at $\rho = 1$

$U=4.0 \ N=8x8$

$N=8x8 \ U=4t \ \mu=0.25t$
Mott Insulator

\( U/t \) large and \( \langle n \rangle = 1 \).

All sites occupied by exactly one \( e^- \).

Hopping causes double occupancy, costs \( U \).

Chemical potential \( \mu \)
- Cost to add particle
- Jumps at \( \rho = 1 \)

\[
\begin{array}{c}
\mu = 0.25t \\
\beta = 4 \\
\beta = 6 \\
\beta = 8 \\
\end{array}
\]

\[
\begin{array}{c}
N = 8 \times 8 \\
U = 4t \\
\end{array}
\]

\[
\begin{array}{c}
\mu = 0.25t \\
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Mott Insulator

$U/t$ large and $\langle n \rangle = 1$.
All sites occupied by exactly one $e^-$. 
Hopping causes double occupancy, costs $U$.
Chemical potential $\mu$
  * Cost to add particle
  * Jumps at $\rho = 1$

$U=4.0$ $N=8x8$

$\beta=4$
$\beta=6$
$\beta=8$

$N=8x8$ $U=4t$ $\mu=0.25t$
Two ways to destroy Mott Insulator:

* Decrease $U/t$: By applying pressure ($\text{MnO}$)
* Shift $\langle n \rangle \neq 1$: Dope chemically (cuprate superconductors)

What is optimal spin arrangement?

Hopping of neighboring parallel spins forbidden by Pauli. Antiparallel arrangement lower in second order perturbation theory.

\[ \Delta E^{(2)} = 0 \quad \Delta E^{(2)} = -t^2/U = -J \]

In Hubbard model insulating behavior and antiferromagnetism go hand-in-hand.
Simple “Stoner” Picture of Magnetic Order

\[
\delta E = \frac{\delta N}{\delta E} \propto \frac{1}{t}
\]

Interaction energy lowered by polarizing the spins:

\[
\delta P E = U(N + \delta N)(N - \delta N) - UN^2 = -U(\delta N)^2 = -UN(E_F)\delta N\delta E
\]

Kinetic energy raised by polarizing the spins:

\[
\delta K E = +\delta N\delta E
\]

Total Energy change:

\[
\delta E = \delta K E + \delta P E = [1 - UN(E_F)]\delta N\delta E
\]

Stoner Criterion: \( UN(E_F) > 1 \rightarrow \text{magnetism!} \)
**Transition Metal Monoxides - The Whole Story?**

- Kinetic Energy: $3d$ bandwidth $t_d$
- Correlation Energy: On-site Coulomb $U_d$
- Multiple orbitals: Hund’s rule (exchange) $J_H$
- Both Mn and O atoms: Charge transfer energy $E_{3d} - E_{2p}$
- Mn in cubic environment: Crystal field splitting $E_{eg} - E_{t_{2g}}$

---

**Diagram:***

- Exchange splitting $> \text{crystal field}$
- Crystal field $> \text{Exchange splitting}$

---

**Loss of moment transition actually a “high-spin to low spin transition”?**

Crystal field splitting decreases below exchange splitting as pressure applied.
High Temperature Superconductor YBa$_2$Cu$_3$O$_{7-\delta}$

Control Mott insulator and antiferromagnetism with $\delta$ (electron density).
Antiferromagnetic when one hole per copper. Neél temperature goes to zero when doped. Superconductivity when doped and temperature lowered (Hg compound shown)

As expected from Hubbard: At 1 hole/Cu: antiferromagnetic and insulating

Unexpected from Hubbard?

* Superconductivity and, in particular, d-wave symmetry
* Charge inhomogeneities
s–wave

\[ \Delta_s^\dagger = c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \]

\[ \Delta_{s^*}^\dagger = c_{j\uparrow}^\dagger \left[ c_{j+x\downarrow}^\dagger + c_{j+y\downarrow}^\dagger + c_{j-x\downarrow}^\dagger + c_{j-y\downarrow}^\dagger \right] \]

\[ \Delta_d^\dagger = c_{j\uparrow}^\dagger \left[ c_{j+x\downarrow}^\dagger - c_{j+y\downarrow}^\dagger + c_{j-x\downarrow}^\dagger - c_{j-y\downarrow}^\dagger \right] \]

Actually, d-wave pairing had been suggested in the Hubbard model before high-\( T_c \) in context of heavy fermion systems.

Mechanism of conventional superconductivity:
Attractive interaction between e\(^-\) mediated by exchange of phonons (lattice vibrations).

Possible mechanism of (un)conventional superconductivity:
Attractive interaction between e\(^-\) mediated by exchange of magnons (vibrations of lattice of antiferromagnetically aligned spins).
“Stripes”: Doped holes are not uniformly distributed.

Are stripes in the Hubbard Hamiltonian?!
Yes! Inhomogeneous Hartree-Fock (Zaanen); Density Matrix Renormalization Group (White).
Again, many ‘real life’ complications

Like TMOs: Oxygen orbitals. 3-band (‘Emery’) model.
Charge transfer versus Mott-Hubbard Insulator

\[
\begin{align*}
&\varepsilon_p - \varepsilon_d \\
U_d &
\end{align*}
\]

Role of number of layers and interlayer atoms

\[
\begin{align*}
La_{1-x}Sr_xCuO_2: & \quad T_c \approx 35^\circ K. \\
Y_{1}Ba_{2}Cu_{3}O_{7-\delta}: & \quad T_c \approx 90^\circ K.
\end{align*}
\]

Hubbard Hamiltonian ‘particle-hole’ symmetry.
Cuprate superconductors: electron doped \(\neq\) hole doped.
Role of phonons
Classical Monte Carlo

Energy of set of degrees of freedom $x_i$:

$$ E = \sum_i^N x_i \sum_{j \in \mathcal{N}(i)} \kappa_{ij} x_j $$

$E$ is often local: $x_i$ couples only to $x_j$ only in some neighborhood $\mathcal{N}(i)$.

Suggest change $x_i \rightarrow x_i'$. 
Throw a random number $0 < r < 1$. If

$$ r < e^{-\Delta E/T}, $$

then accept the change.
If $\mathcal{N}(i)$ is independent of system size, so is time to update $x_i$. 
Quantum Monte Carlo

Classical Boltzmann weight, an exponential of a number, $E$, becomes the exponential of an operator, $\hat{H}$ which can be expressed as a path integral:

$$e^{-\beta E} \rightarrow e^{-\beta \hat{H}} = e^{-\tau \hat{H}} e^{-\tau \hat{H}} e^{-\tau \hat{H}} \ldots e^{-\tau \hat{H}}$$

Extra “imaginary time” dimension of extent $\beta = 1/T$.

If $\hat{H}$ is local, time is still linear in spatial lattice size.

Cost is only extra dimension of lattice, a factor $\propto 1/T$.

This works for quantum spins and bosons (unfrustrated lattices).
But, “sign problem” for fermions. If electron world lines exchange, the contribution to partition function is negative !!!

(Partial) solution: “Determinant” Quantum Monte Carlo. Still have simulation in space and imaginary time, but algorithm scales as cube of spatial size. Worse: Lingering sign problem.

Peter Reynolds, QMC and sign problem for continuum models, eg nodes of He atom wavefunction [PRL 95, 110201 (2005)].
Determinant Quantum Monte Carlo
Magnetic moment formation with $T$ and $U$

$$\langle m_z^2 \rangle = \langle (n_{j\uparrow} - n_{j\downarrow})^2 \rangle$$
Spin Correlations (8x8 lattice)

\[ \langle c(l) \rangle = \langle (n_{j+l\uparrow} - n_{j+l\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle \]

Local moment \( \langle m_z^2 \rangle \) is just \( c(l = 0) \).
Density of States

![Graph showing Density of States](image)

All of the preceding data at “half-filling” (one electron per lattice site).

This is a density where a special “particle-hole” symmetry of the Hubbard Hamiltonian prevents the sign problem.
$s^*$- and $d$-wave pairing vertices when doped away from half-filling
$\Gamma \to -1$ signals superconductivity.

* $d$-wave is dominant superconducting instability
* But cannot reach low enough $T$ (sign problem)

$N=8 \times 8$ lattice

$\langle S \rangle \to 0$ exponentially with $N, 1/T$
Disordered Superconductors

Bi, Pb, Sn, In$_{1-x}$O$_x$ films
Superconductor-Insulator Transition
Tune with:
  - Film thickness
  - O concentration
  - Magnetic field strength
High disorder/field: metal $dR/dT > 0$
Low disorder/field: superconductor $dR/dT < 0$

Is resistance universal at transition??
Mechanism?

Complex superconducting order parameter $\Delta_j = |\Delta_j|e^{i\phi_j}$

- Magnitude of pairing gap vanishes: $|\Delta_j| \rightarrow 0$.
- Phase fluctuations: $\phi_j$ uncorrelated.

M.P.A. Fisher et al suggest bosonic Hubbard model

Alternately, “attractive” ($-|U|$) fermion Hubbard model

Allows interpolation (with $|U|$) between
- Large $|U|$: Short coherence length/bosons/BEC
- Small $|U|$: Large coherence length/fermions/BCS

Particle-hole mapping between attractive and repulsive fermion Hubbard model

\[
\begin{align*}
c_i \downarrow &\quad (-1)^i c_i \uparrow \\
-t \left( c_j \downarrow c_i \downarrow + c_i \uparrow c_j \downarrow \right) &\quad -t \left( c_j \downarrow c_i \downarrow + c_i \uparrow c_j \downarrow \right) \quad \text{(for bipartite lattice)} \\
U(n_i \uparrow - \frac{1}{2})(n_i \downarrow - \frac{1}{2}) &\quad -U(n_i \uparrow - \frac{1}{2})(n_i \downarrow - \frac{1}{2}) \quad \text{(p-h symmetric)} \\
S_j^+ &\quad = c_j^\uparrow c_j \downarrow \\
\Delta_j^\uparrow &\quad = (-1)^j c_j^\uparrow c_j \downarrow \quad \text{SC correlations} \\
S_j^z &\quad = n_j \uparrow - n_j \downarrow \\
&\quad n_j = n_j \uparrow + n_j \downarrow \quad \text{CDW correlations}
\end{align*}
\]
Site disorder term in Hamiltonian

\[ \sum_i v_i n_i \]
\[ -\frac{V}{2} < v_i < +\frac{V}{2}. \]

(s-wave) pair correlations \( P_s(l) = \langle \Delta_{j+l}\Delta_{j}^\dagger \rangle \) driven to zero.
As are Drude-weight \( D \) and superfluid stiffness \( D_s \).
Resistivity $\rho(T)$ also signals the transition

Value of resistance at separatrices is non-universal?

$\rho$ is difficult to obtain from QMC (real time dynamics).
Application of (non-disordered) attractive Hubbard Model to cuprates.

Cuprates exhibit “spin gap”:
   Preformed Cooper pairs (bosons) exist above $T_c$
   Spin up and down cancel: magnetic susceptibility $\chi$ suppressed

Sharp Fermi surface remains.

---

**Left panel:** $\mu(U,T)$ indicates system is degenerate. $\mu$ is much higher than $T$ from the bottom of the band ($-4t$) including Hartree shift.

$$\mu(T,U) + 4t + \langle n \rangle U/2 > T$$

**Right panel:** Yet spin susceptibility $\chi$ is sharply suppressed.
The bosonic Hubbard model

\[ H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i \hat{n}_i (\hat{n}_i - 1) \]

Again, disordered site energies:

\[ + \sum_i v_i n_i \quad - \frac{V}{2} < v_i < + \frac{V}{2}. \]

Extreme limit of attractive fermion Hubbard model.


or with a confining potential:

\[ + \sum_i v_i n_i \quad v_i = V i^2 \]
Phase diagram: Translationally Invariant Case

Quantum Phase Transition

\[ \kappa = \frac{\partial \rho}{\partial \mu} \to |\mu - \mu_c|^{-\nu/2} \text{ as } \mu \to \mu_c \quad \rho_s \sim |\rho - \rho_{Mott}|^{z-d} \]

System sizes ranging from
\[ L = 16 \text{ to } L = 256 \]
Quantum phase transition!
\[ z = 2, \quad \nu = 1 \]
Turn on disorder
New bose glass phase!
\( \rho_s = 0 \) but no Mott gap (incommensurate density).

Figure 7
G.G. Batrouni and R.T. Scalettar
"World Line Simulations of the Bosonic Hubbard Model in the Ground State"

Figure 10
G.G. Batrouni
"Quantum Monte Carlo on a Lattice: The World Line Algorithm"
One dimensional trapped Boson Hubbard model

No globally incompressible Mott plateau in the trapped system! As a whole, the system is always compressible.

$\rho$ and $\kappa$ profiles: Fixed $N_b = 50$

As $U$ is increased, the system **gradually** crosses over to Mott:

No quantum phase transition.
The trapped one dimensional bosonic Hubbard model does not exhibit quantum critical behavior like the uniform system.
CONCLUSIONS

Hubbard Model provides (quite amazing) insight into qualitative physics of strongly interacting solids

- Metal-Insulator Transitions
- Magnetism
- d-wave Superconductivity
- Charge inhomogeneities

No real solid is precisely represented by the Hubbard model.

In general, you can’t solve the fermion Hubbard model with QMC

- Boson Hubbard model is okay
- Fermion Hubbard model at half-filling is okay
- Fermion Hubbard model with $U < 0$ is okay

Challenge/Opportunity for AMO community

- Provide precise realization of Hubbard Model!
- Solve it!