UCDAVIS

Insulator, Metal, or Superconductor: The Criteria

1. Introduction to Tight-Binding Hamiltonians: Metals and Band Insulators
2. Antiferromagnetic and Charge Density Wave Insulators: Mean Field Theory
3. Anderson and Mott Insulators: Disorder and Interactions
4. Formal Definitions
5. Applications of Formal Theory: Quantum Monte Carlo
6. Conductivity and Spectral Functions

Main goal: Insight via solution in simple limits.

Find me any time to chat/ask questions about the book chapter, etc!
Or contact via email: scalettar@physics.ucdavis.edu.

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1. Introduction to Tight-Binding Hamiltonians: Metals and Band Insulators

$$\hat{H} = -t \sum_{\langle \mathbf{ij} \rangle \sigma} (c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) - \mu \sum_{\mathbf{i}\sigma} (n_{\mathbf{i}\sigma} + n_{\mathbf{i}\sigma})$$

- $c^{\dagger}_{\mathbf{i}\sigma}$ ($c_{\mathbf{i}\sigma}$) are fermion creation(destruction) operators, site $\mathbf{i}$, spin $\sigma = \uparrow, \downarrow$.
- Kinetic energy t describes hopping between near-neighbor sites $\langle \mathbf{ij} \rangle$.
- Chemical potential μ controls filling. ($n_{\mathbf{i}\sigma} = c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma}$ is number operator.)

States labeled by site occupation numbers:

$$|\, n \,\rangle \;\; \rightarrow \;\; |\, n_{\mathbf{1}\uparrow}\, n_{\mathbf{2}\uparrow}\, n_{\mathbf{3}\uparrow} \; \ldots \; n_{\mathbf{1}\downarrow}\, n_{\mathbf{2}\downarrow}\, n_{\mathbf{3}\downarrow} \; \ldots \,\rangle .$$

Operators describe fermions: Anticommutation relations: $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$.

$$\{\hat{c}_{\mathbf{j}\sigma}, \hat{c}^{\dagger}_{\mathbf{l}\sigma'}\} = \delta_{\mathbf{j},\mathbf{l}} \delta_{\sigma,\sigma'} \qquad \{\hat{c}^{\dagger}_{\mathbf{j}\sigma}, \hat{c}^{\dagger}_{\mathbf{l}\sigma'}\} = 0 \qquad \{\hat{c}_{\mathbf{j}\sigma}, \hat{c}_{\mathbf{l}\sigma'}\} = 0.$$

$\hat{c}^{\dagger}_{\mathbf{j}\sigma} |\, 0 \,\rangle = |\, 1 \rangle$

$\hat{c}^{\dagger}_{\mathbf{j}\sigma} |\, 1 \,\rangle = \hat{c}^{\dagger}_{\mathbf{j}\sigma} \hat{c}^{\dagger}_{\mathbf{j}\sigma} |\, 0 \rangle = 0.$

Pauli principle! Maximum occupation of a particular site with a given spin is 1.

Anticommutation $\hat{c}^{\dagger}_{\mathbf{j}\sigma}\, \hat{c}^{\dagger}_{\mathbf{l}\sigma} = -\hat{c}^{\dagger}_{\mathbf{l}\sigma}\, \hat{c}^{\dagger}_{\mathbf{j}\sigma}$ ensures wave function antisymmetry.

Two alternate (but equivalent) solutions at $U = 0$ ("band theory").

One works in real space. The other in momentum space.

Start with the real space analysis (useful for disorder later):

$\hat{H}$ commutes with the total number operators $N_\uparrow = \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow}$ and $N_\downarrow = \sum_{\mathbf{j}} n_{\mathbf{j}\downarrow}$

Commutator of the kinetic energy on 'link' of the lattice with density at vertices:

$$[c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}, n_{\mathbf{i}\sigma} + n_{\mathbf{j}\sigma}] = 0$$

Handy identity: $[AB, C] = A\{B, C\} - \{A, C\}B$.

Hopping contains creation and annihilation operators in pairs.

Implication: eigenstates of $\hat{H}$ come in separate sectors of total $N_\uparrow$ and $N_\downarrow$.

Consider single particle sector where $N_\uparrow = 1$ and $N_\downarrow = 0$.

Occupation number basis: $|1\,0\,0\,0\,0\,0\cdots\rangle$, $|0\,1\,0\,0\,0\,0\cdots\rangle$, $|0\,0\,1\,0\,0\,0\cdots\rangle$, $\cdots$.

Example One: Linear chain. $\hat{H}$ moves occupied site to the left or right:

$$\hat{H}\,|0\,1\,0\,0\,0\,0\cdots\rangle = -\mu\,|0\,1\,0\,0\,0\,0\cdots\rangle - t\,|1\,0\,0\,0\,0\,0\cdots\rangle - t\,|0\,0\,1\,0\,0\,0\cdots\rangle$$

Matrix for $\hat{H}$, use periodic boundary conditions (pbc):

$$H = \begin{pmatrix} -\mu & -t & 0 & 0 & \cdots & 0 & -t \\ -t & -\mu & -t & 0 & \cdots & 0 & 0 \\ 0 & -t & -\mu & -t & \cdots & 0 & 0 \\ 0 & 0 & -t & -\mu & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ -t & 0 & 0 & 0 & \cdots & -t & -\mu \end{pmatrix}$$

Mathematical identity: Eigenvalues of NxN tridiagonal matrix (pbc)

$$\lambda_n = -\mu - 2t\cos k_n \qquad k_n = 2\pi n/N \qquad n = 1, 2, 3, \ldots N.$$

Proof: use *ansatz* $v_l = e^{ikl}$ in eigenvalue equation

$$-\mu\, v_l - t\, v_{l-1} - t\, v_{l+1} = \lambda\, v_l.$$
$$\left(-\mu - t\, e^{-ik} - t\, e^{+ik}\right) e^{ikl} = \lambda\, e^{ikl}.$$

Discretization of k arises from pbc, $v_0 = v_N$ and $v_{N+1} = v_1$.

Eigenvalues of $U = 0$ Hubbard Hamiltonian in one particle sector (1d chain):

$$\text{“Energy band”}: \qquad \epsilon(k) = -2t\cos k$$

Eigenvectors $(\vec{v}_k)_l = e^{ikl}$ are Bloch states $\rightarrow$ metal.

Two particle sector: $N_\uparrow = 2$ and $N_\downarrow = 0$.

$N(N-1)/2$ occupation number basis states:

$|1\,1\,0\,0\,0\,0\cdots\rangle$, $|1\,0\,1\,0\,0\,0\cdots\rangle$, $|1\,0\,0\,1\,0\,0\cdots\rangle$, $\cdots$.

Same construction as $N_\uparrow = 1$: Act with $\hat{H}$ on each state. Get the matrix for $\hat{H}$.

Diagonalizing yields $N(N-1)/2$ eigenvalues and eigenvectors.

Eigenvalues are sums of pairs of the eigenvalues of $N_\uparrow = 1$ matrix

with the Pauli Principle restriction (choose distinct eigenvalues).

Similar result for all sectors $N_\uparrow = 3$, 4, 5, ...

Interactions turn the Hubbard Hamiltonian into a *many body problem.*

Second, treatment of $U = 0$ limit ($d = 1$). Canonical transformation:

$$c^\dagger_{k\sigma} = \frac{1}{\sqrt{N}} \sum_l e^{ikl} c^\dagger_{l\sigma}. \qquad\qquad c^\dagger_{l\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{-ikl} c^\dagger_{k\sigma}.$$

Momentum k discretized: same number of $c^\dagger_{k\sigma}$ as $c^\dagger_{l\sigma}$.

Inverse relation follows from orthogonality identities:

$$\frac{1}{N} \sum_l e^{i(k-p)l} = \delta_{k,p} \qquad\qquad \frac{1}{N} \sum_k e^{ik(l-j)} = \delta_{l,j}$$

These are discrete analog of $\int dk\, e^{ikx} = 2\pi\delta(x)$.

Anticommutation relations preserved (suppress spin indices):

$$\begin{aligned}
\{ c_k, c^\dagger_p \} &= \{ \frac{1}{\sqrt{N}} \sum_l e^{-ikl} c_l \ , \ \frac{1}{\sqrt{N}} \sum_m e^{+ipm} c^\dagger_m \ \} \\
&= \frac{1}{N} \sum_{l,m} e^{-ikl} e^{+ipm} \{ c_l \, , c^\dagger_m \} \\
&= \frac{1}{N} \sum_{l,m} e^{-ikl} e^{+ipm} \delta_{l,m} = \sum_l e^{+i(p-k)m} \delta_{l,m} = \delta_{k,p}
\end{aligned}$$

Transform $d = 1$ noninteracting Hubbard Hamiltonian to momentum space:

$$\begin{aligned}
\hat{H} &= -t \sum_l \left(c_{l+1}^\dagger c_l + c_l^\dagger c_{l+1} \right) \\
&= -t \sum_l \frac{1}{N} \sum_k \sum_p \left(e^{ik(l+1)} e^{-ipl} + e^{ikl} e^{-ip(l+1)} \right) c_k^\dagger c_p \\
&= -t \sum_k \sum_p \frac{1}{N} \sum_l e^{il(k-p)} \left(e^{ik} + e^{-ip} \right) c_k^\dagger c_p \\
&= -t \sum_k \sum_p \delta_{k,p} \left(e^{ik} + e^{-ip} \right) c_k^\dagger c_p \\
&= -t \sum_k \left(e^{ik} + e^{-ik} \right) c_k^\dagger c_k \\
\hat{H} &= \sum \epsilon_k c_k^\dagger c_k = \sum \epsilon_k n_k
\end{aligned}$$

Reproduce energy band $\epsilon_k = -2t \cos k$.

Sum of independent (mutually commuting) number operators.

Evident that single particle levels ϵ_k give solution for all particle sectors.

Example Two: (d=1) Hubbard Hamiltonian with staggered potential,

$$\hat{H} = -t \sum_l \left(c^\dagger_{l+1} c_l + c^\dagger_l c_{l+1} \right) + \Delta \sum_l (-1)^l c^\dagger_l c_l$$

Write $(-1)^l = e^{il\pi}$ and go to momentum space.

$$\Delta \sum_l (-1)^l \, c^\dagger_l c_l = \Delta \frac{1}{N} \sum_l e^{i\pi l} \sum_k e^{-ikl} \, c^\dagger_k \sum_p e^{+ipl} \, c_p = \Delta \sum_k c^\dagger_k c_{k+\pi}$$

$\hat{H}$ not fully diagonalized: momenta k and $k+\pi$ mix.

$$H = \sum_k \begin{pmatrix} c^\dagger_k & c^\dagger_{k+\pi} \end{pmatrix} \begin{pmatrix} -2t\cos k & \Delta \\ \Delta & -2t\cos(k+\pi) \end{pmatrix} \begin{pmatrix} c_k \\ c_{k+\pi} \end{pmatrix}$$

k sum is over the reduced Brillouin zone $-\pi/2 < k < \pi/2$.

Diagonalization of 2x2 matrix yields two bands $E_k = \pm\sqrt{(-2t\cos k)^2 + \Delta^2}$.

Band gap 2Δ opens at reduced Brillouin zone boundaries $k = \pm\pi/2$.

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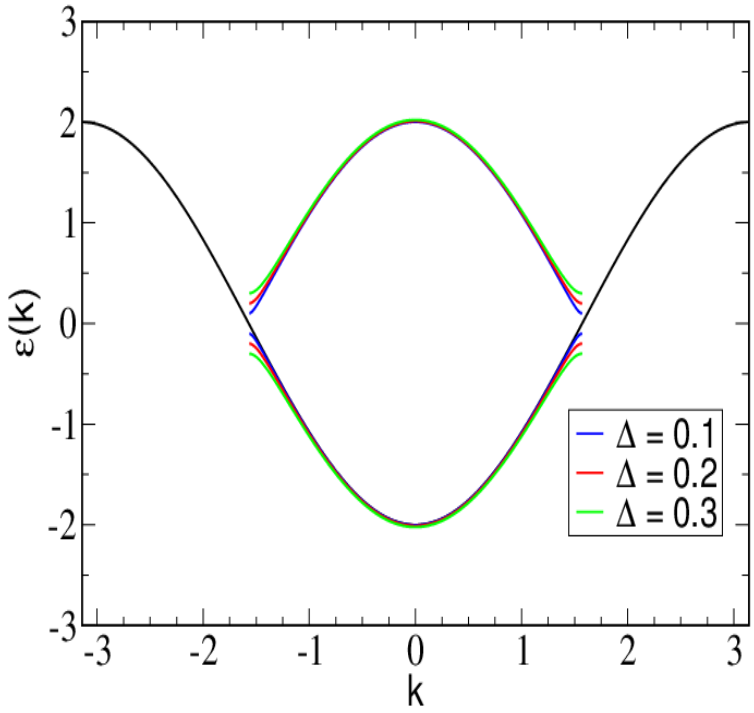

Example of most simple type of Metal-Insulator Transition:

- Fixed $\Delta \neq 0$: Insulator if $-\Delta < \mu < +\Delta$ in gap ($\rho = \frac{1}{2}$). Otherwise Metal.
- At fixed $\rho = \frac{1}{2}$, Insulator if Δ becomes nonzero.

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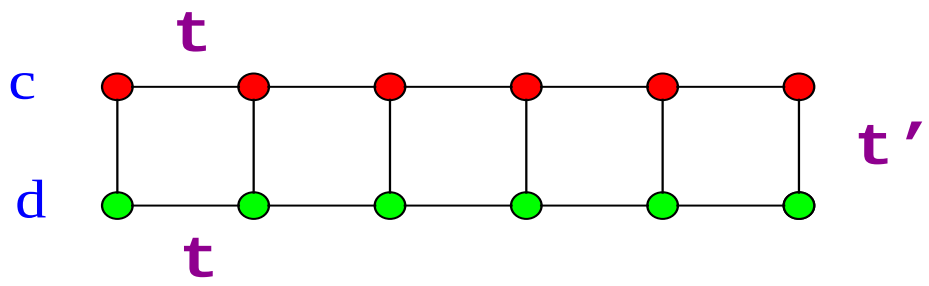

Example Three: Generalize to several orbitals

$$\hat{H} = -t \sum_{\langle \mathbf{j},\mathbf{l} \rangle \, \sigma} (\hat{c}^{\dagger}_{\mathbf{j}\,\sigma} \hat{c}_{\mathbf{l}\,\sigma} + \hat{c}^{\dagger}_{\mathbf{l}\,\sigma} \hat{c}_{\mathbf{j}\,\sigma}) - t \sum_{\langle \mathbf{j},\mathbf{l} \rangle \, \sigma} (\hat{d}^{\dagger}_{\mathbf{j}\,\sigma} \hat{d}_{\mathbf{l}\,\sigma} + \hat{d}^{\dagger}_{\mathbf{l}\,\sigma} \hat{d}_{\mathbf{j}\,\sigma})$$
$$-t' \sum_{\mathbf{j}\,\sigma} (\hat{d}^{\dagger}_{\mathbf{j}\,\sigma} \hat{c}_{\mathbf{j}\,\sigma} + \hat{c}^{\dagger}_{\mathbf{j}\,\sigma} \hat{d}_{\mathbf{j}\,\sigma}) - \mu \sum_{\mathbf{j}} (\hat{n}^{d}_{\mathbf{j}\uparrow} + \hat{n}^{d}_{\mathbf{j}\downarrow} + \hat{n}^{c}_{\mathbf{j}\uparrow} + \hat{n}^{c}_{\mathbf{j}\downarrow}) \; .$$

$\hat{c}^{\dagger}$ and $\hat{d}^{\dagger}$ fermions hop between near-neighbor sites (t).

Inter-orbital hybridization t' converts $\hat{c}^{\dagger}_{\mathbf{j}} \leftrightarrow \hat{d}^{\dagger}_{\mathbf{j}}$ on the same site $\mathbf{j}$.

Momentum space:

$$\hat{H} = \sum_{\mathbf{k}\,\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\,\sigma} \hat{c}_{\mathbf{k}\,\sigma} + \sum_{\mathbf{k}\,\sigma} \epsilon_{\mathbf{k}} \hat{d}^{\dagger}_{\mathbf{k}\,\sigma} \hat{d}_{\mathbf{k}\,\sigma} + t' \sum_{\mathbf{k}\,\sigma} (\hat{d}^{\dagger}_{\mathbf{k}\,\sigma} \hat{c}_{\mathbf{k}\,\sigma} + \hat{c}^{\dagger}_{\mathbf{k}\,\sigma} \hat{d}_{\mathbf{k}\,\sigma})$$
$$= \sum_{k} \begin{pmatrix} c^{\dagger}_{\mathbf{k}} & d^{\dagger}_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} & t' \\ t' & \epsilon_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}} \\ d_{\mathbf{k}} \end{pmatrix} \; .$$

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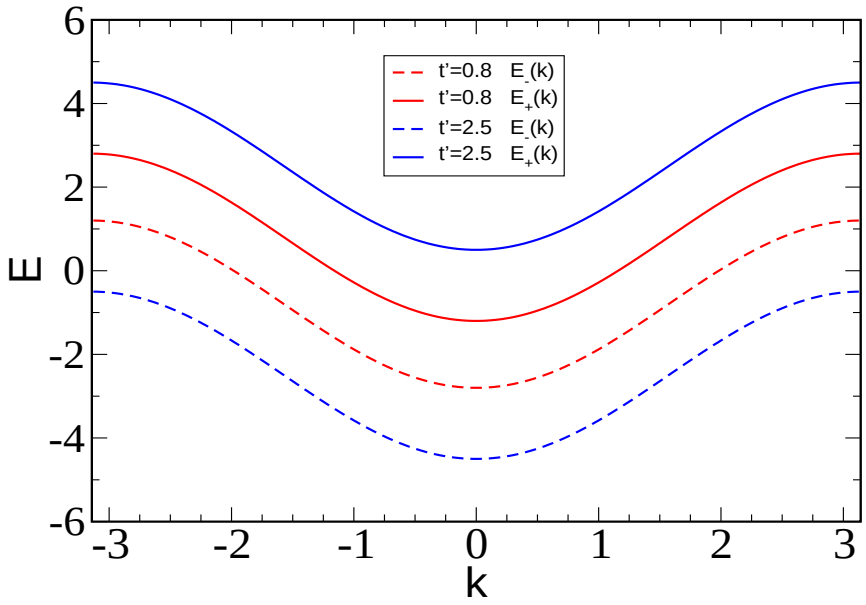


t' just rigidly shifts bands up and down.

The final 2x2 rotation yields the energy levels,

$$E_{\mathbf{k}}^{\pm} = -2t\cos k \pm t' \ .$$

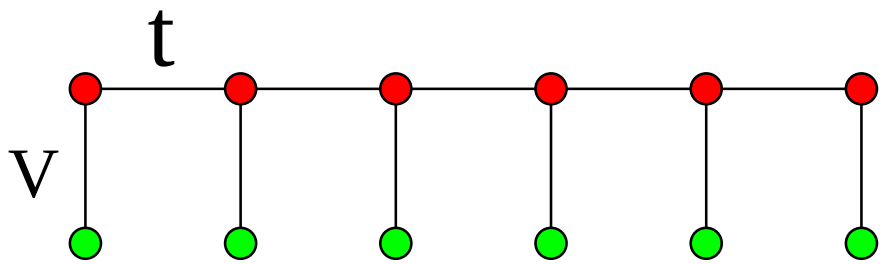
Staggered potential $\Delta(-1)^{\mathrm{j}}$: band gap opens for *any* nonzero Δ.

Here: bands overlap for $t' < 4\,t$ and the system is metallic.

Insulating at $\rho = 1$ if $t' > 4\,t$ (at half-filling).

Also describes 'bilayer' geometries: $c^{\dagger}$ and $d^{\dagger}$ label two distinct spatial layers.

Application of uniaxial strain or pressure to tune t'.



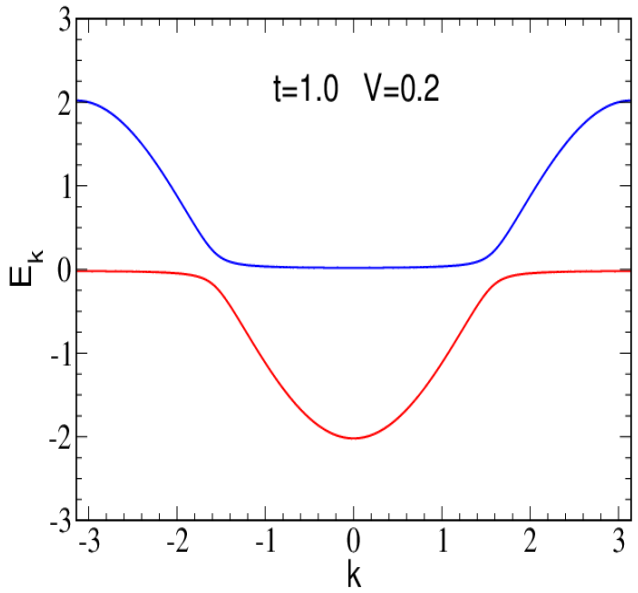
Example Four: Periodic Anderson Model (PAM). One orbital is 'localized'.

No hopping t on d orbitals.

$$H = -t \sum_{\langle \mathbf{j},\mathbf{l} \rangle \sigma} (c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{l}\sigma} + c^{\dagger}_{\mathbf{l}\sigma} c_{\mathbf{j}\sigma}) + V \sum_{\langle \mathbf{j},\mathbf{l} \rangle \sigma} (c^{\dagger}_{\mathbf{j}\sigma} d_{\mathbf{l}\sigma} + d^{\dagger}_{\mathbf{l}\sigma} c_{\mathbf{j}\sigma})$$

Momentum space

$$H = \sum_{k} \begin{pmatrix} c^{\dagger}_{k} & d^{\dagger}_{k} \end{pmatrix} \begin{pmatrix} -2t \cos k & V \\ V & 0 \end{pmatrix} \begin{pmatrix} c_{k} \\ d_{k} \end{pmatrix}$$



Final diagonalization

$$E_k = \tfrac{1}{2}\left(\epsilon_k \pm \sqrt{\epsilon_k^2 + 4V^2}\right)$$

'Hybridization gap'. Dispersionless d repels c band at $k = \pm\pi/2$ crossing.

Summary of these examples:

Simplest (single particle) type of metal-insulator transition:

- Noninteracting fermions on a translationally invariant lattice.
- placement of the chemical potential:

  Within a band: metal

  In gap between bands: insulator.

2. Antiferromagnetic and Charge Density Wave Insulators: Mean Field Theory

Within Mean Field Theory (MFT), insulating behavior arising from interactions and a nonzero order parameter has a very similar mathematical structure!

Hubbard Hamiltonian

$$\hat{H} = -t \sum_{\langle \mathbf{j},\mathbf{l} \rangle \, \sigma} (\hat{c}^{\dagger}_{\mathbf{j}\,\sigma} \hat{c}_{\mathbf{l}\,\sigma} + \hat{c}^{\dagger}_{\mathbf{l}\,\sigma} \hat{c}_{\mathbf{j}\,\sigma}) - \mu \sum_{\mathbf{j}} (\hat{n}_{\mathbf{j}\uparrow} + \hat{n}_{\mathbf{j}\downarrow}) + U \sum_{\mathbf{j}} \hat{n}_{\mathbf{j}\uparrow} \hat{n}_{\mathbf{j}\downarrow} \; .$$

U is an on-site repulsive interaction.

This is a many-body problem (quartic in fermionic operators)

$$U \sum_{\mathbf{j}} \hat{n}_{\mathbf{j}\uparrow} \hat{n}_{\mathbf{j}\downarrow} = U \sum_{\mathbf{j}} c^{\dagger}_{\mathbf{j}\uparrow} c_{\mathbf{j}\uparrow} c^{\dagger}_{\mathbf{j}\downarrow} c_{\mathbf{j}\downarrow}$$

MFT: recast the interaction term so that it is quadratic

$$U \sum_{\mathbf{j}} \left(\hat{n}_{\mathbf{j}\uparrow} \langle \hat{n}_{\mathbf{j}\downarrow} \rangle + \hat{n}_{\mathbf{j}\uparrow} \langle \hat{n}_{\mathbf{j}\downarrow} \rangle - \langle \hat{n}_{\mathbf{j}\uparrow} \rangle \langle \hat{n}_{\mathbf{j}\downarrow} \rangle \right) \; .$$

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$$U \sum_{\mathbf{j}} \left(\hat{n}_{\mathbf{j}\uparrow} \langle \hat{n}_{\mathbf{j}\downarrow} \rangle + \hat{n}_{\mathbf{j}\uparrow} \langle \hat{n}_{\mathbf{j}\downarrow} \rangle - \langle \hat{n}_{\mathbf{j}\uparrow} \rangle \langle \hat{n}_{\mathbf{j}\downarrow} \rangle \right) .$$

An antiferromagnetic (AF) pattern of the fermionic occupations $\langle n_{\mathbf{j}\sigma} \rangle$

$$\langle \hat{n}_{\mathbf{j}\uparrow} \rangle = \rho + (-1)^{\mathbf{j}} m \;\rightarrow\; \left(\rho + (-1)^{\mathbf{j}} m \right) n_{\mathbf{j}\downarrow}$$
$$\langle \hat{n}_{\mathbf{j}\downarrow} \rangle = \rho - (-1)^{\mathbf{j}} m \;\rightarrow\; \left(\rho - (-1)^{\mathbf{j}} m \right) n_{\mathbf{j}\uparrow}$$

looks just like a staggered potential to the opposite spin species $n_{\mathbf{j}-\sigma}$.

m is antiferromagnetic order parameter.

A 'spin density wave' (SDW) opens a band gap and 'Slater' insulator.

Require self-consistent solution. Patterns $\langle \hat{n}_{\mathbf{j}\uparrow} \rangle$, $\langle \hat{n}_{\mathbf{j}\downarrow} \rangle \rightarrow$ energy bands.

What value of m minimizes free energy for these bands?

Optimal m depends on lattice geometry (noninteracting bands); U, T, and ρ.

Generate MFT phase diagram (metallic/insulator regions).

Similar CDW insulators arise when fermions interact with local phonon modes .

Added feature is competition with energy cost to stretch bonds.

3. Anderson and Mott Insulators: Disorder and Interactions

Anderson insulators arising from disorder.

Mott insulators arising from strong repulsive interactions treated outside of MFT.

$d = 1$ hopping Hamiltonian again, with random chemical potentials μ_j:

$$\hat{H} = -t \sum_{j,\sigma} \left(\hat{c}^{\dagger}_{j\,\sigma} \hat{c}_{j+1\,\sigma} + \hat{c}^{\dagger}_{j+1\,\sigma} \hat{c}_{j\,\sigma} \right) - \sum_{j,\sigma} \mu_j \left(n_{j\uparrow} + n_{j\downarrow} \right) \ .$$

Numerically diagonalize real space $\hat{H}$.

$$H = \begin{pmatrix} -\mu_1 & -t & 0 & 0 & \cdots & 0 & -t \\ -t & -\mu_2 & -t & 0 & \cdots & 0 & 0 \\ 0 & -t & -\mu_3 & -t & \cdots & 0 & 0 \\ 0 & 0 & -t & -\mu_4 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ -t & 0 & 0 & 0 & \cdots & -t & -\mu_N \end{pmatrix}$$

Translation invariance broken by impurities. $-\Delta < \mu_j < +\Delta$

Can no longer label the eigenvalues with a momentum index k.

Resulting localized eigenvectors are not extended Bloch states.

'Anderson Insulator': localized states do not conduct.

In one dimension, all eigenstates localized, for any amplitude of disorder.

Also true in two dimensions, although just barely.

In three dimensions:

- Eigenfunctions with largest and smallest eigenvalues: localized.
- Eigenfunctions near center of spectrum: extended.
- Energy separating these two behaviors: mobility edge E_*.

Anderson metal-insulator transitions:

- $\mu < E_*$: only localized eigenfunctions are occupied $\rightarrow$ insulator.
- $\mu > E_*$: extended states become occupied $\rightarrow$ metal.

In contrast to band, SDW, and CDW insulators, no gap in spectrum.

Most powerful approach actually not diagonalization, but transfer matrix.

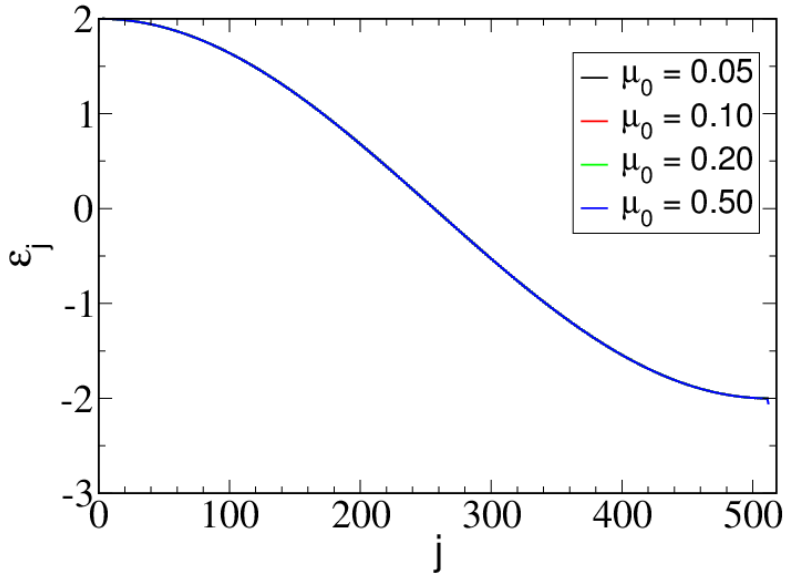
Fairly opaque: physics hidden in diagonalizing random matrix.

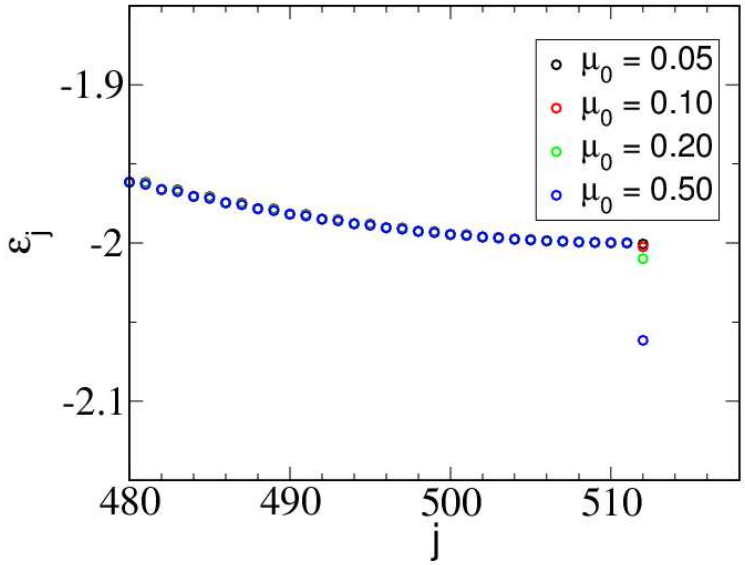
Can develop insight from numeric and analytic solution to single defect problem.

Diagonalize matrix with $\mu_0 \neq 0$ on just one site j_0.

Most eigenvalues continue to look like $-2t\cos k$.

However, one extremal eigenvalue split off from all the others.

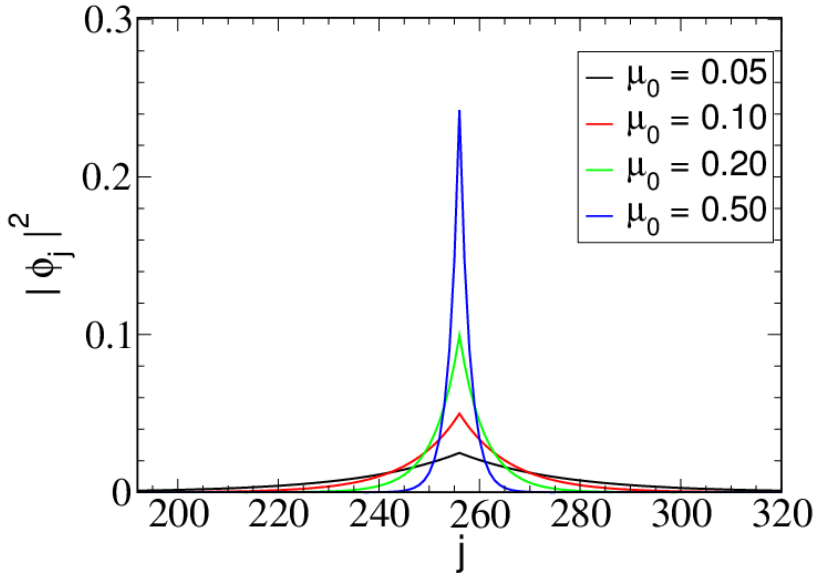




How do we know the associated eigenvector is localized?

Squares of amplitudes of components $\left|\phi_j\right|^2$ are sharply peaked at j_0.

$N = 512$ site chain with defect at $j_0 = 256$.



Formal similarity to localization of vibrations in harmonic chain with defect mass.

Small number of impurities can also be treated analytically.

Single particle eigenstates ϕ and eigenenergies E, in the absence of an impurity:

$$\sum_n L_{mn}\,\phi_n = 0 \qquad\qquad L_{mn} = E\,\delta_{mn} - t\,\delta_{m,n-1} - t\,\delta_{m,n+1}\ ,$$

Nontrivial solution requires $|\,L\,| = 0$.

In the presence of randomness,

$$\sum_n L_{mn}\,\phi_n = \sum_k \delta L_{mk}\,\phi_k \qquad \rightarrow \qquad \big(\,I - G\,\delta L\big)\,\phi = 0\ ,$$

δL is matrix containing local chemical potentials; $G = L^{-1}$. "Solution" is,

$$\phi_n = \sum_{lk} G_{nl}\,\delta L_{lk}\,\phi_k\ .$$

However unknown variables ϕ_n appear on both sides!

Sparsity of δL enormously simplifies the linear algebra problem $|\,I - G\,\delta L\,| = 0$.

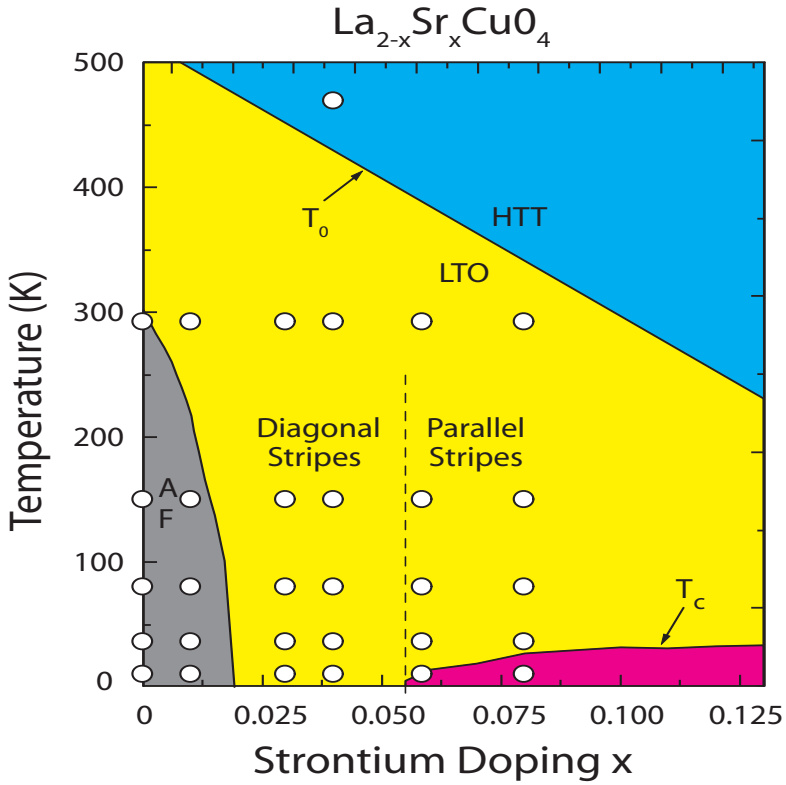
Instead of rank N (number of sites), $I - G\,\delta\,L$ has rank n (number of defects).

Furthermore, we have an explicit expression $G_{nl} = \sum_k e^{ik(n-l)}/E_k$.

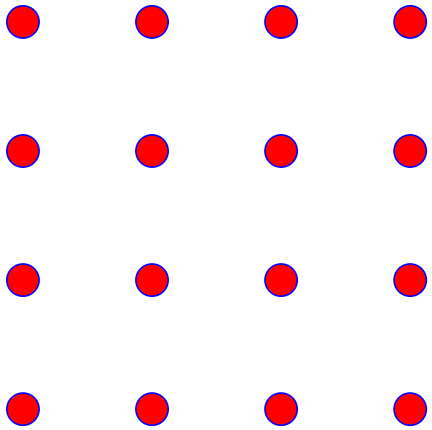
Hubbard-Mott Insulator is the most subtle by far.

Describes qualitative "strong correlation" physics of many-electron materials

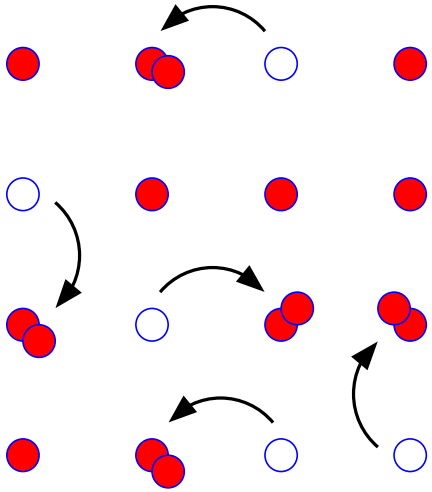
- Transition metal monoxides, cuprate superconductors, ...
- On-site repulsion U sufficiently large $\rightarrow$ Mott Insulator
- Exchange interaction $J \propto t^2/U \rightarrow$ Antiferromagnetism
- Stripes and other charge/spin inhomogeneities.
- d-wave superconductivity ???



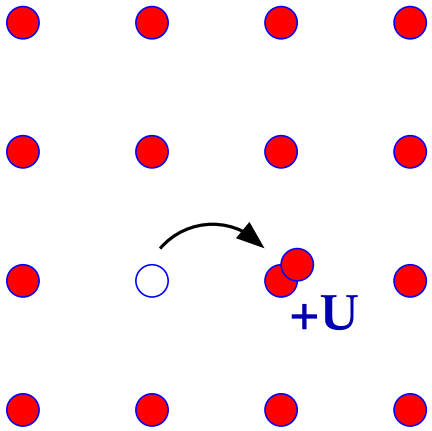
Mott Insulators and Antiferromagnetism: Qualitative Pictures



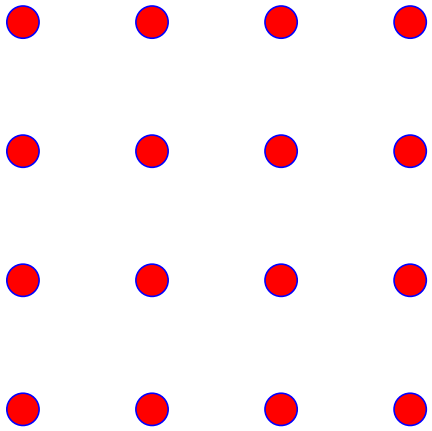
Consider a lattice of sites with
"commensurate filling":
The average number of electrons
is one per site.



"quantum fluctuations" (kinetic energy t)
and thermal fluctuations T, both favor
electrons moving around lattice.
Metal: odd number (one) particle per cell/site.



But what if there were a large repulsive interaction U between electrons on the same site?



A Mott Insulator forms.
Basic physics of parent compounds of cuprate superconductors!

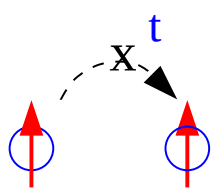
Two ways to destroy Mott Insulator:

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

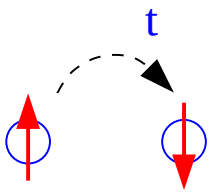
What is optimal spin arrangement?

Hopping of neighboring parallel spins forbidden by Pauli.

Antiparallel arrangement lower in second order perturbation theory.



$\Delta E^{(2)} = 0$

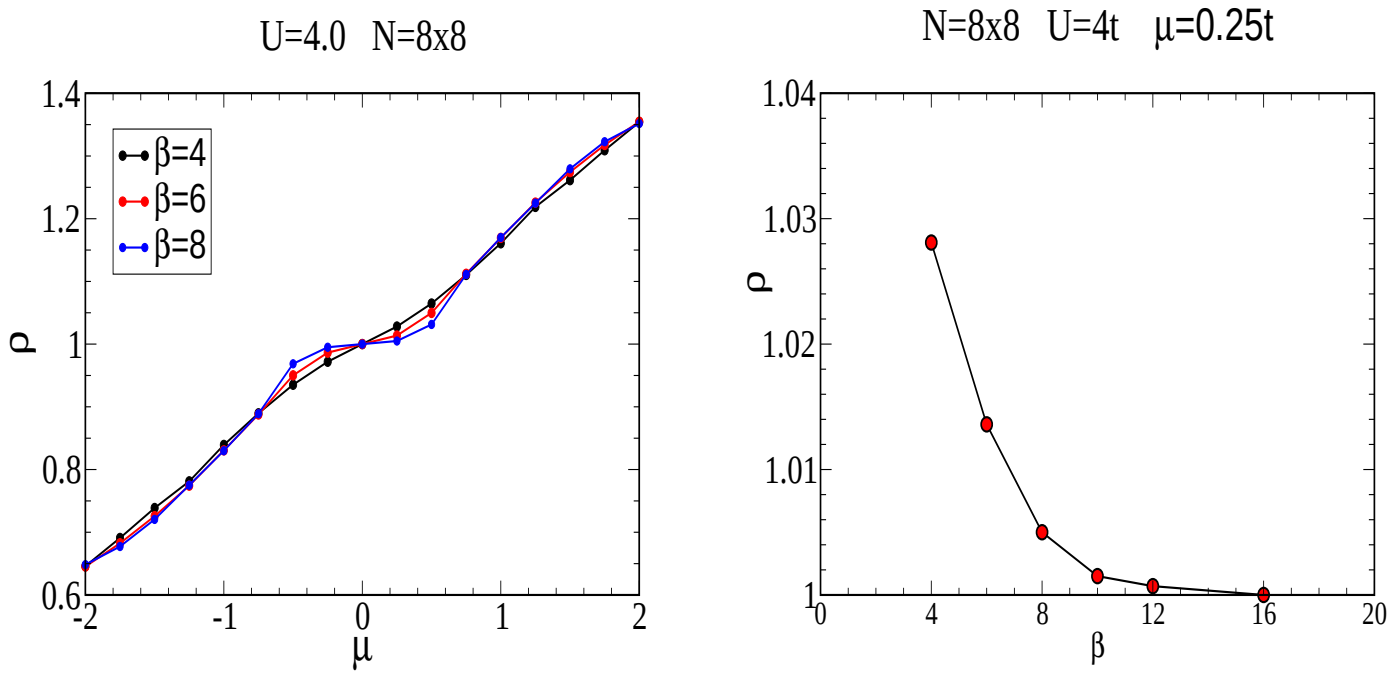


$\Delta E^{(2)} \propto -t^2/U = -J$

Mott insulating behavior and antiferromagnetism go hand-in-hand.
Qualitative picture of cuprate physics before doping.

Still do not fully understand why cuprates superconduct after doping.

Quantum simulation results for the square lattice Hubbard Hamiltonian at $U = 4t$. $\rho(\mu)$ develops a plateau at half-filling signalling Mott insulator has formed.



In many situations Slater insulator forming at small U due to the opening of an AF gap, merges smoothly, as U increases, into Mott insulator.

4. Metals, Insulators, and Superconductors: Formal Definitions

The most natural quantity to distinguish metals and insulators: conductivity σ.

Require response of current to vector potential $A_x(\mathbf{l})$. Modifies hopping,

$$c^\dagger_{\mathbf{l}+x} c_{\mathbf{l}} + c^\dagger_{\mathbf{l}} c_{\mathbf{l}+x} \to e^{ieA_x(\mathbf{l})} c^\dagger_{\mathbf{l}+x} c_{\mathbf{l}} + e^{-ieA_x(\mathbf{l})} c^\dagger_{\mathbf{l}} c_{\mathbf{l}+x} \ .$$

Expand in powers of A.

$$K_A = K - \sum_{\mathbf{l}} \left(e j^p_x(\mathbf{l}) A_x(\mathbf{l}) + \frac{e^2 k_x(\mathbf{l})}{2} A_x(\mathbf{l})^2 \right)$$

$$j^p_x(\mathbf{l}) = it \sum_\sigma \left(c^\dagger_{\mathbf{l}+x\,\sigma} c_{\mathbf{l}\,\sigma} - c^\dagger_{\mathbf{l}\,\sigma} c_{\mathbf{l}+x\,\sigma} \right) \qquad \text{paramagnetic current density}$$

$$k_x(\mathbf{l}) = -t \sum_\sigma \left(c^\dagger_{\mathbf{l}+x\,\sigma} c_{\mathbf{l}\,\sigma} + c^\dagger_{\mathbf{l}\,\sigma} c_{\mathbf{l}+x\,\sigma} \right) \qquad \text{kinetic energy density} \ .$$

Differentiating with respect to $A_x(\mathbf{l})$ yields the total current density,

$$j_x(\mathbf{l}) = -\frac{\delta K}{\delta A_x(\mathbf{l})} = e\, j^p_x(\mathbf{l}) + e^2\, k_x(\mathbf{l})\, A_x(\mathbf{l})$$

Plane wave form for the vector potential,

$$A_x(\mathbf{l},t) = \mathrm{Re}\big(A_x(\mathbf{q},\omega)\, e^{i\mathbf{q}\cdot\mathbf{l}-i\omega t}\big) \ ,$$

results in current,

$$\langle j_x(\mathbf{l},t)\rangle = \mathrm{Re}\big(\langle\, j_x(\mathbf{q},\omega)\rangle\, e^{i\mathbf{q}\cdot\mathbf{l}-i\omega t}\big)$$
$$\langle\, j_x(\mathbf{q},\omega)\rangle = -e^2\Big(\langle k_x\rangle - \Lambda_{xx}(\mathbf{q},\omega)\Big)A_x(\mathbf{q},\omega) \ .$$

Matsubara frequencies $i\omega_m = 2\pi m T$, current-current correlation function

$$\Lambda_{xx}(\mathbf{q},i\omega_m) = \frac{1}{N}\int_0^\beta d\tau e^{i\omega_m\tau}\langle j_x^p(\mathbf{q},\tau) j_x^p(-\mathbf{q},0)\rangle \ ,$$

Analogous to response of magnetization M to an applied Zeeman field.

Susceptibility expressed as magnetization-magnetization correlation function.

$$\chi = \frac{d\langle M\rangle}{dB} = \beta\langle M^2\rangle$$

Final step: Connect Λ to Drude weight D and superfluid density D_s.

Superfluid density determines magnetic field penetration into superconductor.

London's observation:

Meissner effect follows if current density is proportional to the vector potential,

$$j_x(q_y) = -\frac{1}{4\pi}\,\frac{1}{\lambda^2}\,A_x(q_y)\ .$$

Magnetic fields expelled from superconductor beyond penetration depth λ,

$$\frac{1}{\lambda^2} = \frac{4\pi n_s e^2}{mc^2}\ ,$$

which depends on the superfluid density n_s.

Link superfluid weight $D_s = n_s/m$ and current-current correlation function:

$$\frac{D_s}{\pi e^2} = -\langle\, -k_x\,\rangle - \Lambda_{xx}(q_x = 0, q_y \to 0, i\omega_m = 0)\ .$$

Relation between vector potential and electric field, $E_x = -\partial A_x/\partial t$, and between conductivity and electric field yields analogous formula for the Drude weight, the delta function contribution $D\delta(\omega)$ to the conductivity,

$$\frac{D}{\pi e^2} = -\langle\, -k_x \,\rangle - \Lambda_{xx}(q_x = 0, q_y = 0, i\omega_m \to 0) \ .$$

Third limit, longitudinal momentum taken to zero, relates Λ to kinetic energy,

$$\langle\, -k_x \,\rangle = \Lambda_{xx}(q_x \to 0, q_y = 0, i\omega_m = 0) \ .$$

Summary: Depending on the limits in which the momenta and frequency are taken to zero, one can obtain the superfluid density D_s and Drude weight D from the current-current correlation function. Then:

- Insulator: $D = D_s = 0.$
- Metal: $D \neq 0 \quad D_s = 0.$
- Superconductor: $D_s \neq 0.$

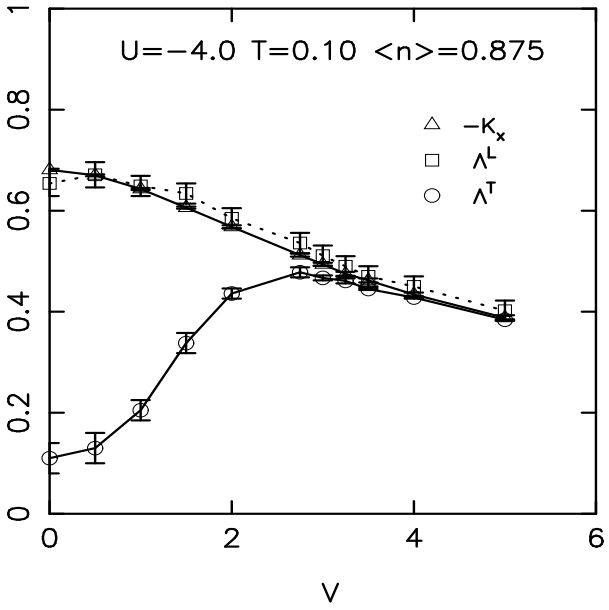
Alternate limits of approaching zero momentum and frequency yield distinct results and profoundly different physical quantities.

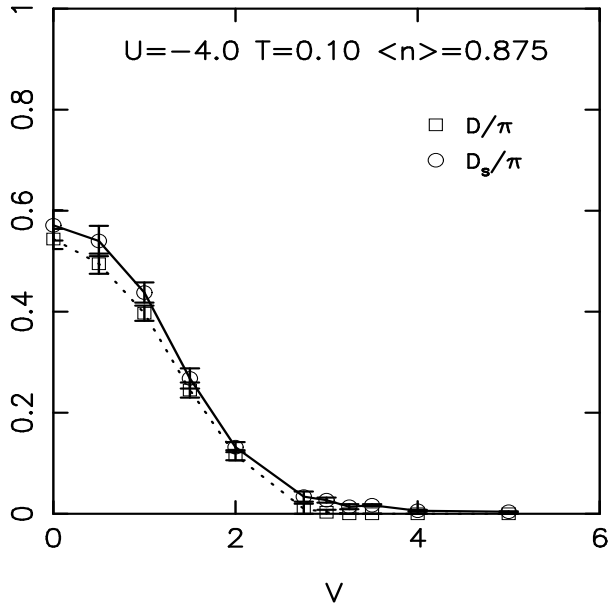
5. Applications of Formal Theory: Quantum Monte Carlo

Can explicitly evaluate Λ and its different limits with Quantum Monte Carlo.

Attractive Hubbard model with disorder of magnitude V. Basic physics:

- If $U < 0$ fermions form pairs which can then condense to a superfluid.
- This superfluid can be destroyed by randomness, which localizes the pairs.





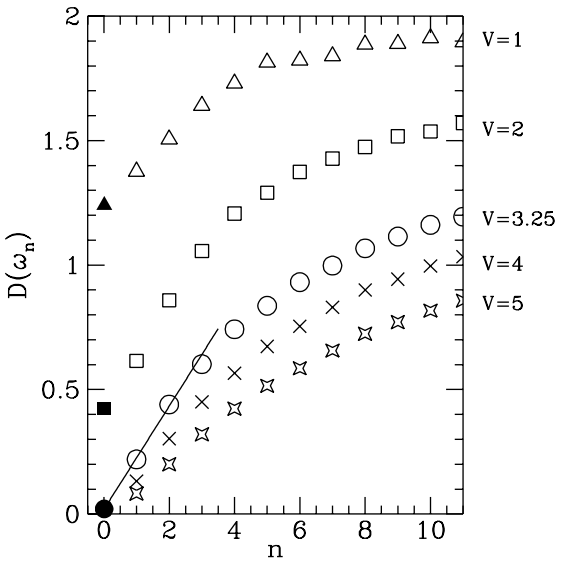
$$\Lambda^{\rm L} \equiv \lim_{q_x \to 0} \Lambda_{xx}(q_x, q_y = 0; i\omega_n = 0) \qquad D_s = \pi[-K_x - \Lambda^T]$$

$$\Lambda^T \equiv \lim_{q_y \to 0} \quad \Lambda_{xx}(q_x = 0, q_y; i\omega_n = 0) \qquad K_x = -\Lambda^L$$

Critical value V_c beyond which $D = D_s = 0$ and the system becomes insulating.

Extrapolation in Matsubara frequencies captures Drude weight, D.

$$D(\omega_m) = \pi\big(\, - K_x - \Lambda_{xx}(q_x = 0, q_y = 0, i\omega_m \, \big)$$



D vanishes at a value consistent with V_c for vanishing of D_s.

Suggests direct superconductor-insulator transition; no intervening metallic phase.

Similar plots showing the momentum extrapolations to verify $\Lambda^L = -\langle \, K_x \, \rangle$.

6. Conductivity and Spectral Functions

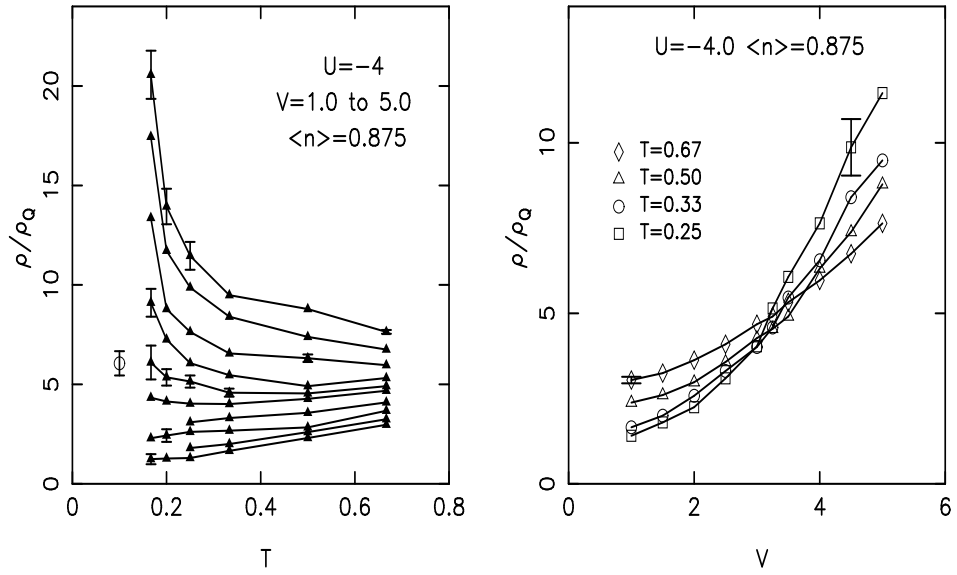
An alternate analysis of conductivity begins with fluctuation-dissipation theorem,

$$\Lambda_{xx}(\mathbf{q},\tau) = \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} \frac{\exp(-\omega\tau)}{1-\exp(-\beta\omega)} \operatorname{Im}\Lambda_{xx}(\mathbf{q},\omega) \ .$$

Inversion of Laplace transform to get $\operatorname{Im}\Lambda_{xx}$, is very ill-conditioned.

If $T << \Omega$, the scale at which ImΛ deviates from Im$\Lambda \sim \omega\,\sigma_{dc}$,

$$\sigma_{\rm dc} = \frac{\beta^2}{\pi}\Lambda_{xx}(\mathbf{q}=0,\tau=\beta/2) \ ,$$



Onset of nonzero D_s:

$$3 \lesssim V_c \lesssim 4.$$

Crossings of ρ_{dc}:

$$V_c \sim 3.5.$$

Analysis of D:

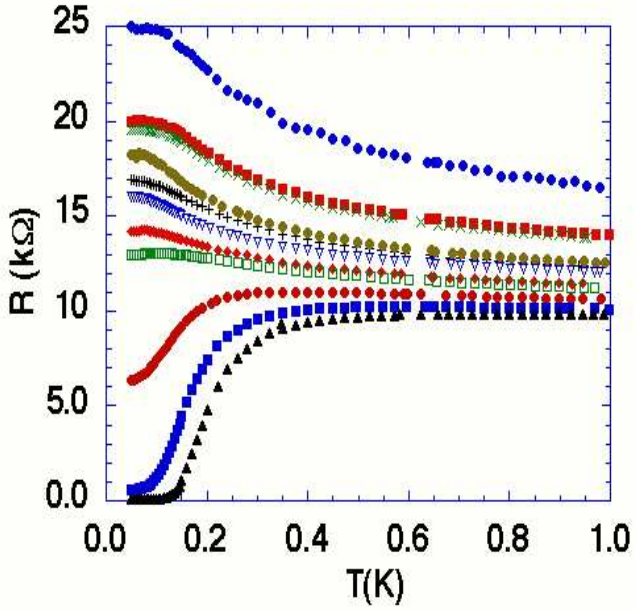
$$V_c \sim 3.25.$$

Data from QMC simulations remarkably similar to experimental literature.

2D superconductor-insulator transition (SIT) in the presence of disorder.

Means to access SIT:

- Changing the degree of microscopic disorder.
- Altering the film thickness.
- Applying a magnetic field
- Changing the carrier density.

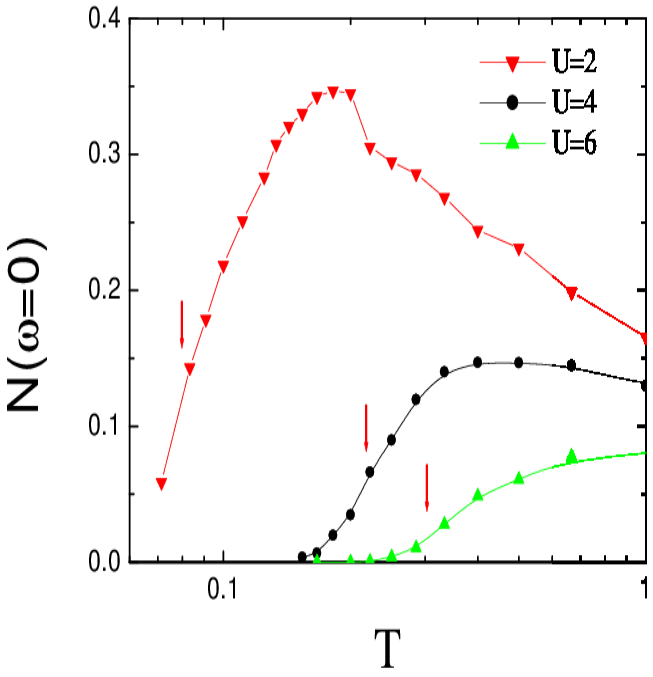


Carrier density tuned SIT in Bi, Pb, Sn, $In_{1-x}O_x$ films.

Distinguishing metals and insulators via momentum-resolved spectral function

$$G(\mathbf{q},\tau) = \int_{-\infty}^{+\infty} d\omega \frac{\exp(-\omega\tau)}{1+\exp(-\beta\omega)} A(\mathbf{q},\omega) \qquad N(\omega) = \sum_{\mathbf{q}} A(\mathbf{q},\omega) \ .$$

Square lattice Hubbard Hamiltonian at half-filling:



$N(\omega = 0) \to 0$ as $T \to 0$

- Small U: Slater insulator driven by SDW order
- Intermediate U crossover to Mott insulator.

Size of insulating gap $\propto$ temperature range over which $N(\omega = 0) = 0$.

Momentum resolution: Track peak in $A(\mathbf{q},\omega)$ to infer dispersion of dressed quasiparticle excitations.

7. Summary

[1] Non-interacting or MFT (quadratic) tight binding Hamiltonians.

Metal to Band Insulator:

Compute single particle energy levels.

Position of chemical potential relaive to gap.

Anderson Insulator:

Driven by disorder; localized eigenstates

Position of chemical potential relative to mobility edge.

[2] Interacting (quartic) tight binding Hamiltonians.

Mott Insulator

Large interactions restrict motion of fermions.

(Very) difficult to solve. Numerics: QMC, DMRG, DMFT

[3] Formal Criteria for Insulator, Metal, Superconductor

Limits of current-current correlation function.