Quick and Dirty Introduction to Mott Insulators

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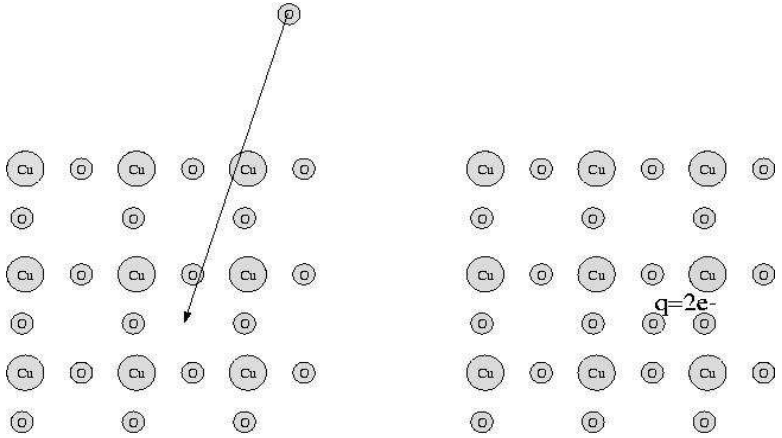
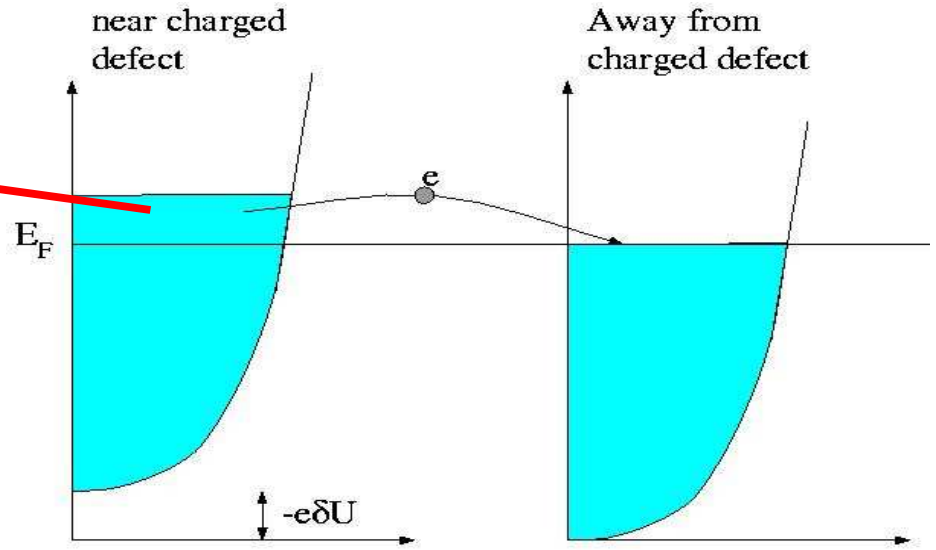
PHYS 624: Introduction to Solid State Physics
http://www.physics.udel.edu/~bnikolic/teaching/phys624/phys624.html

Weakly correlated electron liquid: Coulomb interaction effects



When local perturbation $\delta U(\mathbf{r})$ potential is switched on, some electrons will leave this region in order to ensure constant $\varepsilon_F \simeq \mu$ (chemical potential is a thermodynamic potential; therefore, in equilibrium it must be homogeneous throughout the crystal).

$$\delta n(\mathbf{r}) = eD(\varepsilon_F)\delta U(\mathbf{r})$$



$$\text{assume:} \left| e\delta U(\mathbf{r}) \right| \ll \varepsilon_F$$

$$f(\varepsilon, T \to 0) = \theta(\varepsilon_F - \varepsilon)$$

Thomas -Fermi Screening

- Except in the immediate vicinity of the perturbation charge, assume that $\delta U(\mathbf{r})$ is caused by the induced space charge → Poisson equation: $\nabla^2 \delta U(\mathbf{r}) = -\frac{e\delta n(\mathbf{r})}{\varepsilon_0}$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \Rightarrow \delta U(\mathbf{r}) = \frac{\alpha e^{-r/r_{TF}}}{r}$$

$$r_{TF} = \sqrt{\frac{\varepsilon_0}{e^2 D(\varepsilon_F)}}$$

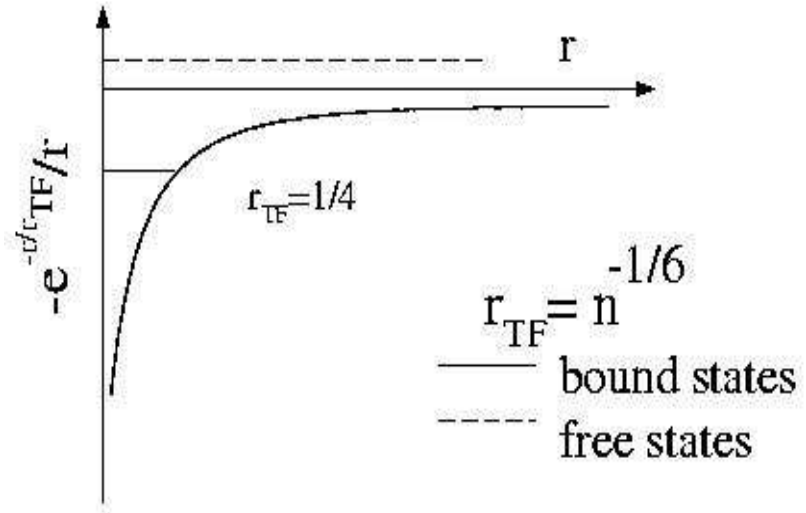
$$r_{TF} \simeq \frac{1}{2}\left(\frac{n}{a_0^3}\right)^{-1/6}, \; a_0 = \frac{4\pi\hbar^2\varepsilon_0}{me^2}$$

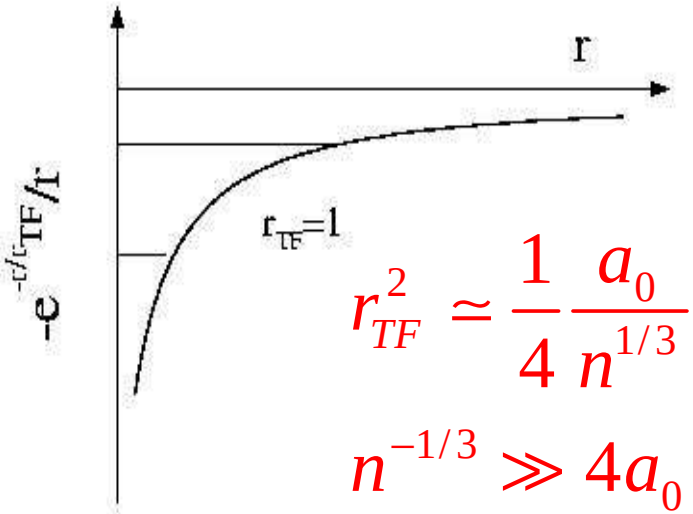
$$n_{Cu} = 8.5\cdot 10^{23} cm^{-3}, \; r_{TF}^{Cu} = 0.55\text{Å}$$

in vacuum: $D(\varepsilon_F) = 0, \; \delta U(\mathbf{r}) = \frac{q}{4\pi\varepsilon_0} = \alpha$

$$D(\varepsilon_F) = \frac{3}{2}\frac{n}{\varepsilon_F} = \frac{1}{2\pi^2}\frac{2m}{\hbar^2}\left(3\pi^2 n\right)^{2/3}, \; \varepsilon_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} \Rightarrow r_{TF}^{-2} = \frac{4}{\pi}\left(3\pi^2\right)^{1/3}\frac{n^{1/3}}{a_0}$$

Mott Metal-Insulator Transition





$$r_{TF}^2 \simeq \frac{1}{4}\frac{a_0}{n^{1/3}} \gg a_0^2$$

$$n^{-1/3} \gg 4a_0$$

- Below the critical electron concentration, the potential well of the screened field extends far enough for a bound state to be formed → screening length increases so that free electrons become localized → Mott Insulators
- Examples: **transition metal oxides, glasses, amorphous semiconductors**

Metal vs. Insulator: Theory

$$\text{Ohm law}: j_\alpha(\mathbf{q},\omega) = \sum_\beta \sigma_{\alpha\beta}(\mathbf{q},\omega) E_\beta(\mathbf{q},\omega)$$

❑**Theoretical Definition of a Metal:**

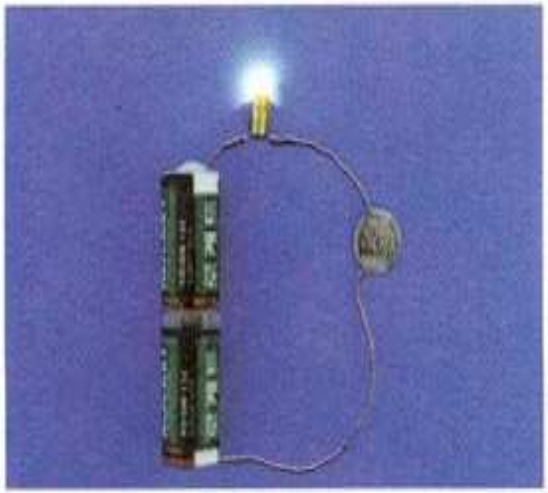
$$\mathrm{Re}\left[\sigma_{\alpha\beta}(T=0,\omega\to 0)\right] = \left(D_c\right)_{\alpha\beta} \frac{\tau}{\pi(1+\omega^2\tau^2)}$$

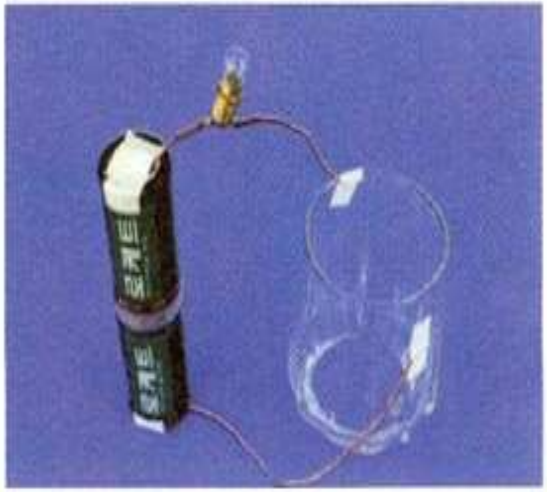
$$\text{Drude: } \left(D_c\right)_{\alpha\beta} = \frac{\pi n e^2}{m^*}\delta_{\alpha\beta}, \quad \mathrm{Re}\left[\sigma_{\alpha\beta}(T=0,\omega\to 0,\tau^{-1}\to 0)\right] = \left(D_c\right)_{\alpha\beta}\delta(\omega)$$

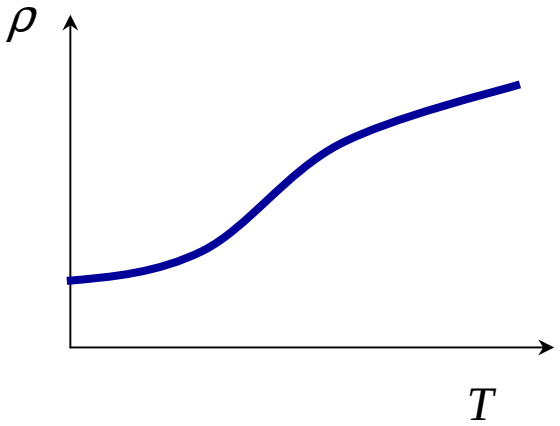
❑**Theoretical Definition of an Insulator:**

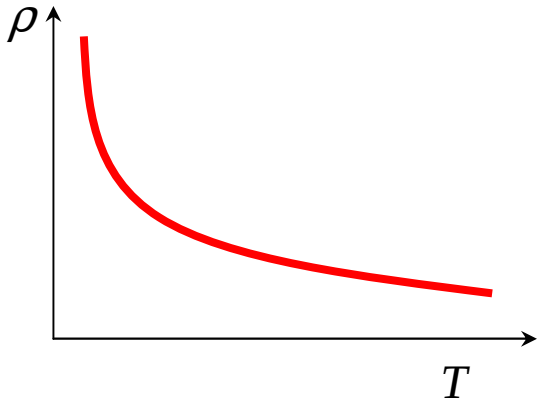
$$\lim_{T\to 0}\lim_{\omega\to 0}\lim_{|\mathbf{q}|\to 0} \mathrm{Re}\left[\sigma_{\alpha\beta}(\mathbf{q},\omega)\right] = 0$$

Metal vs. Insulator: Experiment









Fundamental requirements for electron transport in Fermi systems:

1) Quantum-mechanical states for electron-hole excitations must be available at energies immediately above the ground state (**no gap!**) since the external field provides vanishingly small energy.

2) These excitations must describe delocalized charges (**no wave function localization!**) that can contribute to transport over the macroscopic sample sizes.

Single-Particle vs. Many-Body Insulators

Insulators due to electron-ion interaction (single-particle physics):

- Band Insulators (electron interacts with a periodic potential of the ions → **gap in the single particle spectrum**)
- Peierls Insulators (electron interacts with static lattice deformations → **gap**)
- Anderson Insulators (electron interacts with the disorder=such as impurities and lattice imperfections)

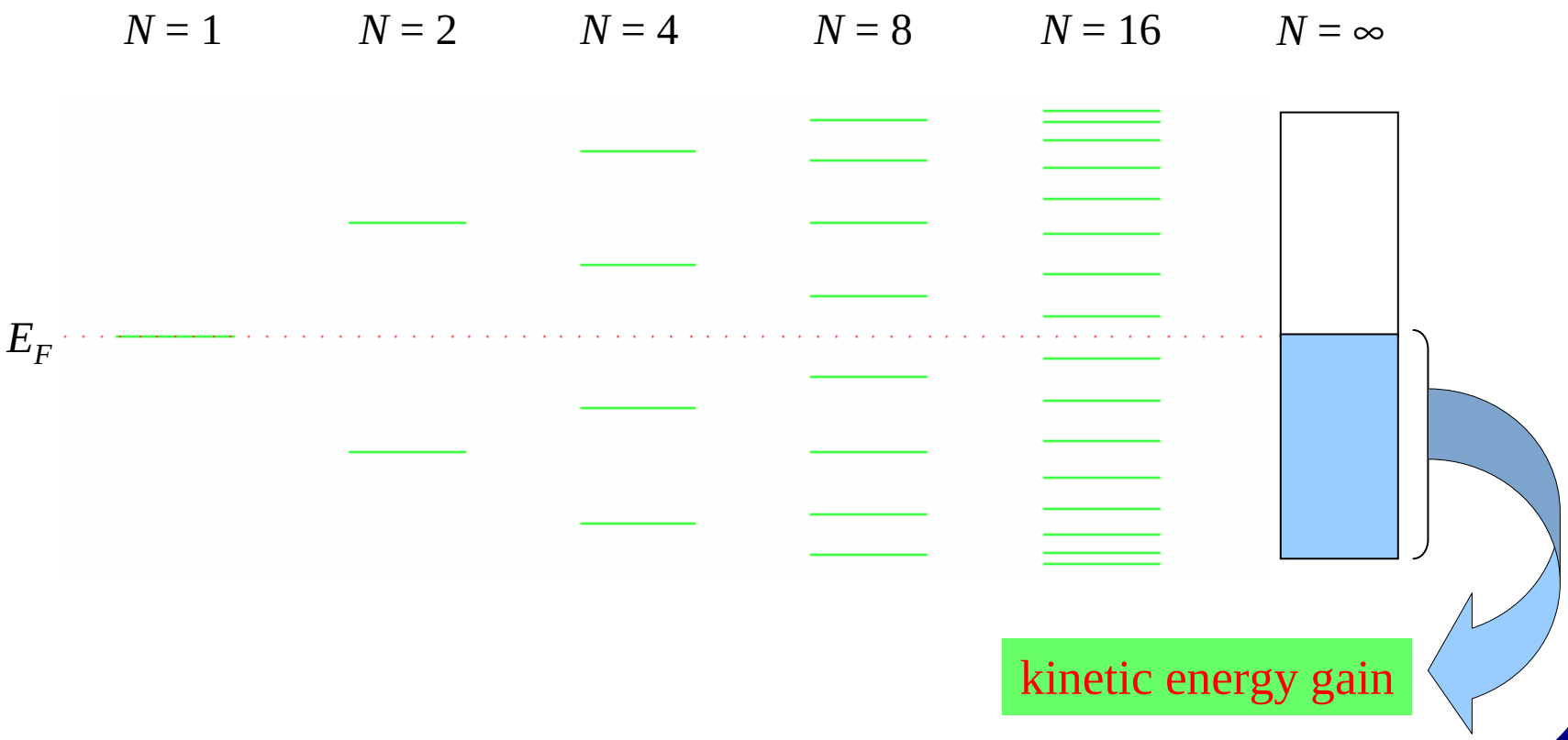
Mott Insulators due to electron-electron interaction (many-body physics leads to the gap in the charge excitation spectrum):

- Mott-Heisenberg (antiferromagnetic order of the pre-formed local magnetic moments below Néel temperature)
- Mott-Hubbard (no long-range order of local magnetic moments)
- Mott-Anderson (disorder + correlations)
- Wigner Crystal (Coulomb interaction dominates at low density of charge, r_s (2D)=$E_{e\text{-}e}/E_F$ =$n_s^{1/2}/n_s$=33 or r_s (3D)=67, thereby localizing electrons into a **Wigner lattice**)

Energy Band Theory

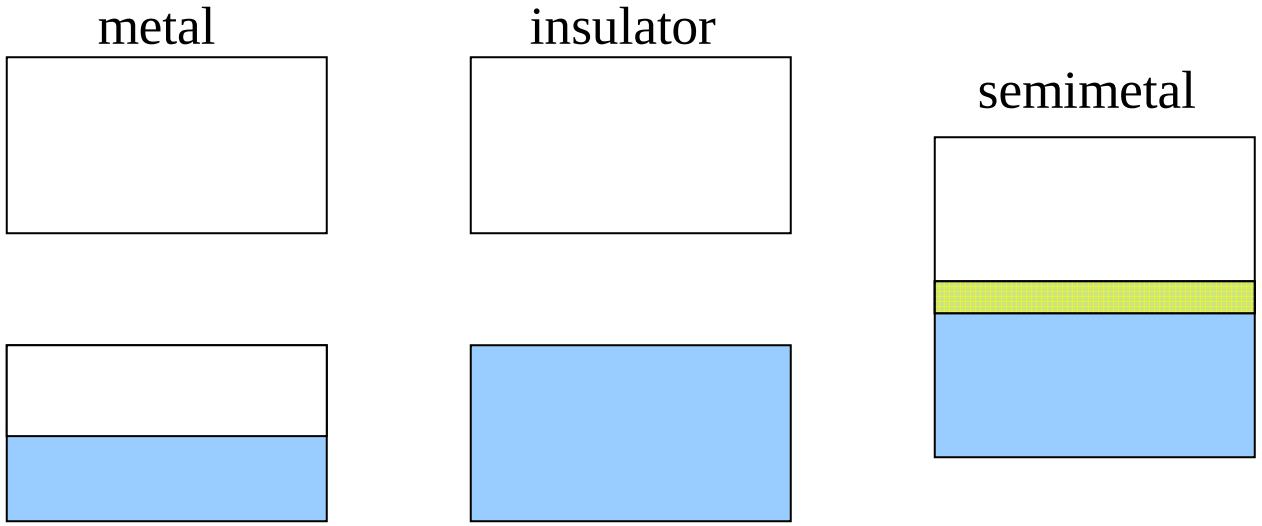
Electron in a periodic potential (crystal)

→ energy band ($\varepsilon(k) = -2t\cos(ka)$: 1-D tight-binding band)



Band (Bloch-Wilson) Insulator

Wilson's rule 1931: partially filled energy band → metal
otherwise → insulator



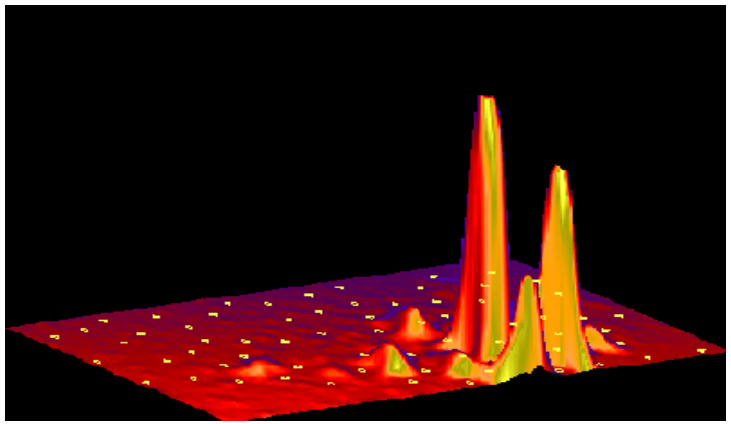
Counter example: transition-metal oxides, halides, chalcogenides

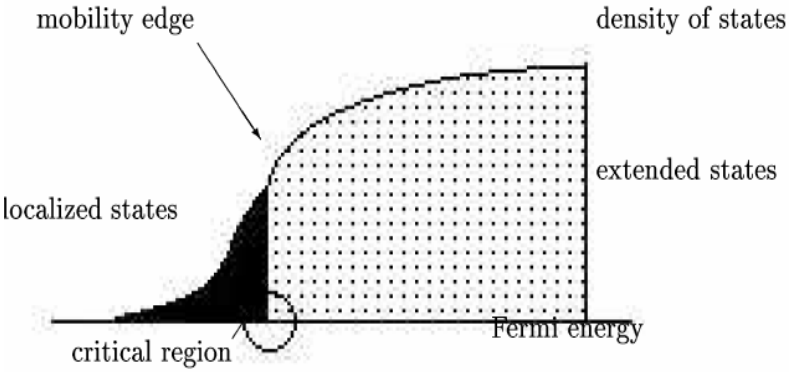
Fe: metal with $3d^6(4sp)^2$

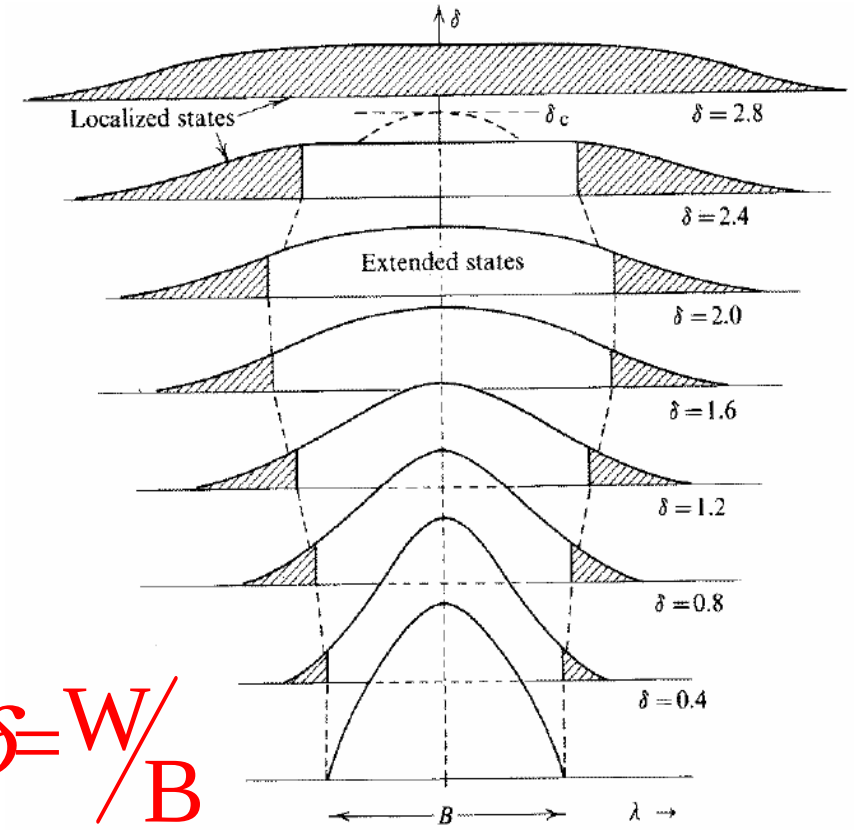
FeO: insulator with $3d^6$

Anderson Insulator

$$\hat{H} = \sum_{\mathbf{m}} \varepsilon_{\mathbf{m}} |\mathbf{m}\rangle\langle\mathbf{m}| + \sum_{\langle \mathbf{m},\mathbf{n} \rangle} t_{\mathbf{mn}} |\mathbf{m}\rangle\langle\mathbf{n}| \quad \text{disorder: } \varepsilon_{\mathbf{m}} \in \left[-\frac{W}{2}, \frac{W}{2} \right]$$

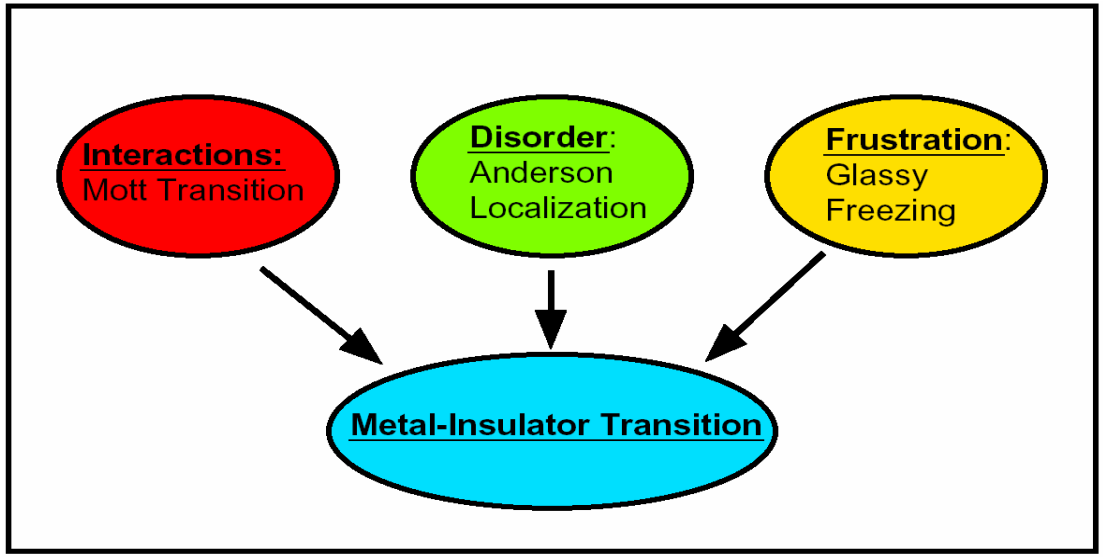






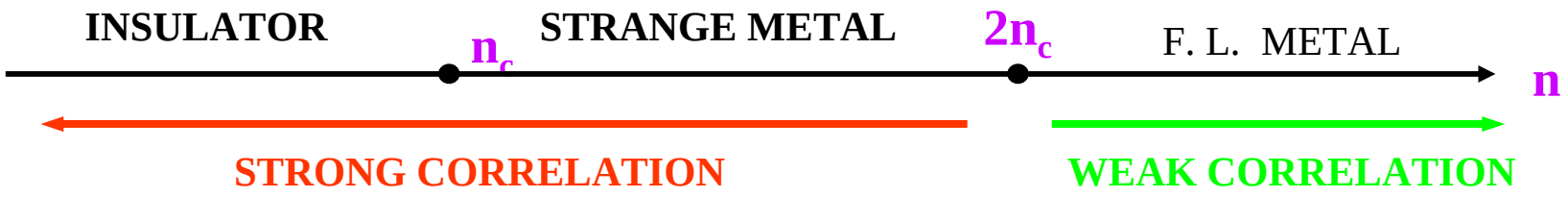
$$\delta = W/B$$

Metal-Insulator Transitions

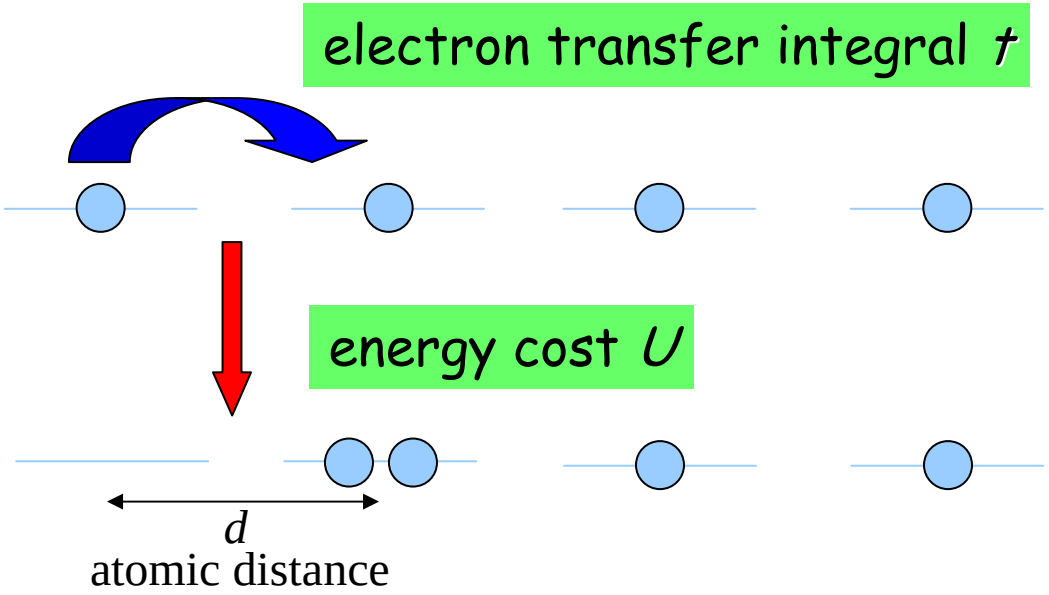


Mott Insulator: A solid in which strong repulsion between the particles impedes their flow → simplest cartoon is a system with a classical ground state in which there is one particle on each site of a crystalline lattice and such a large repulsion between two particles on the same site that fluctuations involving the motion of a particle from one site to the next are suppressed.

From weakly correlated Fermi liquid to strongly correlated Mott insulators



Mott Gedanken Experiment (1949)



$d \to \infty$ (atomic limit: no kinetic energy gain): insulator

$d \to 0$: possible metal as seen in alkali metals

Competition between $W(=2zt)$ and U

$\to$ *Metal-Insulator Transition*

e.g.: V_2O_3, $Ni(S,Se)_2$

Mott vs. Bloch-Wilson insulators

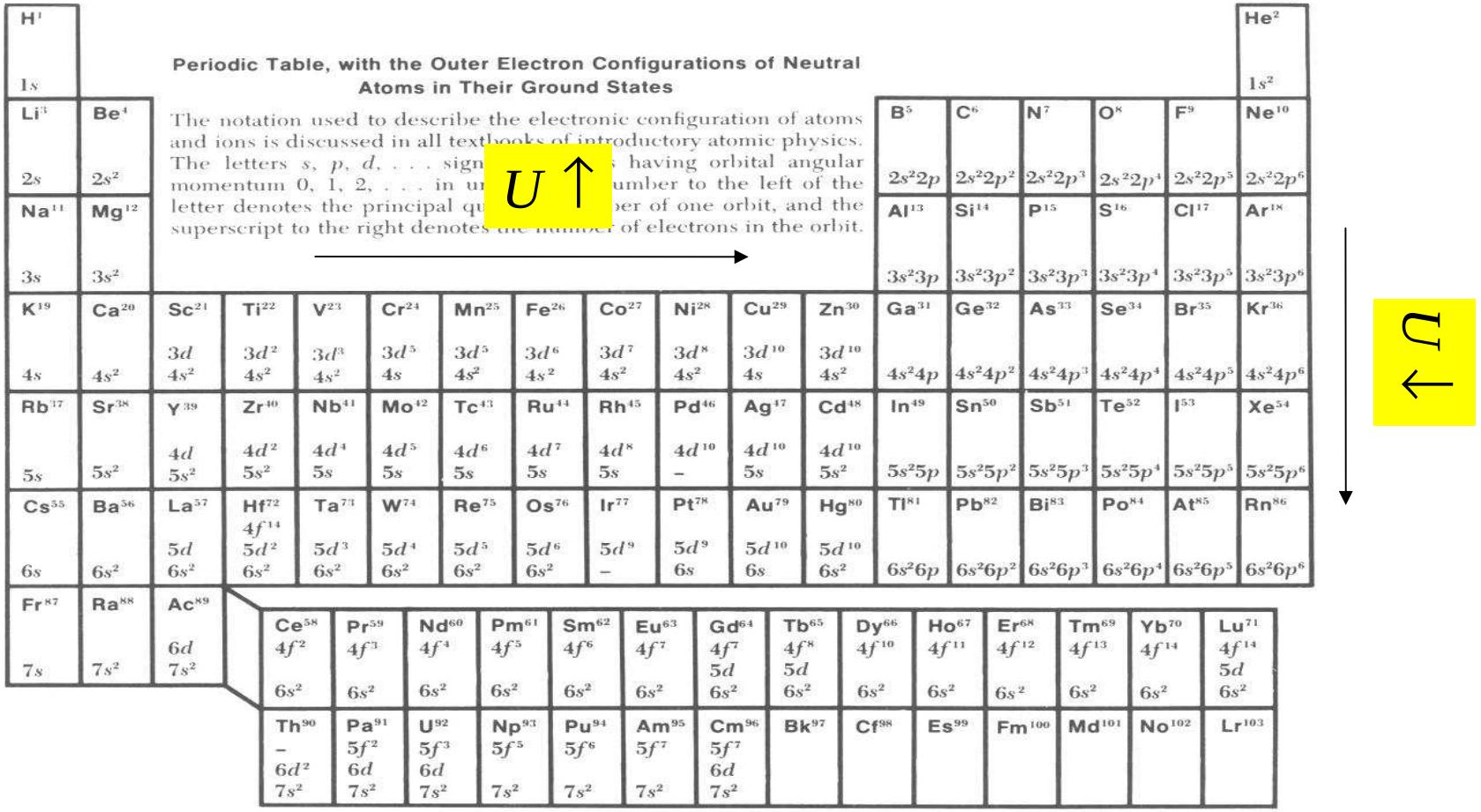
- Band insulator, including familiar semiconductors, is state produced by a subtle quantum interference effects which arise from the fact that electrons are fermions. Nevertheless one generally accounts band insulators to be "simple" because the band theory of solids successfully accounts for their properties.

- Generally speaking, states with charge gaps (including both Mott and Bloch-Wilson insulators) occur in crystalline systems at isolated "occupation numbers" where ν^* is the number of particles per unit cell. $\nu = \nu^*$

- Although the physical origin of a Mott insulator is understandable to any child, other properties, especially the response to doping $\nu \to \nu^* - \delta$ are only partially understood.

- Mott state, in addition to being insulating, can be characterized by: presence or absence of spontaneously broken symmetry (e.g., spin antiferromagnetism); gapped or gapless low energy neutral particle excitations; and presence or absence of topological order and charge fractionalization.

Trend in the Periodic Table



Theoretical modeling: Hubbard Hamiltonian

Hubbard Hamiltonian 1960s:
on-site Coulomb interaction is most dominant

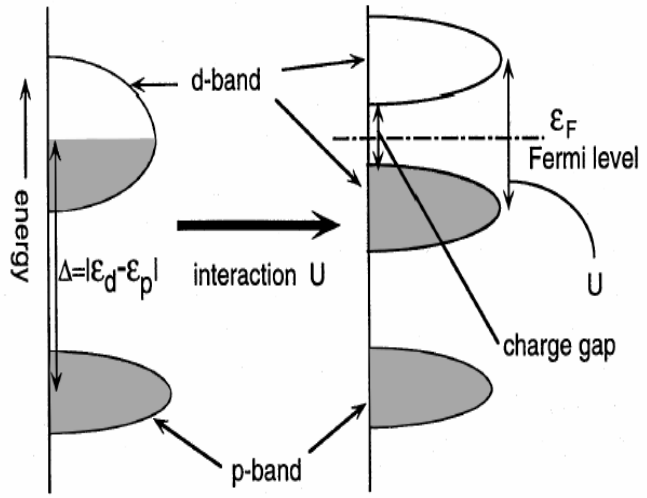
$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

band structure | correlation

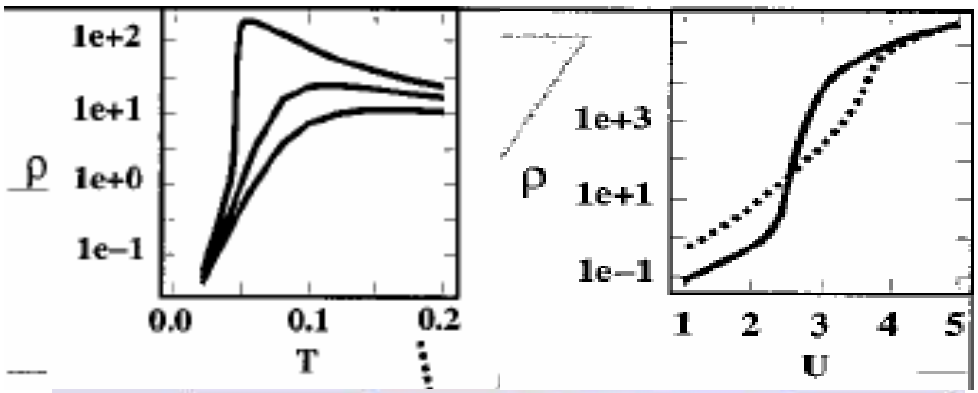
e.g.: $U \sim 5$ eV, $W \sim 3$ eV for most 3d transition-metal oxide such as MnO, FeO, CoO, NiO : Mott insulato

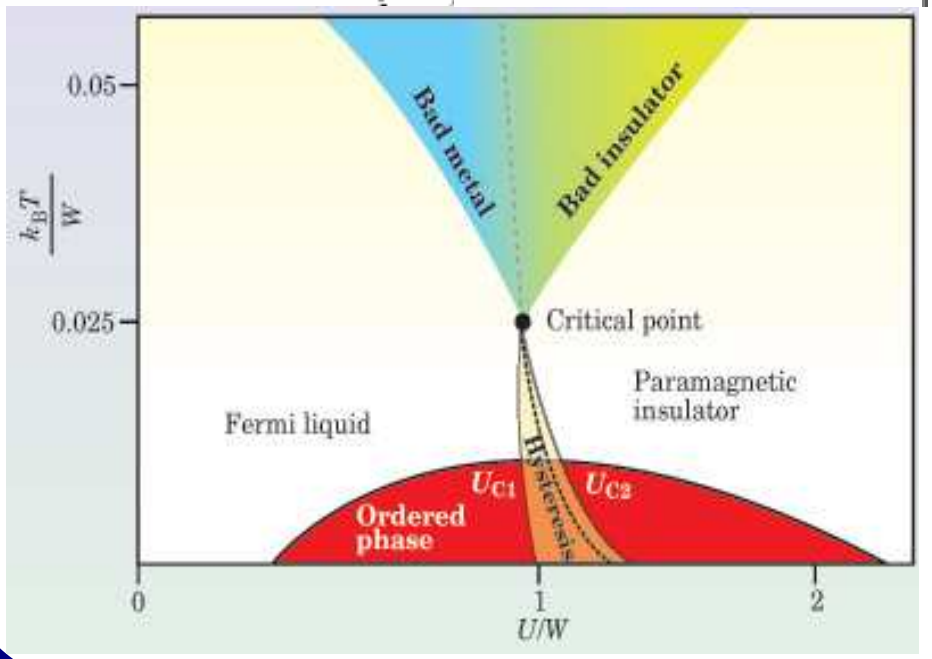
♠ Hubbard's solution by the Green's function decoupling method
→ insulator for all finite U value

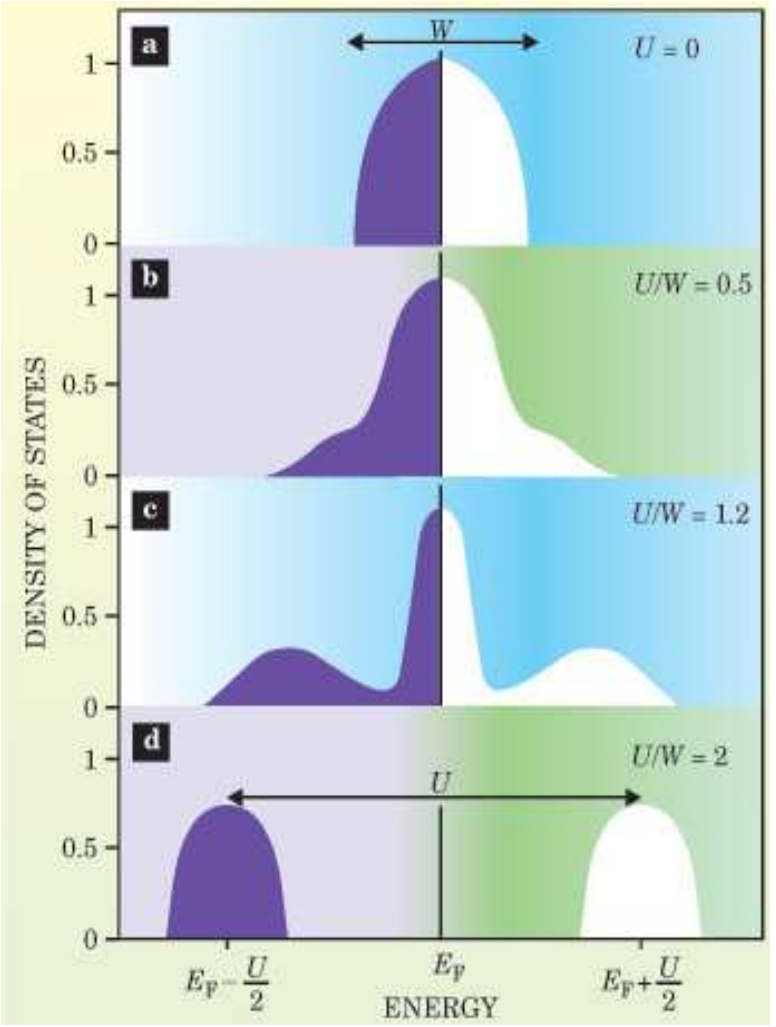
♦ Lieb and Wu's exact solution for the ground state of the 1-D Hubbard model (PRL 68)
→ insulator for all finite U value



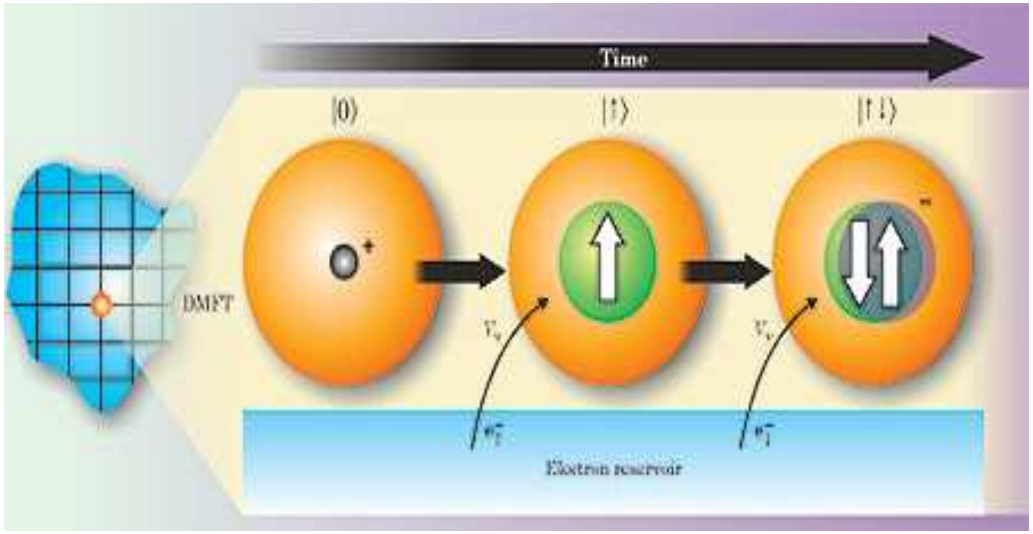
Solving Hubbard Model in ∞ Dimensions







Dynamical Mean-Field Theory in Pictures



- In ∞-D, spatial fluctuation can be neglected.
  → mean-field solution becomes exact.
- Hubbard model → single-impurity Anderson model in a mean-field bath.
- Solve exactly in the time domain
  → "dynamical" mean-field theory

Dynamical mean-field theory (DMFT) of correlated-electron solids replaces the full lattice of atoms and electrons with a single impurity atom imagined to exist in a bath of electrons. The approximation captures the dynamics of electrons on a central atom (in orange) as it fluctuates among different atomic configurations, shown here as snapshots in time. In the simplest case of an s orbital occupying an atom, fluctuations could vary among $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, or $|\uparrow\downarrow\rangle$, which refer to an unoccupied state, a state with a single electron of spin-up, one with spin-down, and a doubly occupied state with opposite spins. In this illustration of one possible sequence involving two transitions, an atom in an empty state absorbs an electron from the surrounding reservoir in each transition. The hybridization V_v is the quantum mechanical amplitude that specifies how likely a state flips between two different configurations.

Static vs. Dynamic Mean-Field Theory

- Static = Hartree-Fock or Density Functional Theory:

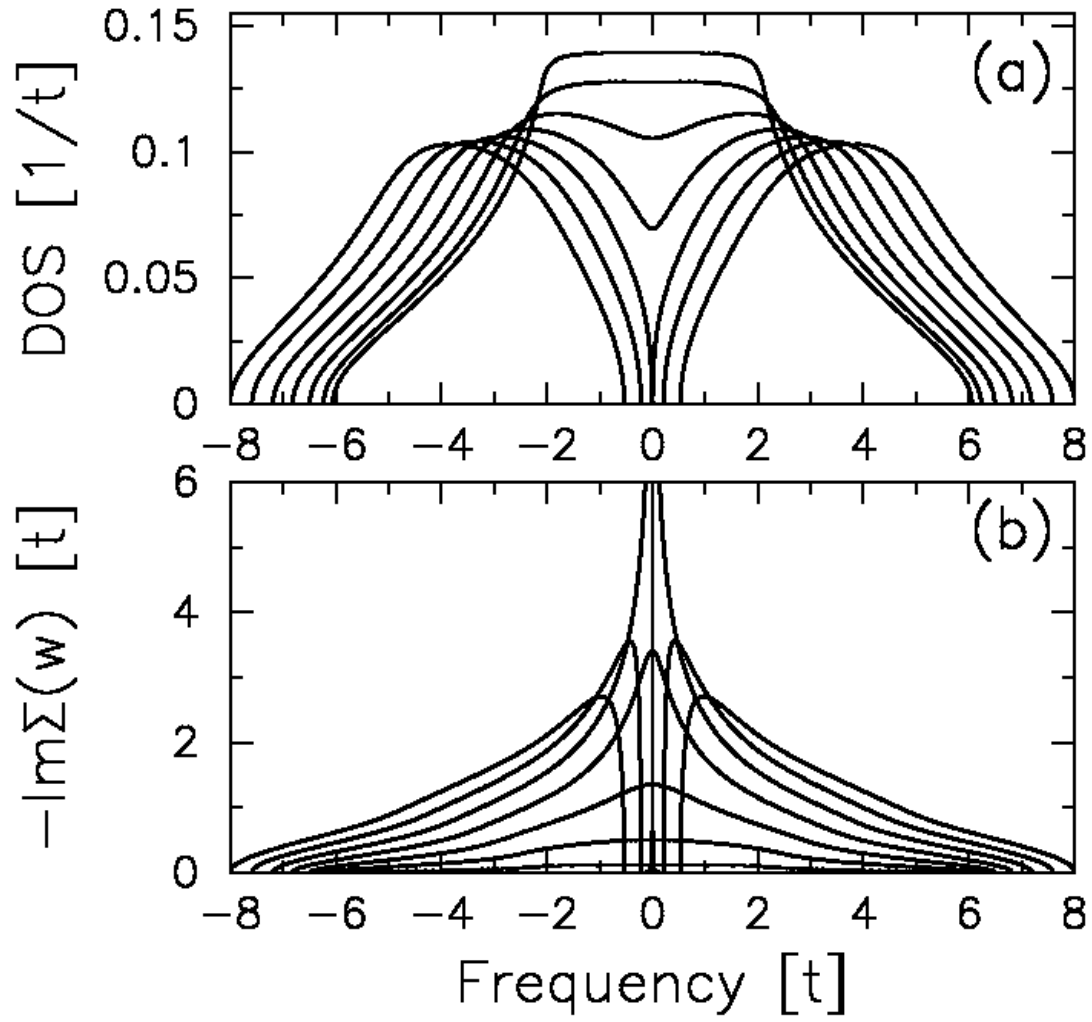
$$\left.\begin{aligned}\Gamma[\rho(\mathbf{r})] &= E_{kinetic}[\rho(\mathbf{r})] + \int V_{ext}(\mathbf{r})\rho(\mathbf{r})d^3\mathbf{r} \\ &+ \frac{1}{2}\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}d^3\mathbf{r}' + E_{exchange}[\rho(\mathbf{r})]\end{aligned}\right\} \Rightarrow \left[\frac{\hbar^2}{2m} + V_{KS}(\mathbf{r})\right]\Psi(\mathbf{r}) = \varepsilon_i\Psi(\mathbf{r})$$

$$V_{KS}[\rho(\mathbf{r})] = V_{ext}(\mathbf{r}) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}' + \frac{\delta E_{exchange}[\rho(\mathbf{r})]}{\delta\rho(\mathbf{r})},\ \rho(\mathbf{r}) = \sum_i f(\varepsilon_i)|\Psi(\mathbf{r}_i)|^2$$

- Dynamic = Dynamical Mean-Field Theory:

$$\left.\begin{aligned}\Gamma[\rho(\mathbf{r}), G] &= E_{kinetic}[\rho(\mathbf{r}), G] + \int V_{ext}(\mathbf{r})\rho(\mathbf{r})d^3\mathbf{r} \\ &+ \frac{1}{2}\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}d^3\mathbf{r}' + E_{exchange}[\rho(\mathbf{r}), G]\end{aligned}\right\} \Rightarrow \begin{cases} G[\Delta(\omega)] = \sum_{\mathbf{k}}\left[\omega - \Sigma[\Delta(\omega)] - t_{\mathbf{k}}\right]^{-1} \\ \Sigma[\Delta(\omega)] \equiv \Delta(\omega) - 1/G[\Delta(\omega)] + \omega \end{cases}$$

Transition from non-Fermi Liquid Metal to Mott Insulator

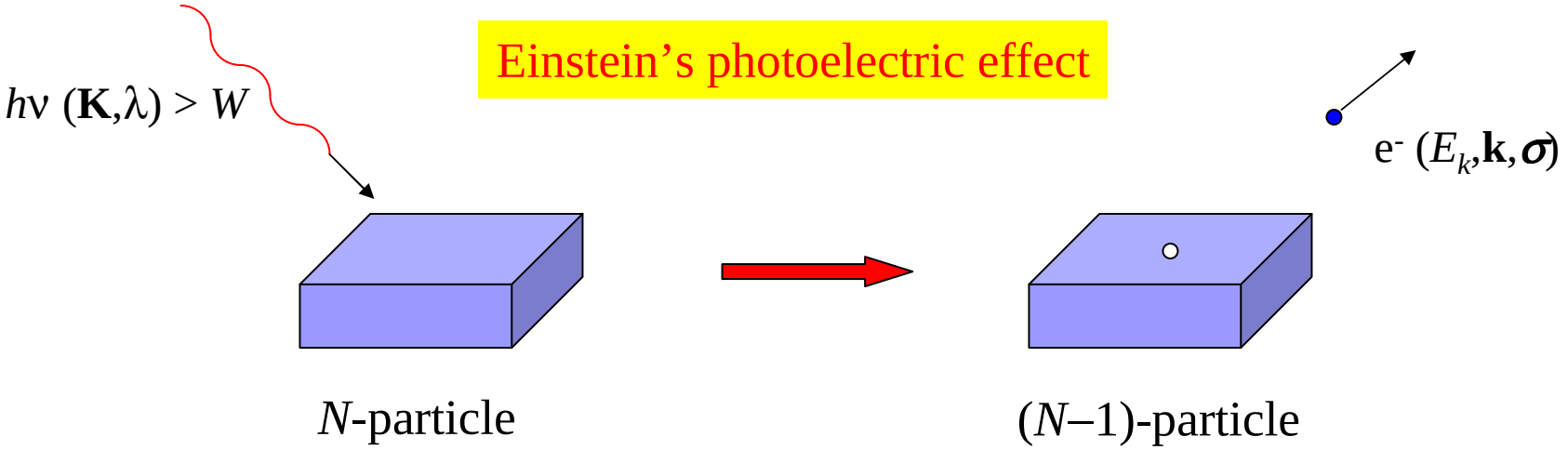


NOTE: DOS well-defined even though there are no fermionic quasiparticles.

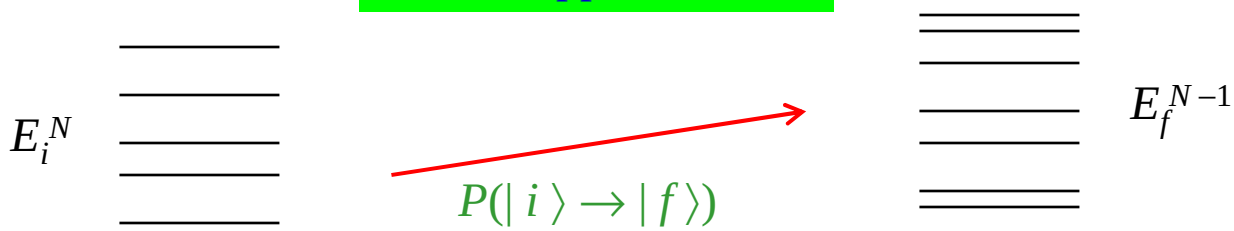
Model: Mobile spin-electrons interact with frozen spin- electrons.

Experiment: Photoemission Spectroscopy

Einstein's photoelectric effect



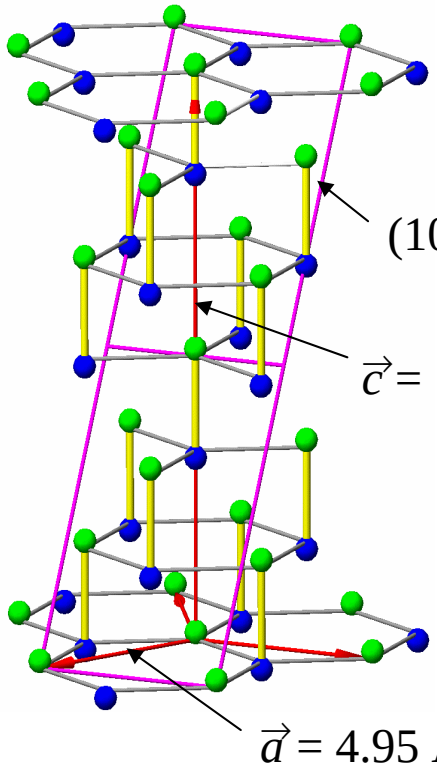
Sudden approximation



Photoemission current is given by:

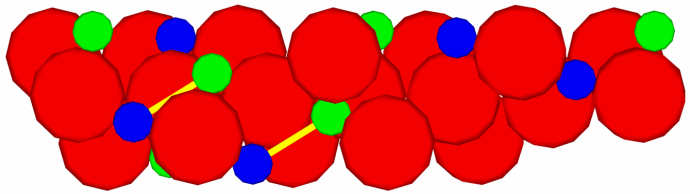
$$A_{-}(\omega) = \frac{1}{Z}\sum_{i,f} e^{-E_i^N/k_BT} \left| < f \,|\, T_r \,|\, i > \right|^2 \delta(\omega + E_f^{N-1} - E_i^N)$$

Mott Insulating Material: V_2O_3

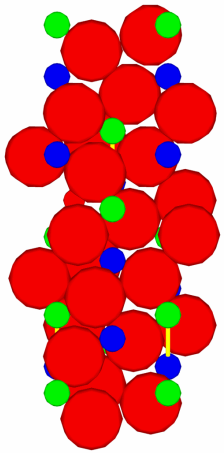


surface-layer thickness =

2.44Å



side view

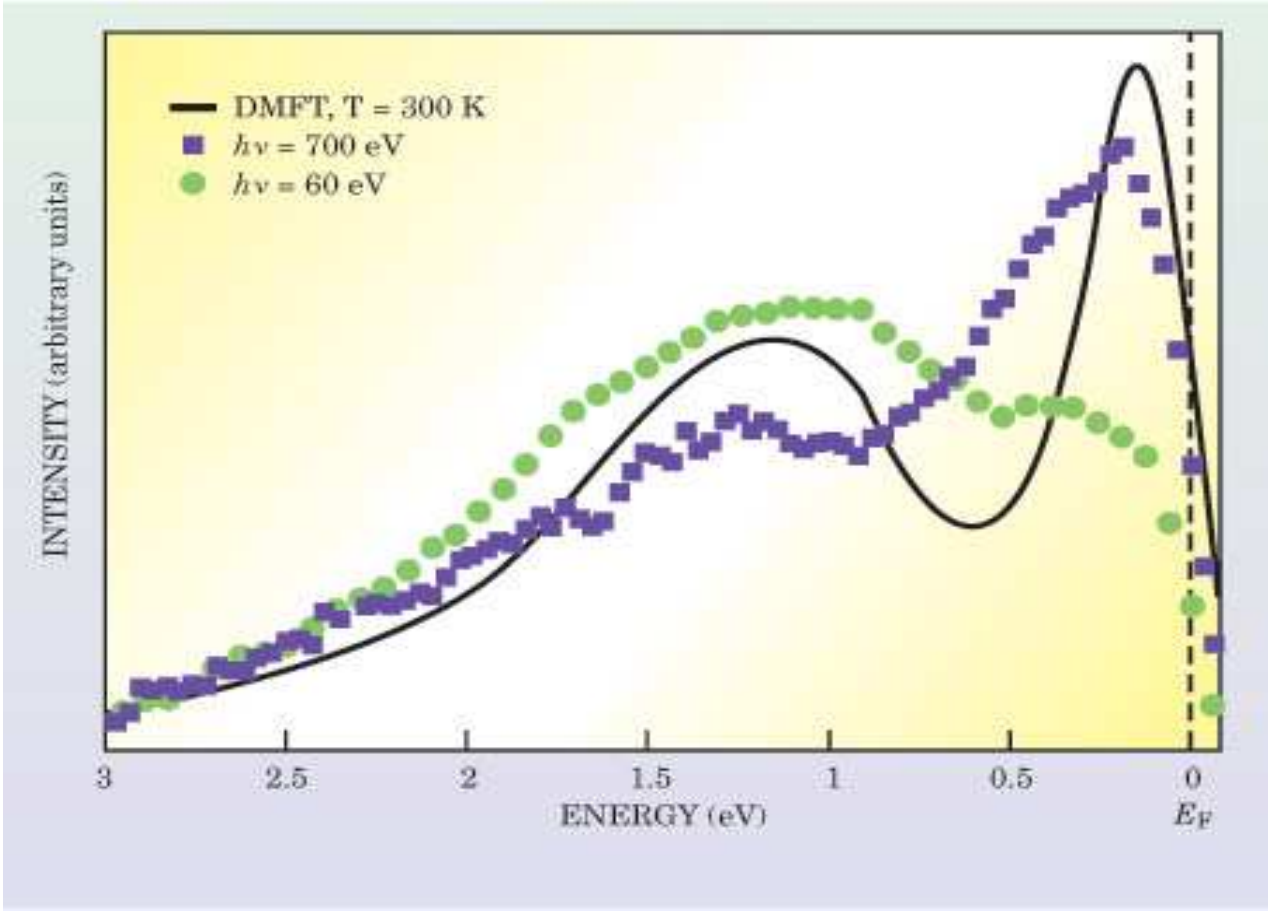


top view

Vanadium

Oxygen

Theory vs. Experiment: Photoemission Spectroscopy



Photoemission spectrum of metallic vanadium oxide V_2O_3 near the metal–insulator transition. The dynamical mean-field theory calculation (solid curve) mimics the qualitative features of the experimental spectra. The theory resolves the sharp quasiparticle band adjacent to the Fermi level and the occupied Hubbard band, which accounts for the effect of localized d electrons in the lattice. Higher-energy photons (used to create the blue spectrum) are less surface sensitive and can better resolve the quasiparticle peak.

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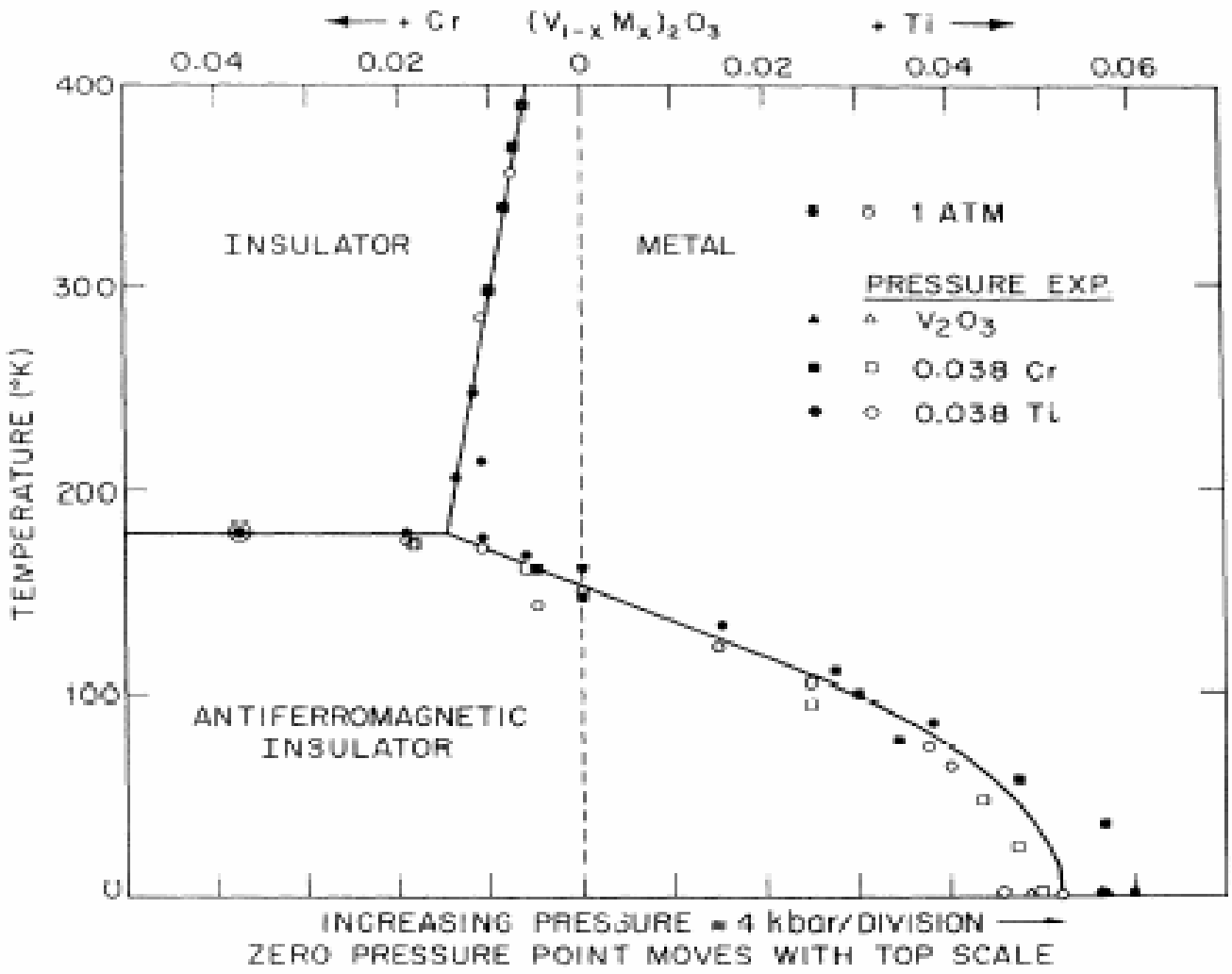
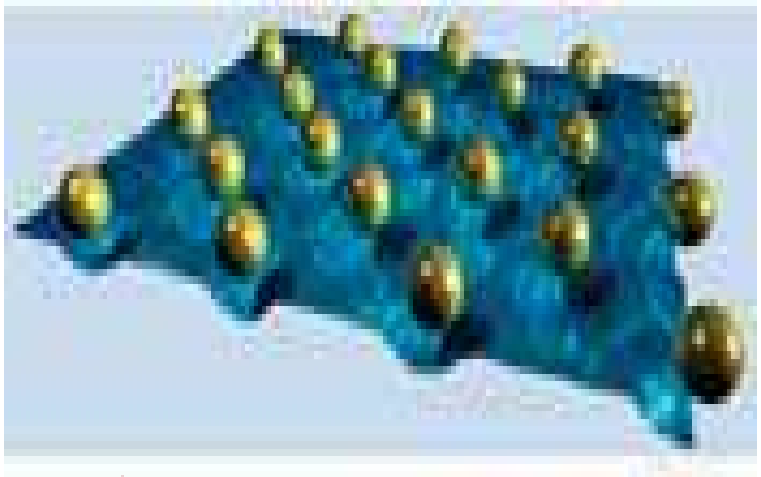
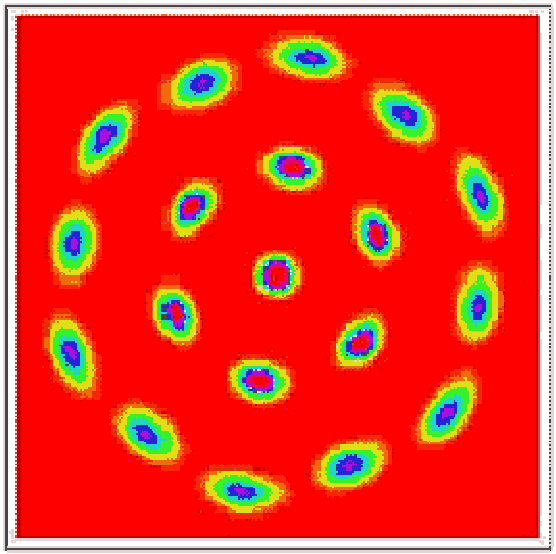
Phase Diagram of V_2O_3



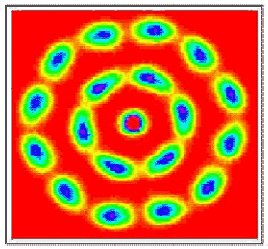
Wigner Crystal

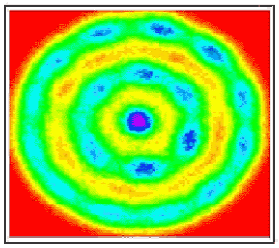




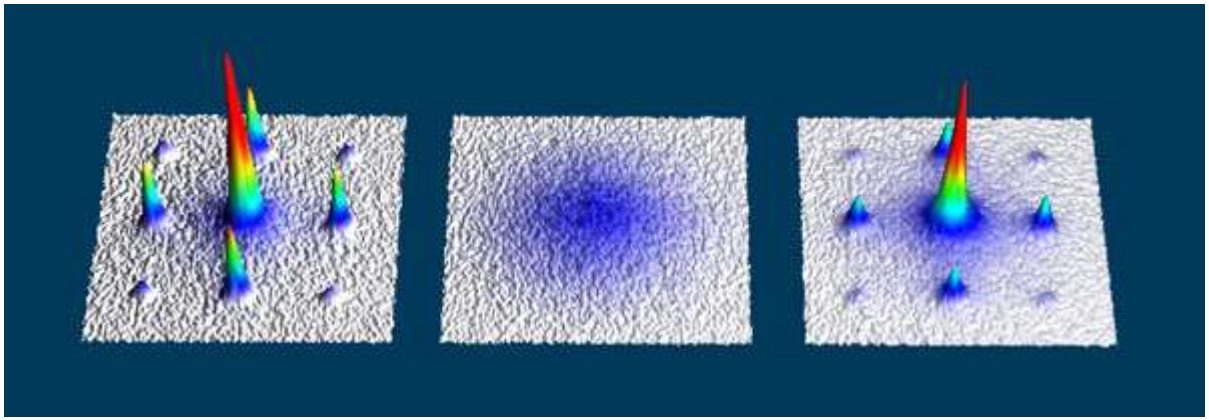
Since the mid-1930s, theorists have predicted the crystallization of electrons. If a small number of electrons are restricted to a plane, put into a liquid-like state, and squeezed, they arrange themselves into the lowest energy configuration possible--a series of concentric rings. Each electron inhabits only a small region of a ring, and this bull's-eye pattern is called a Wigner crystal. Only a handful of difficult experiments have shown indirect evidence of this phenomenon →

Electrons trapped on a free surface of liquid helium offer an excellent high mobility 2D electron system. Since the free surface of liquid He is extremely smooth, the mobility of electrons increases enormously at low temperatures.





Beyond Solid State Physics: Bosonic Mott Insulators in Optical Lattices



❑**EVOLUTION:**
Superfluid state with coherence, Mott Insulator without coherence, and superfluid state after restoring the coherence.