Insulators, metals, and fractionalized states - Berry's phases and the Luttinger theorem

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- Report on recent work that holds the promise to
  - Unify many deep fundamental concepts in condensed matter physics
  - Metals, insulators, fractional statistics, . . .
  - Resolve long-standing issues
  - Open the vista for new phenomena in correlated systems
  - Provide ways to classify and carry out calculations on real problems interacting electron

1867 TM

Specific questions

- Is it possible to have a Mott insulator with no broken symmetry?
  - Spin Liquid?
  - Topological order?

What do these papers have in common?

- Significance of Electromagnetic Potentials in the Quantum Theory,
  Y. Aharonov and D. Bohm, Phys. Rev. 115, 485 (1959)
- Fermi Surface and Some Simple Equilibrium Properties of a System of Interacting Fermions,
  J. M. Luttinger, Phys. Rev. 119, 1153 (1960).
- Two soluble models of an antiferromagnetic chain,
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- Theory of the Insulating State,
  W. Kohn, Phys. Rev. 133, A171 (1964).
- Quantized Hall conductivity in two dimensions,
  R. B. Laughlin, Phys. Rev. 23, 5632 (1981).
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  G. Ortiz, and R. M. Martin, Phys. Rev. B 49, 14202 (1994).
- Quantum Mechanical Position Operator in Extended System,
  R. Resta and S. Sorella, Phys. Rev. Lett. 80, 1800 (1998).
- Polarization and localization in insulators: generating function approach
  I. Souza, T. Wilkens, and R. M. Martin, Phys. Rev. B 62, 1666 (2000).

Which paper is different (apparently)?

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- **Fermi Surface and Some Simple Equilibrium Properties of a System of Interacting Fermions,**
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Recent work unifying fundamental concepts

- Topological Approach to Luttinger's Theorem and the Fermi Surface of a Kondo Lattice,
  M. Oshikawa, Phys. Rev. Lett. 84, 3370 (2000)
- Insulator, Conductor, and Commensurability: A Topological Approach,
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  A. Seidel, H. Fu, D.-H. Lee, J. M. Leinaas, J. Moore, Cond-mat/0509071
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- From Néel long-range order to spin liquids in the multiple-spin exchange model
  W. LiMing, G. Misguich, P. Sindzingre, and C. Lhuillier,
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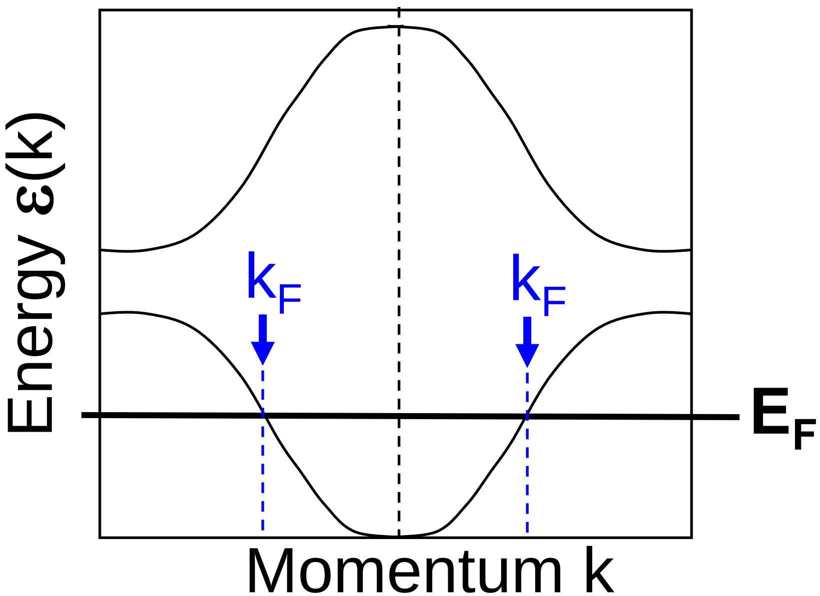
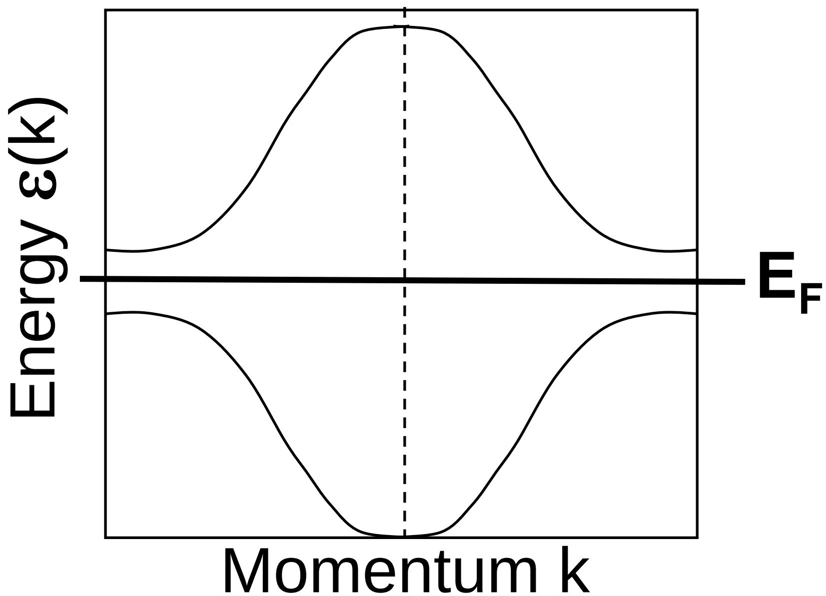
Independent Electrons

- The textbooks we all know and love (Kittel, Ashcroft & Mermin, …) describe metals and insulators in terms of bands:

Metal
partially filled bands

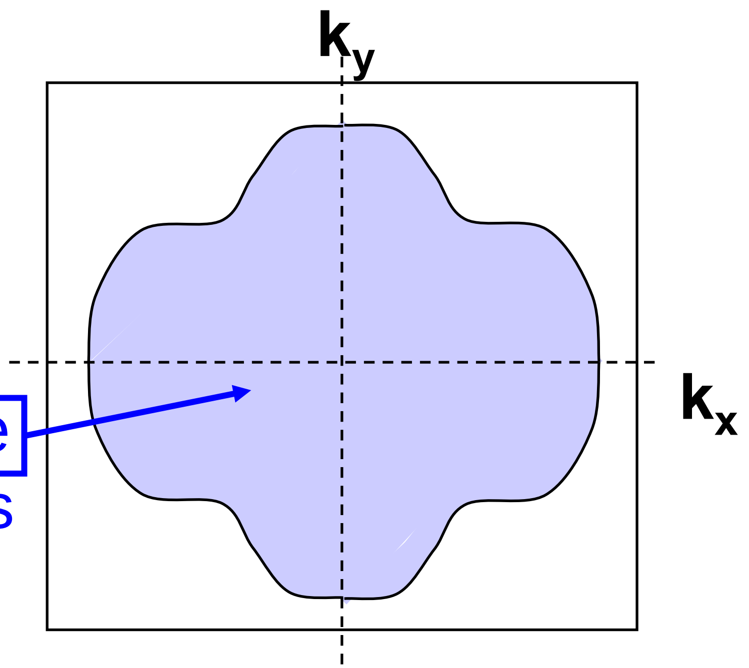


Insulator
filled bands



Independent Electrons

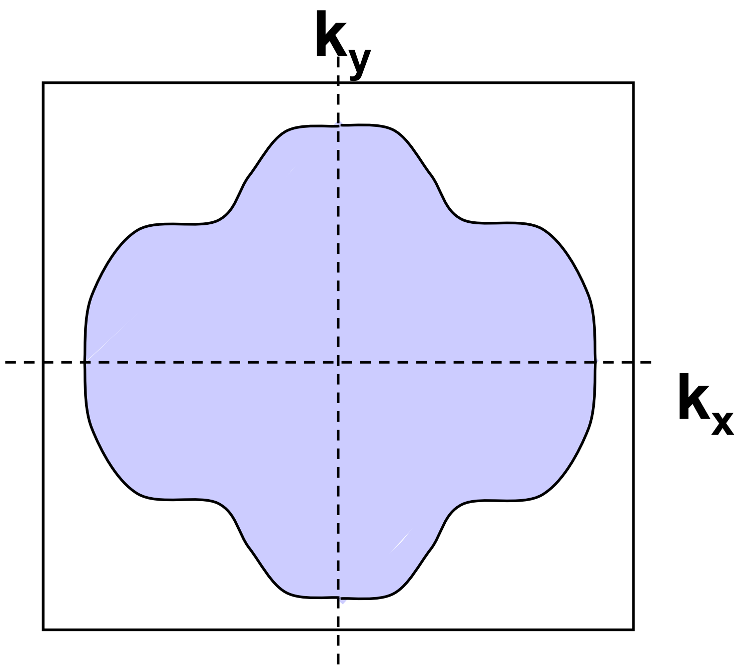
- **Fermi Surface** – surface in **k**-space with $\varepsilon(k) = E_F$
- For independent electrons, the ground state is formed by filling lowest energy states with 1 electron of each spin per state
- Volume enclosed by Fermi surface determined by number of electrons per cell
- Fermi surface for each spin – we will ignore spin-orbit coupling



Metal
partially filled band

Interacting Electrons

- **Luttinger Theorem** – Volume in k-space enclosed by Fermi Surface is not changed
  - determined only by the number of electrons
  – independent of electron-electron interactions
  - Shape may change but total volume enclosed is not changed



Metal
partially filled band

- **Important part of theorem** – volume not changed modulo the volume of the BZ
- A filled band contributes zero since the states occupy the entire BZ

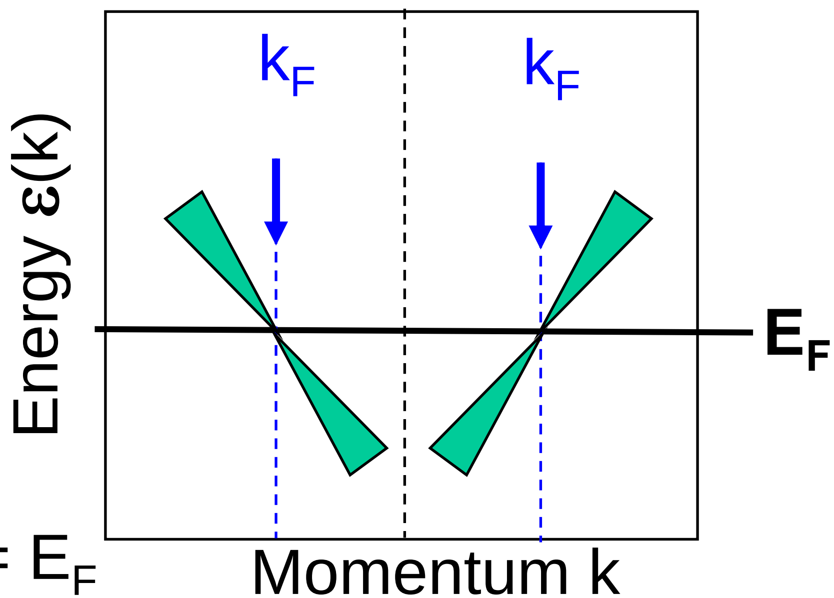
Interacting Electrons

- **Luttinger's derivation** – Perturbation expansion summed to all orders
- Assuming expansion converges, then:
  – The Fermi surface is well-defined
  - Equating two expressions for particle number → theorem
- Quasiparticles well-defined at E_F

$$\mathbf{G_k(z) = \frac{1}{z - \varepsilon_k - \Sigma_k(z)}}$$

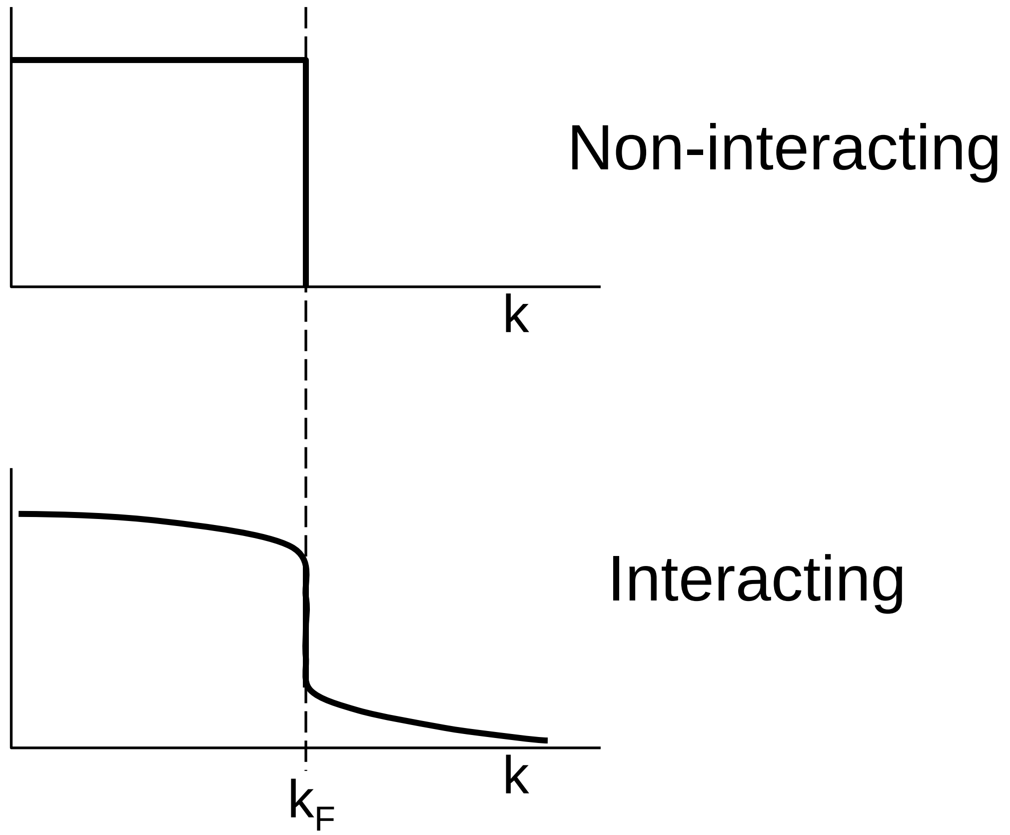
Self-energy $\Sigma_k(\mathbf{z})$ real at z = E_F

Green's function $\mathbf{G_k(z)}$ real at z = E_F and changes sign at k=k_F



Signature of Fermi Surface

- **Momentum distribution** – Can be measured



E_F

Real Solids – Real Experiments

- The well-defined Fermi surface is verified in great detail and many metals by many experiments
  - DeHaas-Van Alfen
  - Angle resolved photoemission
  - . . .
- Experiment provides the evidence for Fermi Liquid theory
- **Are the exceptions?**
  - Strongly correlated systems ?
  - Mott Insulators ?
  - Kondo Lattice ?
  - Hi-Tc ?
  - . . .

Real Calculations

- What calculations will satisfy the Luttinger theorem
  - GW – If done correctly – “conserving approximations”
  - DMFT - in the single site approximation - if done correctly
  - Dynamical Cluster Approximation -- ?
  - . . .
- **Are the exceptions?**
  - More later

Mott Transition

- Metal-insulator transition caused by electron-electron interactions

- Based upon a simple idea

- Consider limits
  - Atoms pushed close together to form a solid – forms bands – if bands are partially filled $\longrightarrow$ metal
  - The same atoms far apart – forms discrete states – electron-electron interactions prevent electrons from moving between atoms $\longrightarrow$ insulator
  - There must be a transition

- Examples – transition metal oxides – MnO, NiO, . . .

Mott transition - example

- **Antiferromagnetic transition**

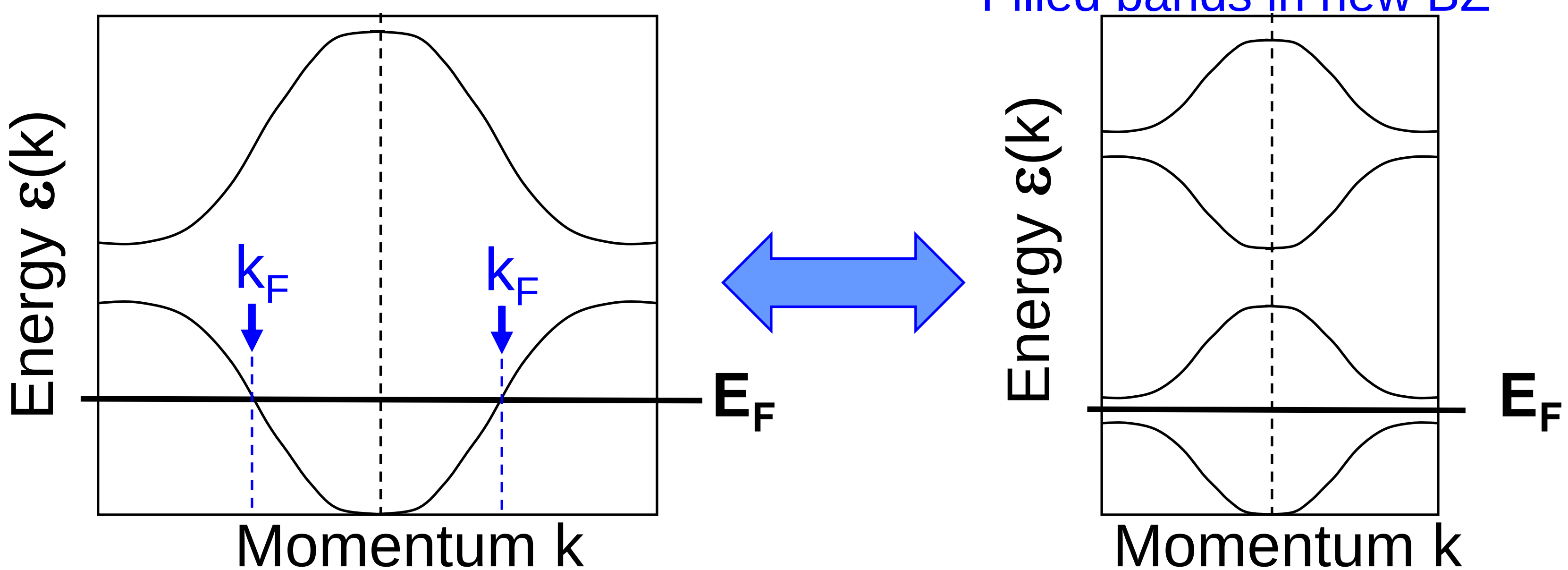
Metal

half filled band

Antiferromagnetic Insulator

Cell doubled – BZ reduced by ½

Filled bands in new BZ



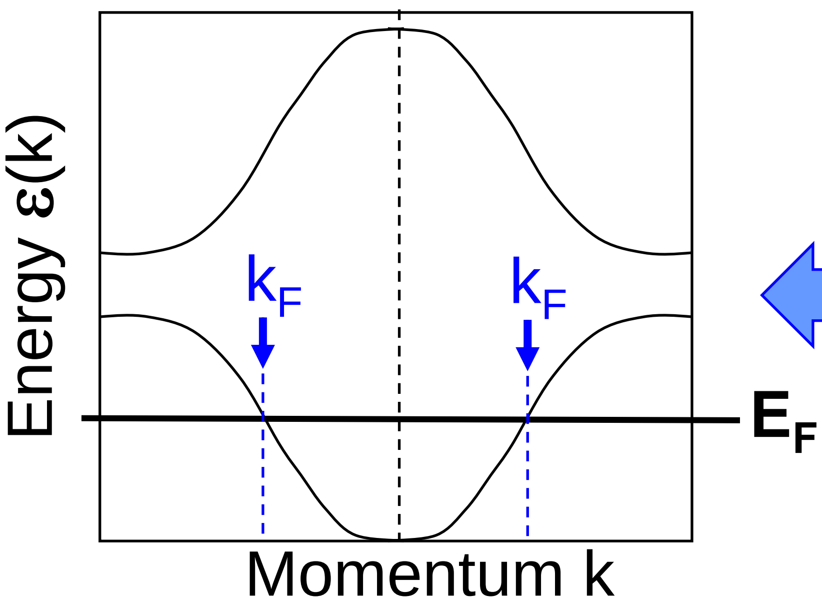
- The Luttinger theorem is consistent with the transition if there is a change in the translation or spin symmetry
- Broken symmetry – phase transition – 1st or 2nd order

Mott Transition - again

- Can there be a metal-insulator transition caused by electron-electron interactions with no broken symmetry ?
  - No magnetic order -- No change in lattice symmetry . . .

Metal

half filled band

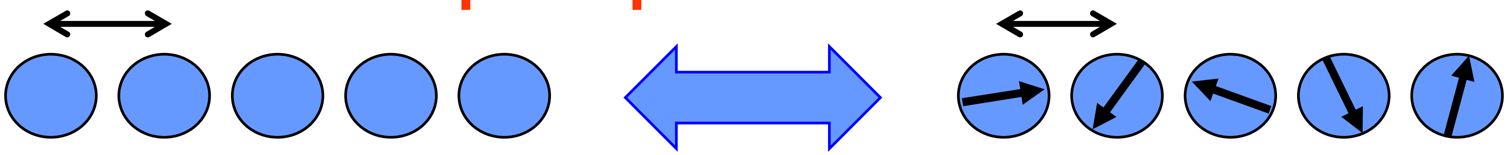


- **Proposals**
  - **Spin Liquids**

? . . .

Spin Liquid

- **Band metal to spin liquid transition**



“Disordered” spins
– no new order
Cell same – BZ same

- A spin liquid is proposed to be a state with no spin order, no change in translation symmetry – yet an insulating state

- The Luttinger theorem – as originally formulated – is inconsistent with an insulating state if there is an odd number of electrons per cell and no change in the translation or spin symmetry

New Analysis based upon Fundamental distinctions Metals, insulators, . . .

W. Kohn (1964) – sensitivity to boundary conditions
Scalapino, White, Zhang - PRB 47, 7995 (1993)
"Insulator, metal, or superconductor: The criteria"

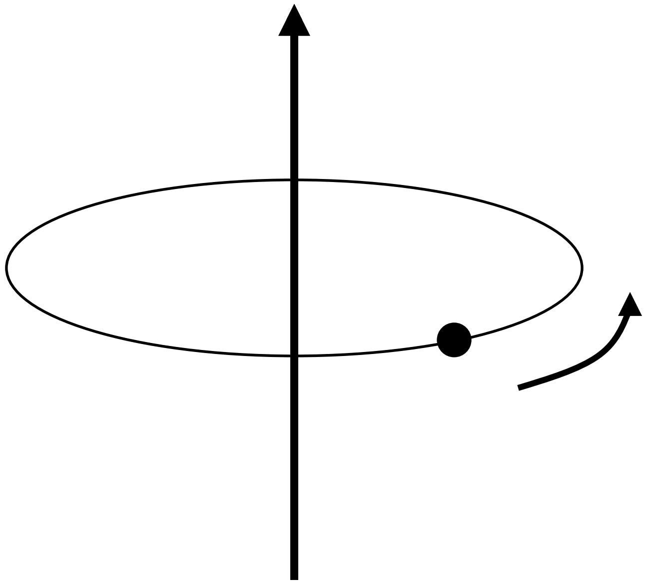
Recent work has identified the key concepts in terms of the Center of Mass Position of the electrons –

$$\mathbf{X} = (1/N)\, \Sigma_i\, \mathbf{x_i}$$

Polarization	**$\langle X \rangle$**	**Berry's curvature (phase)**
Fluctuations	**$\langle X^2 \rangle - \langle X \rangle^2$**	**Quantum Metric**

Ivo Souza, Thesis, UIUC (2000)

Geometric Phases in Quantum Mechanics

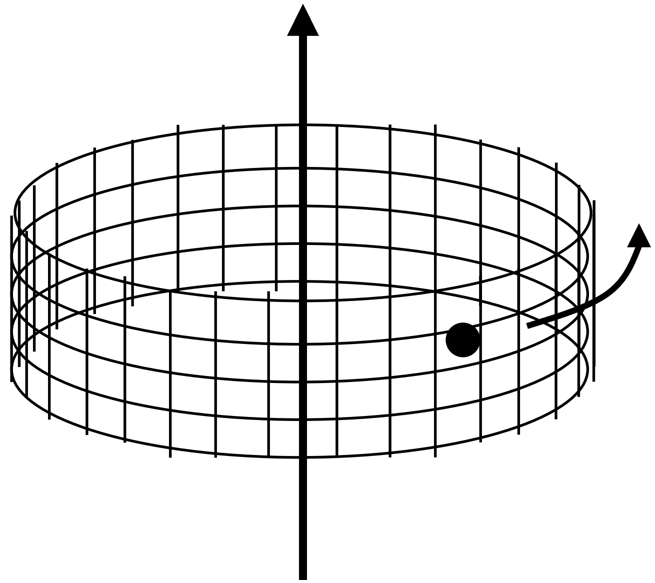


- Example – Aharonov-Bohm Effect:
- Transport a charge around the magnetic flux

$$H = \tfrac{1}{2}(p)^2 \Rightarrow \tfrac{1}{2}(p - (e/c)A)^2$$

- Berry Phase = γ = $(q/\hbar) \int A \cdot dr$ = $q\Phi/(\hbar c)$ (modulo 2π)

Geometric Phases in Quantum Mechanics



- Torus boundary conditions on crystal
- Transport a charge around the supercell

$$H_{\mathbf{k}} = \tfrac{1}{2}(p + k)^2 \Rightarrow \tfrac{1}{2}(p + k - (e/c)A)^2 = \tfrac{1}{2}(p + k + \Delta k)^2$$

- Shift in k equivalent to gauge field
- Idea used by Kohn, . . .

Boundary Conditions

Boundary conditions on a finite cell to describe an infinite system:

"Twisted" b.c. on wave function

$$H\Psi_k = E_k\Psi_k, \qquad \Psi_k(X+L) = e^{ikL}\Psi_k(X)$$

Periodic wave function with k-dependent H

$$\Psi_k(X) = e^{ikX}\Phi_k(X) \qquad \Phi_k(X+L) = \Phi_k(X)$$

$$H_k\Phi_k = E_k\Phi_k \qquad H_k = \tfrac{1}{2}(p + \hbar k)^2 + V$$

Bloch functions for independent electrons

Applies to many-body problem with $X = \Sigma_i x_i$

"Twist operator" – $U(k) = e^{ikX}$

Center of Mass – Position, Fluctuations

- Define **Twist operator**

  $C(k,\alpha) = < \Psi_{\mathbf{k}} |\exp(- i\, \alpha\, \mathbf{X}) | \Psi_{\mathbf{k+\alpha}} > = < \Phi_{\mathbf{k}} | \Phi_{\mathbf{k+\alpha}} >$

  Overlap of Φs

- Simplest case: "Single Point" formula

  (k = 0-- periodic functions)

  $\ln C(\alpha) = \ln < \Phi_{\mathbf{0}} |\exp(- i\, \alpha\, \mathbf{X}) | \Phi_{\mathbf{0}} > = \ln z$

  Non-zero only for $\alpha = (2\pi/L)$ x integer

- It follows that

$$< X\, X\ \ldots >^{c}_{n} = (1/V)\, i^{n}\, (d/d\,\alpha)^{n} \ln C(\alpha)\Big|_{\alpha=0}$$

e.g.,

$$< X > \quad = \quad (i/V)\, (d/d\,\alpha) \ln C(\alpha)\Big|_{\alpha=0}$$

$$< \Delta X^{2} > = -(1/V)\, (d/d\,\alpha)^{2} \ln C(\alpha)\Big|_{\alpha=0}$$

Expeimentally measurable

- From the fluctuation-dissipation theorem:
$$< \Delta P^2 > = (e^2/V) < \Delta X^2 >$$
$$= (h/2\pi^2) \int \mathrm{Re}\,\sigma(\omega)\, d\omega / \omega$$

- Define localization length: $\zeta^2 = (1/N) < \Delta X^2 >$
- Above expressions show
  $\zeta^2 =$ finite for insulators - explicit formula!
  $\zeta^2 =$ infinite for metals

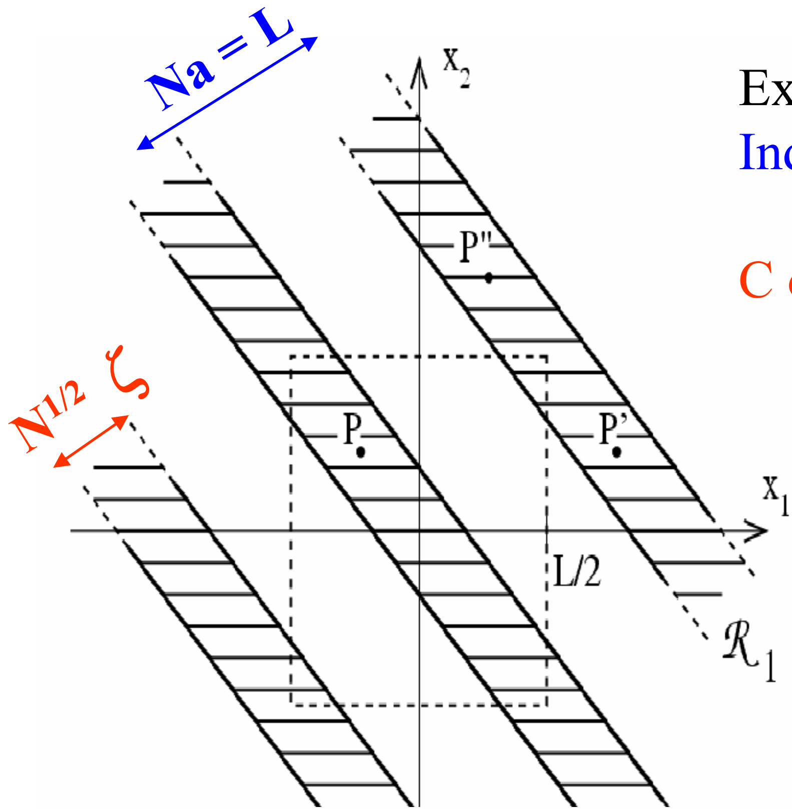
- Souza – Thesis – (2000)

Boundary Conditions

Table 7.2: Comparison between the formulas for the Drude weight and for the localization length, their relation to the optical conductivity, and their asymptotic values in the thermodynamic limit for insulators and conductors at $T = 0$.

	Drude weight D_μ	**Localization length** $\xi_\mu^2(N)$
Formula involving twisted boundary conditions	$\frac{1}{2V} \frac{\partial^2 E(\mathbf{k})}{\partial k_\mu^2}\Big\vert_{\mathbf{k}=0}$	$\frac{1}{N} \frac{\partial^2 \ln C(\boldsymbol{\alpha})}{\partial \alpha_\mu^2}\Big\vert_{\boldsymbol{\alpha}=0}$
Relation to conductivity	$-\frac{1}{2} \lim_{\omega\to 0} \omega \mathrm{Im}\sigma_{\mu\mu}(\omega)$	$\frac{\hbar}{\pi q_e^2 n_0} \int_0^\infty \mathrm{Re}\sigma_{\mu\mu}(\omega) \frac{d\omega}{\omega}$
Asymptotic value $(N, V \to \infty)$		
Insulators	0	Finite
Nonideal conductors	0	∞
Ideal conductors	Finite	∞

Localization of C of M - X



Example of 2 electrons in 1d

Individual electron positions not localized

C of M = X = (1/2)(x_1 + x_2) localized

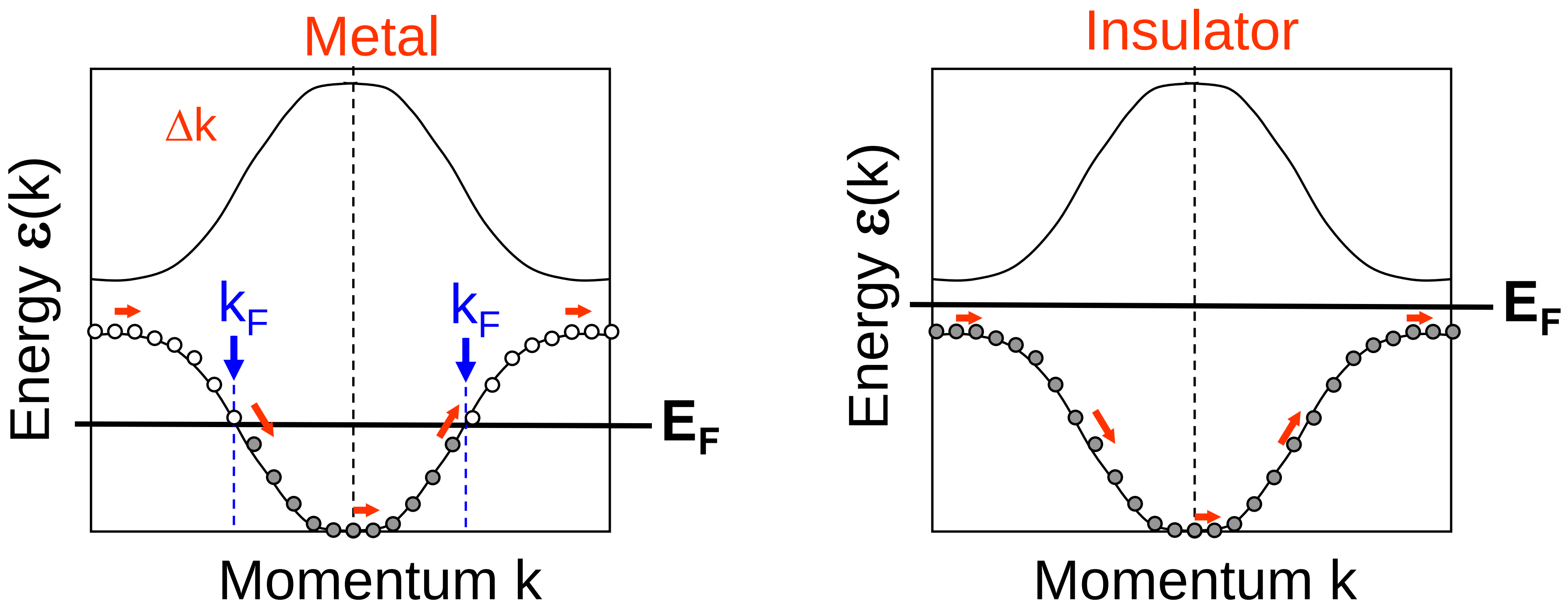
Well separated for large N

Figure by Souza – copied from Kohn, Les Houches Lectures (1968)

Kohn's figure indicating "the nature of the insulating state"

Torus (Bloch) Boundary Conditions

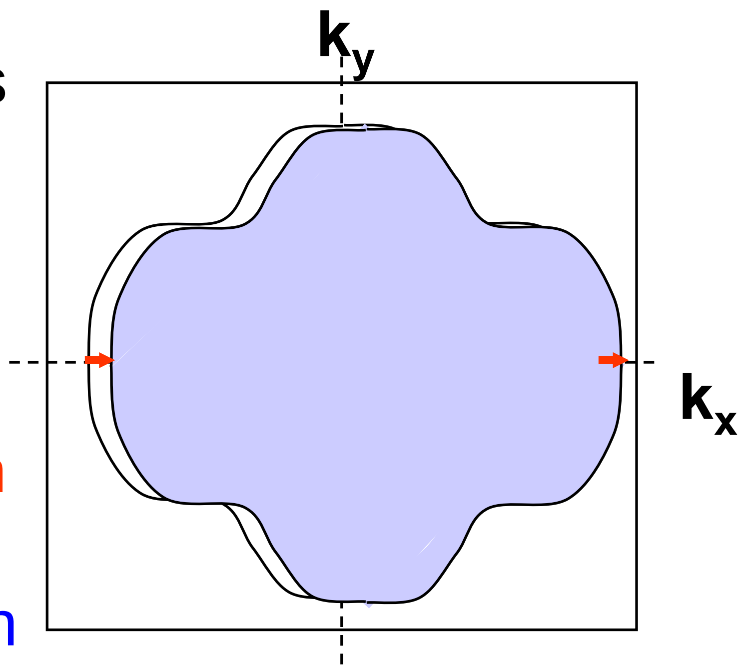
- Change due to the shift in Δk (effect of boundary conditions)



- Kohn(1964) – change in energy – $\Delta E \sim \Delta k^2$ in a metal
- Vanderbilt, Resta, Souza, .. – overlap $\langle \phi_k | \phi_{k+\Delta k} \rangle$ determines polarization, localization, "geometric distance" in an insulator
- Oshikawa, others – change in momentum in a metal

Luttinger Theorem - again

- **Oshikawa derivation – non-perturbative**
- Consider non-interacting electrons
- Shift Δk due to boundary conditions
- All electrons inside Fermi Surface shift by Δk
- Change in total momentum N Δk



- **Interactions conserve momentum**
- Therefore the total momentum is the same independent of electron-electron interactions
- **Since the only low energy excitations are at the Fermi energy ⟶ the Luttinger Theorem for the volume of the Fermi Surface!**

The continuing Saga of the Luttinger Theorem

Commensurability, Excitation Gap, and Topology in Quantum Many-Particle Systems on a Periodic Lattice

Masaki Oshikawa, Phys. Rev. Lett. 84, 1535–1538 (2000)

In combination with Laughlin's treatment of the quantized Hall conductivity, the Lieb-Schultz-Mattis argument is extended to quantum many-particle systems (including quantum spin systems) with a conserved particle number on a periodic lattice in arbitrary dimensions. Regardless of dimensionality, interaction strength, and particle statistics (Bose or Fermi), a finite excitation gap is possible only when the particle number per unit cell of the ground state is an integer.

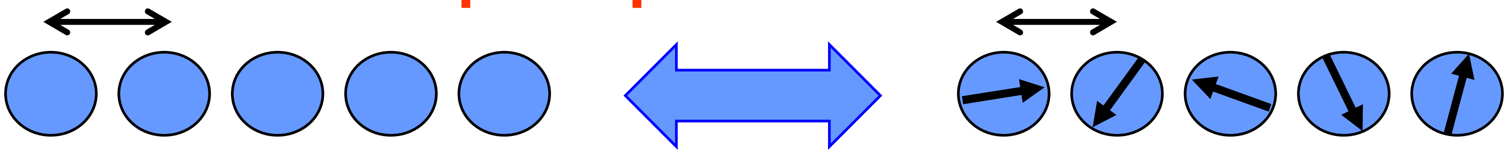
- Appears to rule out the possibility of a Mott Insulator with no broken translation or spin symmetry -----
- BUT there is another possibility – if the ground state is degenerate, the change in the total momentum may include a discrete Δp from the global change in the ground state with boundary conditions

Revised Statement of Luttinger Theorem

- The change in total momentum NΔk with change in boundary conditions is the same independent of electron-electron interactions
- If the ground state is degenerate, the change in the total momentum may include a discrete Δp from the global change ground state with boundary conditions
- Examples:
  - Antiferromagnetic order – doubles unit cell - 2-fold degenerate ground state
  - Peierl's distortion – doubles unit cell - 2-fold degenerate ground state
  - Spin liquid state – **IF** there is a degenerate ground state

Spin Liquid - again

- **Band metal to spin liquid transition**



"Disordered" spins
– no new order
Cell same – BZ same

- The new statement of Luttinger's theorem is consistent with an insulating state if there is an odd number of electrons per cell and there is a topological order
  - Degenerate ground state
  - Even though there is no change in the translation or spin symmetry
  - No local probe can distinguish the degenerate states
  - Distinguished only by global properties
- **Requires topological order in the spin liquid state**

See Paramekanti and Vishwanath, PRB (2004)

Spin Liquid – Examples(?)

- **Z_2 Phase**
  - So called because it has the same 2-fold degeneracy as the Ising model (global up/down symmetry)
  - Several very special models have been constructed See Paramekanti and Vishwanath, PRB (2004)
  - Fractional excitations

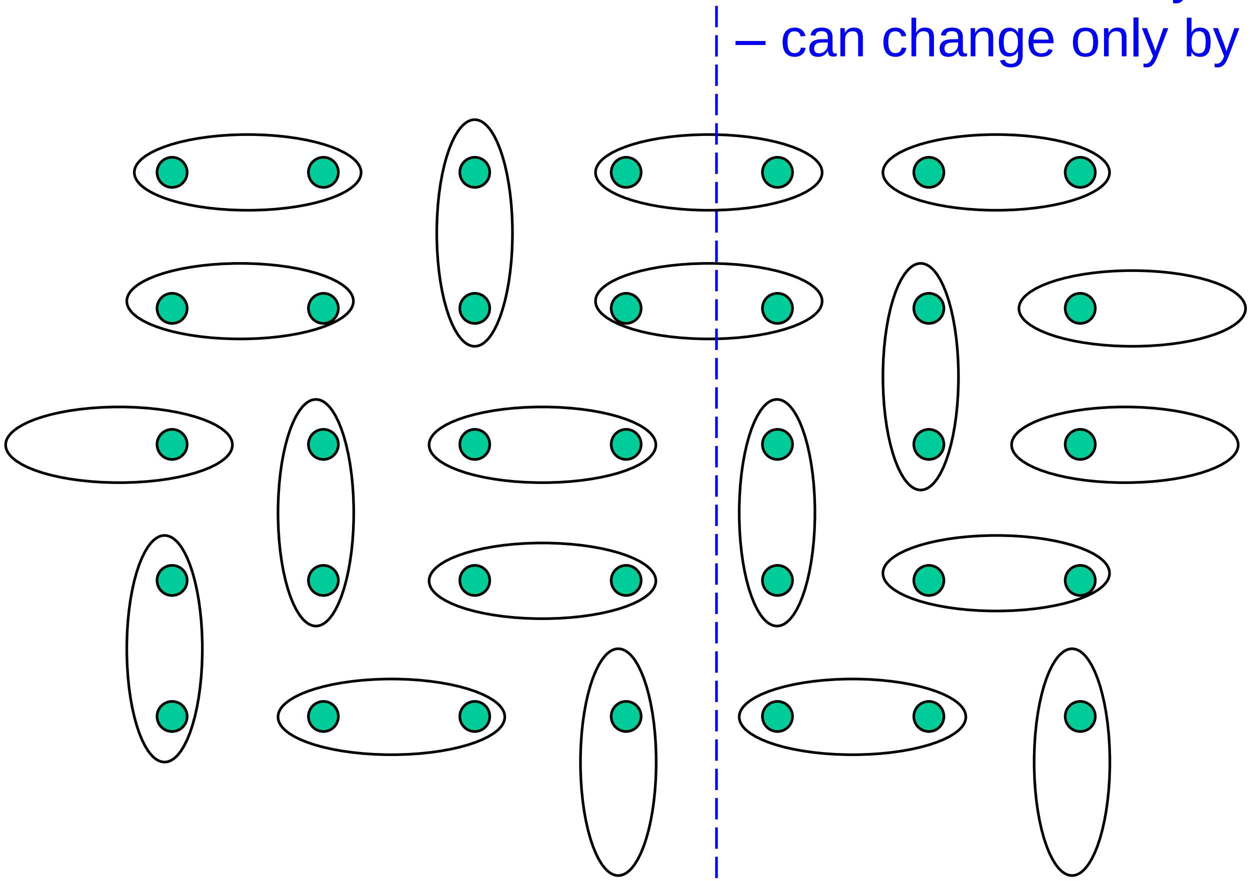
- **Wigner Crystal in 2D**
  - Bernu, Candido, Ceperley PRL (2001)
  - "likely" spin liquid similar to RVB state for ~50 < r_s < ~ 175
  - Ground state is 4-fold degenerate

Resonating Valence Bond (RVB) state

Short-range RVB - Bond formation with no long range order

Linear combination of states with pair bonds – like this example

bonds crossed by line is even or odd
– can change only by a global change



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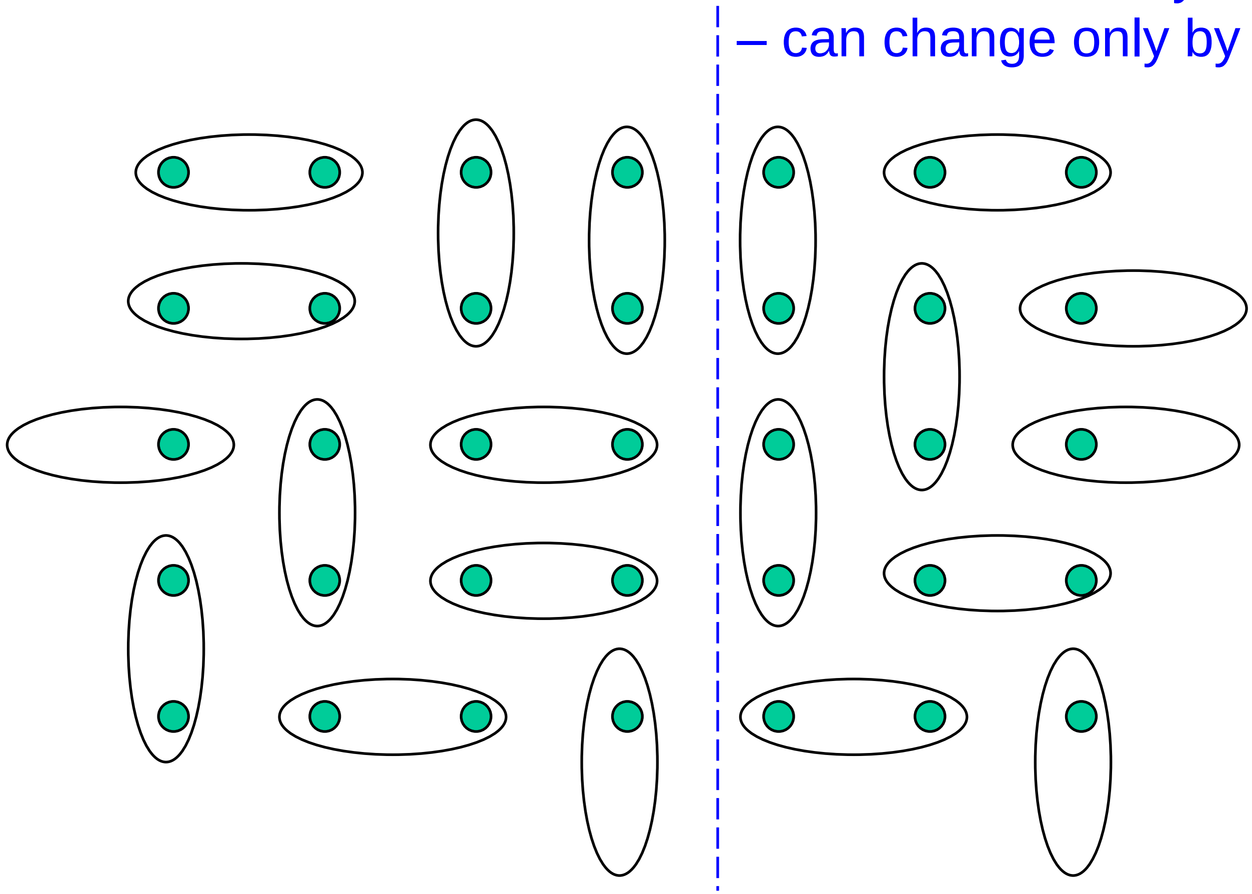


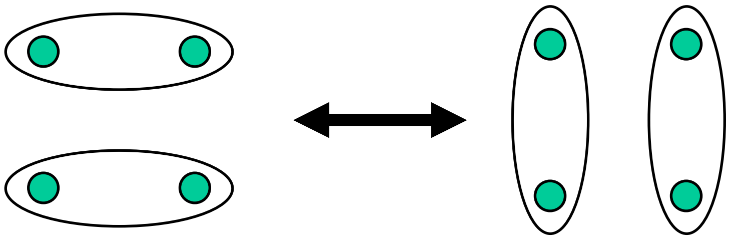
Real Example of Topological Order Fractional Quantum Hall State

- **Laughlin wavefunction**
  - Real example found in experiment
  - Fractional occupation of Landau state – Yet insulating state with a gap
  - Degenerate ground state on a torus
  - Fractional excitations
- **Experimental consequences**
  - A real sample is not a torus
  - Consequence on finite sample with edges – Edge states, . . .

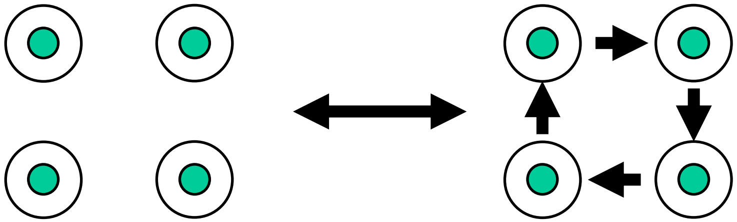
Mott Insulator without broken symmetry

- Proposal by D.-H. Lee and collaborators
  - Consider Hamiltonians that conserve both momentum and center of mass

- Examples:
  - Short Range RVB



  - Ring Exchange



Mott Insulator without broken symmetry

- **Proposal by D.-H. Lee and collaborators**
  - Consider Hamiltonians that conserve both momentum and center of mass

- **U (twist operator) and T (translation operator) commute with H**
  - [U,H] = [T,H] = 0

- **If the system has p/q electrons per site**
  - The ground state and the entire spectrum have q-fold degeneracy
  - Agrees with Oshikawa "theorem"

How can one detect such a state?

- Not from ground state on a torus
- Different boundary conditions

- Edge states, . . .

Conclusions I

- Key theoretical concepts: Global topology
  - Change of ground state with boundary conditions brings together:
    - **Quantum Hall Effect, Fractional QHE**
    - **Spin liquids – degenerate ground states - edge states**
    - **Polarization, Localization in insulators**
    - **Theorems on the Fermi surface of metals**
    - **Possible new topologically ordered states of Fermi Liquids**

- New derivation of a generalized Luttinger theorem
  - Simple, Non-perturbative "momentum balance" argument

- The volume of the Fermi Surface may change for different topologically ordered (degenerate) ground states,
  - Possible realizations of a Mott insulator with no broken translation or spin order

Conclusions II

- What does this have to do with my specialization – “electronic structure” of materials
- Challenge to make quantitative predictions for real systems
  - The theory of electric polarization in terms of “Berry’s phases” is now is the textbooks – widely used
  - Now we are poised to extend the ideas of Kohn and others to new states with interesting topologies
- Fundamental understanding of many-body systems
  - What is a Fermi liquid?
  - Luttinger theorem
  - New ideas on topology of Fermi surface
- New phases of strongly correlated systems
  - Spin liquids, edge states, stripes, superconductors, . . .

What do these papers have in common?

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THE END

The continuing Saga of the Luttinger Theorem

Phys. Rev. Lett. 65, 1490–1493 (1990)
Symmetry breaking in Mott insulators

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We explore the connection between Mott-insulating behavior and the breakdown of lattice-translation symmetry. We find that if a system of hard-core particles in $d=2$ is given to be a Mott insulator, then the charge must form a commensurate charge-density wave. This is true for particles of any statistics. Our result is based on duality arguments and does not seem to depend on the details of the Hamiltonian. For average site-occupation number $n<1$, this implies a breakdown of lattice-translation symmetry.

The continuing Saga of the Luttinger Theorem

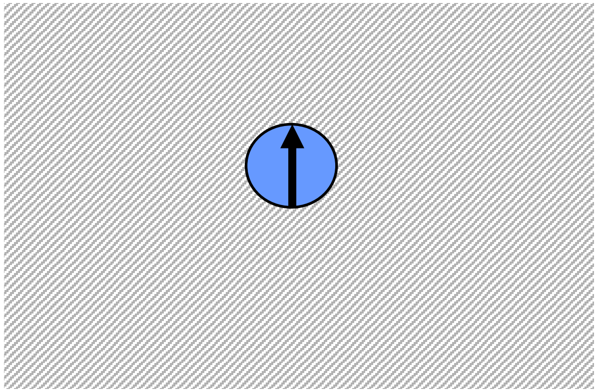
Phys. Rev. Lett. 84, 3370–3373 (2000)
Topological Approach to Luttinger's Theorem and the Fermi Surface of a Kondo Lattice

Masaki Oshikawa

A nonperturbative proof of Luttinger's theorem, based on a topological argument, is given for Fermi liquids in arbitrary dimensions. Application to the Kondo lattice shows that even completely localized spins contribute to the Fermi sea volume as electrons, whenever the system can be described as a Fermi liquid.

Kondo/Anderson Problem

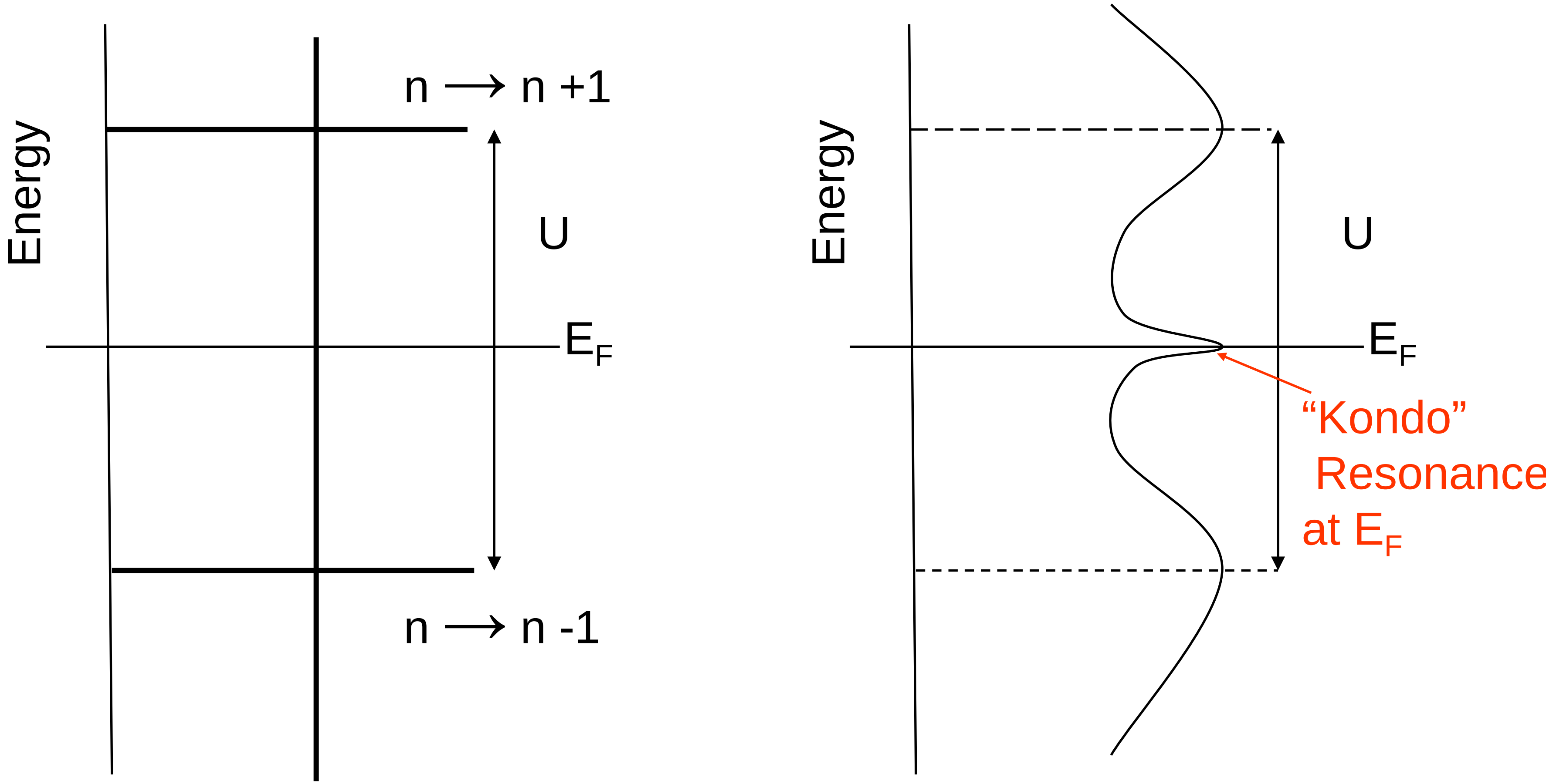
- **Impurity problem**
  - A single impurity in a metal
  - If the impurity were decoupled from the metal it would have a localized state with a spin
  - What happens when the state is coupled to the metal



- **Exact solution**
  - Singlet ground state
  - Friedel Sum rule obeyed – analogy of the Luttinger theorem for impurity
  - States at th Fermi surface are modified so that the localized state counts in the Fermi surface
  - Spin contributes to Fermi surface!

Kondo/Anderson Problem

- **Impurity problem**
  - Density of states

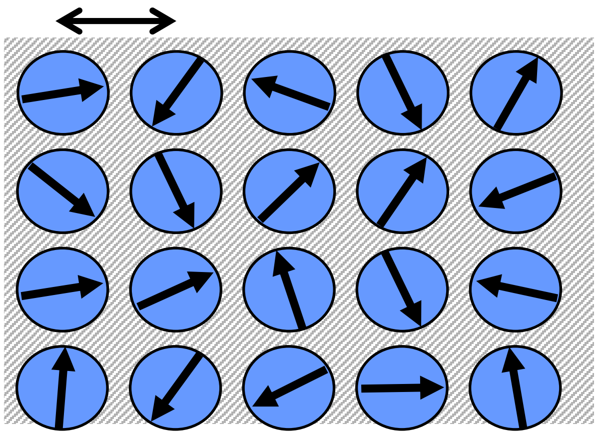


Decoupled

Coupled

Kondo/Anderson Problem

- **Kondo/Anderson Lattice**
  - Spin (localized electrons) on every site
  - Also wide metallic band
  - What happens when spins are coupled to metallic band?

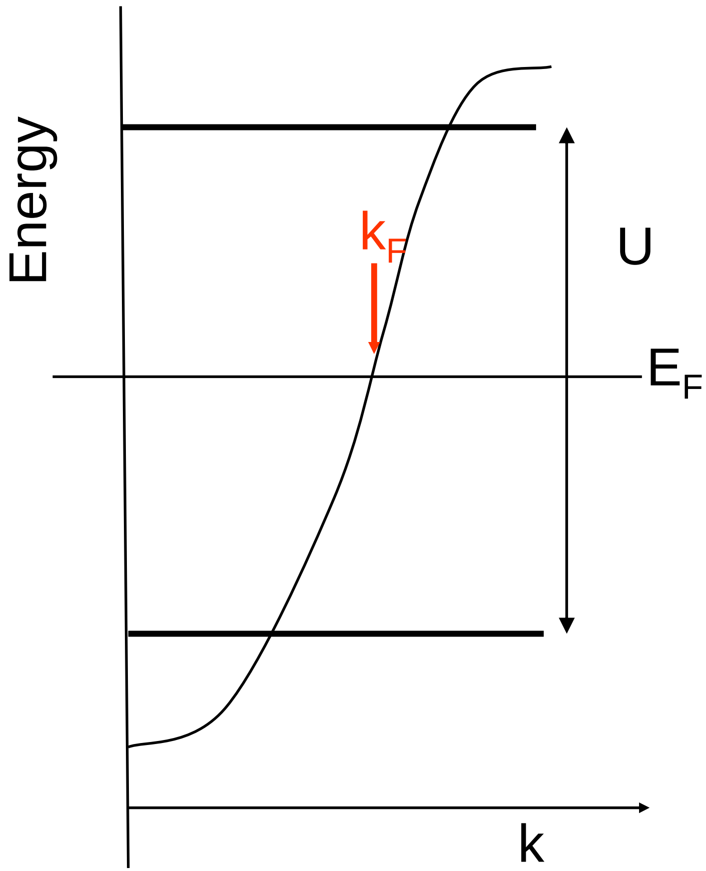


- **Do the spins (localized electrons) count in the Fermi surface?**
  - No exact solutions
  - **YES** – if the Luttinger theorem is satisfied. All the electrons count in the Fermi surface !
  - **No** – If the spins form a spin liquid with a gap. Then they would NOT be counted in the Fermi surface.
  - **Is the Luttinger theorem valid for strongly interacting systems? (Recall that Luttinger's derivation is based upon a perturbation expansion.)**

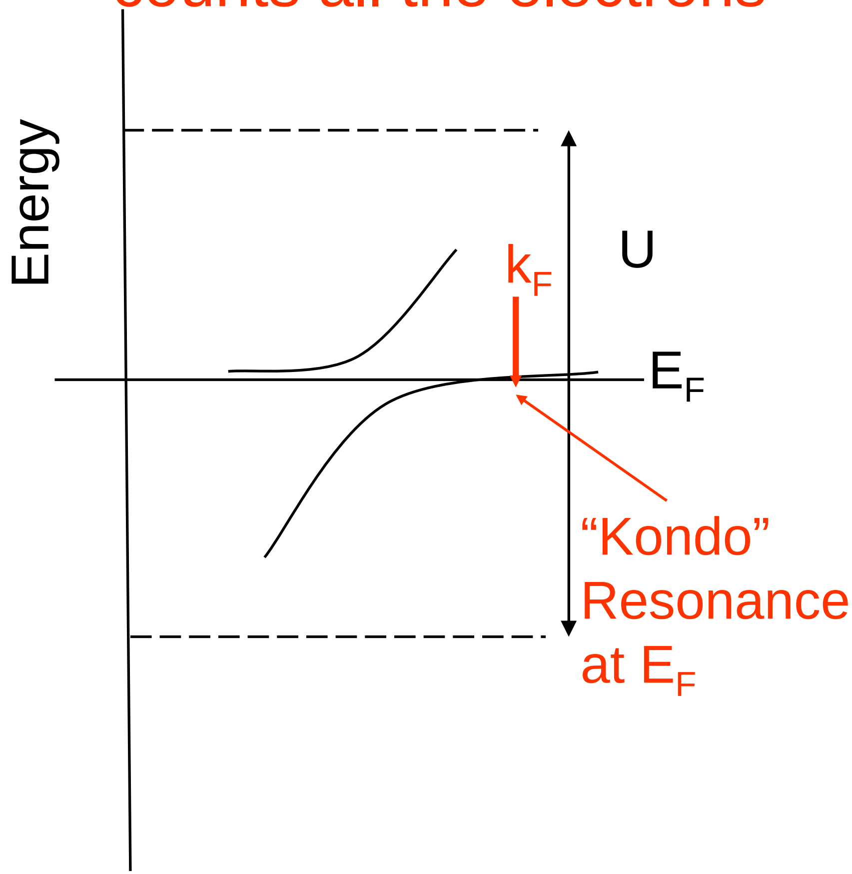
Kondo/Anderson Problem

- **Kondo/Anderson Lattice**
  - Prediction of Luttinger Th.

Fermi Surface Volume counts all the electrons



Decoupled



Coupled