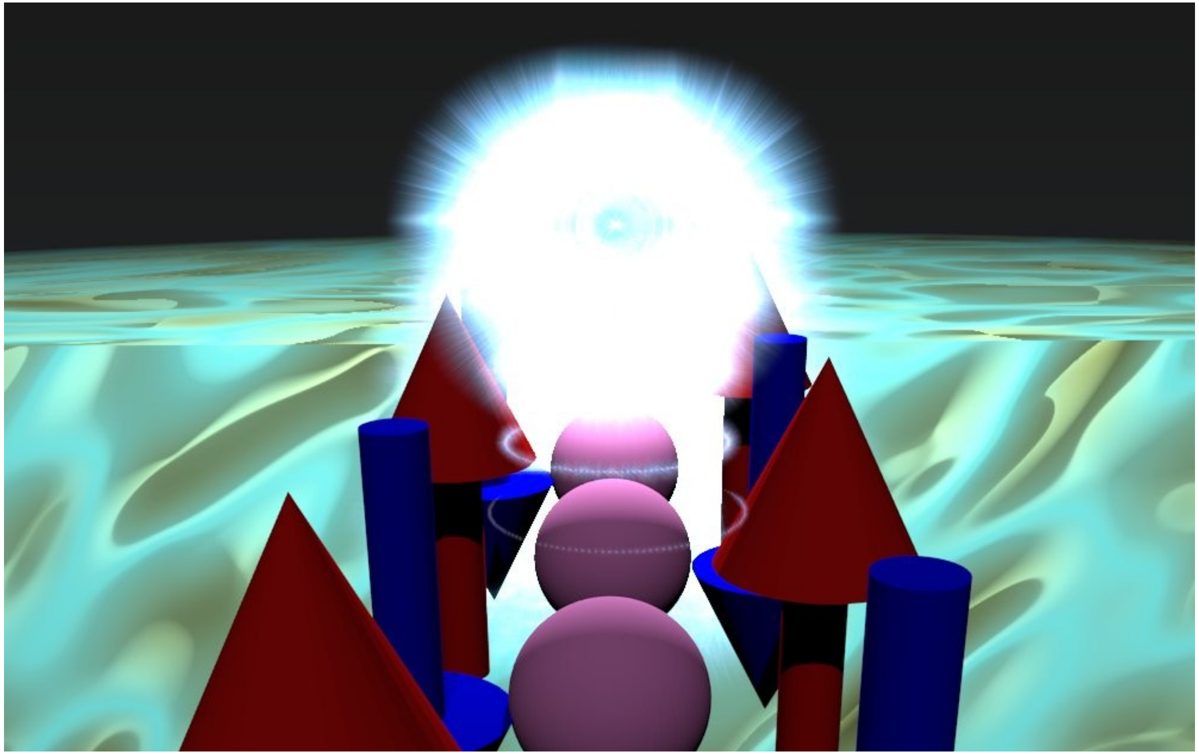
# Linear response theory, Kubo formalism



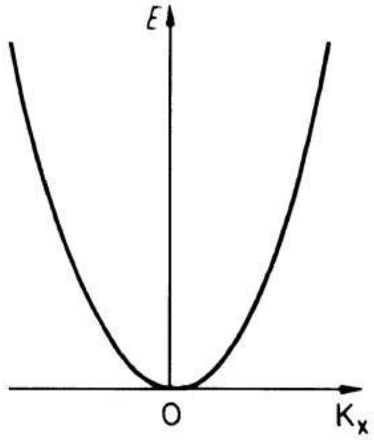
March 22nd 2021

# A reminder from session #3

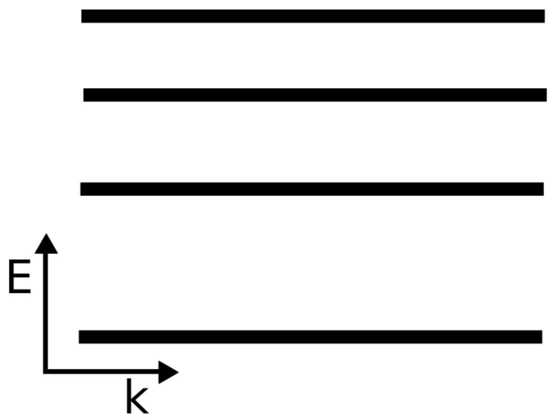
**Hamiltonians with translational symmetry can be diagonalized using Bloch's theorem, yielding a band-structure**

$$H = \sum_{\alpha,k} \epsilon_{\alpha,k} \Psi^{\dagger}_{\alpha,k} \Psi_{\alpha,k}$$

***Parabolic band***




***Flat bands***



# Learning outcomes

- Non-equibrium response can be computed with the equilibrium ground state
- Responses allow to predict instabilities
- Certain responses can be quantized

# Today’s plan

- The response in classical magnets
- Linear response in quantum systems
- Linear response for many electrons and electronic instabilities
- Hall conductivity and Chern invariant

# Response in materials


In general, for a certain observable *A* we will have

$$A(x, x', t, t')$$

**Which kind of perturbation?**

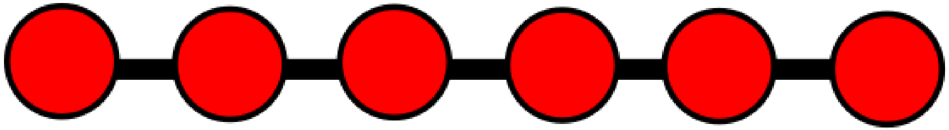
→ Charge (dielectric and conductivity)
→ Spin fluctuation (magnetic susceptibility)
→ Heat (thermal conductance)

# Today’s focus

**We will deal time-independent systems with translational symmetry**

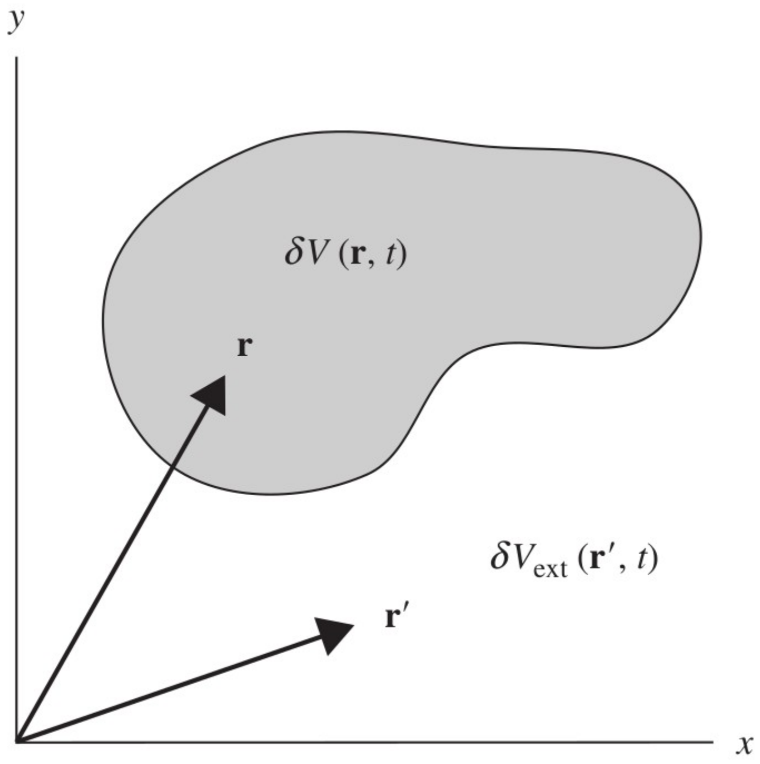
$$A(x, x', t, t') = A(x - x')$$

***(like the one dimensional infinite periodic chain)***



$$H = \sum_{i=-\infty}^{\infty} c_i^\dagger c_{i+1} + h.c.$$

# A simple example: charge response




$$\delta V(\mathbf{r}, t) = \int \epsilon^{-1}(\mathbf{r}, \mathbf{r}', t - t')\delta V_{\text{ext}}(\mathbf{r}', t')d\mathbf{r}'dt'$$

**Change in potential**

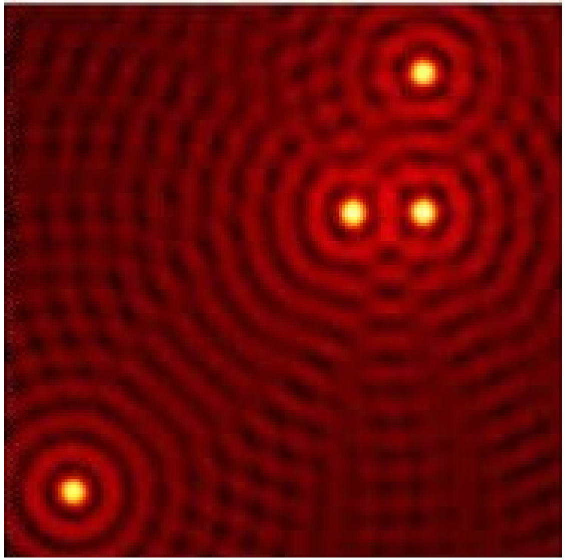
**Perturbation**

Linear response

# Types of responses

**Impurities in a metal**

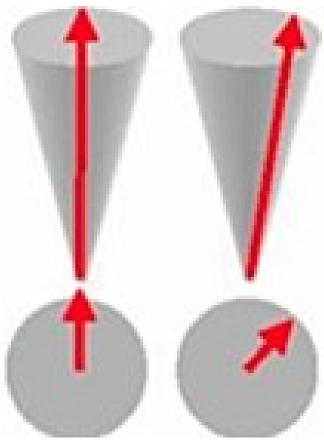
*Friedel oscillation*

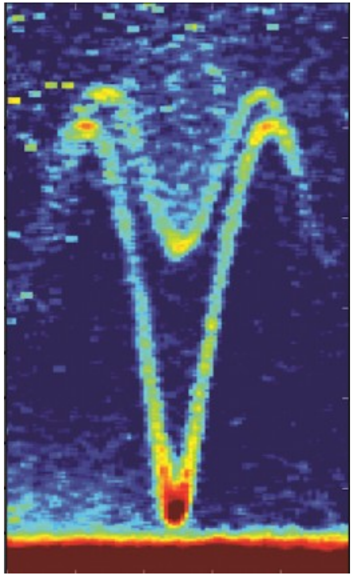


Information on the Fermi surface

**Neutron scattering**

*(Inelastic neutron-matter process)*

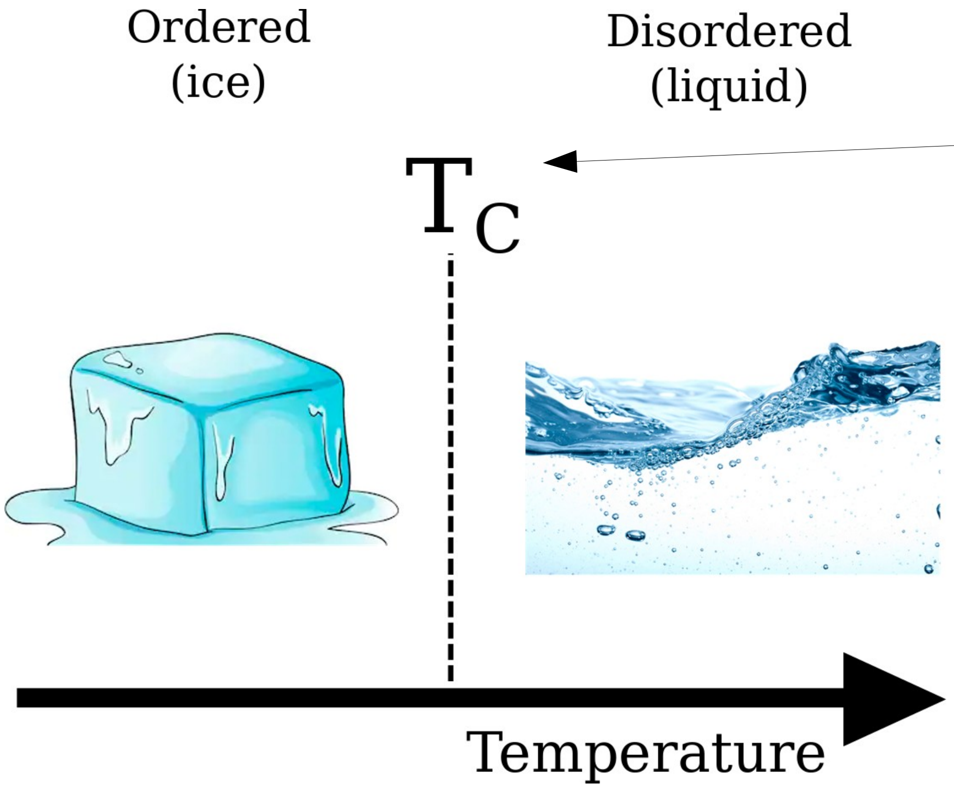




Information on magnetic excitations

# Magnetic response
# in a classical magnet

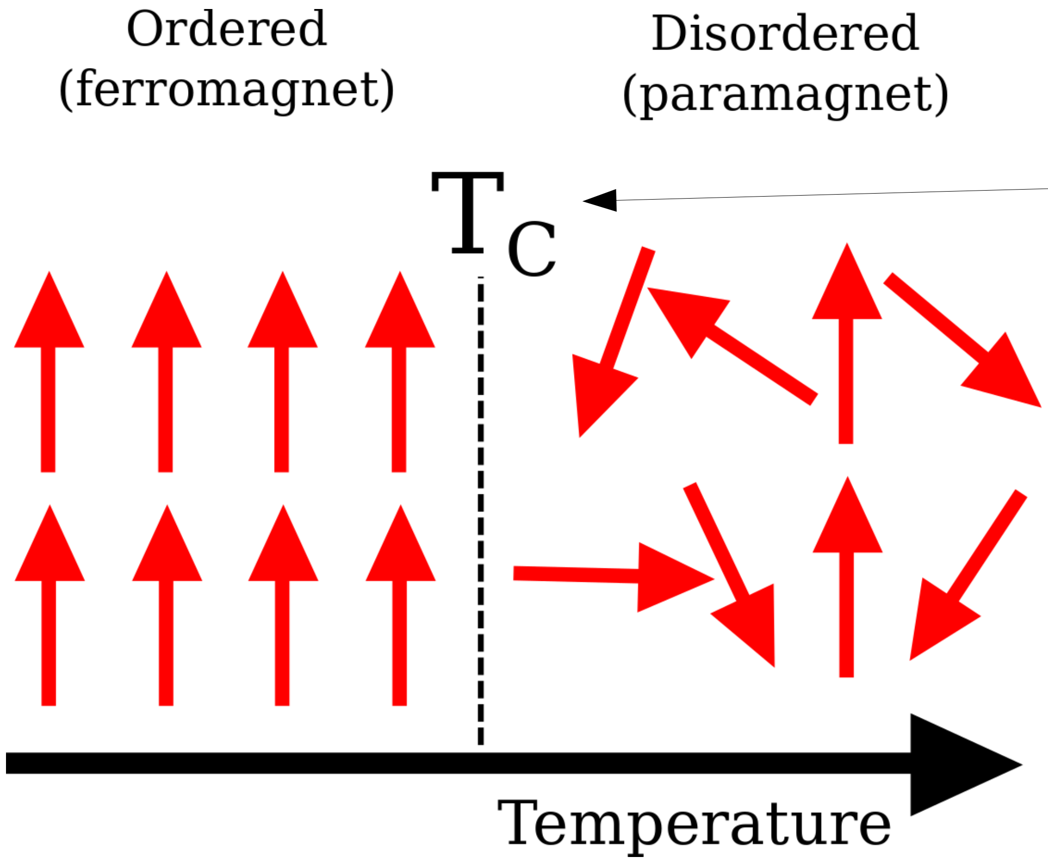
# Classical phase transitions




**Critical temperature**

**Can we know if water freezes by studying water in its liquid state?**

# Classical phase transitions




**Critical temperature**

**Can we know if a system orders from its high temperature behavior?**

# Magnetic susceptibility

$$\vec{M}$$

$$\vec{B}$$

**How does the magnetization of a material change when we apply an external magnetic field?**

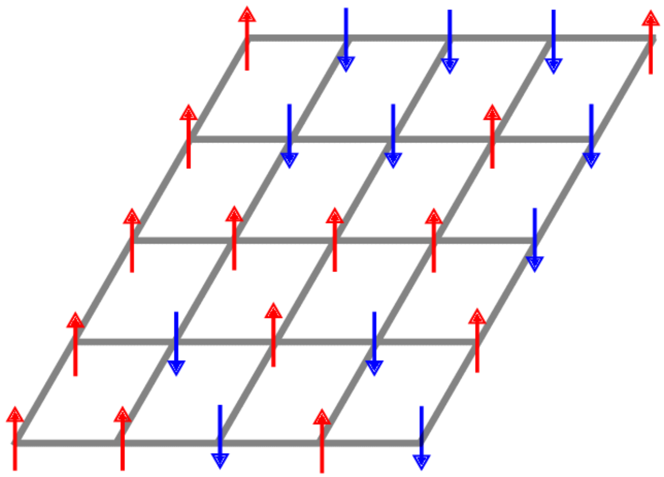
$$\vec{M}(\vec{B})$$

**at high temperatures?**

For small fields, we can perform a linear expansion

$$M_z(B_z) = \chi B_z \qquad \chi = \frac{\partial M_z}{\partial B_z}$$

# Magnetic susceptibility



Take an Ising model

$$H = J\sum_{\langle ij\rangle} S_i^z S_j^z + \sum_i B S_i^z$$

he high-temperature susceptibility (mean field) is $\chi = \frac{\partial M_z}{\partial B_z}$

***Paramagnet***

for $J = 0$

$$\chi \sim \frac{1}{T}$$

***Ferromagnet***

for $J < 0$

$$\chi \sim \frac{1}{T - T_C}$$

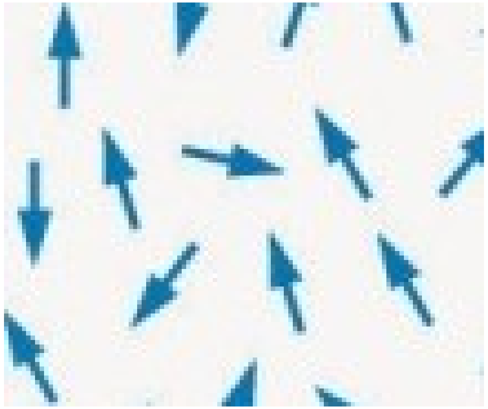
***Antiferromagnet***

for $J > 0$

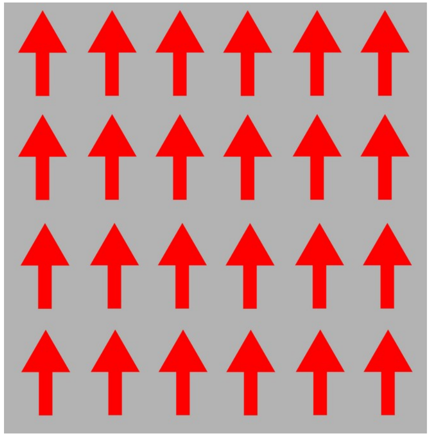
$$\chi \sim \frac{1}{T + T_C}$$

# Three types of magnetic systems

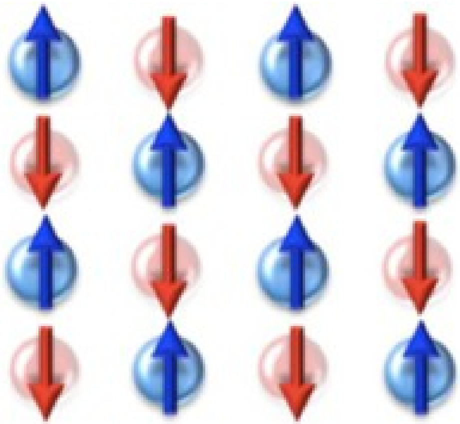
***Paramagnet***
(any T)



***Ferromagnet***
(low T)



***Antiferromagnet***
(low T)



***Paramagnet***

$$\chi \sim \frac{1}{T}$$

***Ferromagnet***

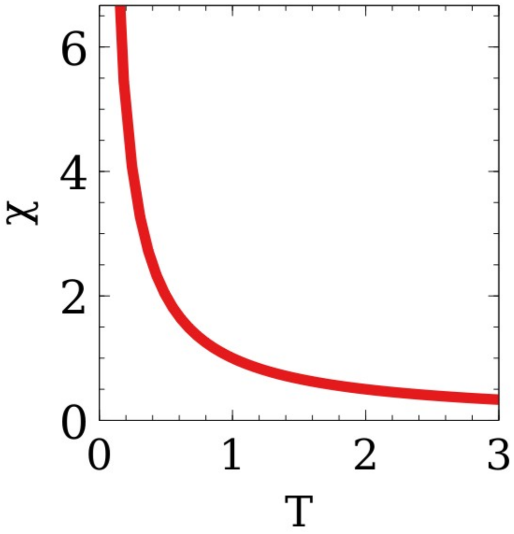
$$\chi \sim \frac{1}{T - T_C}$$

***Antiferromagnet***

$$\chi \sim \frac{1}{T + T_C}$$

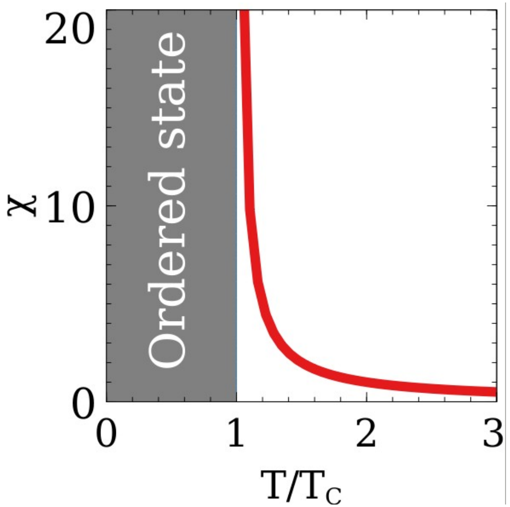
# The high-temperature susceptibility

**The high-T response tells us how the system behaves at low temperatures**



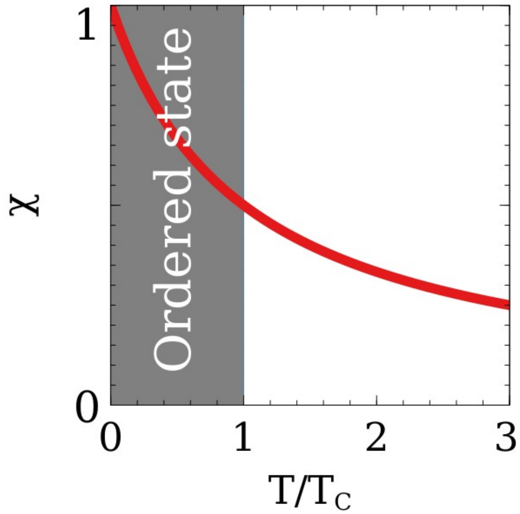

***Paramagnet***

$$\chi \sim \frac{1}{T}$$




***Ferromagnet***

$$\chi \sim \frac{1}{T - T_C}$$




***Antiferromagnet***

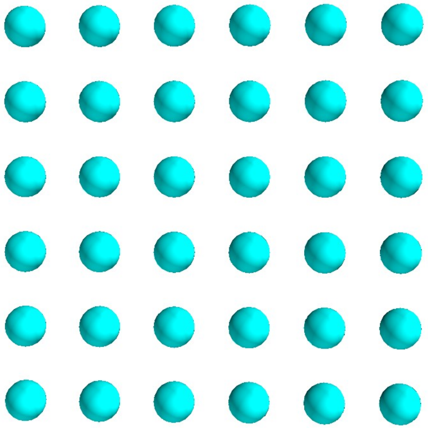
$$\chi \sim \frac{1}{T + T_C}$$

# Linear response in a quantum system

# Unperturbed and perturbed Hamiltonian

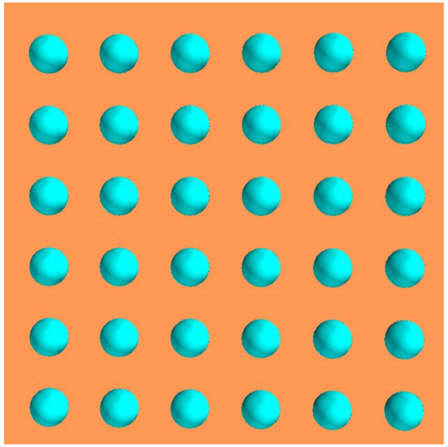
**Unperturbed Hamiltonian**

$$H_0$$



**Perturbed Hamiltonian**

$$H = H_0 + \lambda V$$



**Can we infer the properties of a perturbed Hamiltonian from the unperturbed one?**

# Perturbation theory

Take a Hamiltonian that includes a perturbation V

$$H(\lambda) = H_0 + \lambda V$$

**Every "well behaved" function is linear for small argument**

***Energy***

$$E_{GS}(\lambda)$$

***Observables***

$$\langle A \rangle(\lambda)$$

***Wavefunctions***

$$|\Psi_k\rangle(\lambda)$$

**We will use a Taylor expansion in terms of the parameter** $\lambda$

# Observables in linear response theory

$$H(\lambda) = H_0 + \lambda V$$

Full Hamiltonian

Perturbation

Unperturbed Hamiltonian

**For any observable**

$$A(\lambda) \approx A(\lambda = 0) + \lambda\chi$$

Full value

Unperturbed value

Contribution from the perturbation

**Response of the system**

$$\frac{\partial A}{\partial \lambda} \equiv \chi$$

# Eigenfunctions in linear response theory

$$H(\lambda) = H_0 + \lambda V$$

**Eigenfunctions after the perturbation**

$$|\Psi_i\rangle(\lambda) = |\Psi_i\rangle(\lambda = 0) + \lambda \sum_{j \neq i} \alpha_j |\Psi_j\rangle(\lambda = 0)$$

Eigenfunction after the perturbation

Eigenfunctions before the perturbation

# Eigenfunctions in linear response theory

$$H(\lambda) = H_0 + \lambda V$$

**Correction to the eigenfunctions to first order**

$$|\Psi_i\rangle(\lambda) = |\Psi_i^0\rangle + \lambda \sum_{j\neq i} \alpha_j |\Psi_j^0\rangle$$

**Coefficients**

$$\alpha_j = \frac{\langle\Psi_i^0|V|\Psi_j^0\rangle}{\epsilon_i^0 - \epsilon_j^0}$$

***Notation***

$$|\Psi_i^0\rangle \equiv |\Psi_i\rangle(\lambda = 0)$$

$$H_0|\Psi_i^0\rangle = \epsilon_i^0|\Psi_i^0\rangle$$

**The perturbed eigenfunctions can be expressed in terms of the unperturbed ones**

# Question: perturbation theory for two sites

**Take the full Hamiltonian** $$H = H_0 + \lambda V$$

**with unperturbed term** $$H_0 = \Delta c_1^\dagger c_1 - \Delta c_2^\dagger c_2$$

**and perturbation** $$V = c_1^\dagger c_2 + c_2^\dagger c_1$$

**The unperturbed eigenstates are** $\Psi_1^{0\dagger} = c_1^\dagger \quad \Psi_2^{0\dagger} = c_2^\dagger$

***What are the eigenstates for small*** $\lambda$ ***?***

***Remember*** $$\Psi_i(\lambda) = \Psi_i^0 + \lambda \sum_{j \neq i} \alpha_j \Psi_j^0 \qquad \alpha_j = \frac{\langle \Psi_i^0 | V | \Psi_j^0 \rangle}{\epsilon_i^0 - \epsilon_j^0}$$

# Question: perturbation theory for two sites

$$H = H_0 + \lambda V = \epsilon_1 \Psi_1^\dagger \Psi_1 + \epsilon_2 \Psi_2^\dagger \Psi_2$$

$$H_0 = \Delta c_1^\dagger c_1 - \Delta c_2^\dagger c_2 \qquad V = c_1^\dagger c_2 + c_2^\dagger c_1$$

**Unperturbed eigenstates**

$$\Psi_1^{0\dagger} = c_1^\dagger \quad \Psi_2^{0\dagger} = c_2^\dagger$$

$$\epsilon_1^0 = -\Delta \quad \epsilon_2^0 = \Delta$$

**Using the formula from perturbation theory from the previous slide we get**

$$\Psi_1^\dagger = c_1^\dagger - \frac{\lambda}{2\Delta} c_2^\dagger \qquad \Psi_2^\dagger = c_2^\dagger + \frac{\lambda}{2\Delta} c_1^\dagger$$

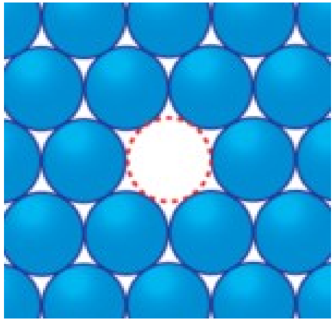
# Breakdown of perturbation theory

$$H(\lambda) = H_0 + \lambda V$$

Is any full many-body ground state perturbative in terms of $\lambda$ ?

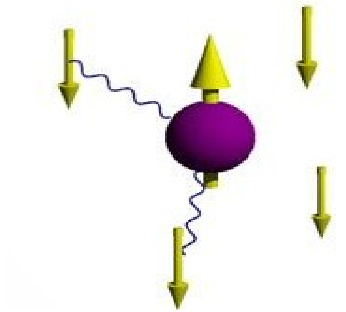
**No! Certain quantum states are intrinsically non-perturbative**

***Impurity in a metal***
***(Orthogonality catastrophe)***



*The many-body ground state*
*Is orthogonal to the original*

***Quantum spin in a metal***
***(Kondo effect)***



*The Kondo temperature*
*is non-perturbative*

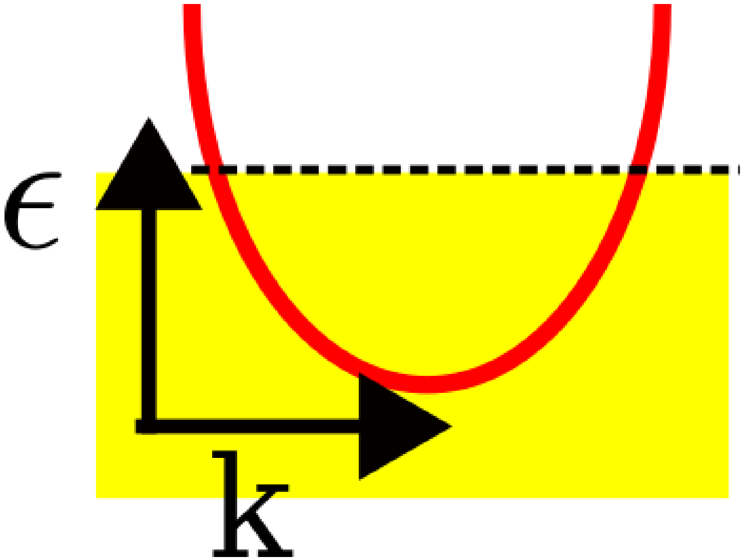
***Superconductivity***
***(BCS limit)***

*The superconducting gap*
*is non-perturbative*

# Many-body response

# The Fermi sea

**Take a certain band-structure**




$$\epsilon_F = 0$$

$$H = \sum_k \epsilon_k \Psi_k^\dagger \Psi_k$$

**States below the Fermi energy are filled**

**The Fermi surface is the set of k-points that cross the Fermi energy**

$$\{\vec{k}\} \text{ with } \epsilon_{\vec{k}} = \epsilon_F$$

# Question: The many-electron energy

**Imagine that we have the following fermionic Hamiltonian**

$$H = \Psi_1^\dagger \Psi_1 - \Psi_2^\dagger \Psi_2 - \Psi_3^\dagger \Psi_3$$

**What is the many-body state with lowest energy $E_{GS}$?**

$$H|GS\rangle = E_{GS}|GS\rangle$$

$$\{\Psi_i^\dagger, \Psi_j\} = \delta_{ij}$$

$$\Psi_i|\Omega\rangle = 0$$

***Option #1***

$$|GS\rangle = \Psi_2^\dagger|\Omega\rangle$$

***Option #2***

$$|GS\rangle = |\Omega\rangle$$

***Option #3***

$$|GS\rangle = \Psi_2^\dagger \Psi_3^\dagger|\Omega\rangle$$

# Question: The many-electron energy

**What is the lowest energy state of this Hamiltonian?**

$$H = \Psi_1^\dagger \Psi_1 - \Psi_2^\dagger \Psi_2 - \Psi_3^\dagger \Psi_3$$

$$H|GS\rangle = E_{GS}|GS\rangle$$

***Option #1***

$$|GS\rangle = \Psi_2^\dagger|\Omega\rangle$$

$$H|GS\rangle = -|GS\rangle$$

$$E_{GS} = -1$$

***Option #2***

$$|GS\rangle = |\Omega\rangle$$

$$H|GS\rangle = 0$$

$$E_{GS} = 0$$

***Option #3***

$$|GS\rangle = \Psi_2^\dagger \Psi_3^\dagger|\Omega\rangle$$

$$H|GS\rangle = -2|GS\rangle$$

$$E_{GS} = -2$$

***This is the state with lowest energy***

# Ground state of an electronic system

**Lets take a fermionic Hamiltonian in diagonal form**

$$H = \sum_k \epsilon_k \Psi_k^\dagger \Psi_k \qquad \{\Psi_i^\dagger, \Psi_j\} = \delta_{ij}$$

***The many body eigenstate with minimum energy (ground state) is***

$$|GS\rangle = \prod_{k \in occ} \Psi_k^\dagger |\Omega\rangle$$

Where *occ* is the set of *k* with $\epsilon_k < 0$

with $\Psi_k|\Omega\rangle = 0$

$$H|GS\rangle = E_{GS}|GS\rangle$$

The total ground state energy is $E_{GS} = \sum_{k \in occ} \epsilon_k$

# Expectation values for the many electron system

**Ground state**

$$|GS\rangle = \prod_{k\in occ} \Psi_k^\dagger|\Omega\rangle$$

**Hamiltonian**

$$H = \sum_k \epsilon_k \Psi_k^\dagger \Psi_k$$

***By definition***

$$\langle GS|\Psi_\alpha^\dagger \Psi_\alpha|GS\rangle = 1 \quad \text{if } \alpha \in occ$$
$$\langle GS|\Psi_\alpha^\dagger \Psi_\alpha|GS\rangle = 0 \quad \text{if } \alpha \notin occ$$

**Ground state energy**

$$E_{GS} = \langle GS|H|GS\rangle = \sum_{k\in occ} \epsilon_k$$

# Perturbation theory for the many electron system

$$H = H_0 + \lambda V$$

$$|GS\rangle = \prod_{k \in occ} \Psi_k^\dagger |\Omega\rangle \qquad V = c_0^\dagger c_0 \qquad H_0 = \sum_k \epsilon_k \Psi_k^\dagger \Psi_k$$

The change in charge in the system is defined as

$$\langle c_n^\dagger c_n \rangle - \langle c_n^\dagger c_n \rangle_{GS} \equiv \chi(n)\lambda$$

Given that we have translational symmetry, we will work with the Fourier transform

$$\chi(q) = \sum_n e^{iqn} \chi(n)$$

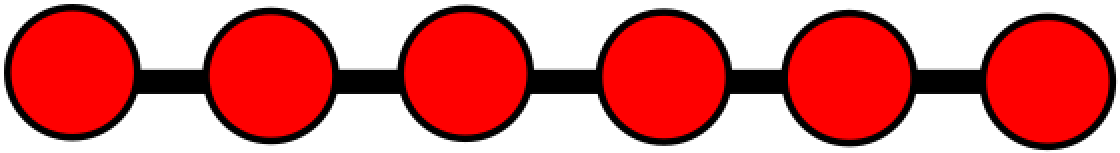
# The Lindhard formula

**Using the formulas from perturbation theory we can show**

$$\chi(q) = \sum_k \frac{n_k - n_{k+q}}{\epsilon_k - \epsilon_{k+q}}$$

$$n_k = \langle GS|\Psi_k^\dagger \Psi_k|GS\rangle$$

$$n_k = 0, 1$$



$$H = \sum_k \epsilon_k \Psi_k^\dagger \Psi_k$$

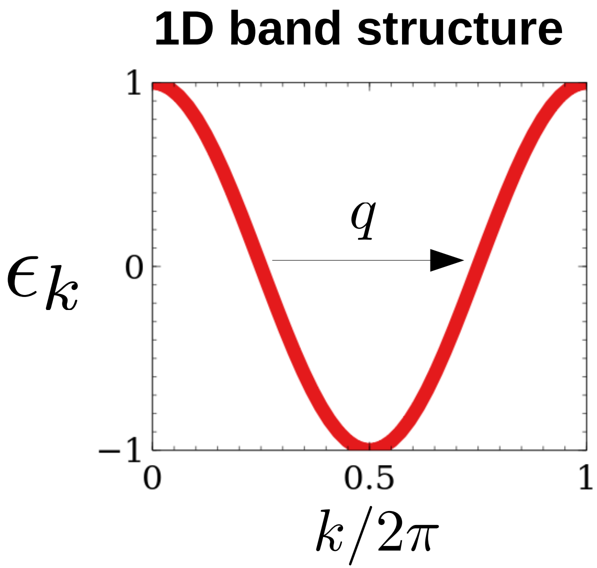
# Instabilities and nesting

***Take the form of the static response***

$$\chi(q) = \sum_k \frac{n_k - n_{k+q}}{\epsilon_k - \epsilon_{k+q}}$$

The response diverges for

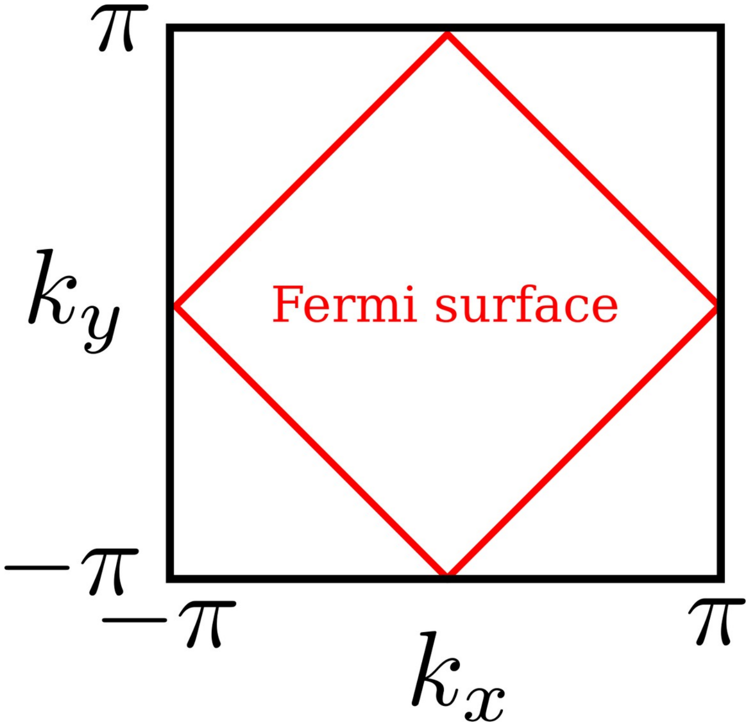
$$\epsilon_k = \epsilon_{k+q}$$




**A very small perturbation creates a huge response in the system, yielding an instability**

# Question: instabilities in the square lattice

**The Fermi surface of the square lattice at half filling has this form**




**Fermi surface for** $\epsilon_k = 0$

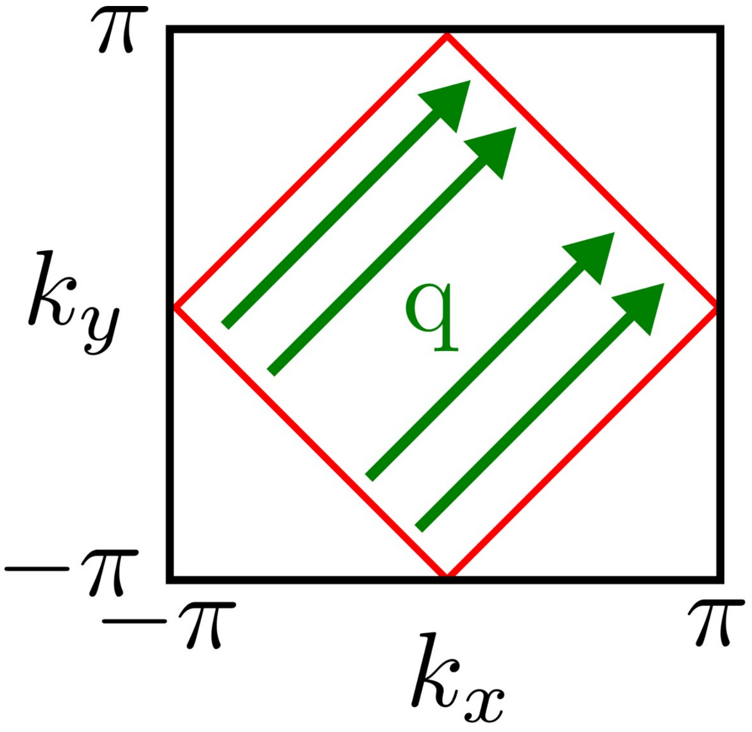
$$\chi(q) = \sum_k \frac{n_k - n_{k+q}}{\epsilon_k - \epsilon_{k+q}}$$

$$n_k = 0, 1$$

**At which q-vector does the response diverge?**

# Question: instabilities in the square lattice

**There is a common q vector that links same energy states**




$$\chi(q) = \sum_k \frac{n_k - n_{k+q}}{\epsilon_k - \epsilon_{k+q}}$$

$$n_k = 0, 1$$

The response diverges at

$$q = \frac{\pi}{2}(1, \pm 1)$$

# Fluctuations and instabilities

**Fluctuation**

**What is the condition for a small perturbation to "break down" a ground state?**

# Classical example of instability

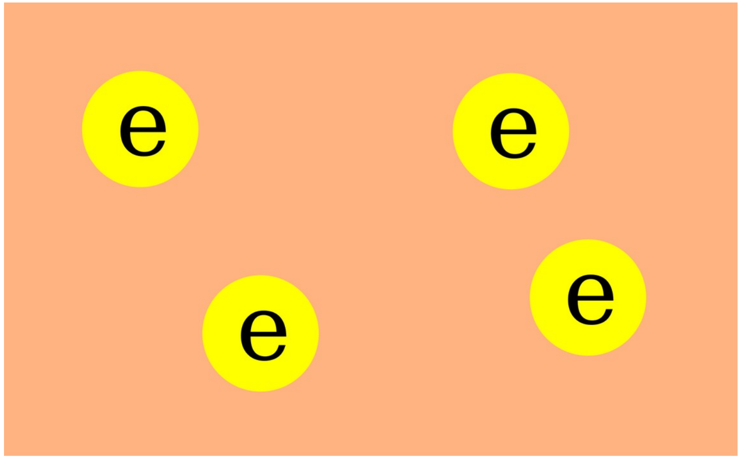
**Supercooled (high purity) water**

https://www.youtube.com/watch?v=_9N-Y2CyYhM

***Below 0 degrees, a perturbation will freeze supercooled water***

# Instability in an electronic system

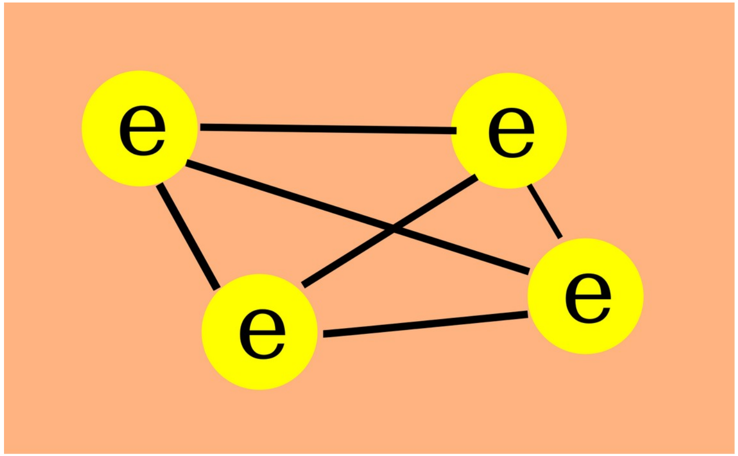
**Without interactions**




**Response of the non-interacting system**

$$\chi_0$$

**With interactions**




**Response of the interacting system**

$$\chi$$

**How to know when a ground state breaks down due to interactions?**

# Instabilities, nesting and interactions

**But what if we now have interactions in the Hamiltonian?**

***Free Hamiltonian*** ***Interactions***

$$H = \sum_{k} \epsilon_k \Psi_k^\dagger \Psi_k + \sum_{k,k' q} v_q \Psi_{k+q}^\dagger \Psi_k \Psi_{k'-q}^\dagger \Psi_{k'}$$

***The random phase approximation (RPA) for the charge response***

Response of the full Hamiltonian

$$\chi(q) \approx \frac{\chi_0(q)}{1 + v_q \chi_0(q)}$$

Response of the free Hamiltonian

**The full response diverges when** $v_q \chi_0(q) = -1$

# Magnetic instabilities of an electron gas

**Spinful Hamiltonian with local interactions**

$$H = \sum_{k,s} \epsilon_k \Psi^\dagger_{k,s} \Psi_{k,s} + \sum_k U c^\dagger_{n\uparrow} c_{n\uparrow} c^\dagger_{n\downarrow} c_{n\downarrow}$$

**RPA for the spin response**

$$\chi^s(0) \approx \frac{\chi^s_0(0)}{1 - U\chi^s_0(0)}$$

***Density of states (DOS)***

$$D(\omega) = \sum_k \delta(\omega - \epsilon_k)$$

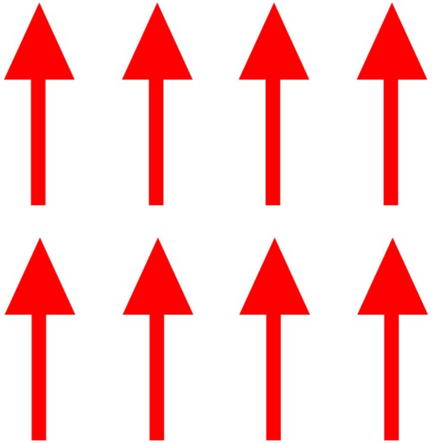
**The Stoner criterion**

$$D(\omega = 0)U = 1$$

**A system can become magnetic when DOS times interactions is sufficiently large**

# Interacting instabilities in materials

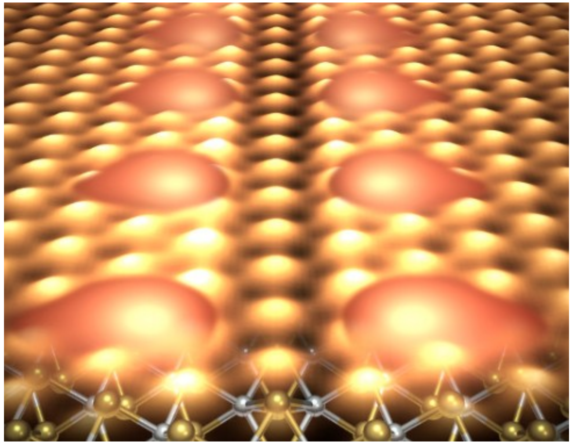
***Magnetism***



*Instability in the*
*spin response*

*(repulsive interaction)*

***Dimerization &***
***charge density wave***



Instability in the
charge/phonon response

*(repulsive interaction)*

**Superconductivity**

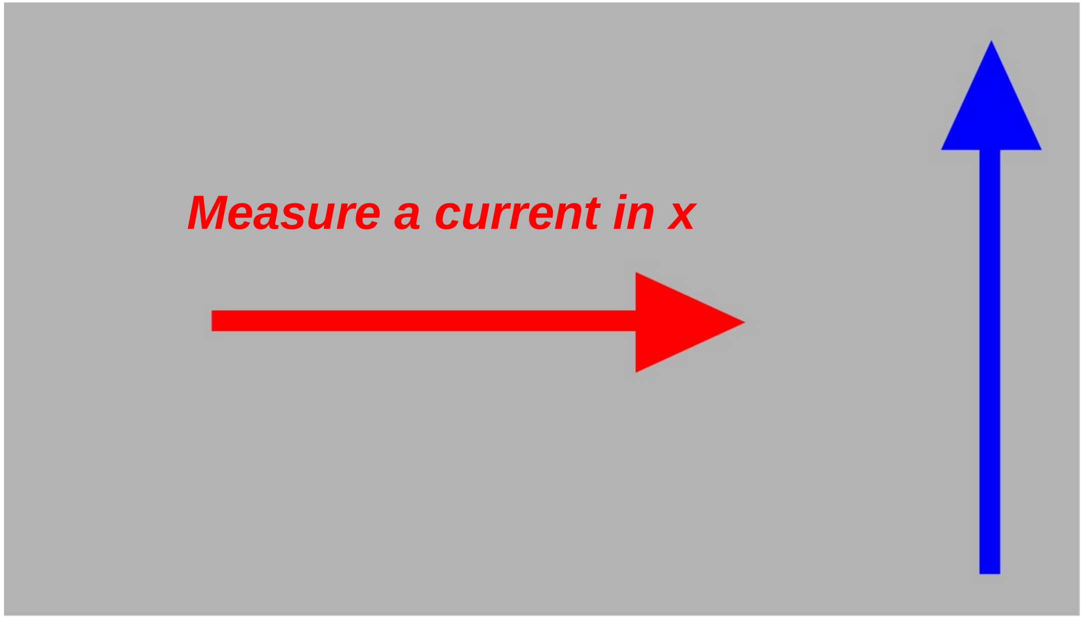
Instability in the
e-e scattering

*(attractive interaction)*

# The Hall conductivity and Chern number

# The transverse conductivity

**Take a two-dimensional material**




***Apply a voltage in y***

$$J_x = \sigma_{xy} V_y$$

***Full Hamiltonian***

$H = H_0 + \lambda V$

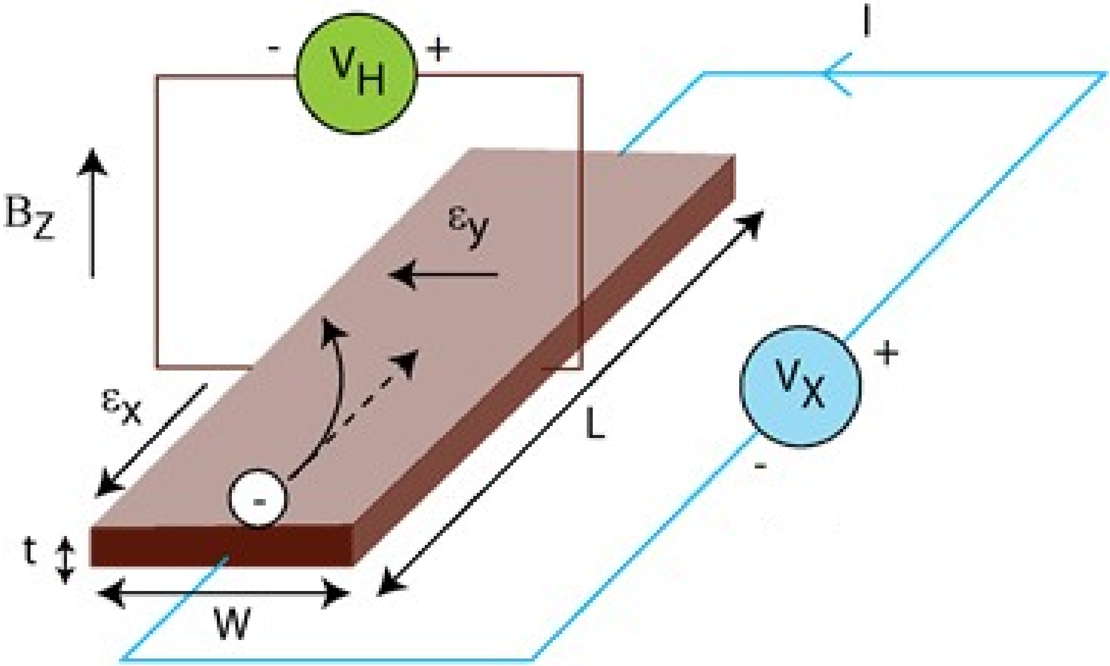
***Perturbation***

$V \sim y \sim i\partial_{k_y}$

***Measure***

$J_x \sim \langle \partial H / \partial k_x \rangle$

# The Hall effect




$$J_x = \sigma_{xy} V_y$$

**Hall conductivity**

**Measure the current perpendicular to a voltage**

# Linear response for transverse current

$$J_x = \sigma_{xy} V_y$$

**The Hall conductivity is obtained as** $$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_\alpha d^2\mathbf{k}$$

with $$\Omega_\alpha(\mathbf{k}) = i \sum_{\beta \neq \alpha} \frac{\langle \Psi_\alpha | \partial H / \partial k_x | \Psi_\beta \rangle \langle \Psi_\beta | \partial H / \partial k_y | \Psi_\alpha \rangle}{(\epsilon_\alpha - \epsilon_\beta)^2} - \alpha \leftrightarrow \beta$$

***Berry curvature of a band***

***Expression coming from perturbation theory***

# The Hall conductivity

**The Hall conductivity is obtained as** $$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_\alpha d^2\mathbf{k}$$

Using $$\langle \Psi_\alpha | \partial H / \partial k_\mu | \Psi_\beta \rangle = \langle \partial_{k_\mu} \Psi_\alpha | \Psi_\beta \rangle (\epsilon_\alpha - \epsilon_\beta)$$

***the Hall conductivity can be expressed in terms of***

**Berry curvature**

$$\Omega_\alpha = \partial_{k_x} A_y^\alpha - \partial_{k_y} A_x^\alpha$$

**Berry connection**

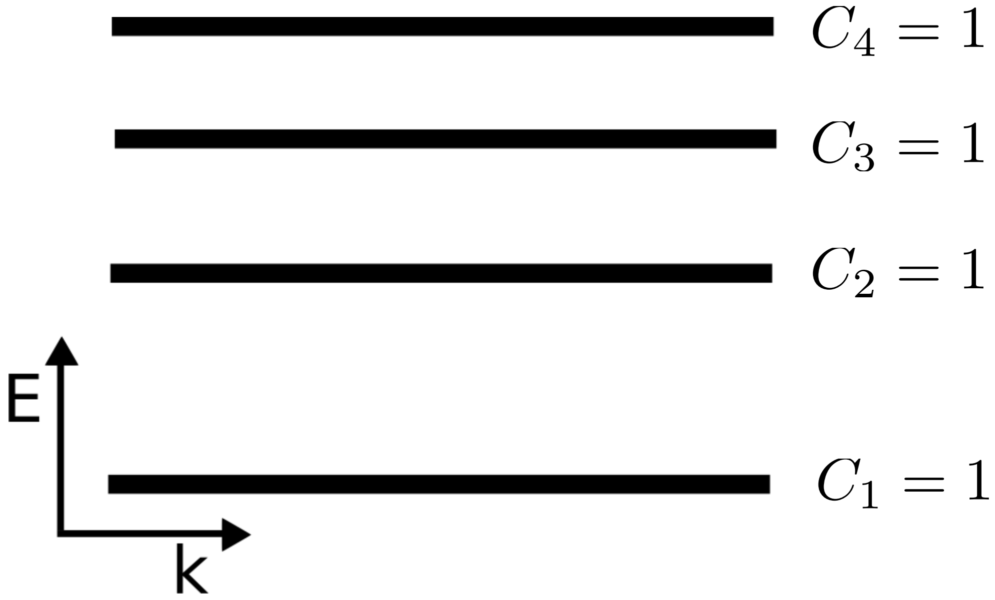
$$A_\mu^\alpha = i \langle \partial_{k_\mu} \Psi_\alpha | \Psi_\alpha \rangle$$

$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_\alpha d^2\mathbf{k} = \sum_\alpha C_\alpha = C$$

Chern number

# Chern numbers in the quantum Hall state

Band-structure in the quantum Hall state




**Hall conductivity**

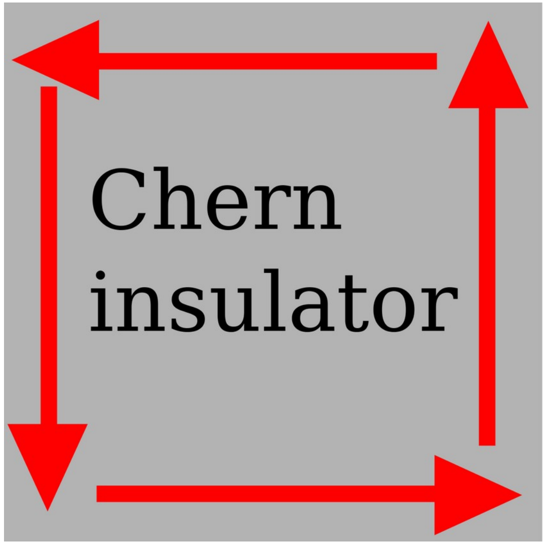
$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_\alpha d^2\mathbf{k} = \sum_\alpha C_\alpha = C$$

**Each band ( a.k.a Landau level), contributes with Chern number +1**

# Hall conductivity in an insulator

$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_\alpha d^2\mathbf{k} = \sum_\alpha C_\alpha = C$$

***The Chern number for each band is quantized*** $$C_\alpha = \int \Omega_\alpha(\mathbf{k}) d^2\mathbf{k} = 0, \pm 1, \pm 2, ....$$




***An insulator can have a finite (and quantized) Hall conductivity***

**This is a simple example of a topological state of matter**

# Take home

- We can predict collective behavior with linear response theory
- Responses of quantum materials allow to predict potential symmetry breaking states
- Reading material:
  - Cohen & Louie, pages 159-164
  - Simon, pages 243-247 and 251-253
  - Bruus & Flensberg, pages 95-104

# In the next session

- Topological materials, beyond the quantized Hall conductance
- The relation between Hamiltonians, cups, dognuts and knots

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j$$