Magnetism in Many-Body Systems

8.512 Theory of solids II (Spring 2022)

Topics:

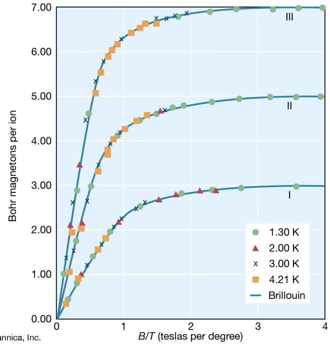
- Quantum exchange interaction
- Long-range order types: ferro- and antiferromagnetic order
- Collective excitations: Spin waves (magnons), Skyrmions
- Band magnetism, Stoner instability
- The Hubbard model and Mott insulators
- Quantum-Hall "ferromagnetic states," spontaneous valley and spin polarization in moiré graphene

Magnetism: microscopic interactions

Need for Quantum Exchange; Why magnetism is quantum

- The word "quantum" in the title is almost redundant, as a simple argument — the Bohr – van Leuwen theorem — demonstrates.
- Indeed, the classical partition function of charged particles coupled to a B field through magnetic vector potential is B-independent!
- $Z_{B\neq 0} = \int d^3pd^3re^{-\beta H(\mathrm{p}-e\mathrm{A}(r))}$. But this equals $Z_{B=0}$ after redefining $\mathrm{p}' = \mathrm{p} - e\mathrm{A}(r)$ (since p and r commute in classical theory)
- No magnetism in classical theory
- Something quantum mechanical is required
- Yet, magnetostatic interactions are too weak. They are present in magnetic materials but mostly irrelevant (except for relatively weak anisotropy effects)

A reminder: magnetism in gases



Magnetization of paramagnetic substances: The approach to saturation in the magnetization of a paramagnetic substance following a Brillouin curve. Curves I, II, and III refer to different ions for which $g = 2$ and $j = 3/2$, $5/2$, and $7/2$, respectively.

Quantum Exchange

- The interactions which provide such strong interactions between magnetic moments are nothing to do with the magnetic nature of the spin degree of freedom, but are to do with its symmetry properties.
- They exist because of the connection between symmetry of spin and spatial wavefunctions for electrons as fermions, and so the energy scales associated with these interactions are the energy scales of the spatial degrees of freedom
- The key players are the electronic kinetic energy and Coulomb interaction.
- To summarize briefly; a given spin configuration restricts the range of possible spatial configurations, and because different spatial configurations can have significantly different energies, there is thus a large energy associated with different spin configurations.

- Within this general framework, there exist two categories of types of magnetic interaction:
- Direct (potential) exchange This is driven by minimizing potential energy, by reducing wavefunction overlap. The overlap is reduced by adding nodes to the wavefunction, producing antisymmetric spatial wavefunctions, and so favors symmetric spins, i.e. ferromagnetic interactions. This case arises when electrons occupy wavefunctions that overlap in space.
- Kinetic exchange. This is driven by minimizing kinetic energy, by reducing gradients of wavefunctions, i.e. allowing delocalization of electrons. This corresponds to using symmetric superpositions of wavefunctions, and so favors antisymmetric spins, i.e. antiferromagnetic interactions. This case generally arises for localized electronic orbitals

Long-range order types: ferro- and antiferromagnetic order

Ferromagnetic order: The Bragg-Williams mean field approach

- Heisenberg model for spin variables on a lattice

$$H = -\tfrac{1}{2}\sum_{\mathrm{x}\neq\mathrm{x}'} J(\mathrm{x}-\mathrm{x}')\hat{s}_{\mathrm{x}}\hat{s}_{\mathrm{x}'}, \quad J(\mathrm{x}-\mathrm{x}') > 0$$

  Ground state at $T = 0$: all spins aligned. Describe the phase transition?
- The mean field method. Start with a single spin in an external field $H = -h\hat{s}_z$. Ensemble-averaged magnetization is found as $m = \langle \hat{s}_z \rangle = L_J(\beta h) = \dots = \left(\sum_{m=-j}^{m=j} m e^{\beta h m}\right) / \left(\sum_{m=-j}^{m=j} e^{\beta h m}\right)$.
- For spin-1/2 case, $j = 1/2$ and $m = \tanh \beta h/2$.
- For many spins, consider one spin (s_{x}) in an effective field of all other spins, $h_{\mathrm{x}} = \sum_{\mathrm{x}'} J(\mathrm{x}-\mathrm{x}')s_{\mathrm{x}}$. Replacing spins by their average values, have

$$h = Um, \quad m = L_J(\beta h)$$

  where $U = \sum_{\mathrm{x}'} J(\mathrm{x}-\mathrm{x}')$. Ensemble average in partition function.
- The equation $m = L_J(\beta U m)$ has zero solution at $\beta U < 1$ and nonzero solutions at $\beta U > 1$. The critical temperature $T_c = U$.
- Susceptibility $\chi = \frac{\partial m}{\partial h} \sim \frac{1}{T - T_c}$ (Curie-Weiss law). Divergence at T_c.

- Heisenberg model for spin variables on a lattice

$$H = -\tfrac{1}{2}\sum_{\mathrm{x}\neq\mathrm{x}'} J(\mathrm{x}-\mathrm{x}')\hat{s}_{\mathrm{x}}\hat{s}_{\mathrm{x}'}, \quad J(\mathrm{x}-\mathrm{x}') < 0$$

  Ground state: two sublattices, spins aligned on each sublattice, antialigned on different sublattices. Phase transition?

- The mean method. Start with a single spin in an external field $H = -h\hat{s}_z$. Ensemble-averaged magnetization is found as $m = \langle \hat{s}_z \rangle = L_J(\beta h) = \ldots$.
- For spin-1/2 case, $j = 1/2$ and $m = \tanh \beta h/2$.
- For many spins, consider one spin (s_{x}) in an effective field of all other spins, $h_{\mathrm{x}} = \sum_{\mathrm{x}'} J(\mathrm{x}-\mathrm{x}')s_{\mathrm{x}}$. Replacing spins by their average values, $+m$ on one sublattice, $-m$ on another sublattice, have

$$h = Um, \quad m = L_J(\beta h)$$

  where $U = \sum_{\mathrm{x}'}(+/-)J(\mathrm{x}-\mathrm{x}')$.

- The equation $m = L_J(\beta Um)$ has zero solution at $\beta U < 1$ and nonzero solutions at $\beta U > 1$. The critical temperature $T_c = U$.
- Susceptibility $\chi = \frac{\partial m}{\partial h} \sim \frac{1}{T+T_c}$ (Néel law). No divergence at T_c.
- Validity: small fluctuations, large spin j

Collective excitations: Spin waves (magnons), Skyrmions

Magnetically ordered states and spin-wave excitations

- Consider a fully polarized ferromagnetic state
$$|S,S\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow \ldots \uparrow\rangle$$
with $S = N/2$, $S_z = N/2$.
- To see that it is an eigenstate let's rewrite the Hamiltonian as
$$H = J\sum_{(ij)} \mathrm{S}_i \cdot \mathrm{S}_j = J\sum_{(ij)} \left[S_i^z S_j^z + \tfrac{1}{2}(S_i^- S_j^+ + S_i^+ S_j^-)\right], \quad J < 0$$
- Generate more states by applying $S^- = \sum_j S_j^-$ to $|S,S\rangle$:
$S^-|S,S\rangle = |S,S-1\rangle = |\downarrow\uparrow\uparrow\uparrow\uparrow \ldots \uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\uparrow \ldots \uparrow\rangle + \ldots |\uparrow\uparrow\uparrow\uparrow\uparrow \ldots \downarrow\rangle$
This state is degenerate with $|S,S\rangle$ because $[H, S^-] = 0$
- A simple modification of the lowering operator can be used to generate an exact spin-wave excited state
$$S_q^- = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{-i\mathrm{q}\cdot\mathrm{R}_j} S_j^-$$
$S_q^-|S,S\rangle$ an eigenstate!
- Excitation energy $\epsilon_q = \frac{\hbar^2 z}{2}|J|(1-\gamma_q)$ with $\gamma_q = \frac{1}{z}\sum_\delta e^{-i\mathrm{q}\cdot\delta}$
- Magnons (spin waves): Collective excitations, elementary excitations, or quasiparticles. Localized spins holding hands. Transporting spin, momentum and energy.

Magnetically ordered states and spin-wave excitations

- Solid as a gas: magnons behave as (nearly) free particles with Bose statistics. Similar to phonons and photons.
- Magnons in FM are soft modes: $\epsilon_q \to 0$ when $q \to 0$
- Mode softness originates from $SU(2)$ symmetry of the Hamiltonian which is spontaneously broken in the ordered state (Nambu-Goldstone theorem)
- Thermal spin fluctuations suppressing long-range order
- At low $T > 0$ estimate magnetization of the ground state using a free boson approximation:

$$M = N/2 - \sum_j b_j^\dagger b_j = N/2 - \sum_q b_q^\dagger b_q = N/2 - \sum_q n_B(\epsilon_q)$$

- with magnon bose operators $b_q^\dagger = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-iqR_j} b_j^\dagger$ and $b_q = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{iqR_j} b_j$ obeying bosonic algebra

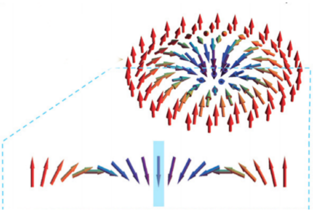
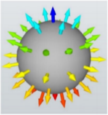
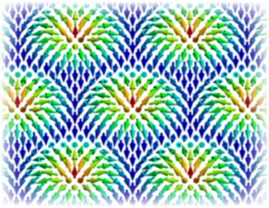
$$[b_q^\dagger, b_{q'}] = \delta_{qq'}, \quad [b_q^\dagger, b_{q'}^\dagger] = [b_q, b_q'] = 0$$

Magnetically ordered states and spin-wave excitations

The lower critical dimension (Hohenberg-Mermin-Wagner theorem)

- At low T only long wavelength magnons are excited, $\epsilon_q = Aq^2$ with A a constant
$$M = N/2 - N \int_{BZ} \frac{d^d q}{(2\pi)^d} \frac{1}{e^{\beta \epsilon_q} - 1}$$
- At $d = 3$ a weak suppression,
$$M = N/2 - CN(T/T_c)^{1/2};$$
- At $d = 2$ a log-divergence:
$$M = N/2 - CN \log(T_c/T)$$
- The HMW theorem: no long-range order at $d \leq 2$ in systems with continuous symmetry
- Seminal exception: topological phase transition in a 2D XY magnet (governed by vortices and antivortices binding/dissociating through Berezinskii-Kosterlitz-Thouless mechanism)

Topological excitations: Magnetic skyrmions

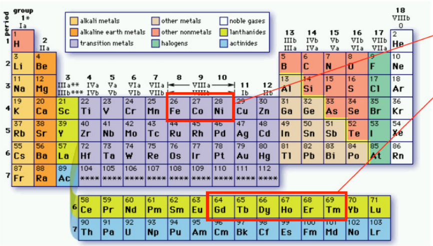




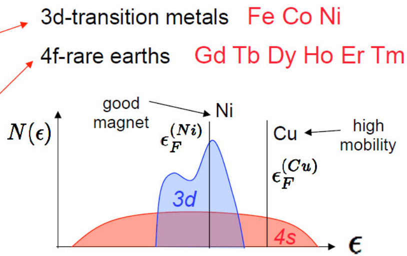
- The long-wavelength degrees of freedom of a Heisenberg ferromagnet in 2D: spin waves only?
- Magnetization slowly varying in space: $\mathrm{m}(x, y)$
- Energy from gradient expansion: $E = \int dxdy \frac{1}{2} J(\partial_\mu \mathrm{m}^\nu)^2$
- Topological invariant: the "wrapping" number (Pontryagin index)
$$n = \frac{1}{4\pi} \int \mathrm{m} \cdot \left(\frac{\partial \mathrm{m}}{\partial x} \times \frac{\partial \mathrm{m}}{\partial y} \right) dxdy$$
- Skyrmions: hedgehog-like textures stabilized by topology. Lowest-energy skyrmions, $n = \pm 1$
- Skyrmyon energy finite, $E \sim J < \infty$. Therefore, skyrmions are thermally activated at any $T < T_c$. No topological phase transition. Finite correlation length $\xi < \infty$ and a long-range-disordered state.

Band magnetism, Stoner instability

Intinerant magnetism: Stoner instability of band electrons

- A magnetic phase transition of a Fermi liquid with net non zero magnetization
- There can be other magnetically ordered states with no net magnetization (eg. AFM) . General class of magnetic transitions is specified by ordering wave vectors $\vec{Q}$. Also inludes Spin Density Waves
- Will focus here on Ferromagnetic Instability. A simple illustration of QPT
- Phase transition occurs on varying a system parameter (Coulombic repulsion U in Stoner case)



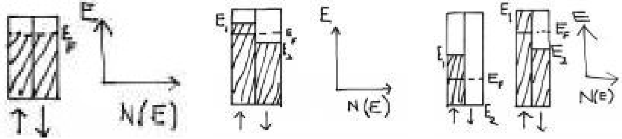


What is Stoner instability?

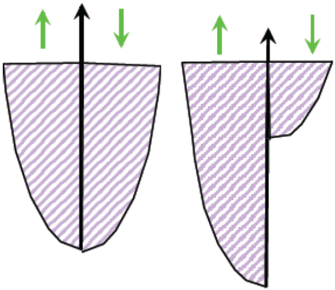
- Consider a 3d transition metal, in which the 3d electrons give rise to magnetism; since the electrons are itinerant (and delocalized) in the metal, the magnetism stems from 3d electron bands.
- The band itself consists of two sub-bands — one for up-spin electrons and another for down-spin electrons. If there are less than ten 3d-electrons in the system, the 3d-band will be partially filled. Further, if the system fills these bands without discrimination, then both the sub-bands will be equally filled.
- If suppose we can define an interaction energy which indicates a reduction in energy if the electrons from one of the sub-bands, say those corresponding to down-spin can be transferred to the up-spin band, then, under certain circumstances it can be shown that this will lead to an instability as discussed below.
- What prevents such an emptying of one of the sub-bands in favor of another is the resultant increase in the electron kinetic energy
- In fact, the total variation in energy in such sub-band transfer of electrons can be shown to be equal to $\Delta E = \frac{n^2 p^2}{N(E_F)}[1 - U_{eff} N(E_F)]$, where, n is the total number of 3d electrons per atom, p is the fraction of atoms that move from down-spin sub-band to up-spin sub-band, U_{eff} is the effective interaction energy, and $N(E_F)$ is the density of energy states at the Fermi level.

What is Stoner instability?

- Thus, if the quantity in square brackets is positive, the state of lowest energy corresponds to $p = 0$ — or, in other words, the metal is non-magnetic. However, if the quantities in the square bracket is negative, the band is "exchange split" — $p > 0$, and hence the metal is ferromagnetic.
- This is known as the Stoner instability, or sometimes ferromagnetic instability. From the equation, it is clear that such band splitting is favored for large exchange interaction energy as well as for large density of states. Since the density of states for s- and p-bands are considerably smaller, which, in turn explains why such band magnetism is restricted to elements with partially filled d-band.
- Here are the schematics explaining band magnetism in partially filled d-electron systems: paramagnetic, weak ferromagnetism, strong ferromagnetism ($n < 5$ and $n > 5$)

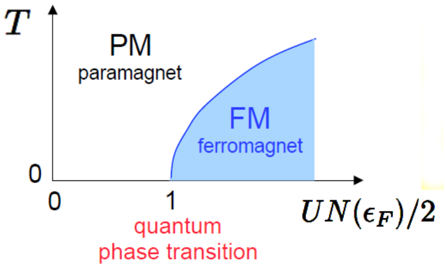


Hubbard model



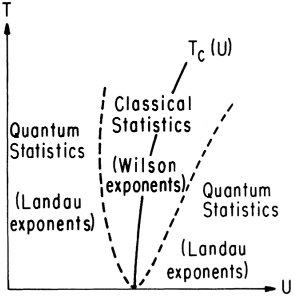
- Hubbard model $\mathscr{H}_{hubbard} = -t \sum_{<ij>} c_i^\dagger c_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$
- Electrons reduce U by favoring magnetic ordering
- Cost: Gain in Kinetic energy

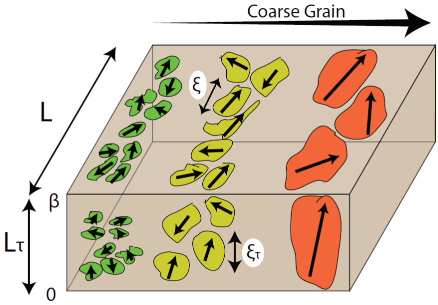
Phase diagram and instability criterion



- Instability occurs when $UN(\epsilon_F)/2 > 1$ (The mean-field approximation).
- Ferromagnetic order at $U > U_c$
- Near critical point spin response function $\chi(q, \omega)$ diverges for $q, \omega \to 0$
- The selfconsistent approach to evaluate $\chi(q, \omega)$

Extend from $T = 0$ to finite T: a quantum critical point

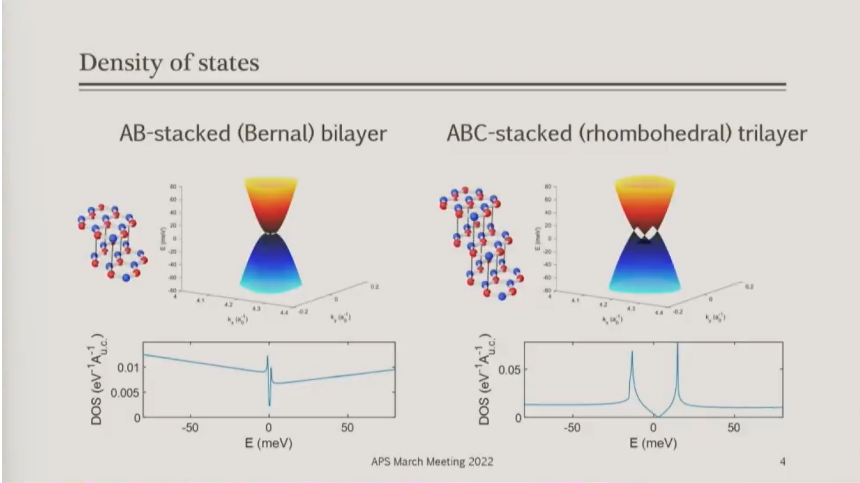




- Fluctuations and scaling at the QCP
- Quantum vs. Classical: Classical $d \leftrightarrow d + 1$
- Close analogy with a 'finite' classical system. A box with infinite d dimensions and a finite $d + 1$th dimension

Spin and valley magnetism in graphene bi- and trilayers

* Atomically thin layers, strong el-el interactions
* Quadratic and cubic Dirac bands
* Four-fold degeneracy in valley and spin



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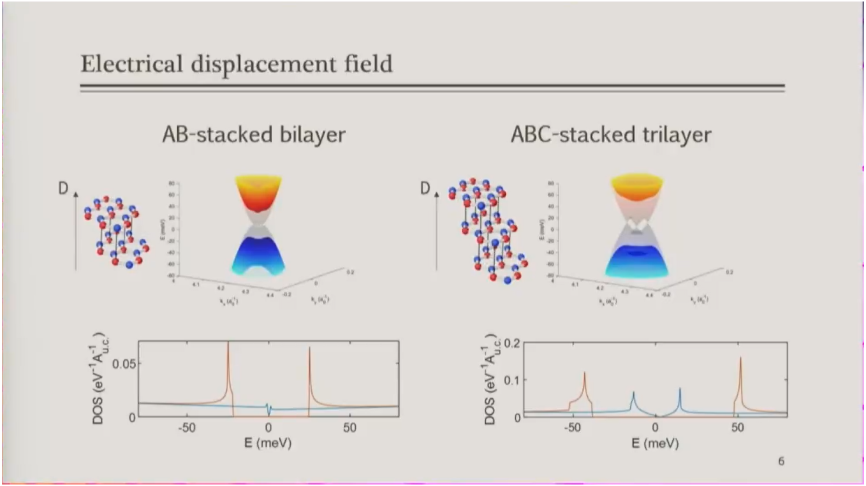

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Density of states at the Fermi surface ρ_F

Ferromagnetism

- Stoner Criterion:

$$U\rho_{\mathrm{F}} > 1$$

U: Strength of the Coulomb repulsion

E. C. Stoner, Proc. R. Soc. A 165, 372–414 (1938)

Superconductivity

- BCS Theory:

$$T_c = T_F e^{-1/g\rho_F}$$

- T_c: Critical temperature
- T_F and g: constant parameters

L. P. Gor'kov, PNAS 113 (17) 4646-4651 (2016)

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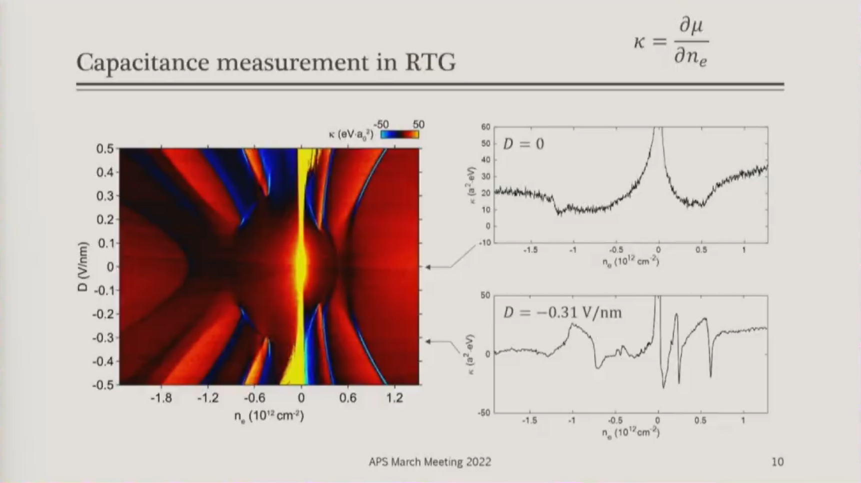
Spin and valley magnetism in graphene bi- and trilayers

* Stoner instability detected by capacitance measurements
* Fully polarized, partially polarized and unpolarized phases
* Phase boundaries tunable by displacement field



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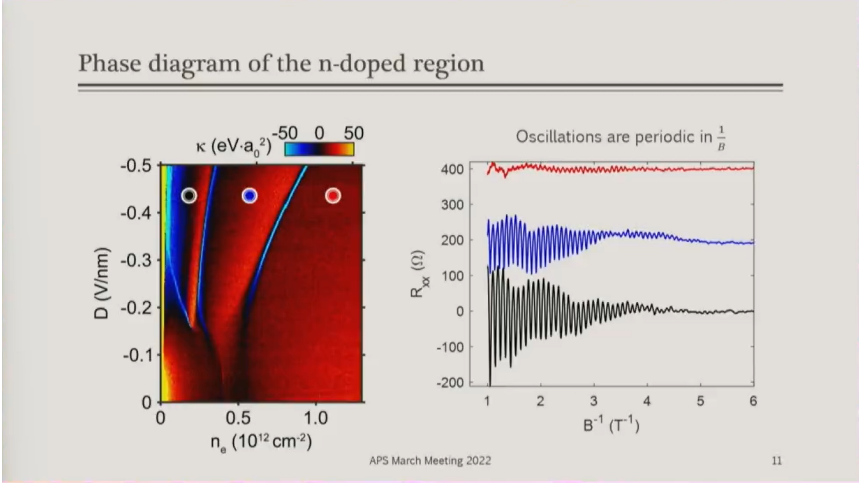

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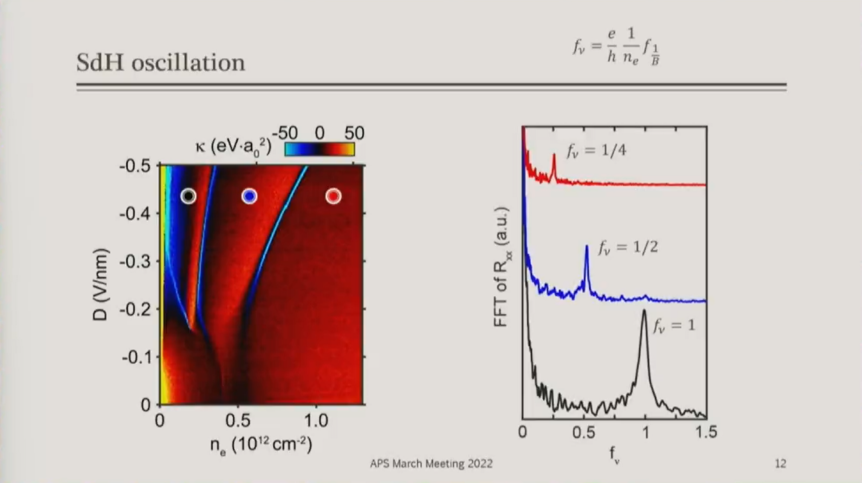

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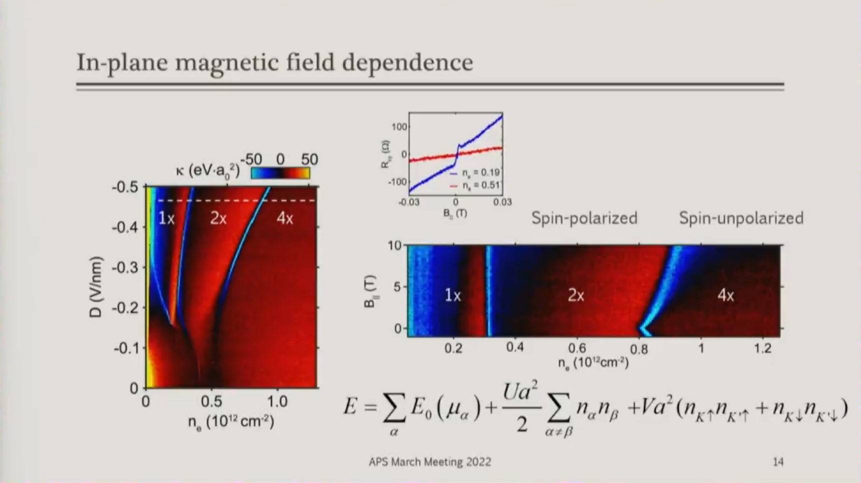
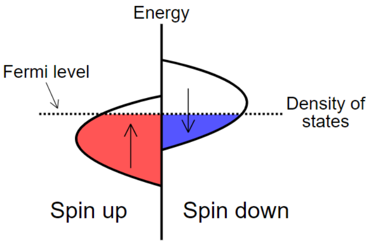
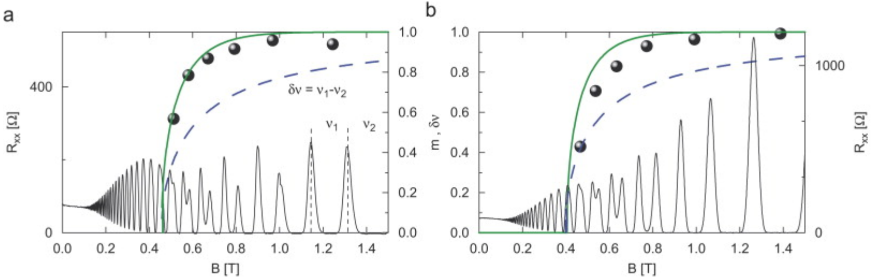


Quantum-Hall "ferromagnetic states"



Magnetic-field-induced Stoner transitions

* Interaction-induced lifting of the two-fold spin degeneracy in the integer quantum Hall effect
* An abrupt transition from spin-unresolved QH to spin-resolved QH
* A Quantum Hall Ferromagnet state in GaAlAs quantum wells



B. A. Piot, et al., Phys. Rev. B 72, 245325 (2005)

Magnetic-field-induced Stoner transitions

Spin-valley Quantum Hall Ferromagnet states in graphene monolayers at charge neutrality (four-fold splitting of the Dirac $n = 0$ Landau level)

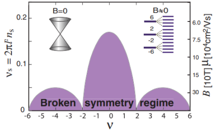
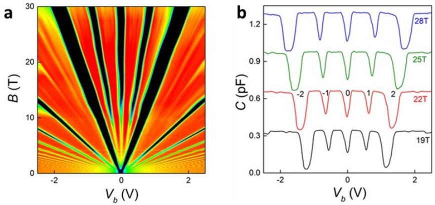
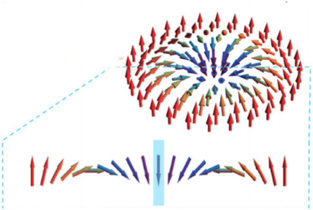


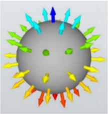
FIG. 1 (color online). Phase diagram for $SU(4)$ quantum Hall ferromagnetism in the $n = 0$ and $n = 1$ Landau levels of graphene. In our model the ordered region is bounded by a maximum value of ν_s, the ratio of the density of Coulomb scatterers to the density of a full Landau level. ν_s is inversely proportional to the product of the sample mobility and the external field strength and order near integer filling factors requires the minimum values for this product indicated on the right-hand vertical axis.



from: Nomura and MacDonald, Phys. Rev. Lett. 96, 256602 (2006); G. L. Yu et al., Nature Physics 10, 525-529 (2014)

Magnetic skyrmions





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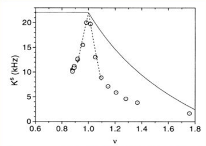
Optically Pumped NMR Evidence for Finite-Size Skyrmions in GaAs Quantum Wells near Landau Level Filling $\nu = 1$

S. E. Barrett,* G. Dabbagh, L. N. Pfeiffer, K. W. West, and R. Tycko†
AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, New Jersey 07974
(Received 19 December 1994)

The Knight shift $[K_s(\nu, T)]$ and spin-lattice relaxation time $[T_1(\nu, T)]$ of the ^{71}Ga nuclei located in n-doped GaAs quantum wells are measured using optically pumped NMR, for Landau level filling $0.66 < \nu < 1.76$ and temperature $1.55 < T < 20$ K. $K_s(\nu)$ [proportional to the electron spin polarization $\langle S_z(\nu)\rangle$] drops precipitously on either side of $\nu = 1$, which is evidence that the charged excitations of the $\nu = 1$ ground state are finite-size Skyrmions. For $\nu < 1$, the data are consistent with a many-body ground state which is not fully spin polarized, with a very small spin excitation gap that increases as $\nu \to \frac{2}{3}$.

Skyrmions are cheapest charge excitations of QHFM

NMR Knight shift data showed charge excitation accompanied by a large spin flip (S~4)

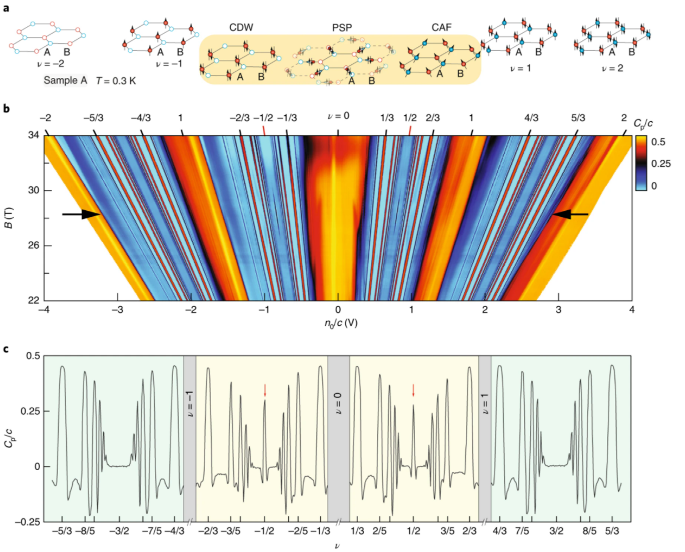


Barrett et al. PRL **74,** 5112 (1995)

Each Skyrmion carries electric charge

$$Q_{\mathrm{e}} = e = \frac{1}{4\pi} \int dx dy \; \boldsymbol{n} \cdot (\partial_x \boldsymbol{n} \times \partial_y \boldsymbol{n})$$

Fractional Quantum Hall states at high B field



from: Zibrov et al., Nature Physics 14, 930-935 (2018)

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The Hubbard model and Mott insulators

- The Hubbard model is a toy model designed to capture the essence of the magnetic effects due to Coulomb interactions. A tight-binding Hamiltonian with the long-range Coulomb interaction replaced by an on-site repulsion (on a square lattice)

$$H = -t \sum_{(ij),\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_j n_{j\uparrow} n_{j\downarrow}, \quad n_{j\sigma} = c^\dagger_{j\sigma} c_{j\sigma}$$

- Note that the Pauli exclusion allows double occupancy only by pairs of electrons of opposite spin; repulsion U penalizes double occupancy.
- The hopping (t) term tends to delocalize electrons through hopping and competes with the interaction (U) term.
- Despite that this model is an extreme simplification, it has resisted the exact solution in dimension $d > 1$
- We'll discuss the features of the physics in the limits that are well understood: $U = 0$, $U = \infty$, large U/t; with the density at and near half-filling, $n = n_\uparrow + n_\downarrow \approx 1$

The Hubbard model and Mott insulators

$$H = -t \sum_{(ij),\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_j n_{j\uparrow} n_{j\downarrow}$$

- We begin our analysis with the case of half-filling $\langle = n_{j\uparrow} + n_{j\downarrow} \rangle = 1$
- In the weak repulsion limit, $U = 0$, the ground state is a Slater determinant made of the free-particle plane wave states each containing two electrons of opposite spin:

$$|\Psi\rangle = \prod_{k,\sigma=\uparrow,\downarrow} \psi^\dagger_{k\sigma} |0\rangle, \quad \psi^\dagger_{k\sigma} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\mathrm{k}\mathrm{R}_j} c^\dagger_{k\sigma}$$

- This is an ordinary nonmagnetic ground state, representing a metallic ground state
- Consider now the case $U = \infty$ for which there can be no double occupancy. Here the state must be of the form

$$|\Psi\rangle = \left(\prod_{j=1}^{N} c^\dagger_{j\sigma_j} \right) |0\rangle, \quad \sigma_j = \uparrow \text{ OR } \downarrow$$

There are 2^N different states according to the choice of spin orientation on each lattice site.

- Since the particles cannot hop to any neighboring sites both the kinetic energy and the interaction energy vanish. The energy eigenvalue is zero and is 2^N-fold degenerate.
- Because of this degeneracy, no particular magnetic order is favored over any other and the system is effectively a nonmagnetic insulator with an infinite charge excitation gap.
- This is a new type of insulator we have encountered. Previously we encountered insulators that can be understood with a free-electron band picture. Such interaction-induced insulators are collectively known as Mott insulators
- Zero compressibility $dn/d\mu = 0$ as for a band-gap insulator but at a "nominally metallic" band filling $1/2$ of an infinite-U Hubbard model
- A parent state for cuprate high-T_c superonductors

The half-filled infinite-U Hubbard model

- Consider what happened if we remove a single electron from this half-filled band. In this case the ground state is given exactly by

$$|\Psi\rangle = \left(\prod_k \psi^\dagger_{k\uparrow} \right) |0\rangle$$

  where the product runs over all allowed ks except a single one corresponding the the highest kinetic energy

- This state is therefore a fully ferromagnetic single Slater determinant with spin $S = \frac{1}{2}(N-1)$ and degeneracy $2S+1$

- This is an eigenstate (since the interaction term vanishes), known as the Nagaoka state

- This is also a ground state (the Nagaoka theorem). Automatically avoids double occupancy because all spins are aligned. The kinetic energy is optimized due to the presence of a hole

- Frustrated states disfavored by the hole stirring effects.

The half-filled infinite-U Hubbard model

- Back to half-filled Mott-insulating state. Consider a large but not infinite U. Now the charge gap is finite and different spin states aren't exactly degenerate.
- It turns out that the ground state has antiferromagnetic Néel order for the square and cubic lattices
- To see how this comes about let's analyze a Hubbard model with only two electrons and two sites (can generalize later)
- States in a two-site Hubbard model:

$$|\uparrow;\uparrow\rangle \quad |\downarrow;\downarrow\rangle \quad |\uparrow;\downarrow\rangle \quad |\downarrow;\uparrow\rangle \quad |\downarrow,\uparrow;-\rangle \quad |-;\downarrow\uparrow\rangle$$

- Perturbation theory carried out in a way that is backwards to the usual one, since $U/t \gg 1$. The unperturbed Hamiltonian is the potential energy $V = U\sum_j n_{j\uparrow}n_{j\downarrow}$ and the kinetic energy $T = -t\sum_{(ij),\sigma}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma})$ will be a perturbation.
- Since V commutes with the total spin $\mathrm{S} = \mathrm{S}_1 + \mathrm{S}_2$ its eigenstates can be labeled by their total spin quantum number $S = 0, 1$
- A triplet and a singlet, both with energy $\epsilon = 0$, and two singlets with energy $\epsilon = U$ because of double occupancy.
- These are all exact eigenstates of V. We are interested in the low-energy states (assuming $U \gg k_B T$)

The half-filled infinite-U Hubbard model

- Because the kinetic energy also commutes with S, $[T, S] = 0$, the perturbation can only mix singlet states among themselves
- The low energy singlet and triplet states obey $\langle\psi|T|\psi\rangle = 0$ (In fact the triplet state is an eigenstate of H)
- Level repulsion will drive the low-energy singlet downwards, lifting the spin degeneracy and leading to an effective antiferromagnetic low-energy spin Hamiltonian

  $$H_{eff} = J\mathrm{S}_1 \cdot \mathrm{S}_2 + C$$

  with $J > 0$ and C a constant.
- To calculate J and C perturbatively in $t/U \ll 1$ note that

  $$T|\psi_0\rangle = -2t\frac{1}{\sqrt{2}}(|\psi_{0L}\rangle - |\psi_{0R}\rangle)$$

  so the second-order energy shift for $|\psi_0\rangle$ equals

  $$\Delta\epsilon = \frac{|\langle\psi_{0L}|T|\psi_0\rangle|^2}{-U} + \frac{|\langle\psi_{0R}|T|\psi_0\rangle|^2}{-U} = -\frac{4t^2}{U}$$
- The energy of the triplet state remains zero, but partial delocalization of the electrons in the singlet case reduces the kinetic energy from zero to $\epsilon = -\frac{4t^2}{U}$

The half-filled infinite-U Hubbard model

- These results allow us to determine J and C using

$$H_{eff} = J\mathbf{S}_1 \cdot \mathbf{S}_2 + C = \frac{1}{2}\left[(S_1 + S_2)^2 - \frac{3}{2}\hbar^2\right] + C$$

- This yields $\epsilon_1 = \frac{J}{4} + C$ for the triplet state, and $\epsilon_0 = -\frac{3J}{4} + C$ for the singlet state. Therefore

$$C = -\frac{t^2}{U}, \quad J = \frac{4t^2}{\hbar^2 U}$$

- For the case of an infinite lattice one obtains an effective Heisenberg spin Hamiltonian

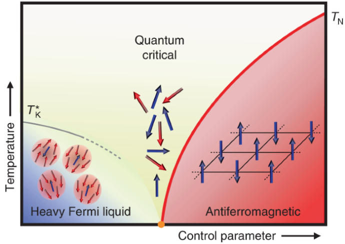
$$H_{eff} = J \sum_{(ij)} \mathbf{S}_i \cdot \mathbf{S}_j$$

  Since the 2nd order perturbation couples only nearest neighbors this result is independent of lattice geometry and spatial dimension

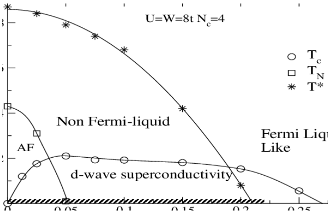
- Discuss once more the sign of the exchange interaction: Here J has its origin in the desire of the electrons to lower their kinetic energy through delocalization. This gives an antiferromagnetic coupling.
- In the case of Stoner instability, the Coulomb energy is lowered due to the so-called direct exchange, and the kinetic energy goes up. In this case the coupling is of a ferromagnetic sign.

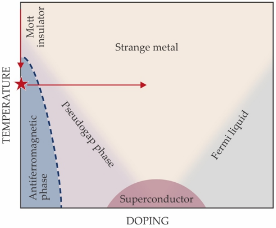
Discuss doped Mott antiferromagnets

Nagaoka theorem: holes polarize AFM state, become magnetic polarons; at a finite doping a Fermi liquid Phase diagram:



Possible relation to the phase diagram of high-T_c superconductors. Phase diagrams:





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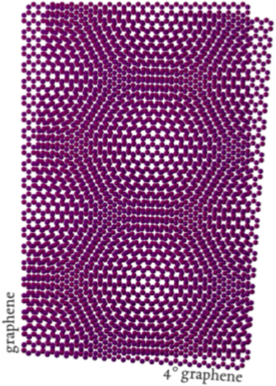
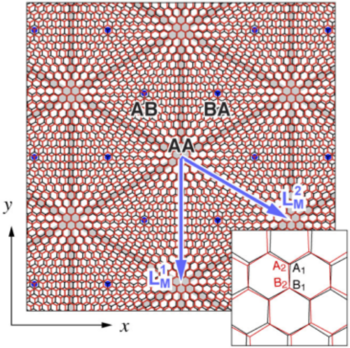
Spontaneous valley and spin polarization in moiré graphene

Flat bands in moire graphene



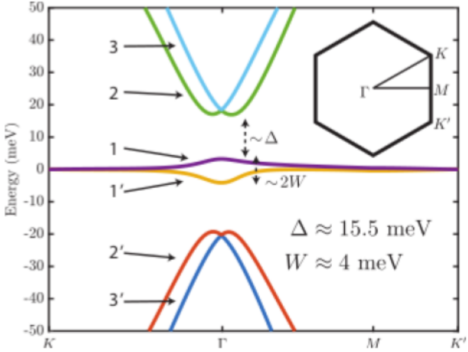
Source: Wikipedia

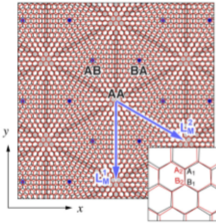


M. Koshino, et. al., Phys. Rev. X 8 031087 (2018)

Flat bands in moire graphene

- Extremely narrow bands at "magic" twist angle θ~1°
- Narrow bandwidth, low Fermi velocity, $v_F/v_{F,0}$~1/100



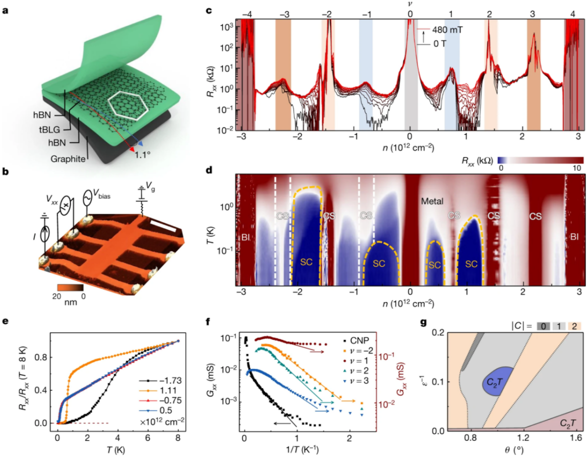


M. Koshino, et. al., Phys. Rev. X 8
031087 (2018)

Correlated states in magic-angle moiré graphene

Mott-insulating states at band fillings $\nu = 0, \pm1, \pm2, \pm3$;
superconducting states in between (resembling high-T_c SC)

From: Superconductors, orbital magnets and correlated states in magic-angle bilayer graphene

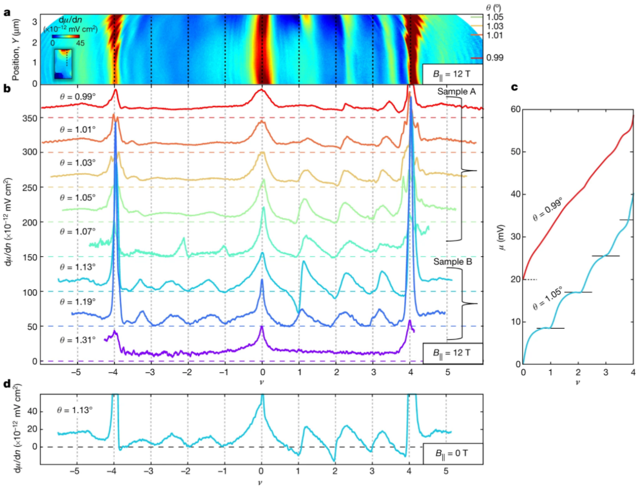


a, Schematic of a typical MAG device. **b**, Atomic force microscopy image and schematic of how various measurements are obtained. Scale bar, 2 μm. **c**, Four-terminal longitudinal resistance plotted against carrier density at different perpendicular magnetic fields from 0 T (black trace) to 480 mT (red

Correlated states in magic-angle moiré graphene

Stoner instability and Dirac resetting/revival transitions

From: Cascade of phase transitions and Dirac revivals in magic-angle graphene



Stoner instability and Dirac resetting/revival transitions

From: Cascade of phase transitions and Dirac revivals in magic-angle graphene