Superconductivity in 2D materials



Jyväskylä Summer School "Emergent Quantum Matter in Artificial Two-dimensional Materials" Tuesday, August 9th 2022

Schedule for the lecture

- 40 min lecture
- 15 min break
- 40 min lecture
- 15 min break
- 40 min lecture



Summer school 2022 "Emergent quantum matter in artificial two-dimensional materials"

Today's plan

- Van der Waals superconductors
- The impact of superconductivity in an electronic structure
- Conventional and unconventional superconductivity
- Impurities in 2D superconductors
- Topological superconductivity

van der Waals materials



Gapped trivial superconductors

Nodal superconductivity Spin-triplet superconductivity Gapped topological superconductors

The role of electronic interactions

Electronic interactions are responsible for symmetry breaking

Broken time-reversal symmetry Classical magnets



 $M \rightarrow -M$

Broken crystal symmetry Charge density wave



 $\mathbf{r}
ightarrow \mathbf{r} + \mathbf{R}$

Broken gauge symmetry Superconductors



 $\langle c_{\uparrow} c_{\downarrow} \rangle \to e^{i\phi} \langle c_{\uparrow} c_{\perp} \rangle$

Quantum matter with interactions

We can consider two broad groups of interacting quantum matter

$$H = \sum_{ij} t_{ij} c_i^{\dagger} c_j + \sum_{ijkl} V_{ijkl} c_i^{\dagger} c_j c_k^{\dagger} c_l$$

With a mean field description
$$H \approx \sum_{ij} \bar{t}_{ij} c_i^{\dagger} c_j + \sum_{ij} \Delta_{ij} c_i c_j$$
Without a mean field description
$$\frac{222}{100} \frac{1}{100} \frac{1}{$$

Approximate guadratic Hamiltonian Effective single particle description

Weakly correlated matter

No good quadratic approximation Requires exact solutions or numerical

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Strongly correlated matter

Macroscopic quantum phenomena

Superconductivity



 $\Phi = \frac{h}{2e} \quad \begin{array}{c} \text{Many-body state} \\ \textbf{Quantization} \text{ of flux} \end{array}$

Quantum Hall effect



The theoretical description of superconductivity

Interactions and mean field



What are these interactions coming from?

- Electrostatic (repulsive) interactions
- Mediated by other quasiparticles (phonons, magnons, plasmons,...)

The net effective interaction can be attractive or repulsive

<u>Superconductivity requires effective attractive interactions</u>

Origin of attractive interactions

Interactions between electrons can be effectively attractive when mediated by other quasiparticles

Conventional superconductors

Phonons

Unconventional superconductors

Antiferromagnetic magnons Ferromagnetic magnons Plasmons Valence fluctuations Charge fluctuations

. . .

A simple interacting Hamiltonian

$$\begin{aligned} \text{Free Hamiltonian} & \text{Interactions} \\ \text{(Hubbard term)} \\ H &= \sum_{ij} t_{ij} [c_{i\uparrow}^{\dagger} c_{j\uparrow} + c_{i\downarrow}^{\dagger} c_{j\downarrow}] + \sum_{i} U c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow} \end{aligned}$$

From now on lets consider we have a spin degree of freedom \uparrow,\downarrow

What is the ground state of this Hamiltonian?

U > 0

Magnetism

U < 0 Superconductivity

The mean-field approximation, superconductivity

Mean field: Approximate four fermions by two fermions times expectation values

Four fermions (not exactly solvable)

Two fermions (exactly solvable)

$$Uc_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow} \approx U\langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}\rangle c_{i\uparrow}c_{i\downarrow} + h.c.$$
$$Uc_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow} \approx \Delta c_{i\uparrow}c_{i\downarrow} + h.c.$$

For U < 0

 $\Delta \sim \langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} \rangle$

is the superconducting order

i.e. attractive interactions

A Hamiltonian for a superconductor

$\begin{array}{ll} \textit{Free Hamiltonian} & \textit{Pairing term} \\ H = \sum_{ij} t_{ij} [c_{i\uparrow}^{\dagger} c_{j\uparrow} + c_{i\downarrow}^{\dagger} c_{j\downarrow}] + \Delta \sum_{i} c_{i\uparrow} c_{i\downarrow} + h.c. \end{array}$

Lets have a look to the term

 $\Delta c_i \uparrow c_i \downarrow$

Superconductivity and symmetries

$$H \sim \Delta c_{i\uparrow} c_{i\downarrow} + h.c.$$

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

This term destroys two electrons



The ground state can not have a well defined number of electrons

$$|GS\rangle \sim |2e\rangle + |4e\rangle + |6e\rangle + \dots |GS\rangle \sim |1e\rangle + |3e\rangle + |5e\rangle + \dots$$

Gauge symmetry and superconductivity

What we know from quantum mechanics

"The phase of a wavefunction (field operator) does not have physical meaning"

This is what we know as gauge symmetry

$$c_n \to e^{i\phi} c_n$$
$$c_n^{\dagger} \to e^{-i\phi} c_n^{\dagger}$$

Terms in the Hamiltonian that do not change under this transformation

$$\begin{array}{c} c_{n}^{\dagger}c_{m} & c_{n,\uparrow}^{\dagger}c_{n,\downarrow} - c_{n,\downarrow}^{\dagger}c_{n,\downarrow} & c_{n,\downarrow}^{\dagger}c_{m,\downarrow} & c_{n,\uparrow}^{\dagger}c_{m,\downarrow} \\ \hline \textit{Hopping} & \underline{\textit{Magnetism}} & \underline{\textit{Spin-orbit coupling}} & \underline{\textit{Interactions}} \end{array}$$

Superconductivity and gauge symmetry breaking

Gauge symmetry

$$c_n \to e^{i\phi} c_n$$

$$c_n^\dagger \to e^{-i\phi} c_n^\dagger$$

How does the superconducting order transform under a gauge transformation?

$$\Delta = \langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} \rangle$$

Superconductivity and gauge symmetry breaking

Gauge symmetry

$$c_n \to e^{i\phi} c_n$$

$$c_n^\dagger \to e^{-i\phi} c_n^\dagger$$

How does the superfluid density transform under a gauge transformation?

$$\Delta \to e^{-2i\phi} \Delta$$

A superconductor breaks gauge symmetry

The electronic structure of a superconductor

The Nambu representation

How do we solve a Hamiltonian of the form $H = \sum_{\mathbf{k},s} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},s} c_{\mathbf{k},s} + \sum_{\mathbf{k}} \Delta c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k},\downarrow} + h.c.$



The Hamiltonian in the Nambu basis is quadratic and can be diagonalized

$$H = \Psi_{\mathbf{k}}^{\dagger} \mathcal{H} \Psi_{\mathbf{k}}$$

The original Hamiltonian

$$H = \sum_{\mathbf{k},s} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},s} c_{\mathbf{k},s} + \sum_{\mathbf{k}} \Delta c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k},\downarrow} + h.c.$$

 $\left| \right\rangle$

Can be rewritten as

$$H = \frac{1}{2} \Psi_{\mathbf{k}}^{\dagger} \mathcal{H} \Psi_{\mathbf{k}} \qquad \Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\downarrow} \\ c_{-\mathbf{k}\downarrow}^{\dagger} \\ -c_{-\mathbf{k}\uparrow}^{\dagger} \end{pmatrix} - \text{Electron sector}$$

with
$$\mathcal{H} = \begin{pmatrix} \epsilon_{\mathbf{k}} & 0 & \Delta & 0 \\ 0 & \epsilon_{\mathbf{k}} & 0 & \Delta \\ \Delta & 0 & -\epsilon_{\mathbf{k}} & 0 \\ 0 & \Delta & 0 & -\epsilon_{\mathbf{k}} \end{pmatrix}$$

Single orbital in the square lattice

$$H = \sum_{\mathbf{k},s} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},s} c_{\mathbf{k},s}$$





Single orbital in the square lattice



Single orbital in the square lattice



Impact of superconductivity in the electronic structure

Let us take the electronic structure of a triangular lattice



Impact of superconductivity in the electronic structure

A uniform superconducting terms opens up a gap in the electronic structure



Impact of superconductivity in the electronic structure

Let us take the electronic structure of a square lattice



Impact of superconductivity in the electronic structure

A uniform superconducting terms opens up a gap in the electronic structure



Nodal superconductivity

Let us now take a square lattice, and add a nodal superconducting order parameter



Some parts of the Fermi surface get a gap, while others remain gapless

Gapped and gapless superconductivity

The electronic structure is modified differently depending on the type of superconductivity



Square lattice

Gapped and gapless superconductivity

The electronic structure is modified differently depending on the type of superconductivity



Triangular lattice



10-15 min break

(optional) to discuss during the break

What is the correct sign for this equality, and why?

$$\langle c_{k,\uparrow}^{\dagger}c_{-k,\uparrow}^{\dagger}\rangle = \langle c_{-k,\uparrow}^{\dagger}c_{k,\uparrow}^{\dagger}\rangle \qquad \qquad \langle c_{k,\uparrow}^{\dagger}c_{-k,\uparrow}^{\dagger}\rangle = -\langle c_{-k,\uparrow}^{\dagger}c_{k,\uparrow}^{\dagger}\rangle$$

Unconventional superconductivity

Generic forms of superconductivity

A generic superconducting Hamiltonian

$$\widehat{H}' = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \widehat{c}_{\boldsymbol{k},\sigma}^{\dagger} \widehat{c}_{\boldsymbol{k},\sigma} - \frac{1}{2} \sum_{\boldsymbol{k}}' \sum_{\sigma_{1},\sigma_{2}} \left[\Delta_{\boldsymbol{k},\sigma_{1}\sigma_{2}} \widehat{c}_{\boldsymbol{k},\sigma_{1}}^{\dagger} \widehat{c}_{-\boldsymbol{k},\sigma_{2}}^{\dagger} + \Delta_{\boldsymbol{k},\sigma_{1}\sigma_{2}}^{*} \widehat{c}_{\boldsymbol{k},\sigma_{1}} \widehat{c}_{-\boldsymbol{k},\sigma_{2}} \right]$$

Can be characterized by a superconducting matrix

$$\Delta_{\boldsymbol{k}} = \begin{pmatrix} \Delta_{\boldsymbol{k},\uparrow\uparrow} & \Delta_{\boldsymbol{k},\uparrow\downarrow} \\ \Delta_{\boldsymbol{k},\downarrow\uparrow} & \Delta_{\boldsymbol{k},\downarrow\downarrow} \end{pmatrix}$$

The symmetry of the SC order determines the nature of the SC order

Superconducting momentum symmetries

A generic type of a superconductor is characterized by the order parameter

Real space

Reciprocal space

 $\Delta_{\uparrow\downarrow}(\mathbf{r},\mathbf{r}')\sim\langle c_{\mathbf{r}\uparrow}c_{\mathbf{r}\downarrow}\rangle\qquad\qquad\Delta_{\uparrow\downarrow}(\mathbf{k})\sim\langle c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}\rangle$

The superconducting state can be characterized by the symmetry of $~~\Delta_{\uparrow\downarrow}({f k})$

Singlet and triplet superconductors

The superconducting order inherits a symmetry property

$$\Delta_{\vec{k},s_{1}s_{2}} = -\Delta_{-\vec{k},s_{2}s_{1}} = \begin{cases} \Delta_{-\vec{k},s_{1}s_{2}} = -\Delta_{\vec{k},s_{2}s_{1}} & \text{even} \\ -\Delta_{-\vec{k},s_{1}s_{2}} = \Delta_{\vec{k},s_{2}s_{1}} & \text{odd} \end{cases}$$

 $\begin{array}{ll} \textit{Spin-singlet (even)} & \textit{Spin-triplet (odd)} \\ \Delta_{\uparrow\downarrow}(\mathbf{k}) = \Delta_{\uparrow\downarrow}(-\mathbf{k}) & \Delta_{\uparrow\uparrow}(\mathbf{k}) = -\Delta_{\uparrow\uparrow}(-\mathbf{k}) \end{array}$

The symmetry of the superconducting order characterizes the superconductor

Generating a spin-triplet superconductor

Let us take a Hamiltonian breaking time-reversal with attractive interactions

$$H = t \sum_{\langle ij \rangle} c_{i,s}^{\dagger} c_{j,s} + J_z \sum_{i} \sigma_z^{s,s'} c_{i,s}^{\dagger} c_{j,s'} + V_1 \sum_{\langle ij \rangle} \sum_{s} (c_{i,s}^{\dagger} c_{i,s}^{\dagger}) \sum_{s'} (c_{j,s'}^{\dagger} c_{j,s'}^{\dagger})$$

kinetic

exchange

attractive interactions

At the mean-field level, this may generate

$$H \sim \sum_{\langle ij \rangle} \Delta_{\uparrow\uparrow} c^{\dagger}_{i,\downarrow} c^{\dagger}_{j,\downarrow} + h.c. + \dots$$
Generating a spin-triplet superconductor

We start with a ferromagnetic 2D material, and see if interactions create superconductivity

$$H = t \sum_{\langle ij \rangle} c^{\dagger}_{i,s} c_{j,s} + J_z \sum_{i} \sigma^{s,s'}_{z} c^{\dagger}_{i,s} c_{j,s'} \qquad \overset{\text{by}}{\underset{-1}{\overset{-1}{\overset{-2}{\overset{2}}{\overset{2}}{\overset{2}}{\overset{2}}{\overset{2}}{$$

A spin-triplet superconductor



A spin-triplet superconductor, in a strip



A ferromagnetic superconductor can develop edge modes

Gapped and gapless superconductors

Let us focus on the superconducting order $~~\Delta_{\uparrow\downarrow}({f k})$

Fully gapped

$$|\Delta_{\uparrow\downarrow}(\mathbf{k})|^2 > 0$$

Gapless

$$|\Delta_{\uparrow\downarrow}(\mathbf{k}_{\alpha})|^2 = 0$$

Twisted trilayer graphene



Superconducting momentum symmetries

The superconducting state can be characterized by the symmetry of $\Delta({f k})$



(driven by phonons)

(driven by FE magnons)

(driven by AF magnons)



Some superconducting symmetries in the square lattice

Some superconducting symmetries in the square lattice



Some superconducting symmetries in the triangular lattice

Some superconducting symmetries in the triangular lattice



Gapped superconducting orders can be radically different



While both orders are gapped, they have different topological properties

Gapped superconducting orders can be radically different



The topological superconducting gap leads to protected edge excitations

Pair breaking effects in superconductors

Impurities in 2D superconductors

So-far we considered pristine superconductors, but what happens when we put impurities?





How detrimental are defects in superconductors?

Impurities in 2D superconductors

A non-magnetic impurity



Several non-magnetic impurities



A magnetic impurity



Several magnetic impurities



Non-magnetic impurity, conventional s-wave superconductor



A non-magnetic impurity does not affect conventional s-wave superconductors

Non-magnetic disorder, conventional s-wave superconductor



Non-magnetic disorder does not impact a conventional s-wave superconducting gap

The interplay between magnetism and superconductivity



Magnetic impurities create in-gap states in fully gapped superconductors



The interplay between magnetism and superconductivity

The exchange coupling controls the energy of the in-gap state



The effect of magnetic disorder in superconductors



Magnetic disorder decreases the gap of conventional superconductors

The interplay between impurities and unconventional superconductivity



Non-magnetic impurities create in-gap states in fully gapped unconventional superconductors

Summer school 2022 "Emergent quantum matter in artificial two-dimensional materials" The impact of non-magnetic disorder in unconventional superconductors

Non-magnetic disorder in unconventional superconductors decreases the gap



Non-magnetic impurities in nodal superconductors



Non-magnetic impurities create in-gap states in nodal unconventional superconductors



10-15 min break

(optional) to discuss during the break

What type of superconducting order is each one?

$$c_{n,\uparrow}^{\dagger}c_{n,\downarrow}^{\dagger}$$
 $c_{n,\uparrow}^{\dagger}c_{n+1,\downarrow}^{\dagger}$ $c_{n,\uparrow}^{\dagger}c_{n+1,\uparrow}^{\dagger}$

and which symmetries do they break?

One-dimensional topological superconductivity

The Nambu representation

How do we solve a Hamiltonian of the form

$$H = \sum_{\mathbf{k},s} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},s} c_{\mathbf{k},s} + \sum_{\mathbf{k}} \Delta c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k},\downarrow}$$

Define a Nambu spinor



The Hamiltonian in the Nambu basis is quadratic and can be diagonalized

$$H = \Psi_{\mathbf{k}}^{\dagger} \mathcal{H} \Psi_{\mathbf{k}}$$

Majorana excitations

A very special type of fermion is a so-called Majorana fermion

 $\Psi^{\dagger}=\Psi$

Which by definition it is its own antiparticle

Majorana fermion do not appear naturally in materials, as we only have electrons

Yet, mathematically, each electron can be written as two Majoranas

$$c = \Psi_{\alpha} + i\Psi_{\beta}$$
 $c^{\dagger} = \Psi_{\alpha} - i\Psi_{\beta}$ $\Psi_{\alpha}^{\dagger} = \Psi_{\alpha}$ $\Psi_{\beta}^{\dagger} = \Psi_{\beta}$

Can we isolate a single Majorana in a material?



Excitations in superconductors are combinations of electrons and holes, for instance

$$\Psi \sim c_n + c_n^{\dagger}$$

But this excitation is by definition a Majorana fermion

 $\Psi^{\dagger} = \Psi$

Can we have superconductors in nature that show these excitations?

Summer school 2022 "Emergent quantum matter in artificial two-dimensional materials" The minimal model for a 1D topological superconductor

One dimensional spinless p-wave superconductor (Kitaev model)

$$H = \sum_{n} t c_{n+1}^{\dagger} c_n + \Delta c_n c_{n+1} + c.c.$$

p-wave superconductivity

$$c_k = \sum_{n} e^{ikn} c_n$$

$$H = \sum_{k} \epsilon_k c_k^{\dagger} c_k + i\Delta \left[c_{-k} c_k \sin k - c_{-k}^{\dagger} c_k^{\dagger} \sin k \right]$$

Summer school 2022 "Emergent quantum matter in artificial two-dimensional materials" A model Hamiltonian for topological superconductivity

Spinless fermions in a 1D chain (Kitaev model)

$$H = \sum c_n^{\dagger} c_{n+1} + c_n c_{n+1} + h.c.$$

Can be transformed into

n

 $c_n = \gamma_{2n-1} + i\gamma_{2n}$

$$H = i \sum \gamma_{2n} \gamma_{2n+1}$$

n

 γ Majorana operators



A model Hamiltonian for topological superconductivity

Infinite one dimensional chain



A model Hamiltonian for topological superconductivity



For finite systems, topological superconductivity gives rise to zero modes

Majorana states as topological surface modes

Generalized Kitaev model $H = \sum_{n} c_{n}^{\dagger} c_{n+1} + \Delta c_{n} c_{n+1} + \mu c_{n}^{\dagger} c_{n} + h.c.$ p-wave SC Chemical potential

- Large chemical potential render the system filled, and topologically trivial
- p-wave SC promotes a topological phase with Majorana states

The emergence of Majorana states is associated to non-trivial topology

The two phases of the Kitaev model





Taking the surface states of a quantum spin-Hall (QSH) insulator



Summer school 2022 "Emergent quantum matter in artificial two-dimensional materials" A Simple way of building a topological superconductor with Majorana modes

Gap some of the helical modes with a magnet



Summer school 2022 "Emergent quantum matter in artificial two-dimensional materials" A simple way of building a topological superconductor with Majorana modes



Two-dimensional artificial topological superconductivity

Engineering unconventional superconductors with conventional ones

CrBr₃/NbSe₂

Van der Waals superconductor

Van der Waals ferromagnet


Engineering helical states



With Rashba SOC, a spin-dependent spin splitting appears

Engineering helical states

$H_{kin} + H_J + H_{SOC}$



With Rashba SOC and exchange, helical states appear

Engineering a topological superconductor



An s-wave superconducting gap opens up a tropological gap in the heterostructure

Artificial topological superconductivity C=1, bulk electronic structure

Bulk electronic structure



The combination of SOC and exchange creates helical states Superconductivity gaps out the helical states in a non-trivial way

Artificial topological superconductivity C=1, ribbon electronic structure



Artificial topological superconductivity C=3, bulk electronic structure



The combination of SOC and exchange creates helical states Superconductivity gaps out the helical states in a non-trivial way

Artificial topological superconductivity C=3, ribbon electronic structure





As we the value of the exchange coupling is changed, a transition from trivial to topological emerges



A gap closing appears at a critical value of the exchange field



As we the value of the exchange coupling is changed, a transition from trivial to topological emerges



A gap closing (and edge states) appear at a critical value of the exchange field

For the exercise session this afternoon

Download the Jupyter-notebook from

https://github.com/joselado/jyvaskyla_summer_school_2022/blob/main/sessions/session2.ipynb

The tasks during the exercise sessions

You will see examples with the code



You have to modify them, and answer questions

Exercise

- Discuss why an f-wave order is a triplet superconducting order parameter
- · Discuss in which points of the Brillouin zone the triplet order (odd order parameter) must have nodes