P-Wave Superconductivity

in Extremely Correlated 2d metal

Current Trends in Condensed Matter Physics
NISER, Bhubaneswar
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The Institute of Mathematical Sciences

G Baskaran

Chennai 600113

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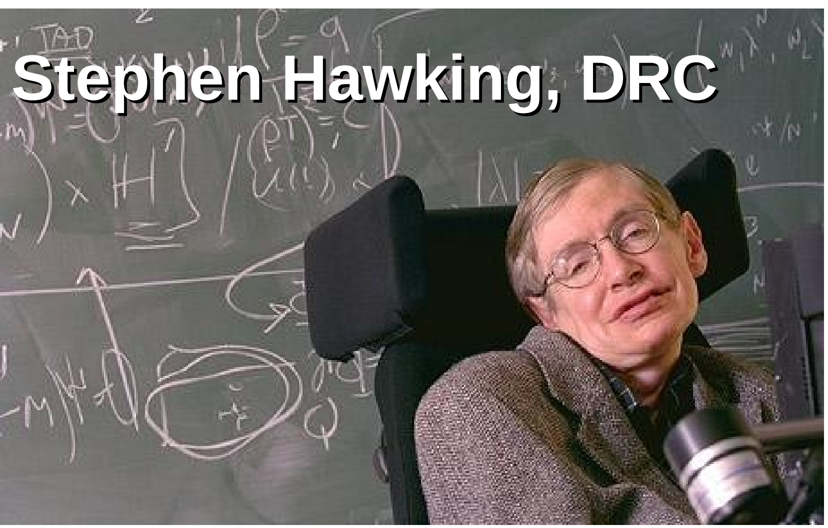

Lou Gehrig's disease

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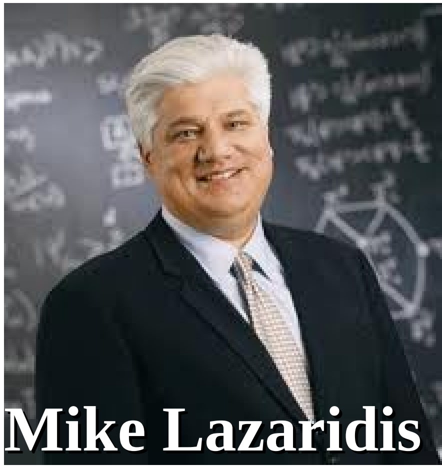
**An example of respect by an individual
for theoretical physics as something
that helps transform society
(other examples – Kavli, Yuri Millner, Simons
Tata, Alagappa, Birla, Mehta, A C Muthiah, …)**



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Plan of the Talk

Chiral P-wave superconductors, Vortices, Manorana Zero Modes

Braiding of vortices & Topological Quantum Computation

P-wave superconducting instability in Half Metal Fermi Liquids
From charge and spin current coupling

Infinite U repulsive Hubbard Model on a Honey Comb Lattice,
Nagaoka Ferromagnetism (Half metal) coexisting with
p-wave superconductivity **(Grassman Tensor Network approach)**

Possible Experimeental Realization

p-Wave Superconductivity

Attraction in the spin triplet channel

Orbital part is antisymmetric. Spin part symmetric

He^3 is a well known p-wave superfluid
Some heavy fermions are believed to be p-wave superconductors

Sr_2RuO_4 is a good example of a 2-dimensional p-wave superconductor with a good experimental support

Pairing in nuclei and neutron stars have p-wave character

Sr_2RuO_4

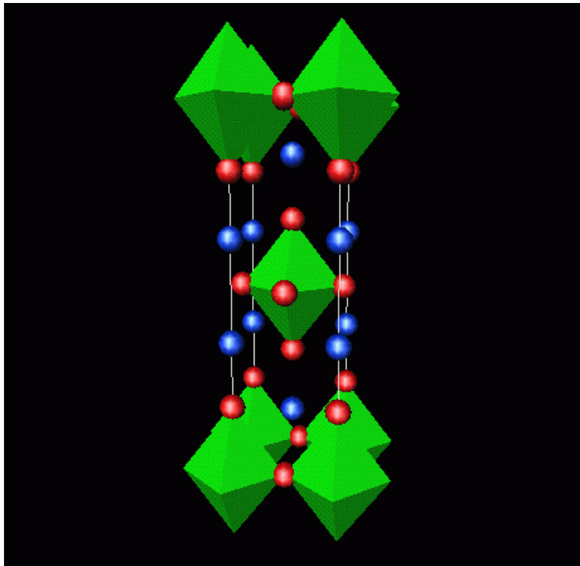
structurally similar to

La_2CuO_4

- **Theoretical Prediction of p-Wave Superconductivity**
- **T. M. Rice, M. Sigrist**, *J. Phys. Cond. Matter* **7**, L643 (1995)
- **G. Baskaran**, *Physica B* ***223-224****, 490 (1996); Trieste Workshop July 1995*

Superconducting Tc ~ 1 K,   very low !

Story: Piers Coleman's Challenge at Trieste
and GB's response



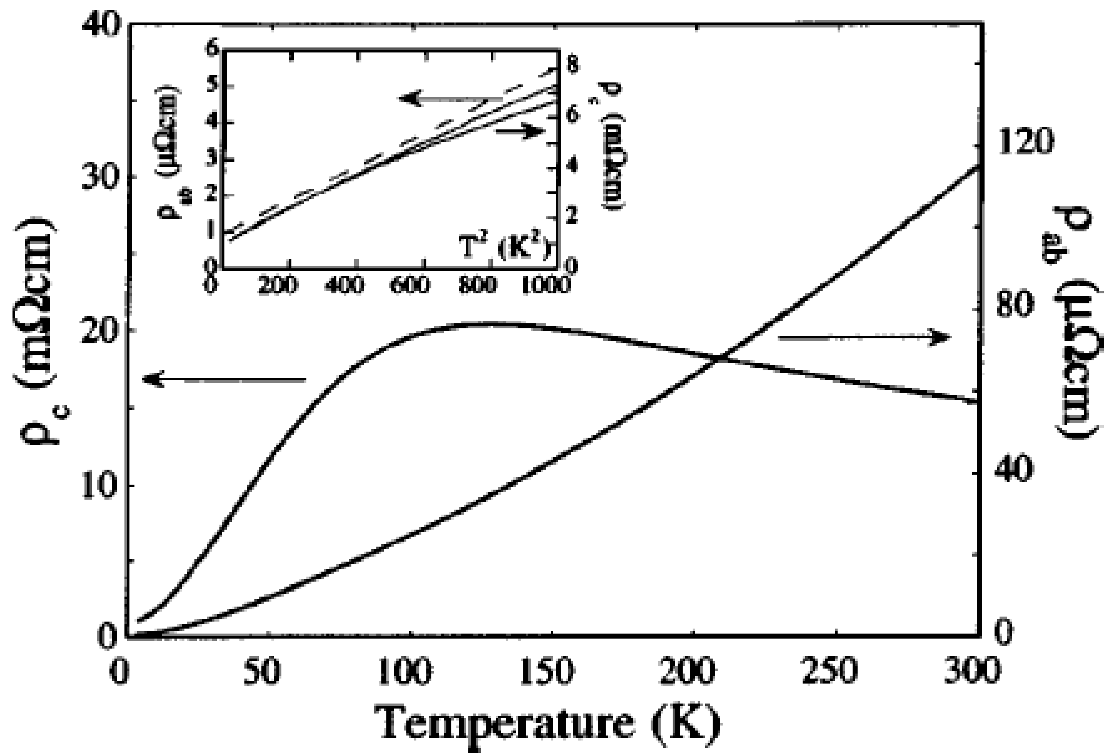
BCS@50 50th ANNIVERSARY

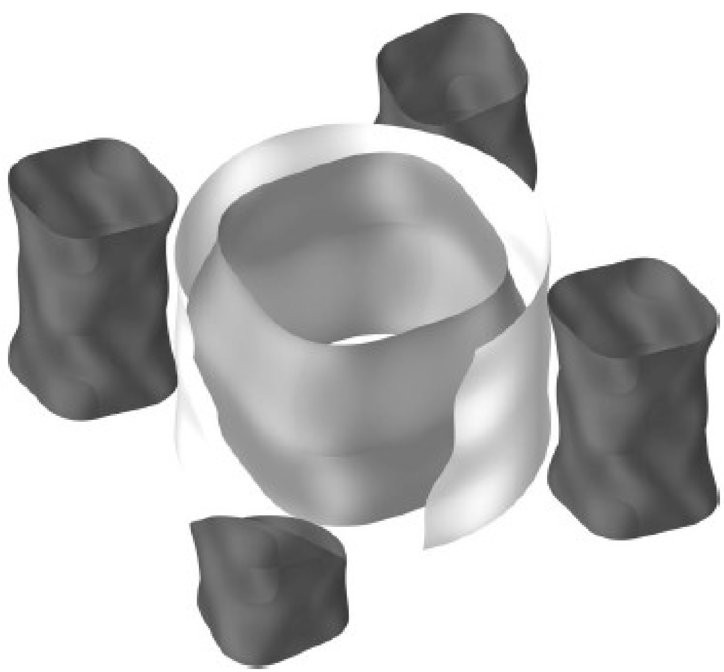
ILLINOIS UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

SUPERCONDUCTIVITY AND ELECTRON CORRELATIO IN RUTHENATES

BECKMAN AUDITORIUM

Dr. Mackenzie will review the physics of ruthenate superconductivity, a field which was kick-started by the experimental discovery of Yoshiteru Maeno and colleagues in 1994 and further fueled soon afterwards by the inspired suggestions by Rice, Sigrist, and (independently) Baskaran th Sr_2RuO_4 was a candidate for spin triplet pairing. He will discu the evidence that has accumulated supporting that hypothe and try to give an objective assessment of the current state knowledge regarding the gap symmetry. He will particularly

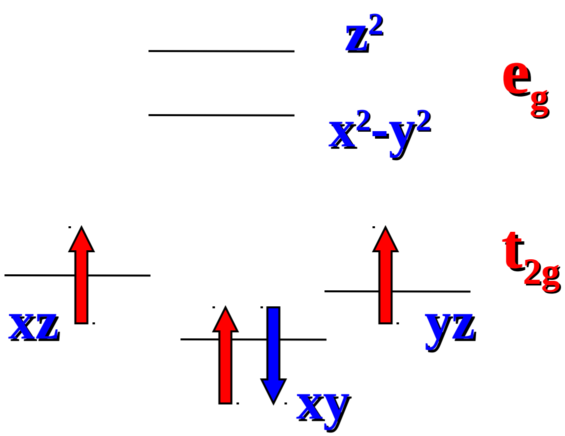




dHvA oscillation and experimental Fermi surface

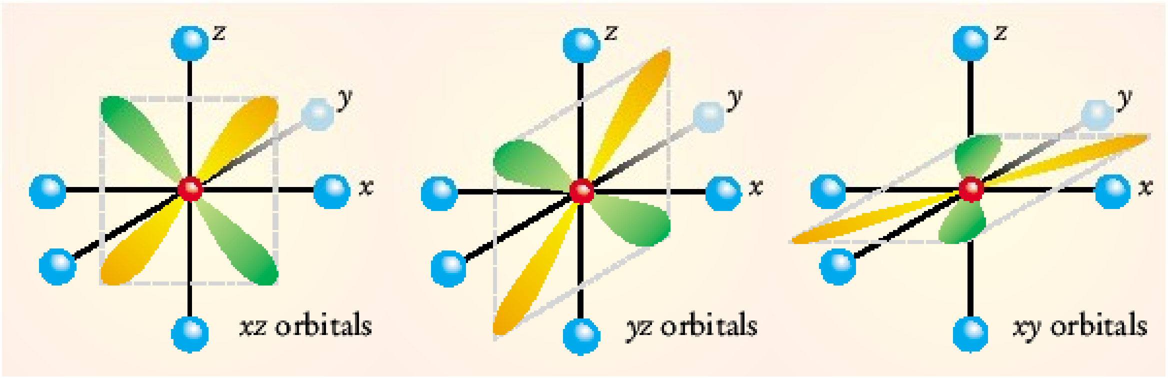
$(Sr^{2+})_2\ Ru^{4+}\ (O^{2-})_2$ Ru^{4+} is in $4d^4$ configuration

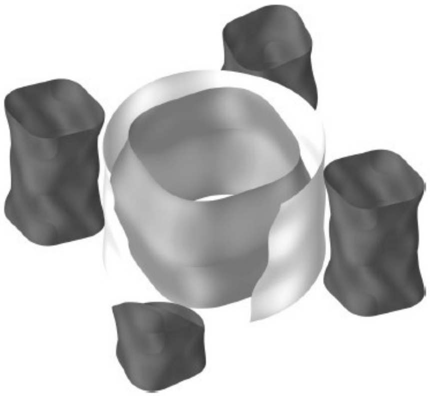
Sister compound Sr_2FeO_4 is a spin-1 Mott insulator



So coulomb correlations and Hund coupling are likely to be very important (GB)

Spin triplet pairing ($p_x + ip_y$) was predicted





Orbital part can have p_x , p_y or p_z symmetry or
linear combinations such as $p_x + i\,p_y$ or $p_x - i\,p_y$
(in 2D this will be favored, because of in plane orbital motion)

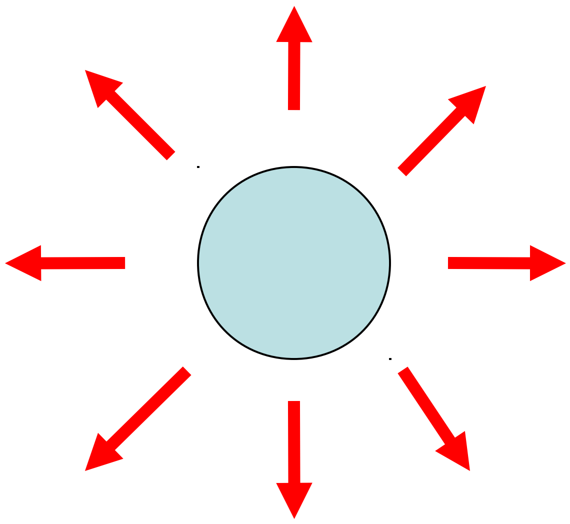
Spin part has to be symmetric under interchange. So it will be one of the three triples or linear combinations.

Cooper pair amplitude (Superconducting order parameter is not a scalar

$$\Psi = e^{i\varphi}[d_x(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) + i d_y(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) + d_z(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)](k_x + i k_y).$$

direction $\hat{\mathbf{d}}$ of triplet pairing

Excitations of 2D supercondctors



Bogoliubov quasi particles and quantized vortices

Traditionally one views the phase as a 2d vector

In a quantized vorex carrying flux quanta $\frac{hc}{2e}$

The phase of the order parameter φ winds by 2π as we go around the vortex once

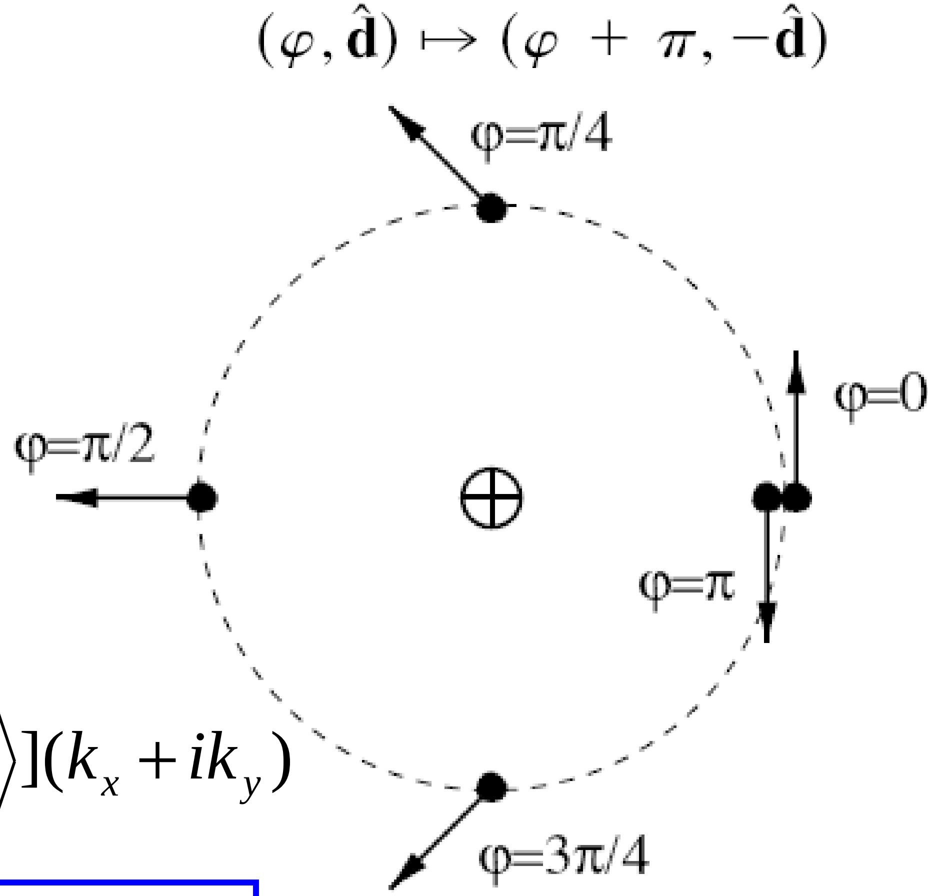
There is a normal core at the center of the vortex of dimension ξ , the coherence length.

The size of the magnetic flux is λ the London peneteration length

Single quantum vortex located at the origin in 2D s-wave superconductor

$$\Delta(r,\theta) = \Delta_0 f(r) e^{i\theta}$$

Half Quantum Vortex



$$\Psi(r,\theta) = \Delta(r) e^{\frac{i\theta}{2}} [e^{\frac{i\theta}{2}} \left|\uparrow\uparrow\right\rangle + e^{\frac{-i\theta}{2}} \left|\downarrow\downarrow\right\rangle](k_x + ik_y)$$

$$\Psi(r,\theta) = \Delta(r)[e^{i\theta} \left|\uparrow\uparrow\right\rangle + \left|\downarrow\downarrow\right\rangle](k_x + ik_y)$$

Order parameter remains single valued

In the absence of vortices Bogoliubov quasiparticles are Bloch waves
They are positive energy excitations with a finite gap

S-wave superconductors are nodeleess and generically have a gap
(Extended-S can have nodes)
P_x or p_y states has a node because of they have odd parity

$$\Delta(k_x, k_y) = \Delta_0 k_x$$

Time reversal symmetry is not broken
only parity symmetry is broken

States such as $p_x + i\,p_y$ or $p_x - i\,p_y$ are gapless and do note have a node

$$\Delta_{\pm}(k_x, k_y) = \Delta_0 \times (k_x \pm i k_y)$$

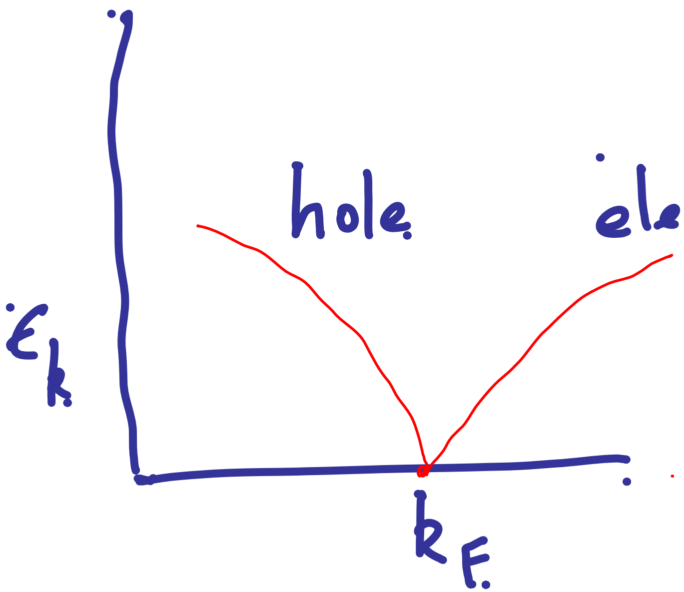
They violate both parity and time reversal symmetry (PT violation)

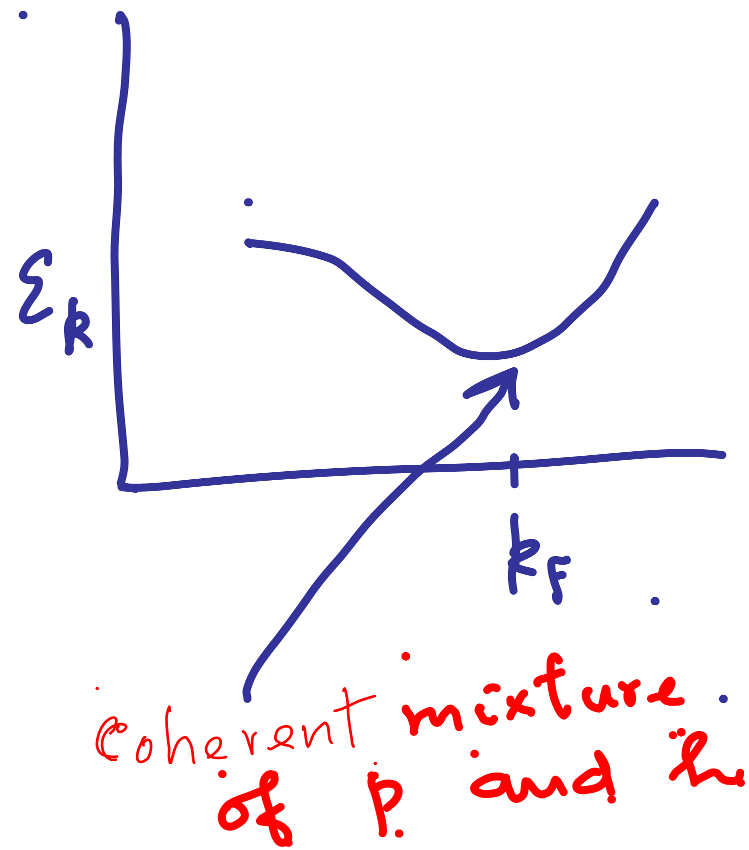
The orbital motion produces magnetic field perpendicular to the plane which has been measured, for the case of Sr_2RuO_4 , by muon spin rotation

Bogoliubov quasi particle is a linear combinations of an electron and a hole of opposite spin Their chrges are defined only module 2

$$\alpha_{k\sigma} = u_k c_{k\sigma} + \sigma v_k c^{+}_{-k\bar{\sigma}}$$

$$\alpha^{+}_{k\sigma} = u_k c^{+}_{k\sigma} + \sigma v_k c_{-k\bar{\sigma}}$$





How does one study quantized vortices and see how quasi particle states get modified in the presence of vortices ?

Use Bogoliubov de Gennes Equations, derivable from mean field BCS Hamiltonian

$$H = \int d^2\mathbf{r}\Big[\Psi^\dagger\Big(-\frac{\nabla^2}{2m} - \varepsilon_F\Big)\Psi \quad + \Psi^\dagger[e^{i\theta}\Delta(r) * (\nabla_x + i\nabla_y)]\Psi^\dagger + \text{H.c.}\Big]$$

$[A * B = (AB + BA)/2]$ $\qquad$ r and θ are the polar coordinates

$$i\hbar\partial_t\Psi = [H,\Psi] = -\frac{\hbar^2}{2m^*}(\partial_x{}^2 + \partial_y{}^2)\Psi + g\Delta\Psi^*$$

$$i\hbar\partial_t\Psi^* = [H,\Psi^*] = -\frac{\hbar^2}{2m^*}(\partial_x{}^2 + \partial_y{}^2)\Psi^* + g\Delta^*\Psi$$

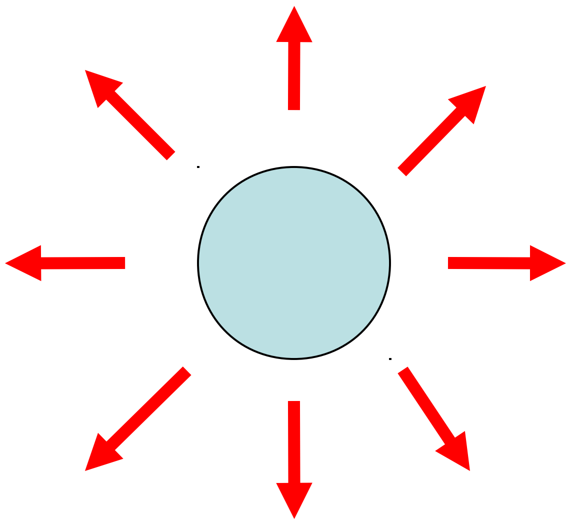
$\begin{pmatrix} u \\ v \end{pmatrix}$ Nambu spinor

The combination $\qquad \gamma^\dagger = u\Psi^\dagger + v\Psi$

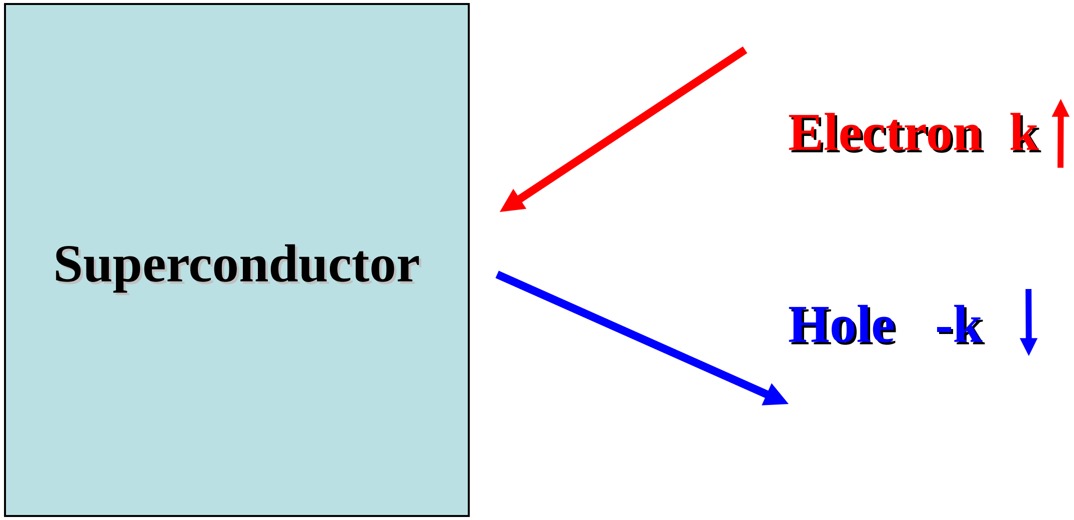
Solves the BGD equation $\qquad [H, \gamma^\dagger] = E\gamma^\dagger$

$$E \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} h & \frac{i}{2}\left\{\Delta(\mathbf{r}), \partial_x + i\partial_y\right\} \\ \frac{i}{2}\left\{\Delta^*(\mathbf{r}), \partial_x - i\partial_y\right\} & -h \end{pmatrix} \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix}$$

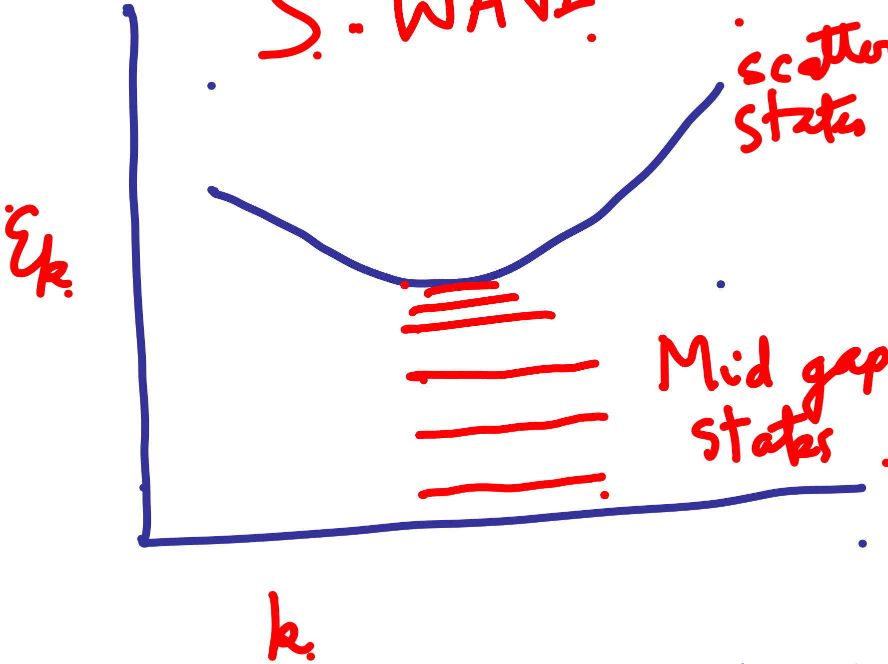
Normal state quasi particles at the vortex core get Andreev reflected at the boundary of the core and establish bound quasi particle states in the gap of the quasi particle spectrum



Because the boundary has a non trivial topology for the phase of the order parameter the bound qp-states could have non-trivial topological and robust character



S-WAVE



s-wave

de Gennes Marticoni

$$E_n \sim E_0 \left(n + \tfrac{1}{2}\right)$$

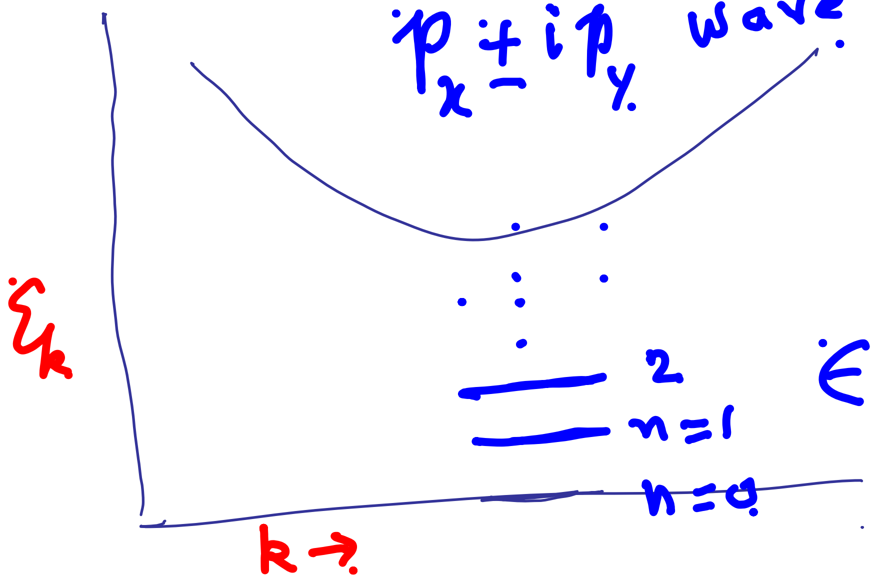
$$E_0 \sim \frac{\Delta^2}{E_F}$$

p-wave

Kopnin, Salomaa

Volovick ...

$p_x \pm i p_y$ wave SC



$$E_n \sim E_0 n \qquad n = 0, 1, 2 \ldots$$

Nature of localized quasi particle states in Half vortices

$$\gamma^{\dagger}(E) = \gamma(-E)$$

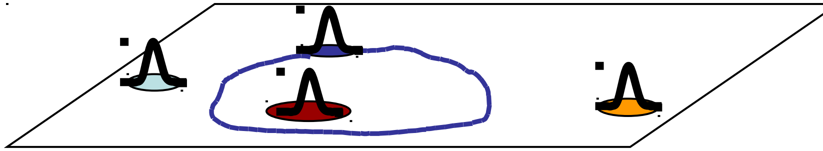
Number of degree of freedom (number of fermi oscillators) is half as that of a single vortex

The zero-energy level becomes a self-conjugate **Majorana Fermion**

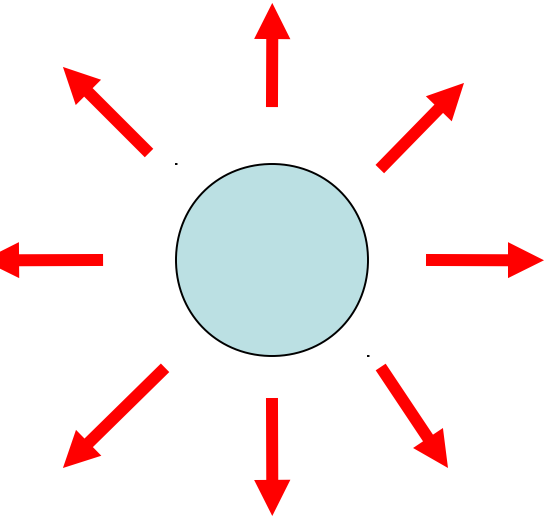
$$\gamma^{\dagger}(E=0) = \gamma(E=0)$$

Contrast it with midgap states in domain walls in polyacetylene

The Majorana Fermion zero mode is stable against local perturbations such as external scalar, electromagnetic vector potentials, spin orbit coupling, local variation of the order parameter etc.

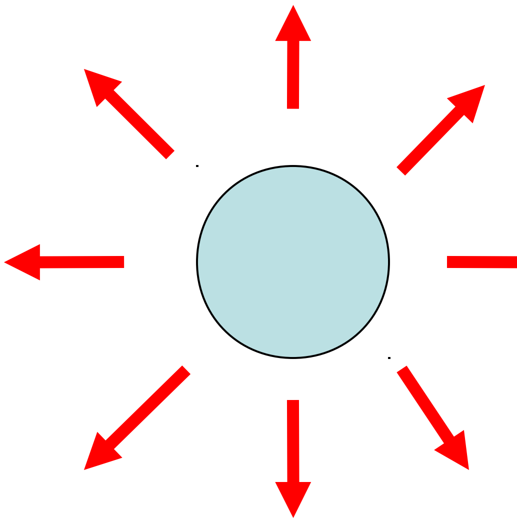


$$\gamma_i = \int dr\left[\; g(r-R_i)\psi(r) \quad + \quad g^*(r-R_i)\psi^+(r)\;\right]$$



$$\Psi = \gamma_1 + i\gamma_2$$

A complex fermion mode whose
Real and imaginary parts are
Well separated spacially !



γ_1

Majorana mode

γ_2

Majorana mode

How Majorana fermion transforms under U(1) gauge transformation

A overall phase of the superconducting gap shifts by $\frac{\varphi}{2}$

is equivalent to rotating the electronic creation and annihilation 0perators by

$$\Psi_\alpha \mapsto e^{i\phi/2}\Psi_\alpha, \ \Psi_\alpha^\dagger \mapsto e^{-i\phi/2}\Psi_\alpha^\dagger$$

Equivalently the solution (u,v) transforms accordingly $(u, v) \mapsto (ue^{i\phi/2}, ve^{-i\phi/2})$

The important consequence of this transformation rule is that under change of the phase of the order parameter by 2π the Majorana fermion in the vortex changes sign: $\gamma \mapsto -\gamma$. This is an obvious consequence of the fact that the quasiparticle is a linear combination of fermionic creation and annihilation operators carrying charge ± 1.

Considere a system of 2n vortices, far from each other at distances $l >> \xi \approx \frac{v_F}{\Delta}$

To each vortex there is a bound zero energy Majorana mode

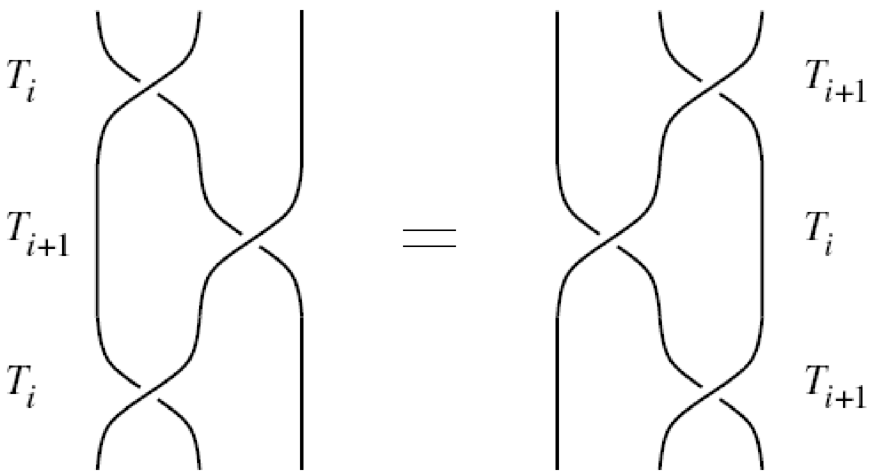
Denoted by the operator γ_i **i = 1,2, ….., 2n**

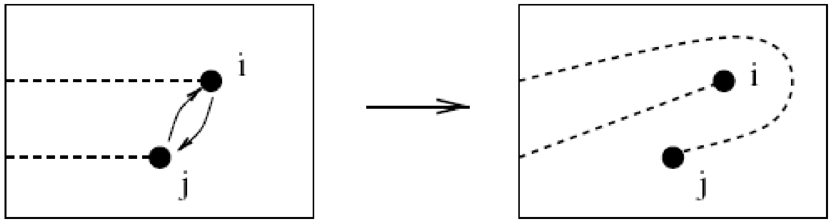
They can be combined to give n complex fermion operators
Therefore the ground state degeneracy is 2^n
(each fermion level may be full or empty)

If the vortices move adiabatically slowly so that we can neglect transitions between subgap levels, the only possible effect of such vortex motion is a unitary evolution in the space of ground states.

Let us fix the initial positions of vortices. Consider now a permutation (braiding) of vortices which returns vortices to their original positions (possibly in a different order). Such braid operations form a braid group B_{2n} (multiplication in this group corresponds to the sequential application of the two braid operations) This group is generated by elementary interchanges T_i of neighboring particles ($i = 1, \ldots, 2n - 1$) modulo the relations

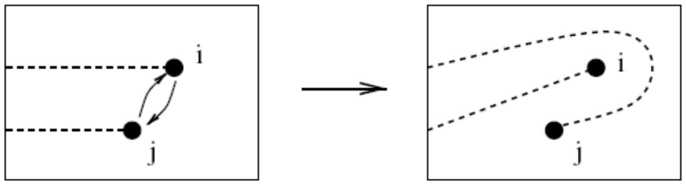
$$T_i T_j = T_j T_i, \qquad |i - j| > 1\,,$$
$$T_i T_j T_i = T_j T_i T_j, \qquad |i - j| = 1\,.$$





We seek a (projective) representation of the braid group B_{2n}

Since the Majorana fermions γ_i change sign under a shift of the superconducting phase by 2π, we introduce *cuts* connecting vortices to the left boundary of the system



$$T_i : \begin{cases} \gamma_i \mapsto \gamma_{i+1} , \\ \gamma_{i+1} \mapsto -\gamma_i , \\ \gamma_j \mapsto \gamma_j & \text{for } j \neq i \text{ and } j \neq i+1 \end{cases}$$

Now the action of operators T_i may be extended from *operators* to the Hilbert space. Since the whole Hilbert space can be constructed from the vacuum state by fermionic creation operators, and the mapping of the vacuum state by T_i may be determined uniquely up to a phase factor, the action (6) of B_{2n} on operators uniquely defines a projective representation of B_{2n} in the space of ground states.

We need to construct operators

$\tau(T_i)$ obeying $\tau(T_i)\gamma_j[\tau(T_i)]^{-1} = T_i(\gamma_j)$, where $T_i(\gamma_j)$ is defined by (6)

Recall $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$ **then (upto a phase factor)**

$$\tau(T_i) = \exp\left(\frac{\pi}{4}\gamma_{i+1}\gamma_i\right) = \frac{1}{\sqrt{2}}(1 + \gamma_{i+1}\gamma_i)$$

In the case of two vortices, the two Majorana fermions may be combined into a single complex fermion as $\Psi = (\gamma_1 + i\gamma_2)/2$, $\Psi^\dagger = (\gamma_1 - i\gamma_2)/2$. The ground state is doubly degenerate, and the only generator of the braid group T is represented by

$$\tau(T) = \exp\left(\frac{\pi}{4}\gamma_2\gamma_1\right) = \exp\left[i\frac{\pi}{4}(2\Psi^\dagger\Psi - 1)\right]$$
$$= \exp\left(i\frac{\pi}{4}\sigma_z\right), \tag{8}$$

In the case of 4 vortices we have two complex fermions

$$\Psi_1 = (\gamma_1 + i\gamma_2)/2, \Psi_2 = (\gamma_3 + i\gamma_4)/2 \text{ (and similarly for } \Psi_1^\dagger \text{ and } \Psi_2^\dagger)$$

The ground state degeneracy is 4 and 3 generators T_1 , T_2 and T_3 are given by

$$\tau(T_1) = \exp\left(i\,\frac{\pi}{4}\,\sigma_z^{(1)}\right) = \begin{pmatrix} e^{-i\pi/4} & & & \\ & e^{i\pi/4} & & \\ & & e^{-i\pi/4} & \\ & & & e^{i\pi/4} \end{pmatrix}$$

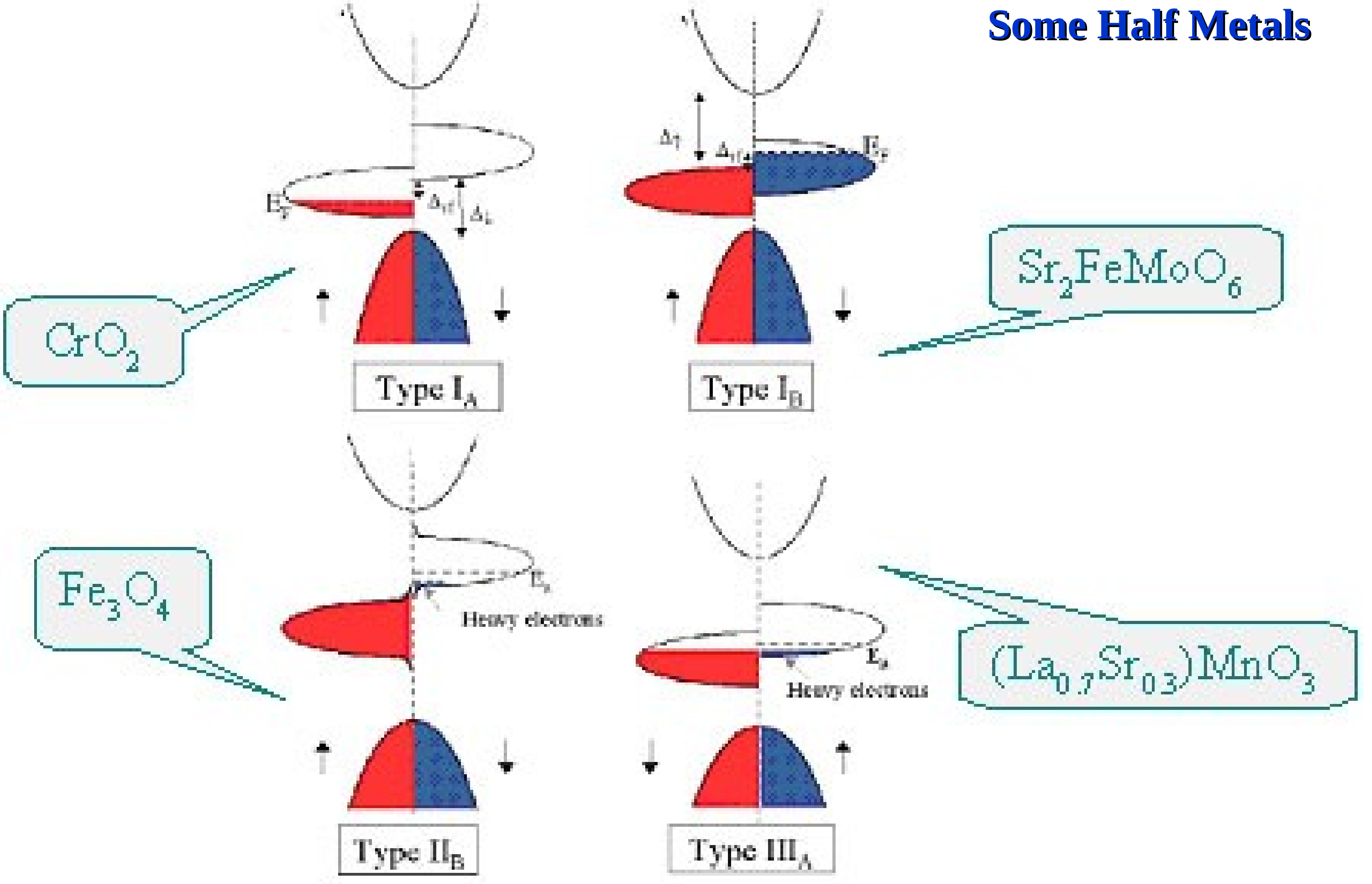
$$\tau(T_3) = \exp\left(i\,\frac{\pi}{4}\,\sigma_z^{(2)}\right) = \begin{pmatrix} e^{-i\pi/4} & & & \\ & e^{-i\pi/4} & & \\ & & e^{i\pi/4} & \\ & & & e^{i\pi/4} \end{pmatrix}$$

$$\tau(T_2) = \exp\left(\frac{\pi}{4}\,\gamma_3\gamma_2\right) = \frac{1}{\sqrt{2}}(1 + \gamma_3\gamma_2) = \frac{1}{\sqrt{2}}[1 + i(\Psi_2^\dagger + \Psi_2)(\Psi_1^\dagger - \Psi_1)] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & -i \\ 0 & 1 & -i & 0 \\ 0 & -i & 1 & 0 \\ -i & 0 & 0 & 1 \end{pmatrix}$$

The matrices are written in the basis $(|0\rangle,\ \Psi_1^\dagger|0\rangle,\ \Psi_2^\dagger|0\rangle,\ \Psi_1^\dagger\Psi_2^\dagger|0\rangle)$

Half Metallic Ferromagnets

Some Half Metals



Coey et al. J. Phys. D (2002)

Instability of the Half Metal Ferromagnet

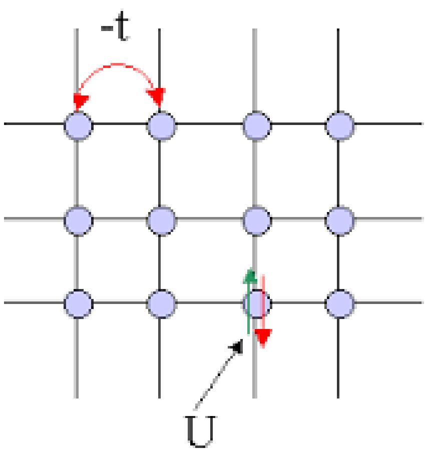
Majority spin electrons

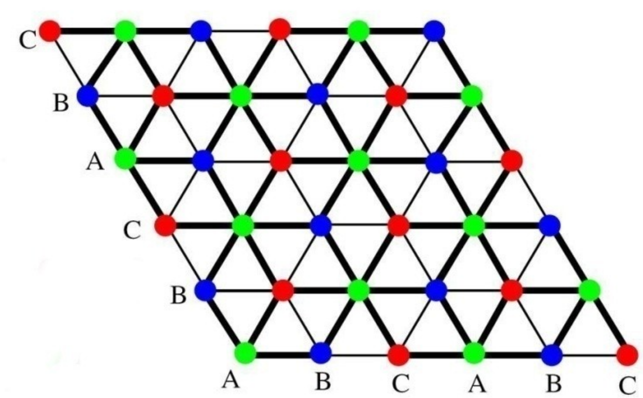
A small density of minorty spin electrons

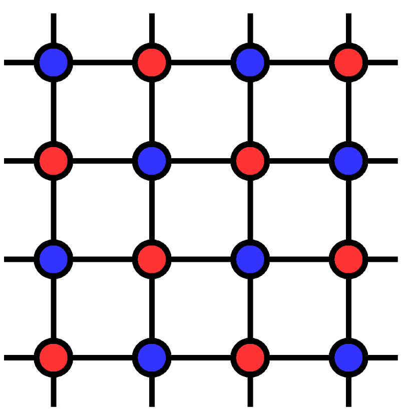
How do they couple ?

Hubbard Model

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow},$$

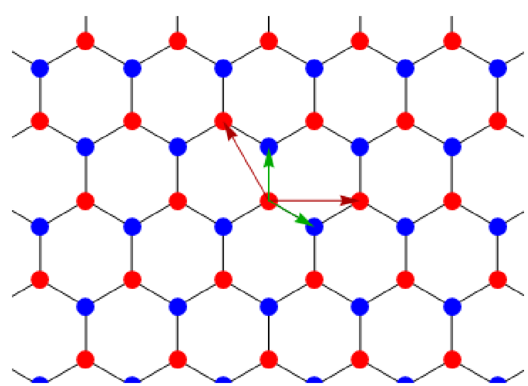






sublattice A

sublattice B



Infinite U Repulsive Hubbard Model

$$H = - \; t \sum_{\langle ij \rangle, \sigma} (\tilde{c}^{\dagger}_{i,\sigma} \tilde{c}_{j,\sigma} + h.c.) \cdot$$

$$\tilde{c}_{i,\sigma} \equiv c_{i,\sigma}(1 - n_{i,\bar{\sigma}})$$

Infinite repulsive U Hubbard model at Half Filling
is an insulator with dangling or fee spins.
Ground state has a 2^N fold spin degeneracy.

Nagaoka Theorem:
For bipartite lattices with nearest neighbor hoping a single hole removes the massive degeneracy and creates a fully spin polarized Ferromagnetic ground state.

How about finite density of holes ?
Theoretical studies indicate that ferromagnetism might survive upto about 20 % of doping.

All focus in the literature has been on Nagaoka Ferromagnet, a half metallic state

Instability of half metallic Fermi Liquid (GB, Zhengcheng Gu, Hong-Chen Jiang) 2015)

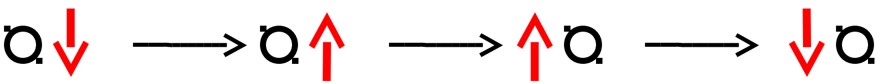
$$H = t\sum_{\langle ij\rangle}(1-n_{i\downarrow})c^\dagger_{i\uparrow}c_{j\uparrow}(1-n_{j\downarrow}) + h.c.$$
$$+\ t\sum_{\langle ij\rangle}(1-n_{i\uparrow})c^\dagger_{i\downarrow}c_{j\downarrow}(1-n_{j\uparrow}) + h.c.$$

$$(1-n_{i\uparrow})c^\dagger_{i\downarrow} = c_{i\uparrow}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} = S^-_i c^\dagger_{i\uparrow}$$

$$c_{j\downarrow}(1-n_{j\uparrow}) = c_{j\downarrow}c_{j\uparrow}c^\dagger_{j\uparrow} = c_{j\uparrow}S^+_j$$

Where $S^-_i \equiv c^\dagger_{i\downarrow}c_{i\uparrow}$ **etc.**

$$H = t\sum_{\langle ij\rangle}(1-n_{i\downarrow})c^\dagger_{i\uparrow}c_{j\uparrow}(1-n_{j\downarrow}) + h.c. + t\sum_{\langle ij\rangle}c^\dagger_{i\uparrow}c_{j\uparrow}S^-_i S^+_j + h.c.$$



$$H = t(1-\delta_0)^2\sum_{\langle ij\rangle}(c^\dagger_{i\uparrow}c_{j\uparrow} + h.c.)$$
$$+\ \frac{1}{2}t\sum_{\langle ij\rangle}(c^\dagger_{i\uparrow}c_{j\uparrow} + c^\dagger_{j\uparrow}c_{i\uparrow})(S^-_i S^+_j + S^-_j S^+_i)$$
$$+\ \frac{1}{2}t\sum_{\langle ij\rangle}(c^\dagger_{i\uparrow}c_{j\uparrow} - c^\dagger_{j\uparrow}c_{i\uparrow})(S^-_i S^+_j - S^-_j S^+_i)$$

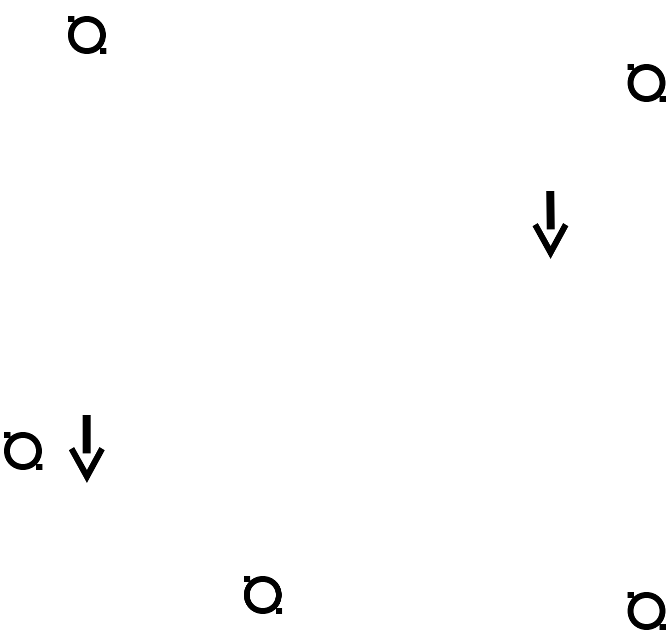
$$(S^-_i S^+_j + S^-_j S^+_i) \equiv (S^i_x S^j_x + S^i_y S^j_y)$$

$$(S^-_i S^+_j - S^-_j S^+_i) \equiv \vec{z}\cdot(\vec{S}_i \times \vec{S}_j)$$

$$
\begin{aligned}
H \;=\;& t(1-\delta_0)^2 \sum_{\langle ij\rangle} (c^\dagger_{i\uparrow} c_{j\uparrow} + h.c.) \\
&+ \frac{1}{2} t \sum_{\langle ij\rangle} (c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{j\uparrow} c_{i\uparrow})\,(S^i_x S^j_x + S^i_y S^j_y) \\
&+ \frac{1}{2} t \sum_{\langle ij\rangle} (c^\dagger_{i\uparrow} c_{j\uparrow} - c^\dagger_{j\uparrow} c_{i\uparrow})[\,\vec{z}\cdot(\vec{S}_i \times \vec{S}_j)\,]
\end{aligned}
$$

Charge kinetic energy -
Spin-kinetic energy coupling

Charge current –
Spin Chirality current coupling



Dilute gas of holes ○ ↓
and down spins in the
background of dense up spins

Spin current excitations are topological and carry non-zero chirality
Skyrmions in 2 dimensions and Monopoles in 3-dimensions

Skyrmions are capable of binding a single hole and
Gain energy through charge and spin current interaction
Skyrmions form pairs and provide opportunity for pairing of two holes bound to them

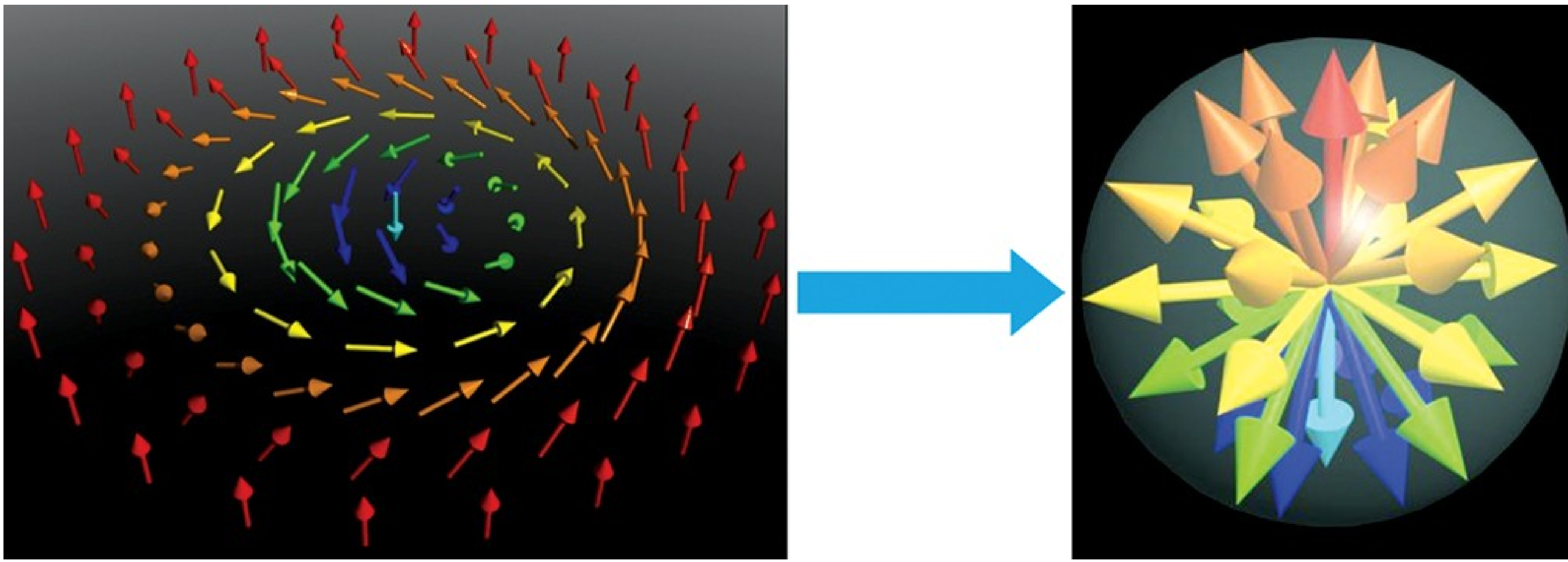
This is a spin triplet cooper pair
having unit orbital angular momentum ($l_z = +1$ or -1)

The system gains energy by having a small and optimal density of
Skyrmions in the ground state. ($N_{skyrmion} / N_{hole} << 1$)

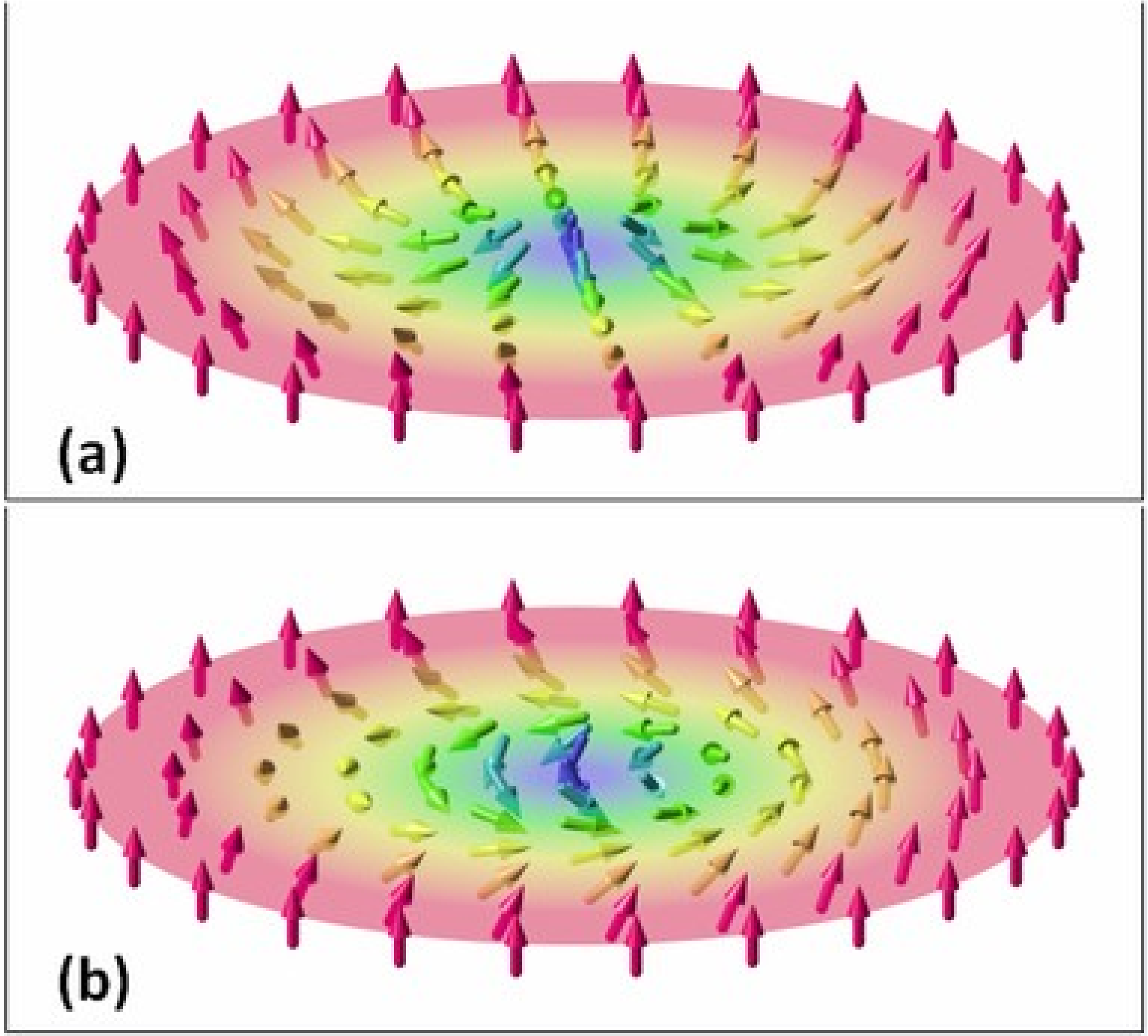
p + i p and p – i p order parameter symmetry correspond to
Chiral spin liquids with opposite macroscopic chirality

Skyrmion and anti Skyrmion:

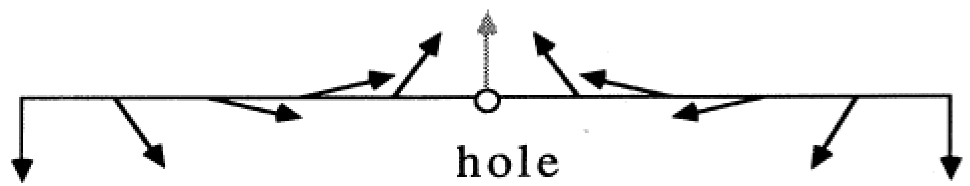
Mapping of spins in the plane R^2 ⟶ Unit sphere S^2



http://www.riken.jp/en/research/rikenresearch/highlights/6527



http://www.revolvy.com/main/index.php?s=Skyrmion



A hole in a twisted spin configuration

Doucot and Wen, Phys Rev B (2002)

GrassmannTernsor Product States – A variational approach

(a new and powerful variational approach for strongly interacting fermions developed by Verstraete, Cirac, Wen, Gu and others following DMRG, matrix product and tensor network states)

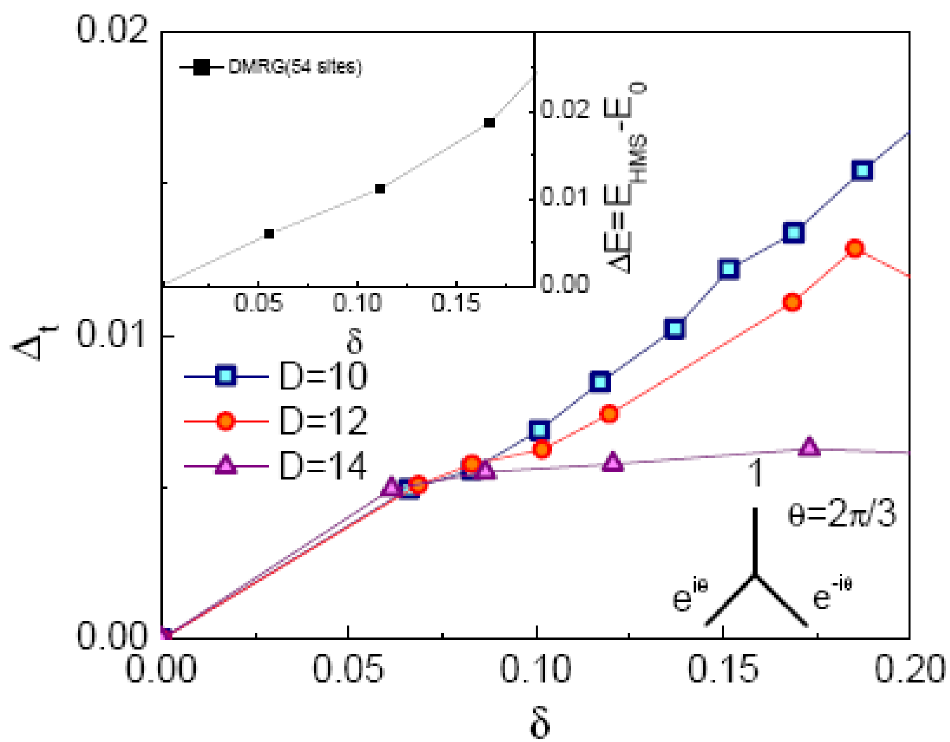


FIG. 2: (Color online)Triplet SC order parameters as a function of doping. Insert: "condensation energy" ΔE as a function of doping.

Gu, Jiang, GB

arXiv:1408.6820

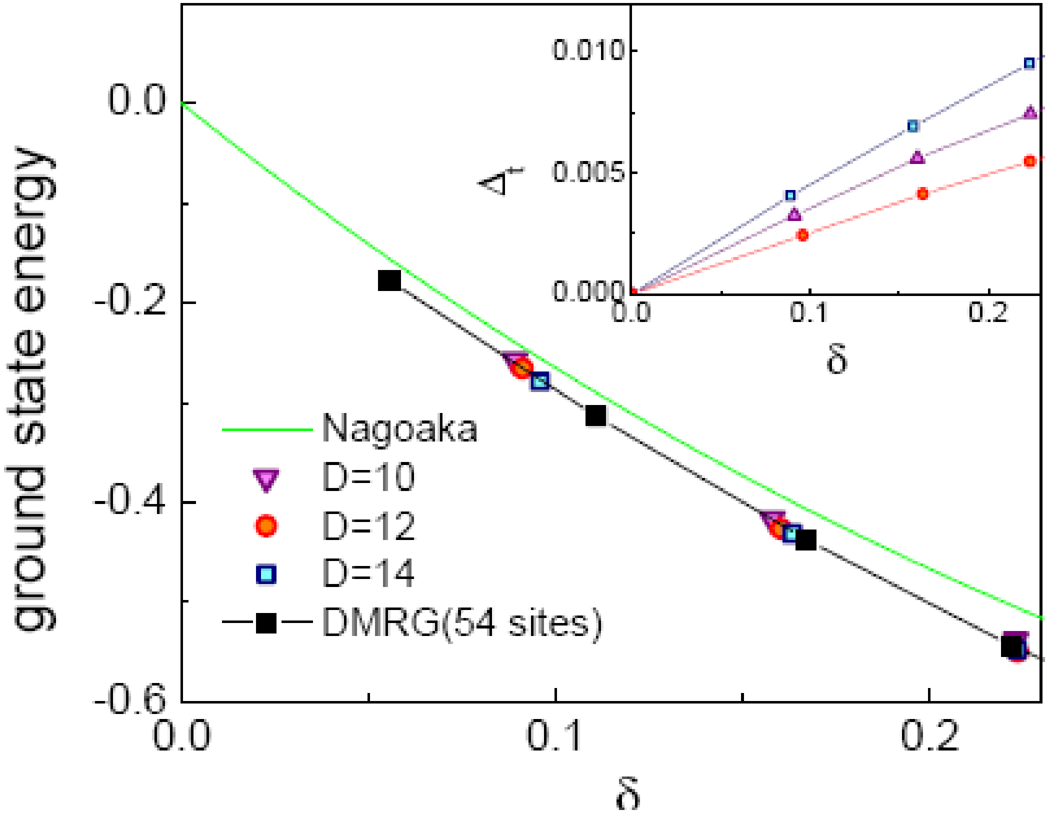


FIG. 3: (Color online) Ground state energy as a function of doping for $t-J$ model at $t/J=30$. As a benchmark, we performed DMRG calculation for a small cluster with $N=54$ sites under PBC. Insert: $p+ip$ SC order parameter as a function of doping.

Gu, Jiang, GB

arXiv:1408.6820

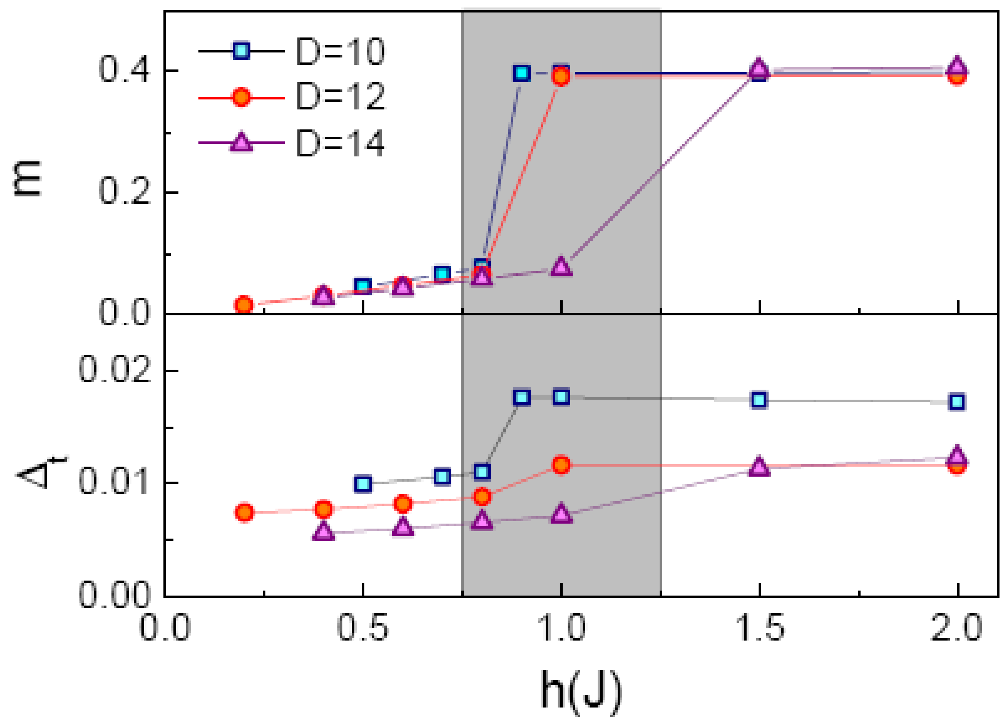


FIG. 4: (Color online)FM magnetization m and triplet SC order parameters Δ_t as a function of Zeeman field for $\delta \sim 0.2$.

Gu, Jiang, GB

arXiv:1408.6820

Possible Experimental Realizations

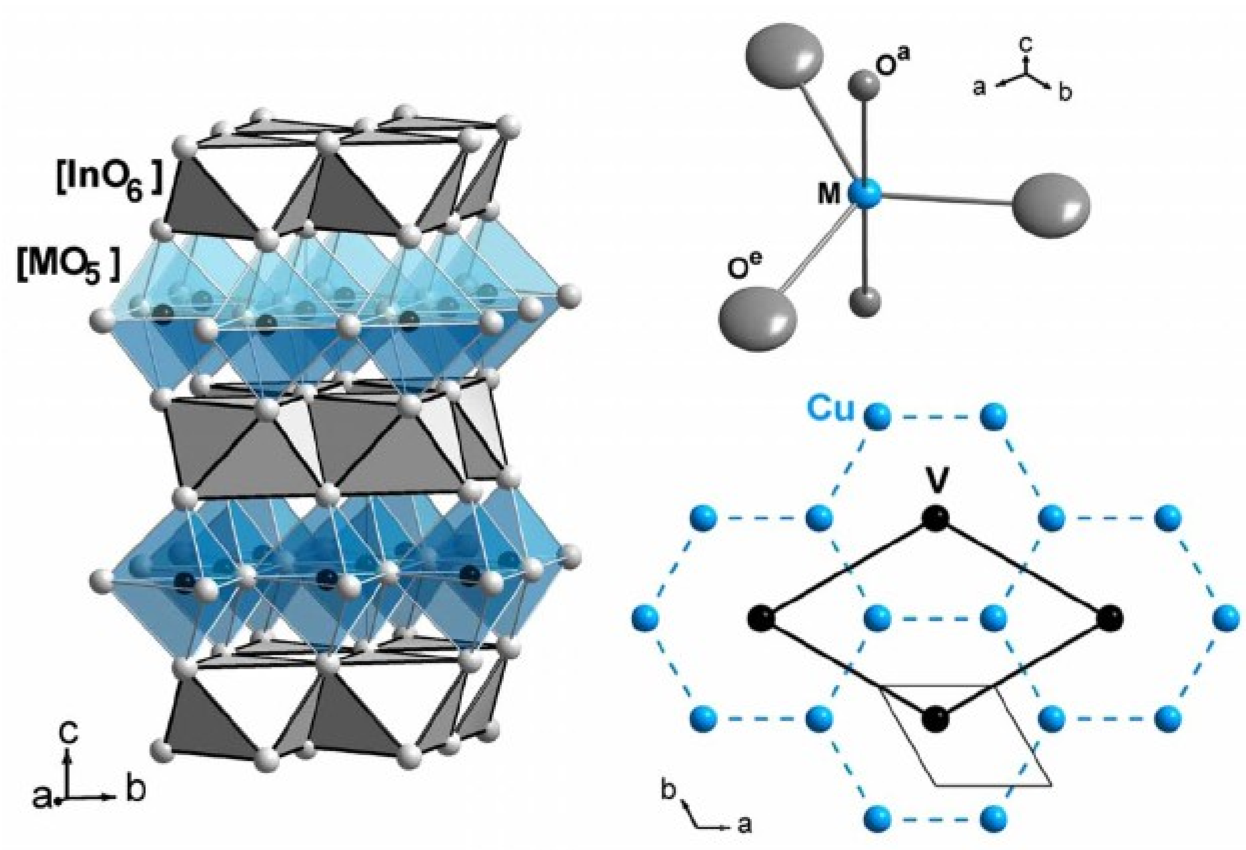
Moller et al. PHYSICAL REVIEW B **78**, 024420 (2008)

He^3 on graphene (Hiroshi Fukuyama et al. PRL 2012)

Ferromagnetic

Long-range magnetic order in a purely organic 2D layer adsorbed on epitaxial graphene

Garnica et al., Nat. Phys. 9, 368 (2013)

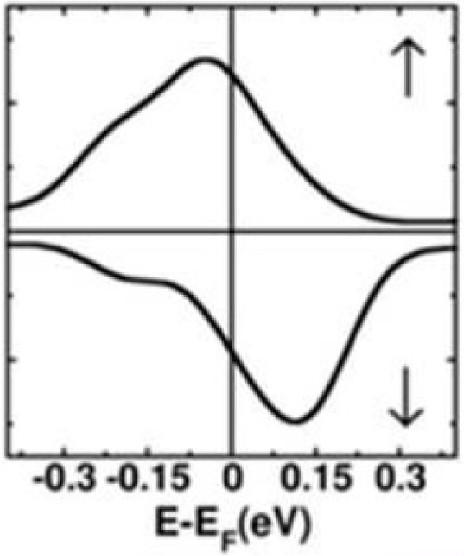


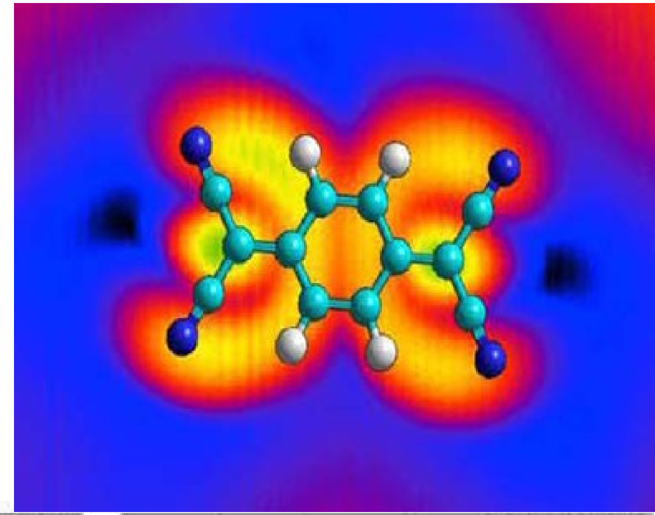
$InCu_{2/3}V_{1/3}O_3$ with $[InO_6]$ and $[MO_5]$ polyhedra (left)

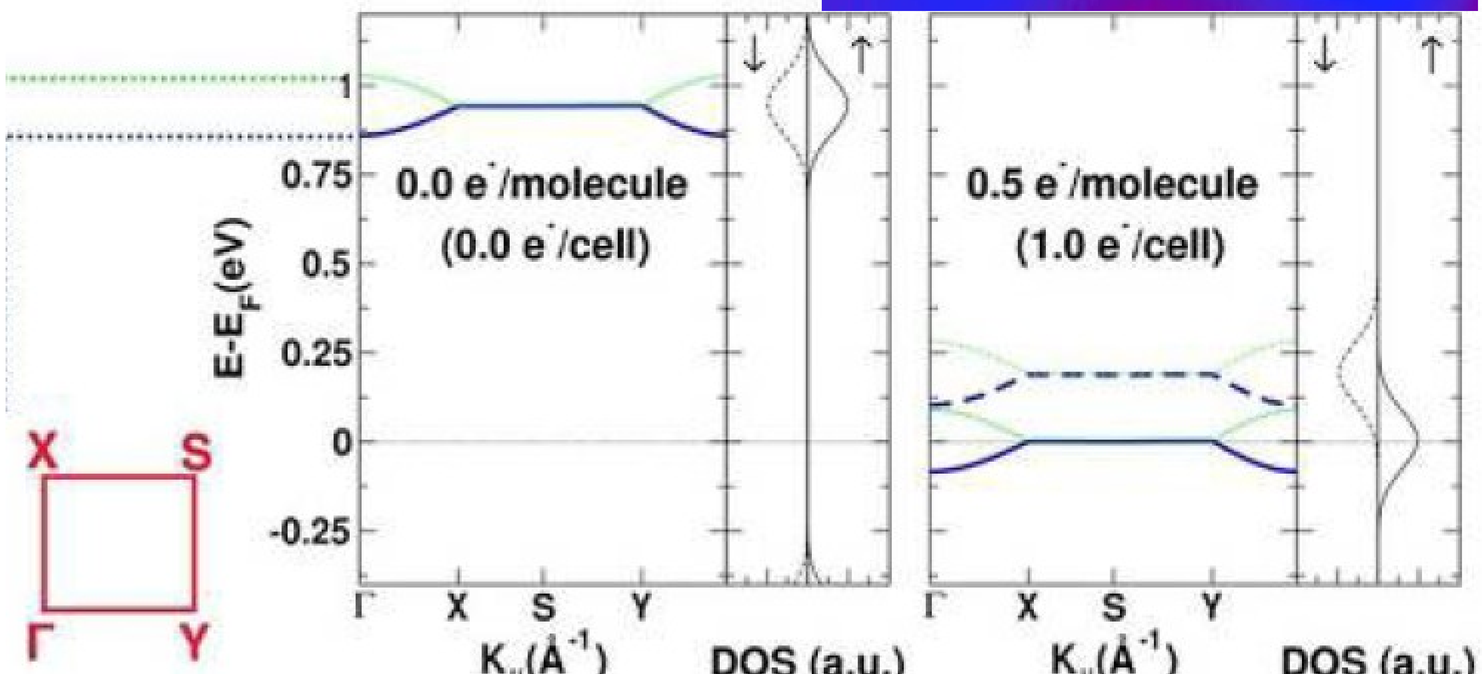
Long-range magnetic order in a purely organic 2D layer adsorbed on epitaxial graphene

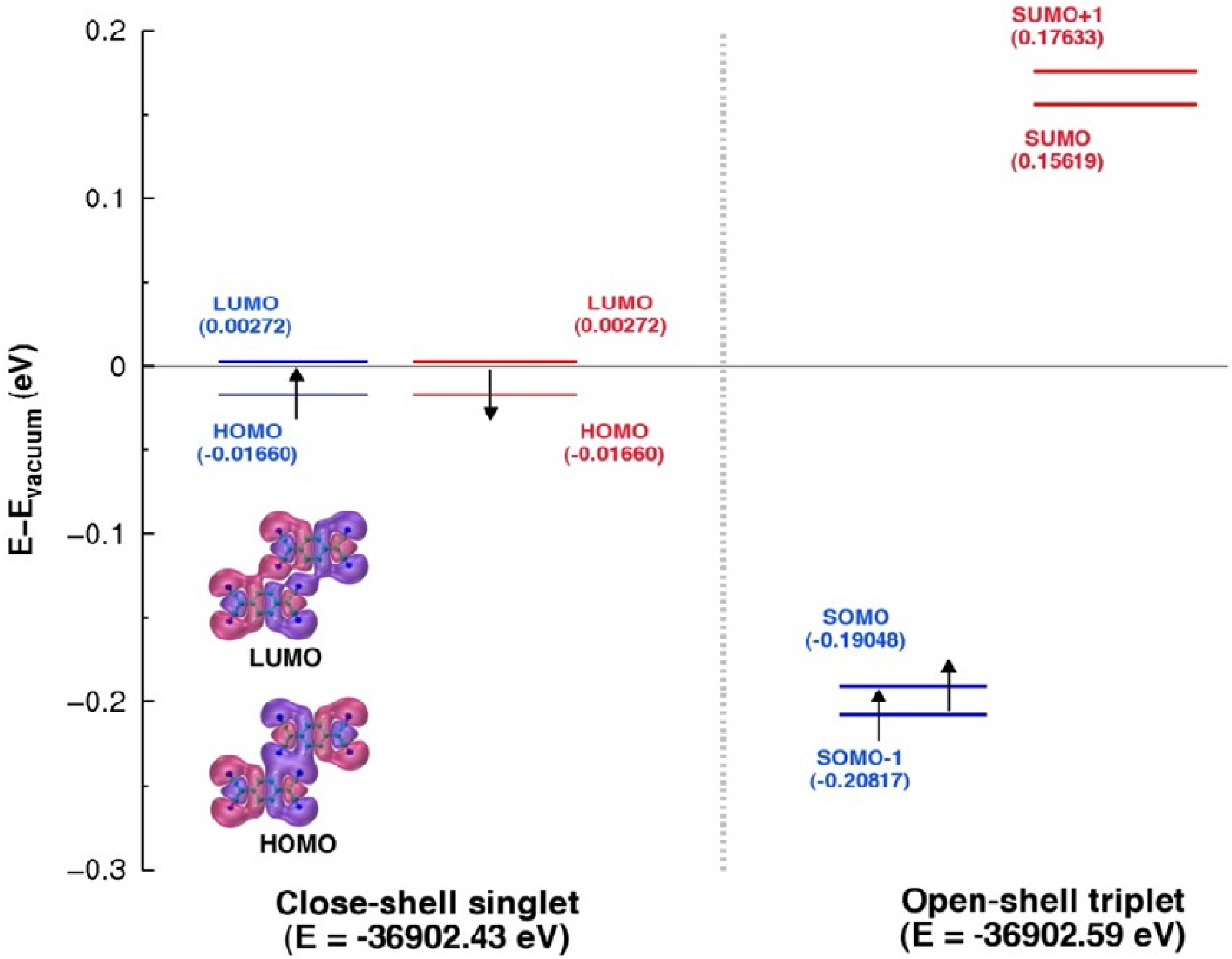
Garnica et al., Nat. Phys. 9, 368 (2013)

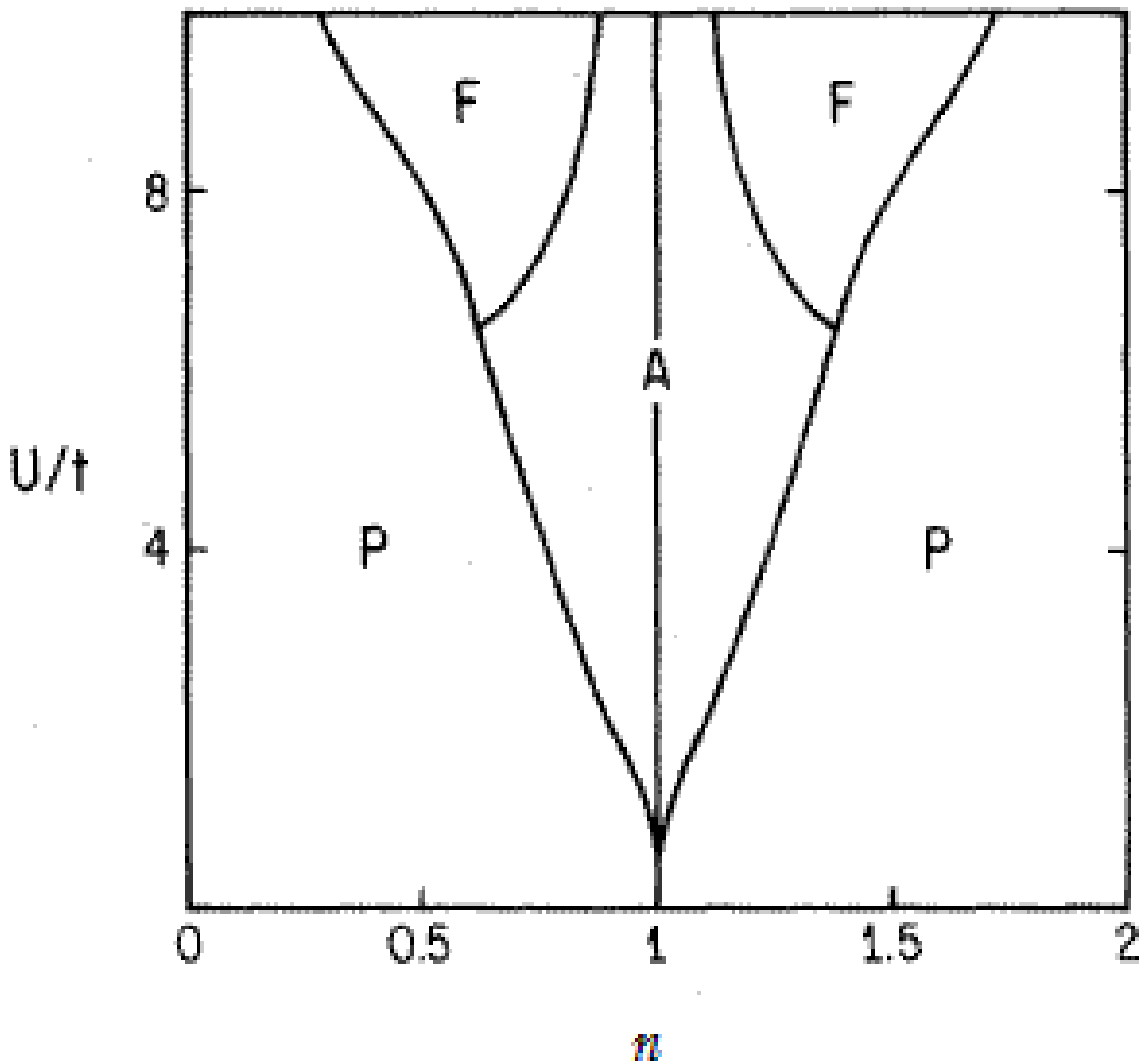
Spin Resolved STM Study of TCNQ lattice





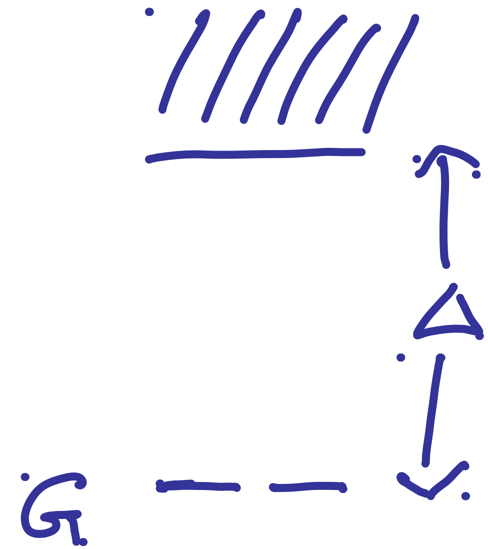



0.2
0.1
0
−0.1
−0.2
−0.3
E–E$_{vacuum}$ (eV)
LUMO
(0.00272)
HOMO
(-0.01660)
LUMO
(0.00272)
HOMO
(-0.01660)
LUMO
HOMO
SUMO+1
(0.17633)
SUMO
(0.15619)
SOMO
(-0.19048)
SOMO-1
(-0.20817)
Close-shell singlet
(E = -36902.43 eV)
Open-shell triplet
(E = -36902.59 eV)



F
F
A
P
P
U/t
8
4
0
0.5
1
1.5
2
n

Topological Degeneracy



Emergence of Ground State degeneracy
Without spontaneous symmetry breaking

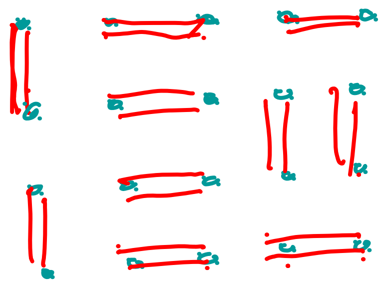
Quantum Order
No local order parameter description
Quantum Rigidity

The degeneracy is visible in torus geometry

This degeneracy leads to anyon quasi particles and quantum number fractionization in 2d

Quantum Dimer Model

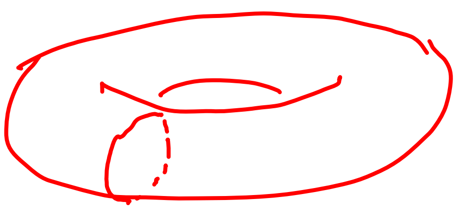
Kivelson
Rokhsar



Bond bosons. Hard core repuls

$$H = J \sum | \,|\,|\, \rangle \langle = | + V$$

Periodic BC



Two SECTORS

Blue curve cuts
i) even no. of bonds
ii) Odd no. of bonds

H does not mix the 2 sectors

$$|G_A\rangle = \sum_{C_A} |C_A\rangle$$

$$|G_B\rangle = \sum_{C_B} |C_B\rangle$$

DISORDERED GROUND STATES

A ——— ——— B

Ordinary Superconductor in 2D
& Laughlin fQH states
have topological degeneracies

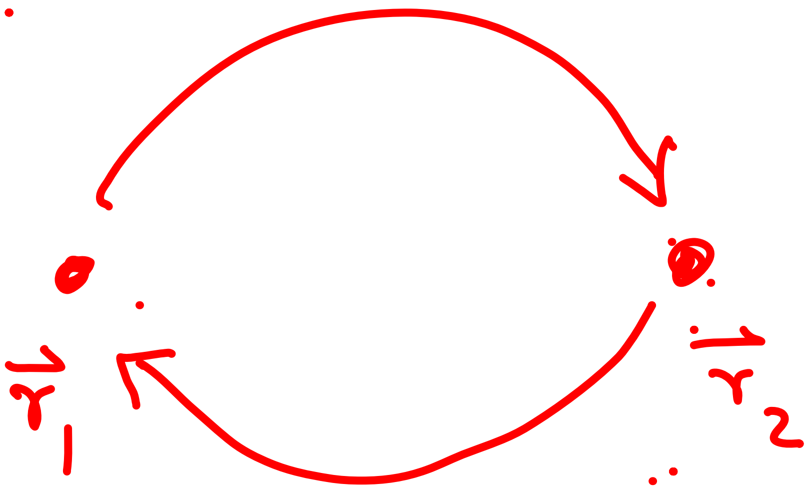
Quantization of Center of Mass degree of freedom

TD's have consequences in the excitation spectrum

Anyons in 2D

$$\psi(\vec{r}_1, \vec{r}_2) \longrightarrow e^{i\theta}\psi(\vec{r}_2, \vec{r}_1)$$

$\theta = \pi$
semion

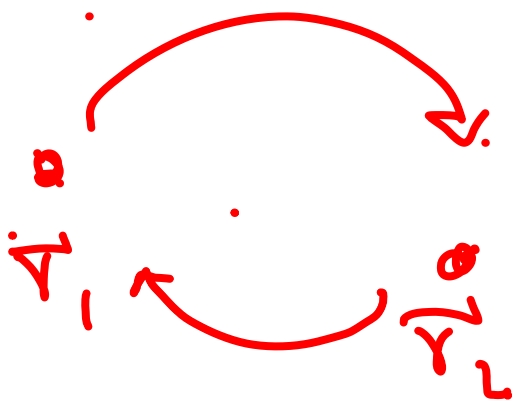


Non-Abelian Anyons

$\psi_a(r_1, r_2, \dots, r_N)$ $\quad a = 1, 2, \dots, M$

ground state (degeneracy)

$$\psi_a(r_1, r_2) \longrightarrow \sum_b D_{ab}\, \psi_b(r_2, r_1)$$

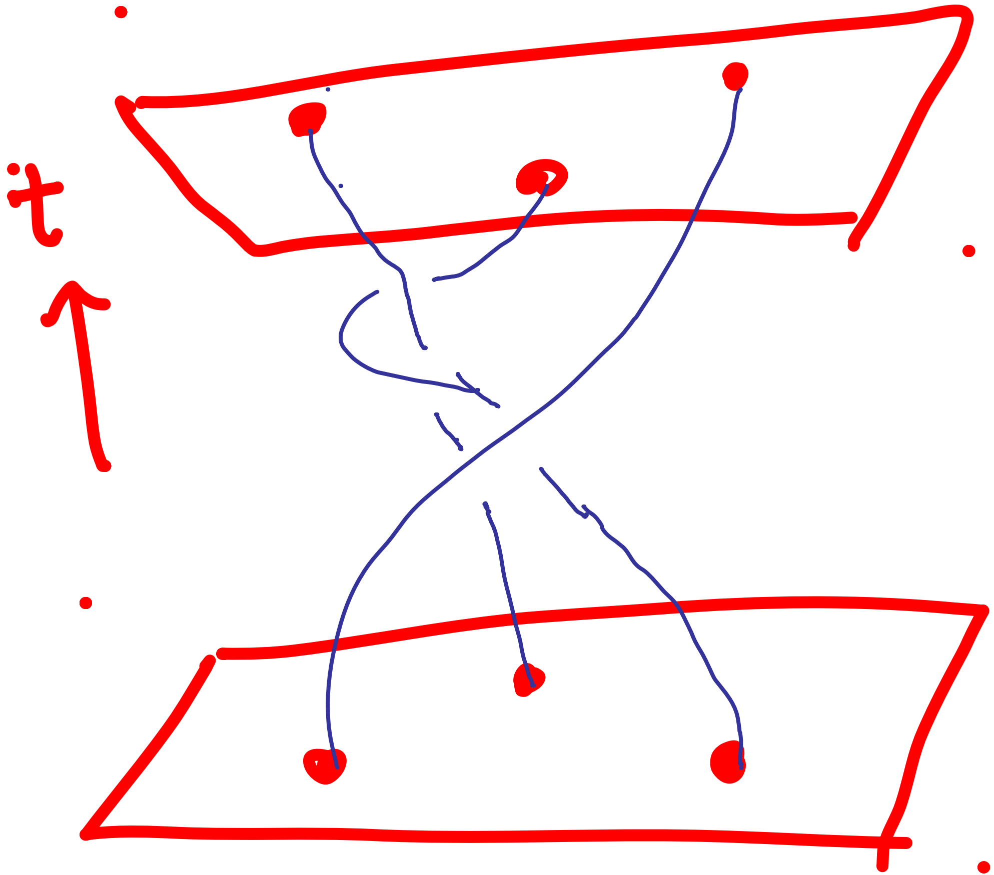


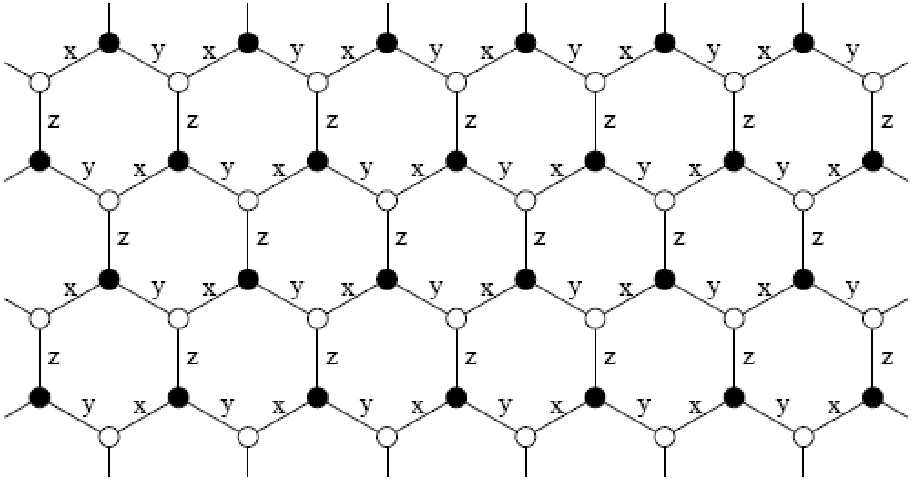
Braiding

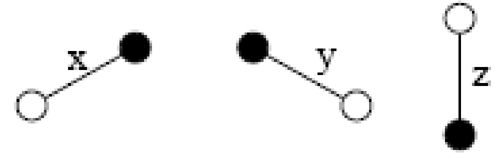
$\psi \longrightarrow \hat{\mathcal{D}}\,\psi$

$\psi \to \hat{\mathcal{D}}_1 \hat{\mathcal{D}}_2 \hat{\mathcal{D}}_3\,\psi$

non commuting



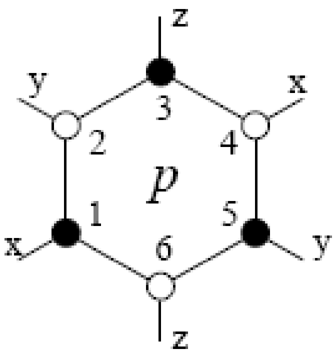




It is a highly Frustrated Quantum Spin System

$$H = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z$$

Local Conserved Quantities



$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

$W_p^2 = 1$

Eigen values of W_p = 1, -1

$$K_{jk} = \begin{cases} \sigma_j^x \sigma_k^x, & \text{if } (j,k) \text{ is an } x\text{-link;} \\ \sigma_j^x \sigma_k^y, & \text{if } (j,k) \text{ is an } y\text{-link;} \\ \sigma_j^x \sigma_k^z, & \text{if } (j,k) \text{ is an } z\text{-link.} \end{cases}$$

$W_p^2 = 1$

Eigen values of W_p = 1, -1

$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z = K_{12} K_{23} K_{34} K_{45} K_{56} K_{61}$$

$$[K_{ij}, W_p] = 0 \quad \forall i,j,p \quad \Rightarrow \quad [H, W_p] = 0\,, \quad [W_q, W_p] = 0 \quad \forall q,p$$

Number of unit cell 2N **Number of sites N** **Number of Plaquettes N**

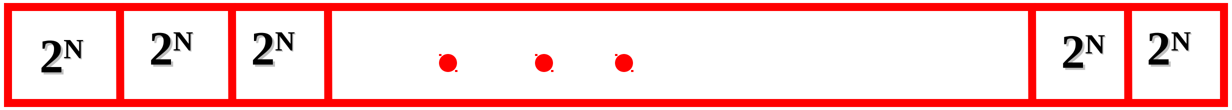
Number of spins 2N

Hilbert space dimension 2^{2N} **Number of W_p's is N** **They can take 2^N different values**

So ther are 2^N different W_p sectors

$2^{2N} = 2^N + 2^N + \ldots\ldots + 2^N$

2N different Wp sectors



Dirac or complex Fermion

$\{\psi_i, \psi_j^\dagger\} = \delta_{ij}$

$|0\rangle, \quad |1\rangle$

$\psi = \frac{1}{2}(\zeta + i\eta)$

Majorana or Real fermions

$\{\zeta_i, \zeta_j\} = \delta_{ij}$

$\eta^2 = \zeta^2 = 1$

Hilbert space dimensions

$D_\zeta = \sqrt{2}$

$D_F = D_\zeta \times D_\xi = \sqrt{2} \times \sqrt{2} = 2$

$D_\xi = \sqrt{2}$

Majorana Fermions

A system with n fermionic modes is usually described by the annihilation and creation operators a_k, $a_k^\dagger$ $\quad (k = 1, \ldots, n)$.

Instead, one can use their linear combinations,

$$c_{2k-1} = a_k + a_k^\dagger, \qquad c_{2k} = \frac{a_k - a_k^\dagger}{i},$$

which are called Majorana operators.

The operators c_j $(j = 1, \ldots, 2n)$ are Hermitian and obey

$$c_j^2 = 1, \qquad c_j c_l = -c_l c_j \ \text{ if } j \neq l.$$

Hilbert space enlargement

Used in RVB theory (GB, Anderson, Zou, 1987)

$$\left\{a_\uparrow, a_\uparrow^\dagger, a_\downarrow, a_\downarrow^\dagger\right\}$$

$$\{|\uparrow\rangle, |\downarrow\rangle\} \longrightarrow \left\{|00\rangle_{\uparrow\downarrow}, |11\rangle_{\uparrow\downarrow}, |01\rangle_{\uparrow\downarrow}, |10\rangle_{\uparrow\downarrow}\right\}$$

$\sigma_i^+ = a_{i\uparrow}^+ a_{i\downarrow}$ $\quad \sigma_i^- = a_{i\downarrow}^+ a_{i\uparrow}$ $\quad n_{i\uparrow} + n_{i\downarrow} = 1$

$$b^x = a_\uparrow + a_\uparrow^\dagger, \quad b^y = -i\left(a_\uparrow - a_\uparrow^\dagger\right), \quad b^z = a_\downarrow + a_\downarrow^\dagger, \quad c = -i\left(a_\downarrow - a_\downarrow^\dagger\right)$$

Dimension of enlarged Hilbert space is 4^{2N} compared to physical Hilbert space dimension 2^{2N}

$$\sigma_j^x \mapsto -ib_j^y b_j^z, \quad \sigma_j^y \mapsto -ib_j^z b_j^x, \quad \sigma_j^z \mapsto -ib_j^x b_j^y$$

Local Constrant

$$D_j|\xi\rangle = |\xi\rangle \text{ for all } j \qquad D_j = b_j^x b_j^y b_j^z c_j$$

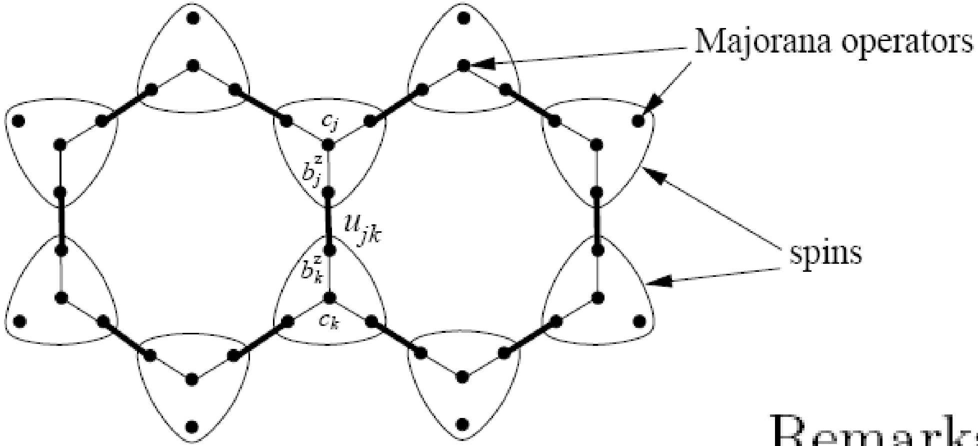
$$K_{jk} = \sigma_j^\alpha \sigma_k^\alpha \longrightarrow \widetilde{K}_{jk} = (ib_j^\alpha c_j)(ib_k^\alpha c_k) = -i\,(ib_j^\alpha b_k^\alpha)\,c_j c_k$$

α takes values x, y or z

$$\hat{u}_{jk} = ib_j^\alpha b_k^\alpha \longrightarrow \hat{u}_{kj} = -\hat{u}_{jk}$$

$$\widetilde{H} = \frac{i}{4}\sum_{j,k} \hat{A}_{jk} c_j c_k, \qquad \hat{A}_{jk} = \begin{cases} 2J_{\alpha_{jk}}\hat{u}_{jk} & \text{if } j \text{ and } k \text{ are connected,} \\ 0 & \text{otherwise,} \end{cases}$$

$$\hat{u}_{jk} = ib_j^{\alpha_{jk}} b_k^{\alpha_{jk}}.$$



$u_{ij}^2 = 1$

Eigen values $u_{ij} = 1, -1$

Remarkably, the operators $\hat{u}_{jk}$ commute with the Hamiltonian and with each other

A two body interaction term (four fermion term) is reduced to a two body term

$$\widetilde{K}_{jk} = (ib_j^\alpha c_j)(ib_k^\alpha c_k) = -i\,(ib_j^\alpha b_k^\alpha)\,c_j c_k \longrightarrow i\,(u_{jk})\;c_j c_k$$

RVB mean field factorisation becomes exact !

We have **free majorana fermion** hopping Hamiltonian

$$\widetilde{H} = \frac{i}{4}\sum_{j,k} \hat{A}_{jk} c_j c_k, \qquad \hat{A}_{jk} = \begin{cases} 2J_{\alpha_{jk}} \hat{u}_{jk} & \text{if } j \text{ and } k \text{ are connected} \\ 0 & \text{otherwise,} \end{cases}$$

A complex interacting Hard core boson problem is reduced to a Free majorana fermion problem **Hilbert space dimension 2^{2N}**

Sufficient to solve a one particle problem on a Honey comb lattice !

Hilbert space dimension 2N

From this we can build the many particle Fock space of dimension 2^{2N}

To satisfy local Constrant and go to physical Hilbert space we need to do some projection (similar to Gutzwiller projection in RVB theory)

$$|\Psi_w\rangle = \prod_j \left(\frac{1+D_j}{2}\right)|\widetilde{\Psi}_u\rangle \in \mathcal{L}$$

However, to calculate physical quantities such as energy spectrum spin-spin correlation functions etc., no such projection is necessary !

This follows from an emergent local Z_2 Gauge symmetry in the problem

$u_{ij} \longrightarrow \tau_i u_{ij} \tau_j \qquad \tau_i = \pm 1$

$c_i \longrightarrow \tau_i c_i$

gauge invariant

$\prod_p u_{ij} = W_p$

Wilson loop

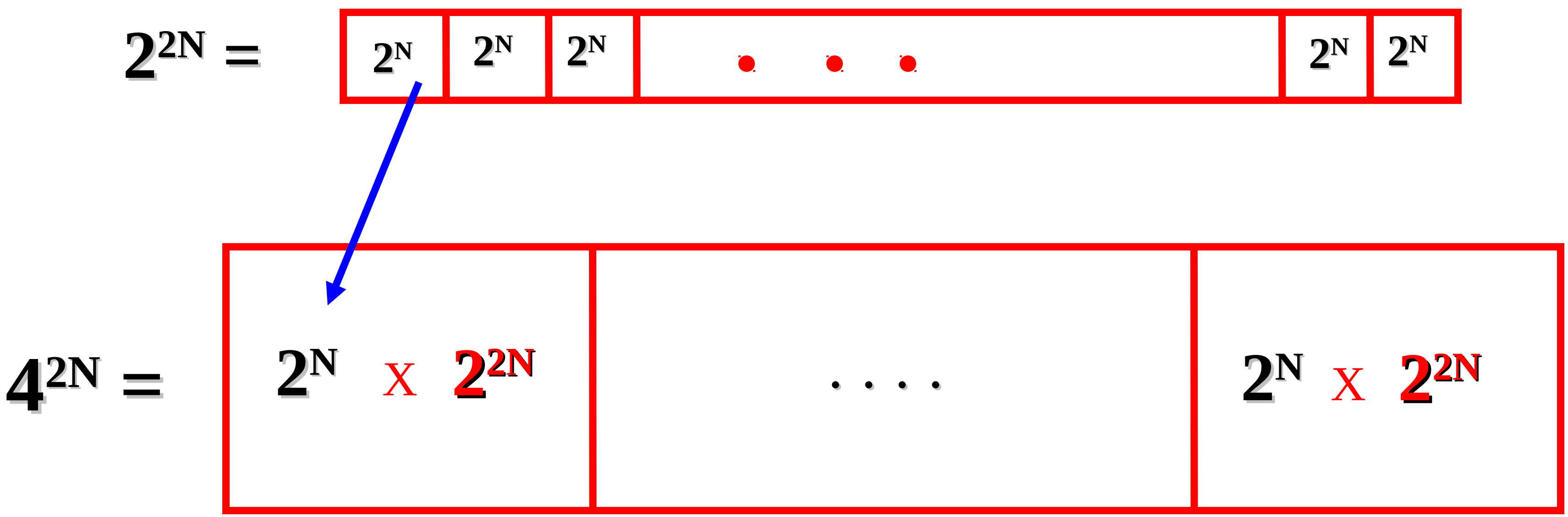
$\prod_c u_{ij} = W_c$

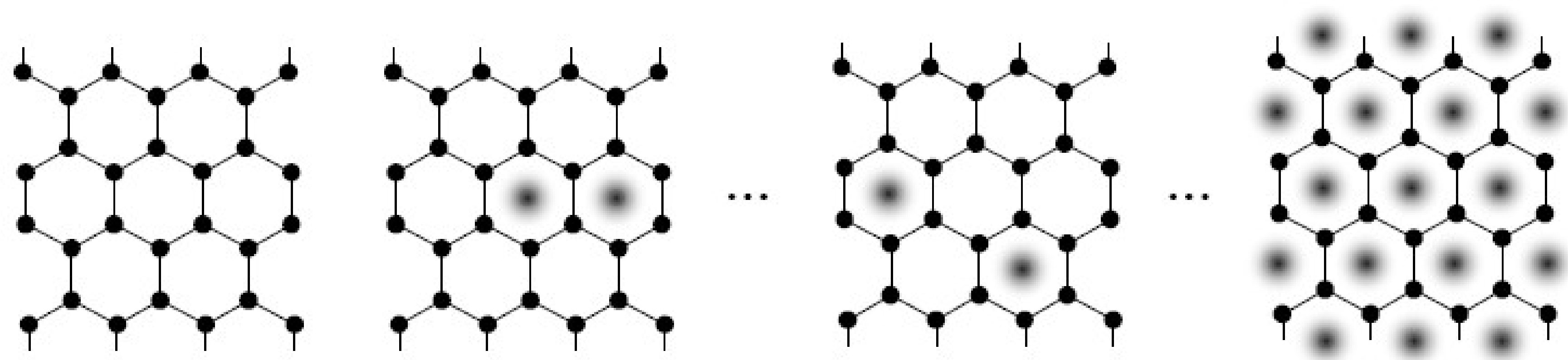
Dimension of enlarge Hilbert space is 4^{2N} compared to physical Hilbert space dimension 2^{2N}

No. of possible values of $\{\tau_i\}$ is $2^{2N} \longrightarrow$ This is the no. of gauge copies

Each W_p sector has 2^{2N} gauge copies.

Gauge invariant quantities are the physical observables





vortex free sector

examples from two-vortex sectors

full vortex sector

W_p = -1 is defined as a vortex excitation

Solving the free Majorana problem in different W_p sectors

$$\widetilde{H}_u = \frac{i}{4}\sum_{j,k} A_{jk} c_j c_k$$

A is a real skew-symmetric matrix

$$H_{\text{canonical}} = \frac{i}{2}\sum_{k=1}^{m} \varepsilon_k b'_k b''_k = \sum_{k=1}^{m} \varepsilon_k \left(a_k^\dagger a_k - \tfrac{1}{2}\right), \qquad \varepsilon_k \geqslant 0$$

$$(b'_1, b''_1, \ldots, b'_m, b''_m) = (c_1, c_2, \ldots, c_{2m-1}, c_{2m})\, Q$$

$$A = Q \begin{pmatrix} 0 & \varepsilon_1 & & & \\ -\varepsilon_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & \varepsilon_m \\ & & & -\varepsilon_m & 0 \end{pmatrix} Q^T$$

$$\begin{pmatrix} a^\dagger \\ a \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}\begin{pmatrix} b' \\ b'' \end{pmatrix}$$

$$a_k|\Psi\rangle = 0 \text{ for all } k$$

$$E = -\frac{1}{2}\sum_{k=1}^{m} \varepsilon_k = -\frac{1}{4}\operatorname{Tr}|iA|$$

Absolute ground state energy is obtained in the Sector where $W_p = 1$ in all plaquettes (Lieb's Theorem)

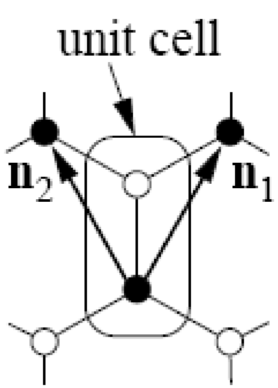
The spectrum of free fermions is obtained by Fourier transform If we use periodic boundary condition

$$H = (i/4)\sum_{s,\lambda,t,\mu} A_{s\lambda,t\mu} c_{s\lambda} c_{t\mu}$$

$$H = \frac{1}{2}\sum_{\mathbf{q},\lambda,\mu} i\widetilde{A}_{\lambda\mu}(\mathbf{q}) a_{-\mathbf{q},\lambda} a_{\mathbf{q},\mu}$$

$$\widetilde{A}_{\lambda\mu}(\mathbf{q}) = \sum_t e^{i(\mathbf{q},\mathbf{r}_t)} A_{0\lambda,t\mu}$$

$$a_{\mathbf{q},\lambda} = \frac{1}{\sqrt{2N}}\sum_s e^{-i(\mathbf{q},\mathbf{r}_s)} c_{s\lambda}$$



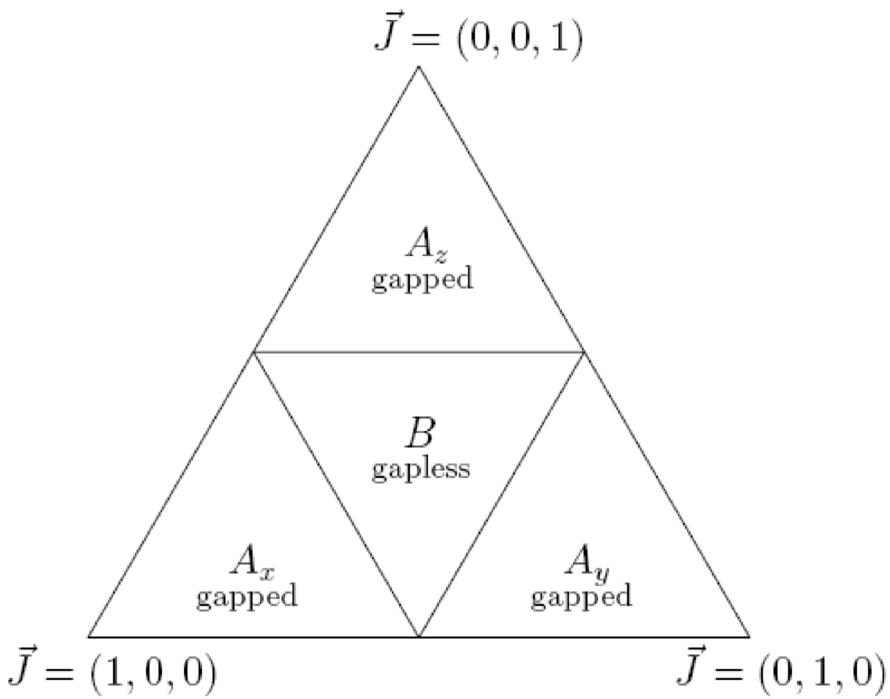
$$i\widetilde{A}(\mathbf{q}) = \begin{pmatrix} 0 & if(\mathbf{q}) \\ -if(\mathbf{q})^* & 0 \end{pmatrix}$$

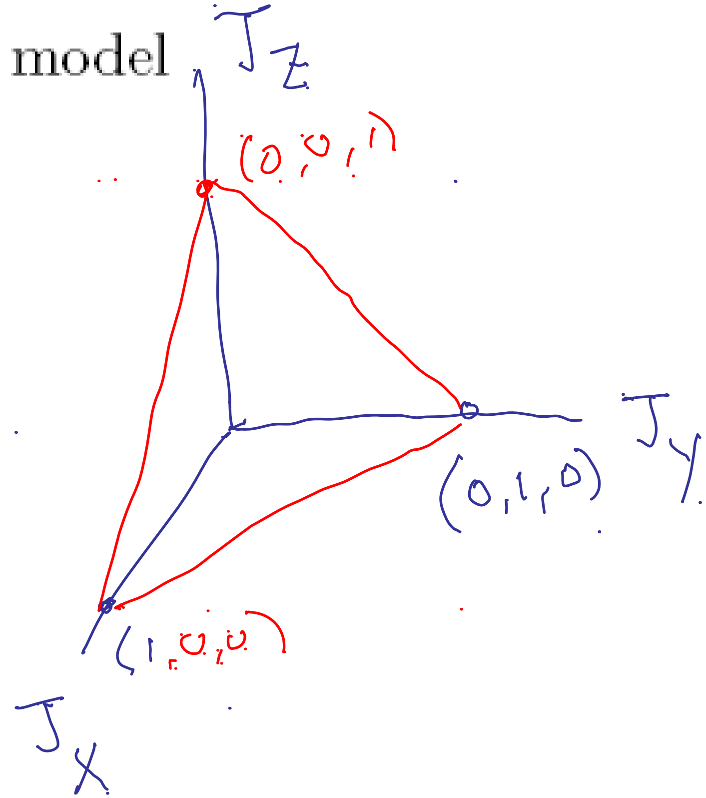
$$f(\mathbf{q}) = 2\left(J_x e^{i(\mathbf{q},\mathbf{n}_1)} + J_y e^{i(\mathbf{q},\mathbf{n}_2)} + J_z\right)$$

$$\varepsilon(\mathbf{q}) = \pm|f(\mathbf{q})|$$

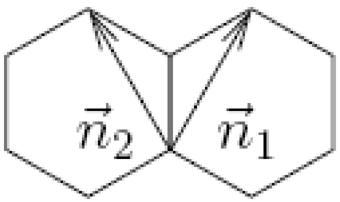
$$\mathbf{n}_1 = \left(\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}\right), \;\; \mathbf{n}_2 = \left(-\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}\right)$$

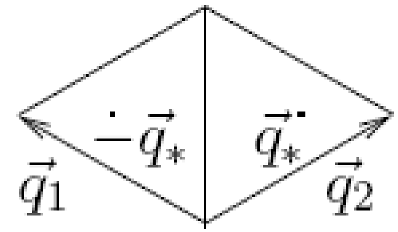
Phase diagram of the model





The triangle is the section of the positive octant $(J_x, J_y, J_z \geqslant 0)$ by the plane $J_x + J_y + J_z = 1$



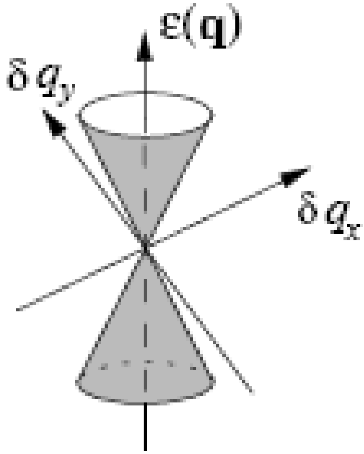


$J_x = J_y = J_z$

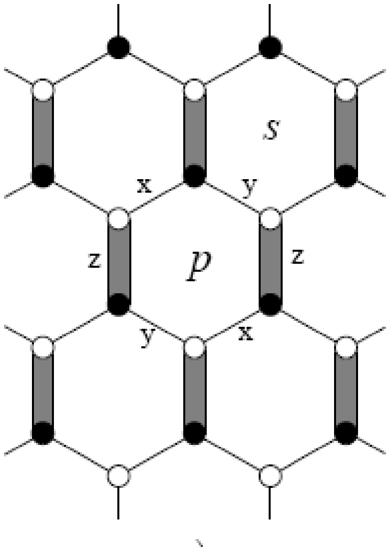
GRAPHENE LIKE SPECTRUM

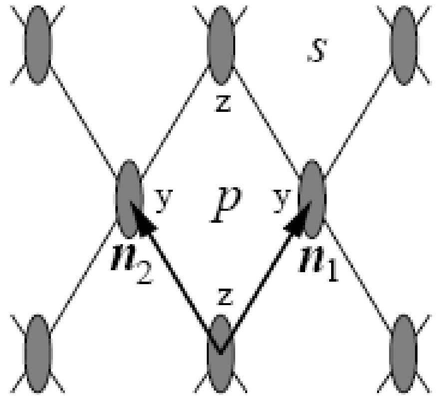
(ONLY PARTICLES & NO HOLES)

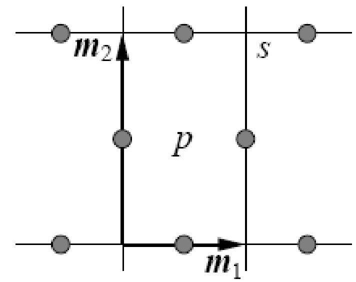
A particle is its own antiparticle!

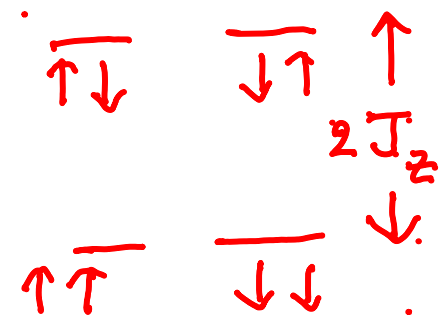


Toric Code Hamiltonian as a limit of Kitaev Model in the gaped phase





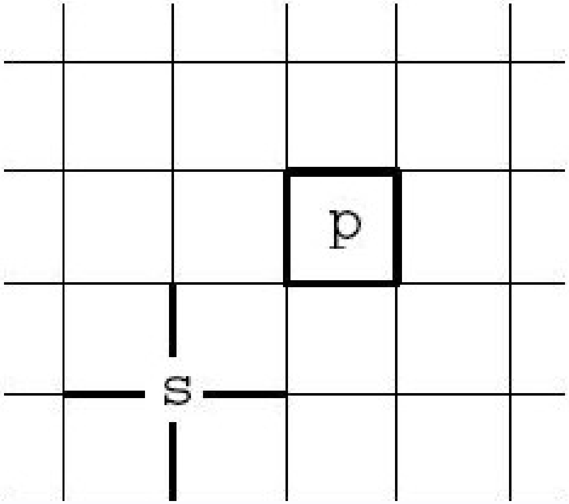




Perturbation theory in powers of the ratios J_x/J_z and J_y/J_z

$$H_{\mathrm{eff}} = -\frac{J_x^2 J_y^2}{16|J_z|^3} \sum_p Q_p \longrightarrow -J_{\mathrm{eff}} \left(\sum_{\mathrm{vertices}} A_s + \sum_{\mathrm{plaquettes}} B_p \right)$$

$$Q_p = \sigma^y_{\mathrm{left}(p)} \sigma^y_{\mathrm{right}(p)} \sigma^z_{\mathrm{up}(p)} \sigma^z_{\mathrm{down}(p)}$$



$$H_{eff} = -J_{eff}\left(\sum_{vertices} A_s + \sum_{plaquettes} B_p\right)$$

$$A_s = \prod_{j\in star(s)} \sigma_j^x, \qquad B_p = \prod_{j\in boundary(p)} \sigma_j^z$$

$$[A_s, B_p] = [B_p, B_q] = [A_s, A_r] = 0$$

To create a pair of *e*, or move an *e* through a path t we must apply:

$$S^z(t) = \prod_{j\in t} \sigma_j^z$$

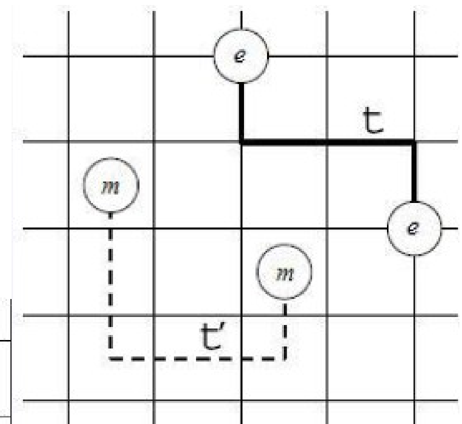
To create a pair of *m*, or move an *m* through a path t' we must apply:

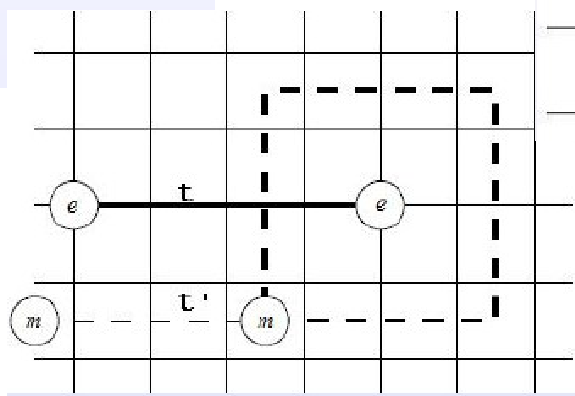
$$S^x(t') = \prod_{j\in t'} \sigma_j^x$$

e and m are bosons;

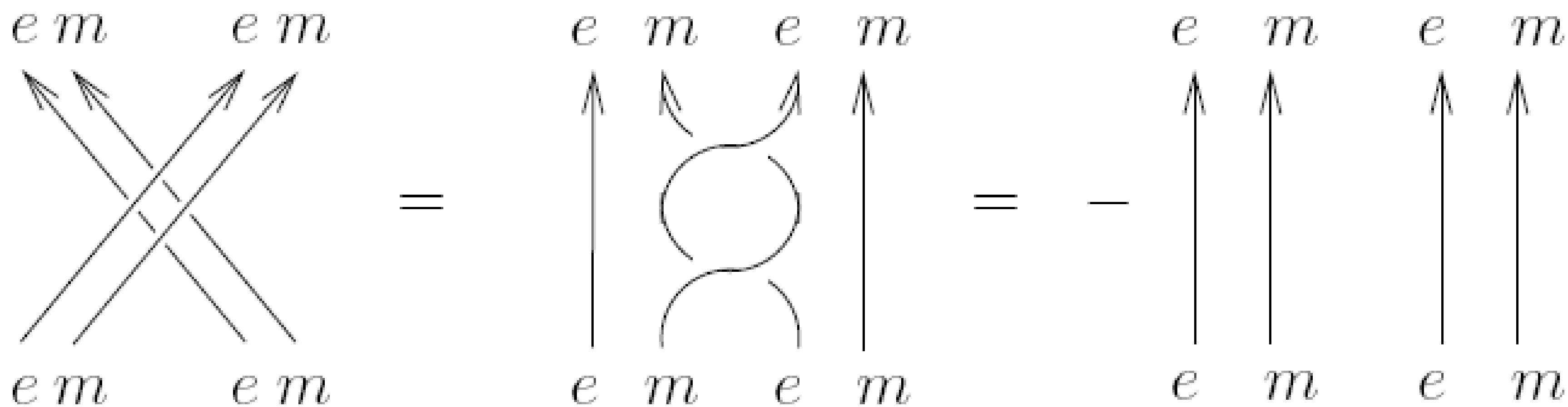
Moving an e around an m yields -1

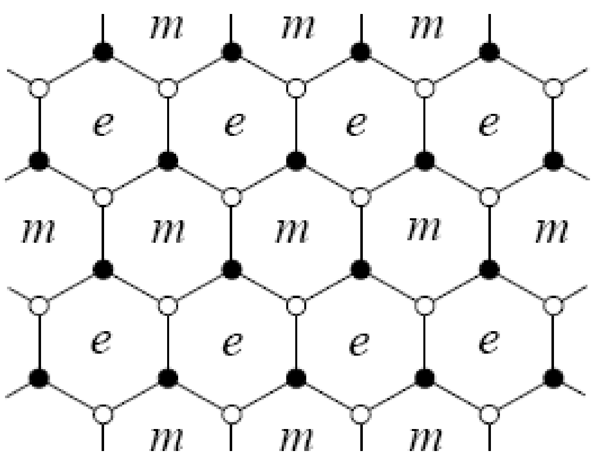
em composite is a fermion





em composite is a fermion





In the gapful phase we have only Abelian Anyons

Application of an external magnetic field

or addition of a specific 3 spin interaction term

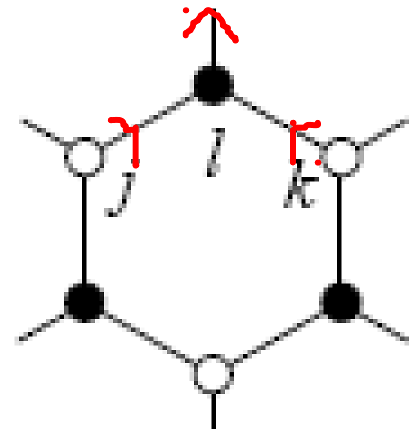
Produces a phase where there are

Non Abelian Anyons

3 spin interaction term

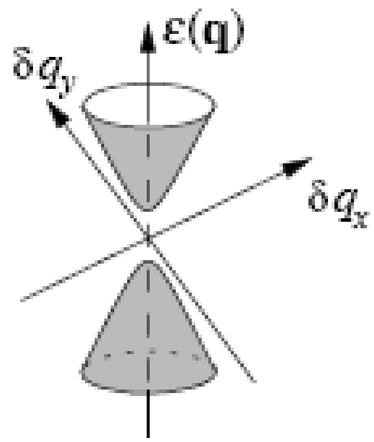
(model continues to be exactly solvable and all W_p commute with the full Hamiltonian)

$\sigma_j^x \sigma_k^y \sigma_l^z$ = $u_{jl}\, u_{kl}\, c_j\, c_k$



$$H = \frac{i}{4} \sum_{\langle j,k \rangle} A_{jk} c_j c_k$$

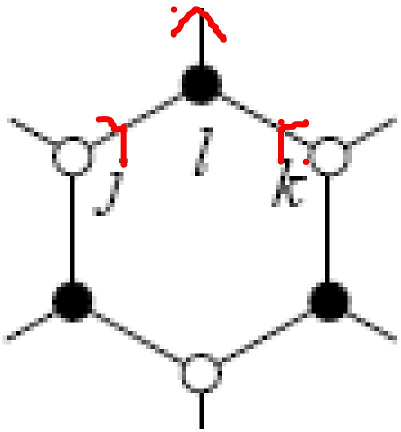
$$i\widetilde{A}(\mathbf{q}) = \begin{pmatrix} \Delta(\mathbf{q}) & if(\mathbf{q}) \\ -if(\mathbf{q})^* & -\Delta(\mathbf{q}) \end{pmatrix}$$



$$f(\mathbf{q}) = 2J\left(e^{i(\mathbf{q},\mathbf{n}_1)} + e^{i(\mathbf{q},\mathbf{n}_2)} + 1\right)$$

$$\Delta(\mathbf{q}) = 4\kappa\left(\sin(\mathbf{q},\mathbf{n}_1) + \sin(\mathbf{q},-\mathbf{n}_2) + \sin(\mathbf{q},\mathbf{n}_2 - \mathbf{n}_1)\right)$$

$$\varepsilon(\mathbf{q}) \approx \pm\sqrt{3J^2\,|\delta\mathbf{q}|^2 + \Delta^2}$$



$$\sum_{(i,j,k)\in p} K_{ijk}\sigma_i^x\sigma_j^y\sigma_k^z = K_{123}\sigma_1^z\sigma_2^y\sigma_3^x + K_{234}\sigma_2^x\sigma_3^z\sigma_4^y + K_{345}\sigma_3^y\sigma_4^x\sigma_5^z + K_{456}\sigma_4^z\sigma_5^y\sigma_6^x$$

$$+K_{561}\sigma_5^x\sigma_6^z\sigma_1^y + K_{612}\sigma_6^y\sigma_1^x\sigma_2^z.$$

How do we get Non Abelian anyons ?

We start with spins but end up with
two types of emergent elementary constituents in the problem

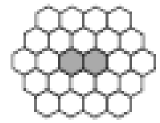
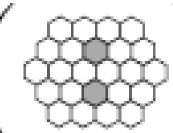
flux excitation

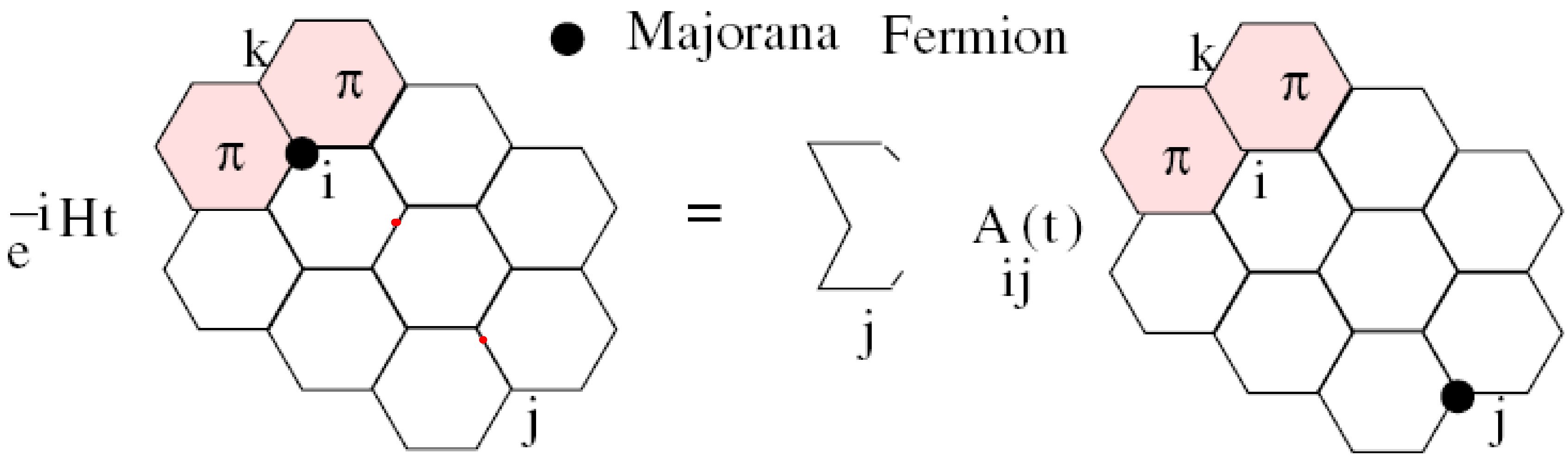
Majorana fermion

The physical spectrum for a given flux configuration contains
only propagating complex (Dirac) fermion excitations
(linear combination of majorana fermions)

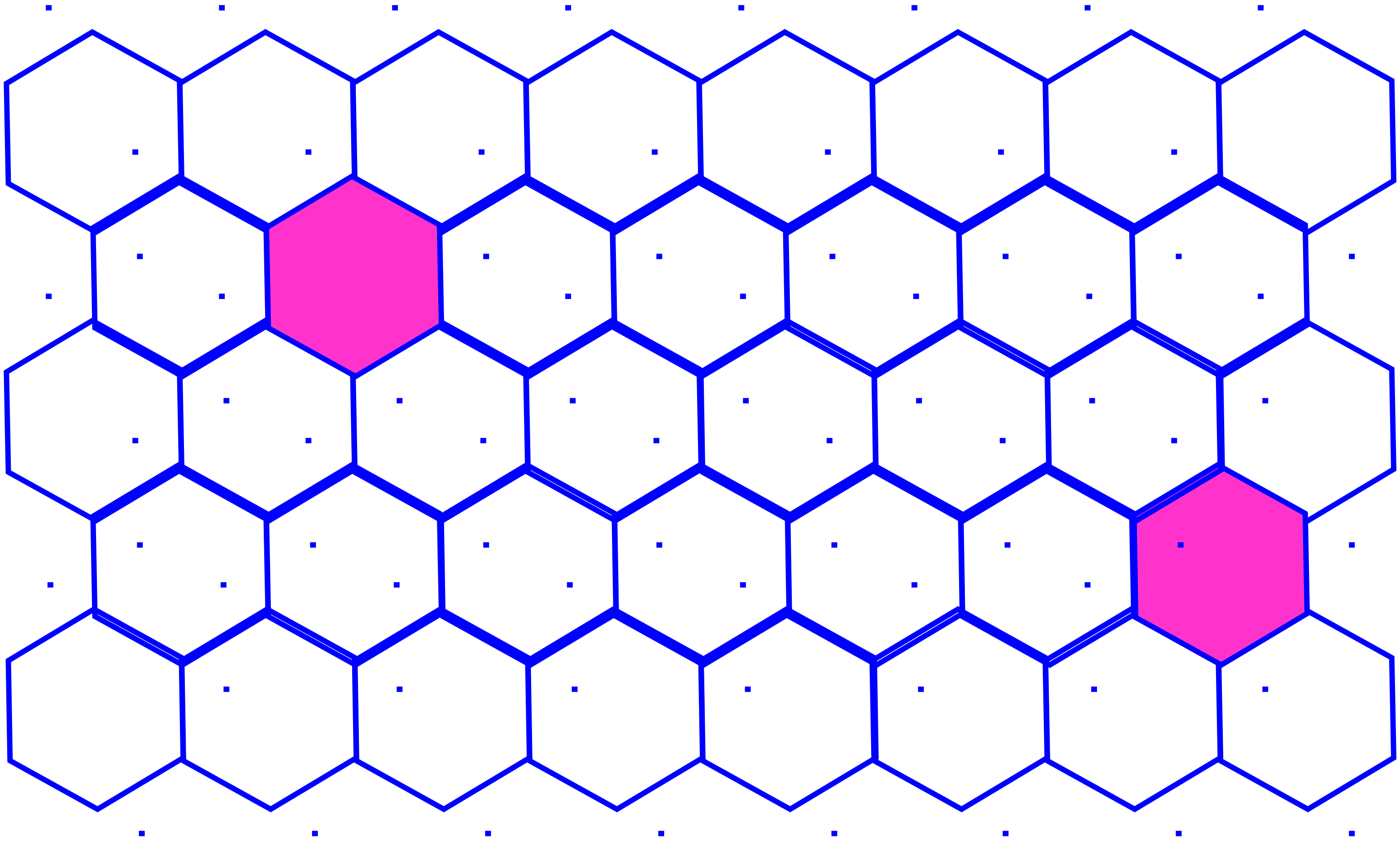
However, on introduction of the 3 spin interaction term
a flux excitation binds a single localized majorana fermion mode
for J's near the isotropic point $J_x = J_y = J_z$

The Majorana Fermion Flux composite is our Non Abelian Anyon

$E_{\text{vortex}} \approx 0.1536, \quad \Delta E\Big($  $\Big) \approx -0.04, \quad \Delta E\Big($  $\Big) \approx -0.07.$

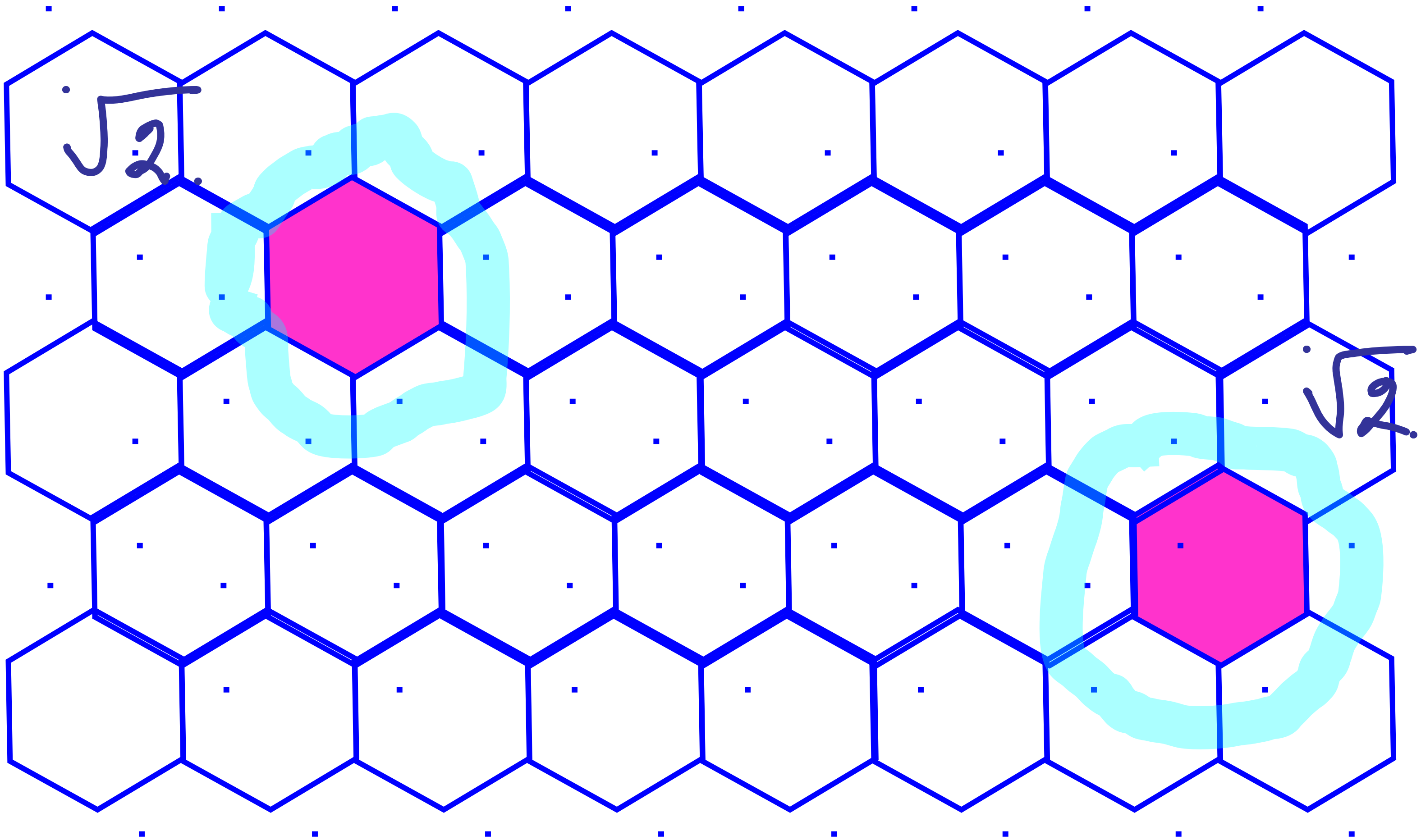


In the Abelian phasd two well isolated vortices have a non degenerate ground state



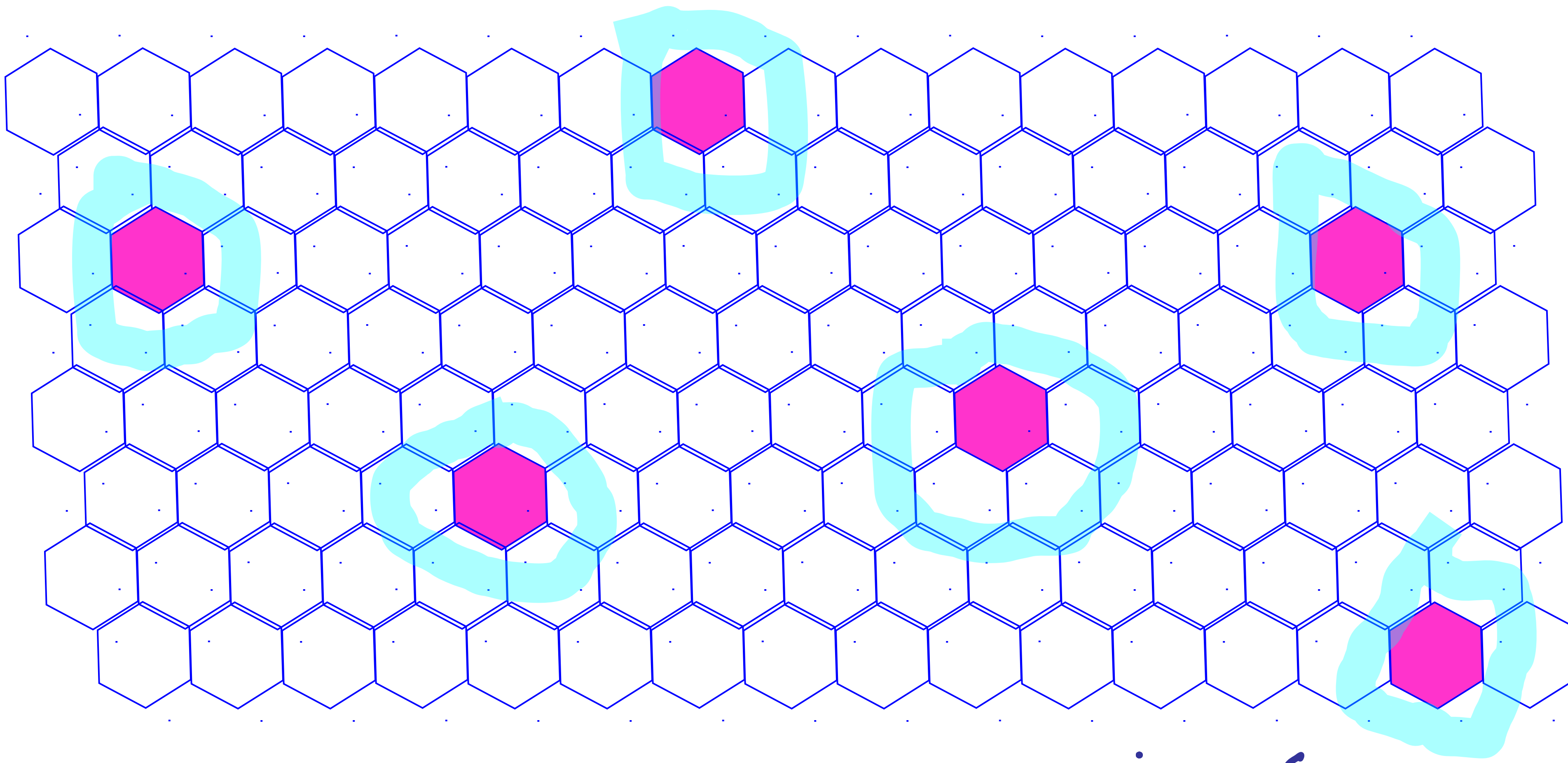
The vortices interact and the degeneracy is in general split.
However, the splitting vanishes exponentiall as a function of separataion

In the Non Abelian phasd two well isolated vortices have a doubly degenerate ground state



2 well separated vortices   Ground state degeneracy is $(\sqrt{2})^2 = 2$

M well separated vortices Ground state degeneracy is $(\sqrt{2})^M$



6 well separated vortices Ground state degeneracy is $(\sqrt{2})^6 = 8$

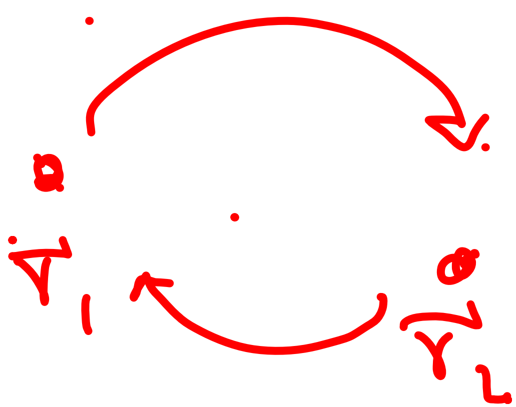
For M well separated vortices   Ground state degeneracy is $(\sqrt{2})^M$

Let us denote the ground states by

$$\psi_a(r_1, r_2 \cdots r_M) \qquad a = 1, 2, \ldots (\sqrt{2})^M$$

ground state (degeneracy)

$$\psi_a(r_1, r_2) \longrightarrow \sum_b D_{ab}\, \psi_b(r_2, r_1)$$

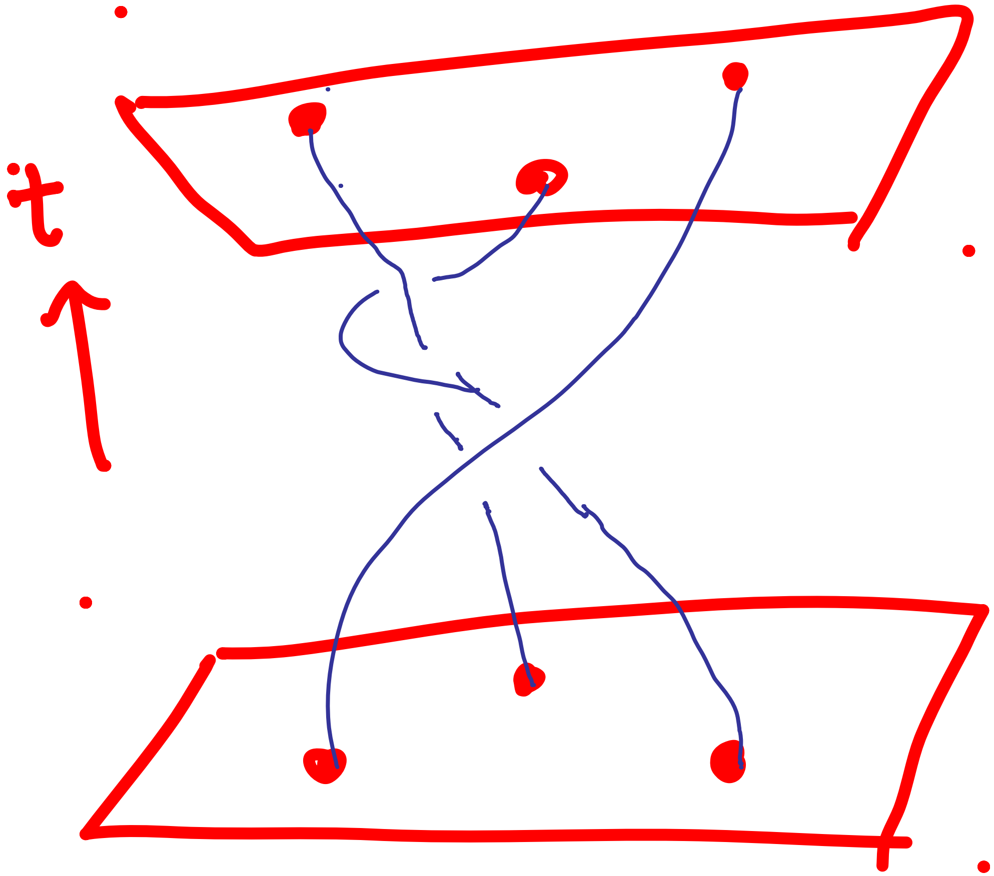


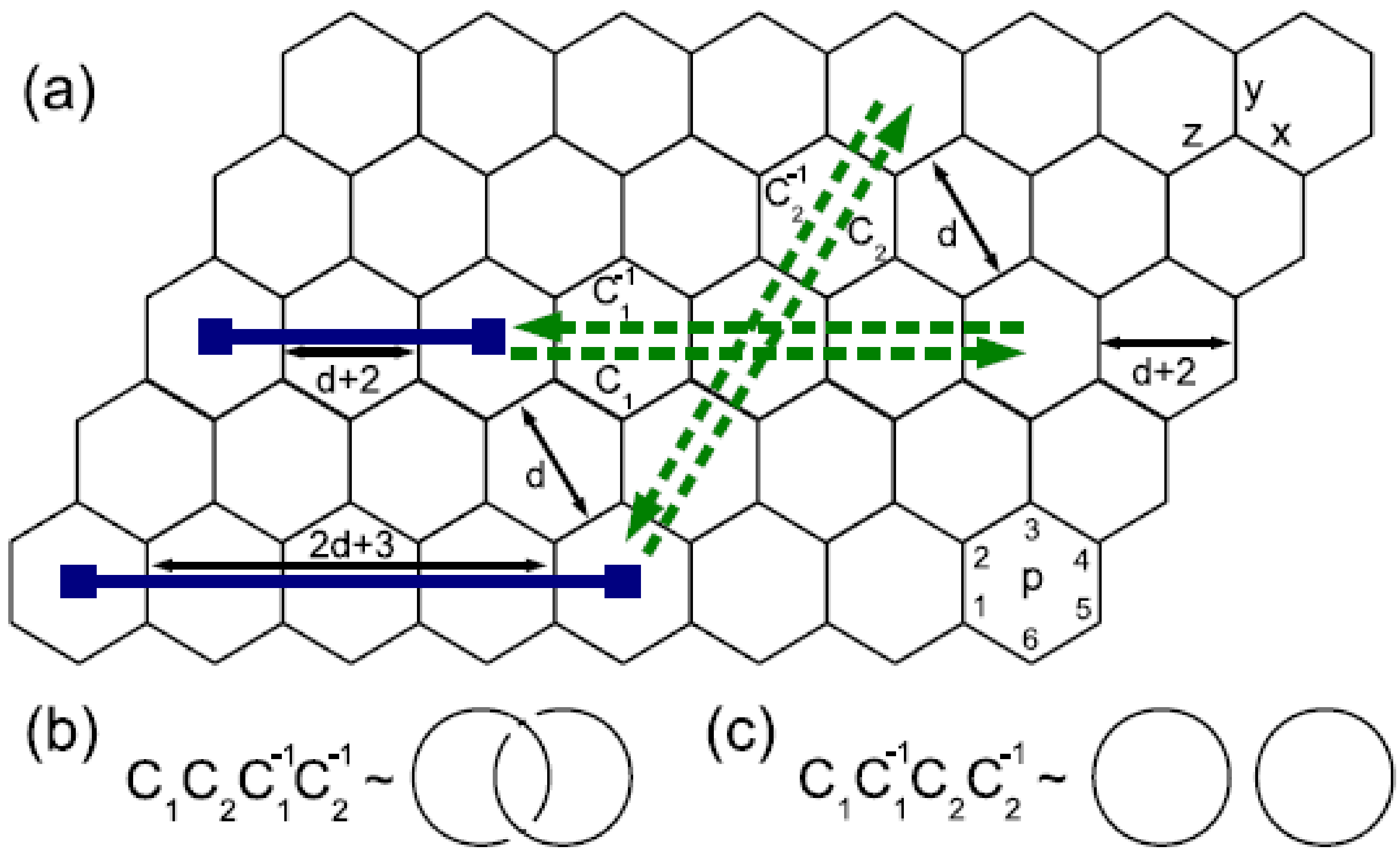
Braiding

$$\psi \longrightarrow \hat{\mathcal{B}}\,\psi$$

$$\psi \to \hat{\mathcal{B}}_1 \hat{\mathcal{B}}_2 \hat{\mathcal{B}}_3\, \psi$$

non commuting





(a)
y
z
x
C_2^{-1}
C_2
d
C_1^{-1}
C_1
d+2
d+2
d
2d+3
3
2
4
p
1
5
6
(b)
$C_1C_2C_1^{-1}C_2^{-1}$ ~
(c)
$C_1C_1^{-1}C_2C_2^{-1}$ ~

Superselection sectors: 1 (vacuum), ε (fermion), σ (vortex).

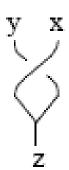
Quantum dimension:	$d_1 = 1,$	$d_\varepsilon = 1$	$d_\sigma = \sqrt{2};$
Topological spin:	$\theta_1 = 1,$	$\theta_\varepsilon = -1,$	$\theta_\sigma = \theta = \exp\left(\frac{\pi}{8} i\nu\right);$
Frobenius-Schur indicator:	$\varkappa_1 = 1,$	$\varkappa_\varepsilon = 1,$	$\varkappa_\sigma = \varkappa = (-1)^{(\nu^2-1)/8}.$

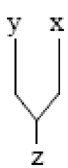
Global dimension: $\mathcal{D}^2 \stackrel{\text{def}}{=} \sum_u d_u^2 = 4.$

Fusion rules: $\varepsilon \times \varepsilon = 1, \qquad \varepsilon \times \sigma = \sigma, \qquad \sigma \times \sigma = 1 + \varepsilon.$

Braiding rules:

Definition of R_z^{xy}:



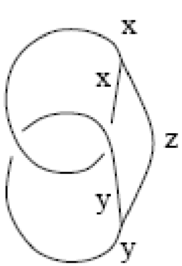
$= R_z^{xy}$


;

$$R_1^{\varepsilon\varepsilon} = -1, \qquad R_1^{\sigma\sigma} = \varkappa \exp\left(-\tfrac{\pi}{8} i\nu\right),$$

$$R_\sigma^{\varepsilon\sigma} = R_\sigma^{\sigma\varepsilon} = -i^\nu, \qquad R_\varepsilon^{\sigma\sigma} = \varkappa \exp\left(\tfrac{3\pi}{8} i\nu\right).$$

Topological S-matrix:

$(S_z)_{xy} \stackrel{\text{def}}{=} \dfrac{1}{\mathcal{D}}$


;

$$S_1 = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \qquad (S_\varepsilon)_{\sigma\sigma} = \exp\left(-\tfrac{\pi}{4} i\nu\right)$$

Anomalous spin-spin correlation function and Quatnum number fractionization

GB, Mandal, Shankar PRL 2007

$$\langle \sigma_i^\alpha \sigma_j^\beta \rangle = \delta_{\alpha\beta}\, \delta_{\langle ij \rangle \alpha}\, A$$

Two spin correlation fn vanishes identically beyond nearest neighbour separation

The best short range Q spin liquid known so far

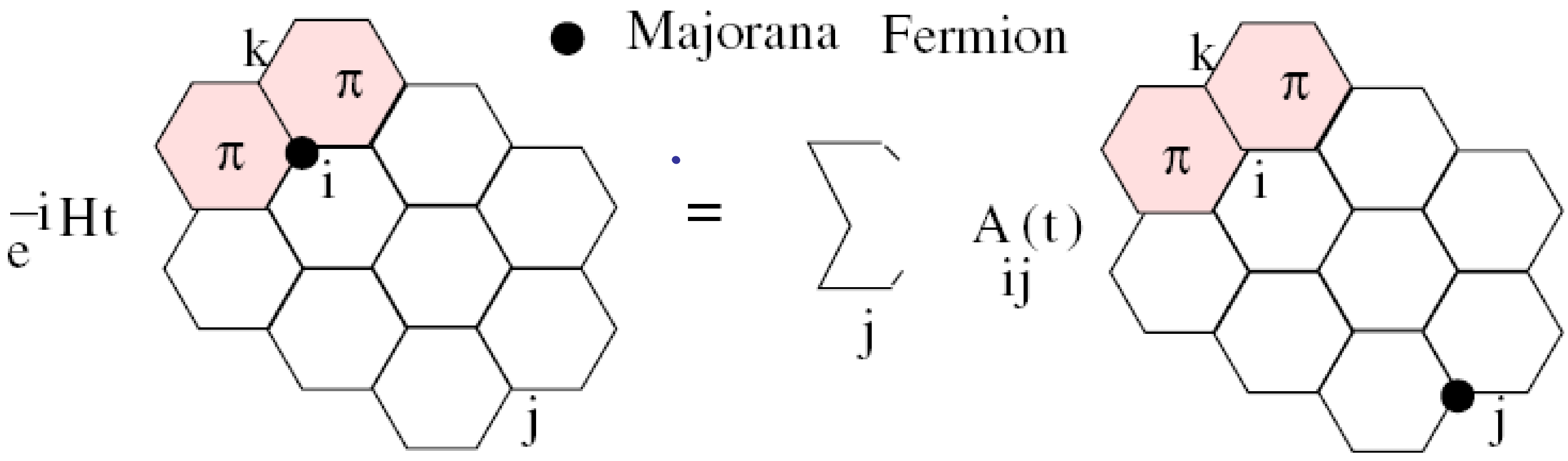
We could also calculate $\langle \sigma_i^\alpha(0)\, \sigma_j^\beta(t) \rangle$ (related to $S(q,\omega)$)

A gapless system that has short range spin correlation !

Any one of the component of Pauli spin operators create a Composite of a Majorana Fermion a pair of flux excitations, while on acting on the ground state.

$$\sigma_i^\alpha |G\rangle \cong \hat{\pi}_{\alpha_1} \hat{\pi}_{\alpha_2} c_i |G\rangle$$

This state evolves in time. The fluxes stay localized. The Majorana fermion gets delocalized.



Non-Abelian Statistics of Half-Quantum vortices in p-Wave Superconductors
D.A. Ivanov, *Phys. Rev. Lett.* **86,** 268 (2001)

Superconductivity in Sr_2RuO_4
Y. Maeno et al., *Nature **372**, 532 (1994)*

- **Theoretical Prediction of p-Wave Superconductivity**
- **T. M. Rice, M. Sigrist**, *J. Phys. Cond. Matter* **7**, L643 (1995)
- **G. Baskaran**, *Physica B **223-224**, 490 (1996); Trieste Workshop July 1995*

- **The intriguing superconductivity of strontium ruthenate**
- **Y. Maeno, T. M. Rice, M. Sigrist**, *Physics Today* (p 42-47), Jan 2001

- **The superconductivity of Sr_2RuO_4 and the physics of spin-triplet pairing**
- **A.P. Mackenzee, Y. Maeno,** *Rev. Mod. Phys.* **75**, 657 - 712 (2003)