Nobel Lecture, Aula Magna, Stockholm University, December 8, 2016

Topological Quantum Matter

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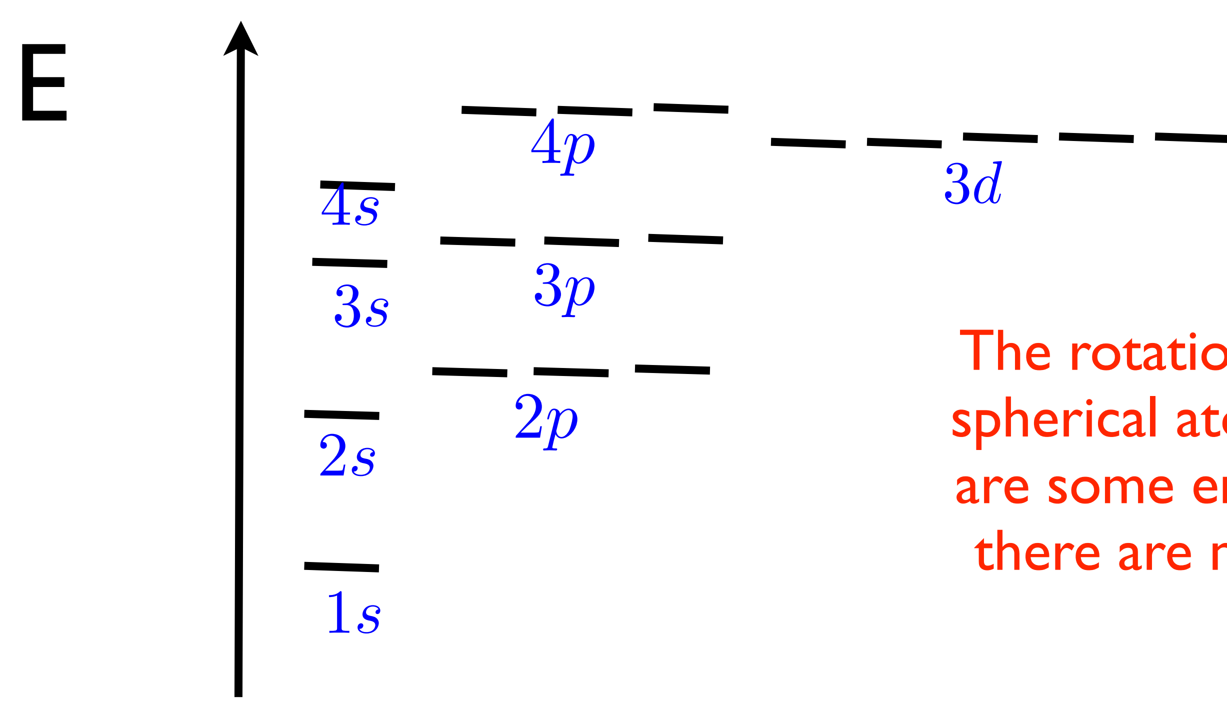
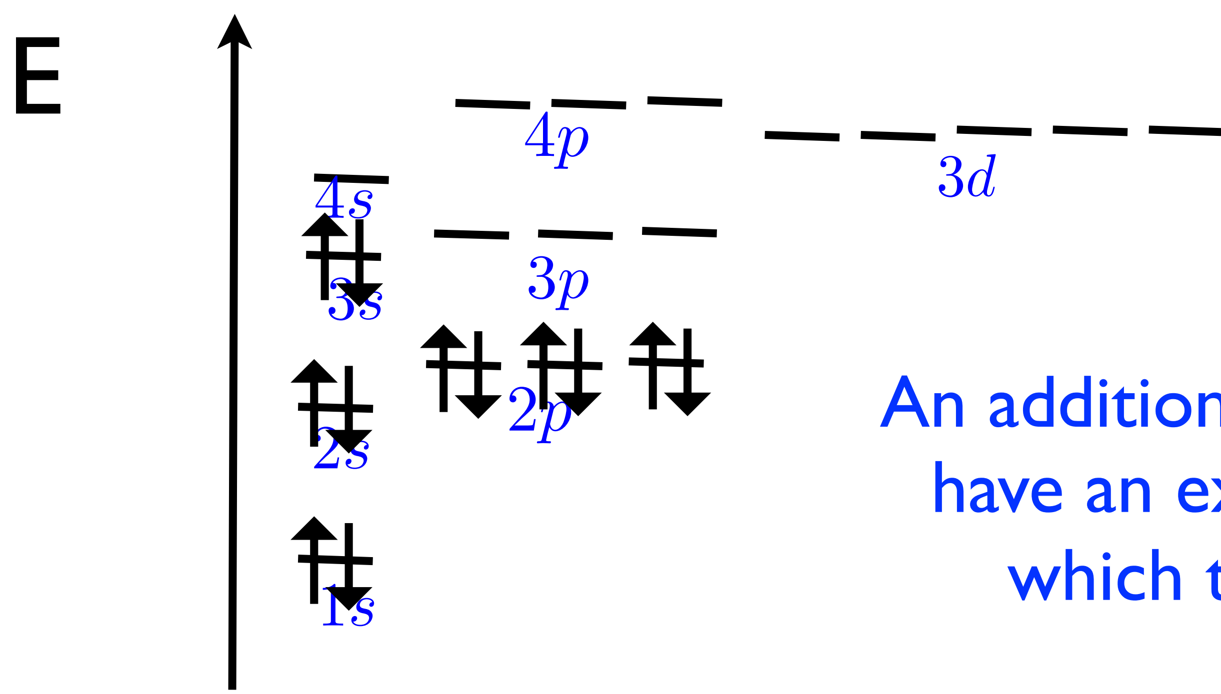
- The TKNN formula (on behalf of David Thouless)
- The Chern Insulator and the birth of "topological insulators"
- Quantum Spin Chains and the "lost preprint"

- In high school chemistry, we learn that electrons bound to the nucleus of an atom move in closed orbits around the nucleus , and quantum mechanics then fixes their energies to only be one of a discrete set of energy levels.



The rotational symmetry of the spherical atom means that there are some energy levels at which there are more than one state

- This picture (which follows from the **Heisenberg uncertainty principle**) is completed by the **Pauli exclusion principle**, which says that no two electrons can be in the same state or “orbital”



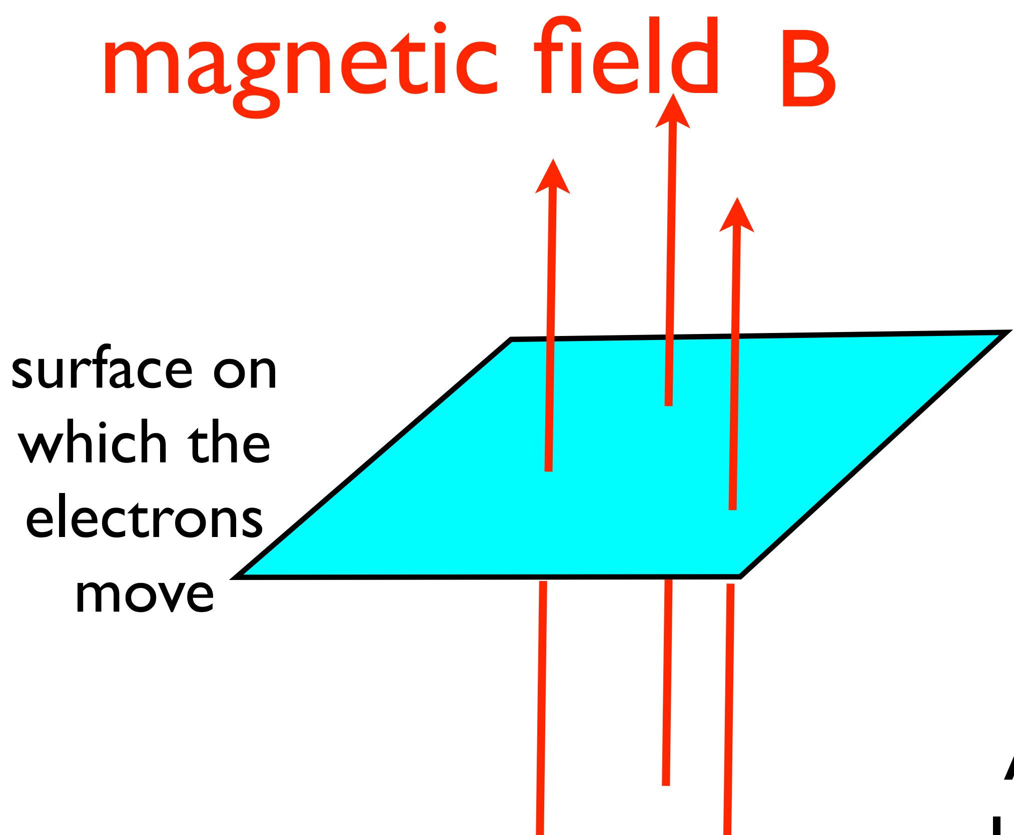
Occupied orbitals of the Calcium atom (12 electrons)

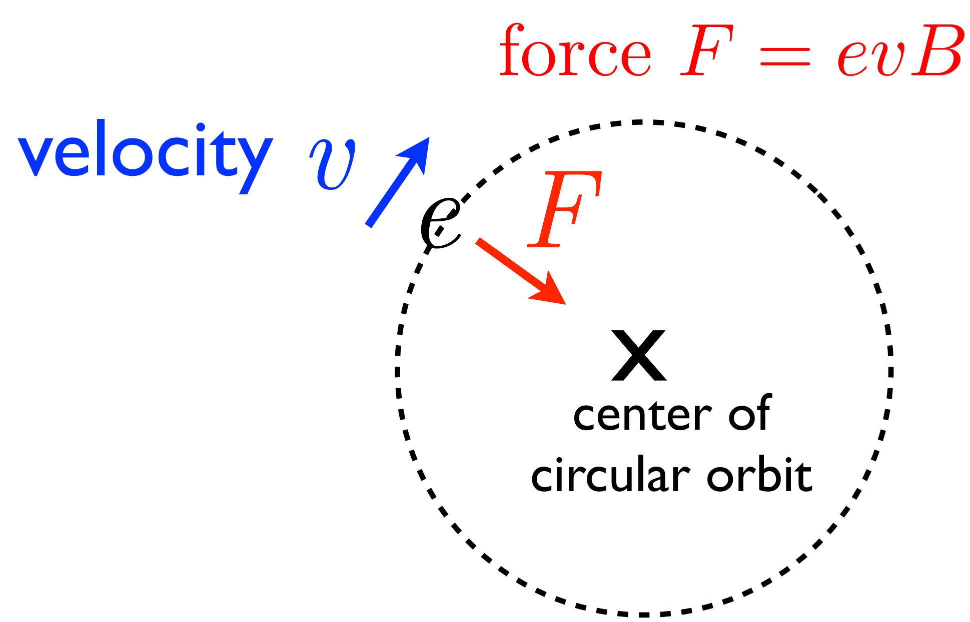
An additional ingredient is that electrons have an extra parameter called “spin” which takes values “up” (↑) and “down” (↓)

This allows <u>two</u> electrons (one ↑, one↓) to occupy each orbital

- If electrons which are not bound to atoms are free to move on a two-dimensional surface, with a magnetic field normal to the surface, they also move in circular orbits because there a magnetic force at right angles to the direction in which they move

- In high magnetic fields, all electrons have spin ↑ pointing in the direction of the magnetic field

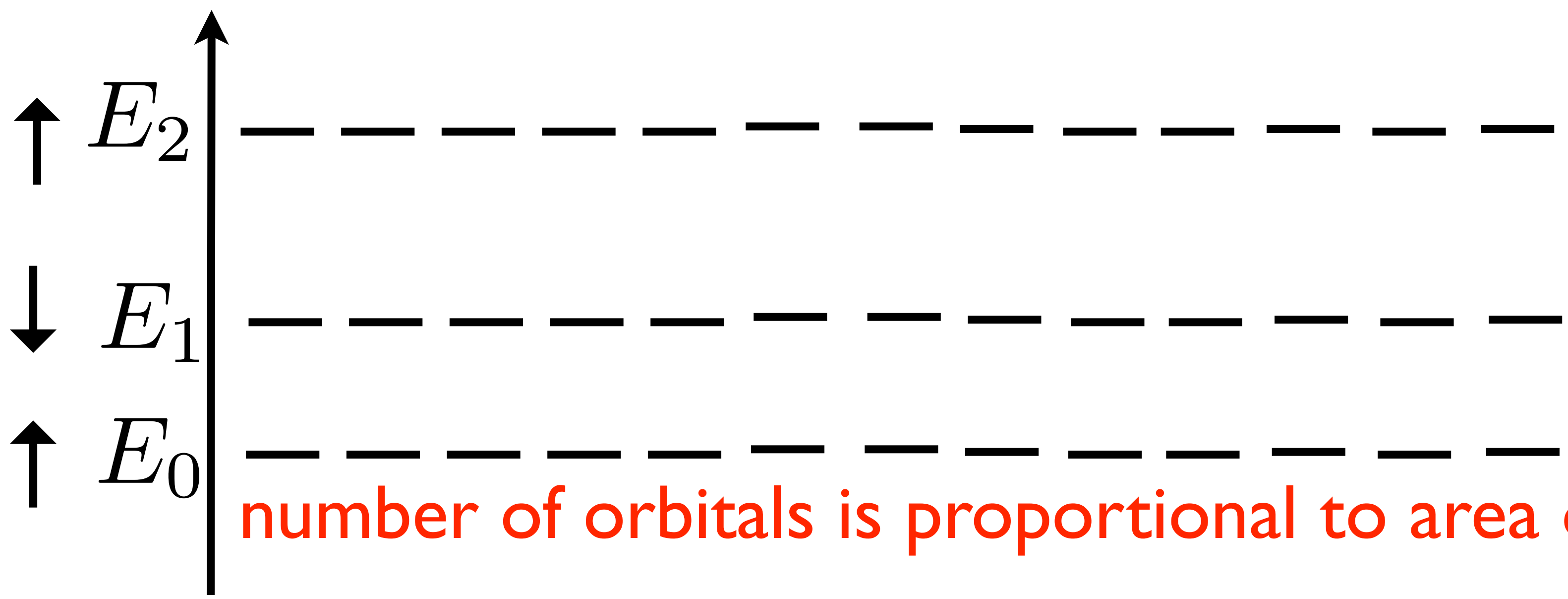




As in atoms, the (kinetic) energy of the electron can only take one of a finite set of values, and now determines the radius of the orbit (larger radius = larger kinetic energy)

- As with atoms, we can draw an energy-level diagram:

(spin direction is fixed in each level)

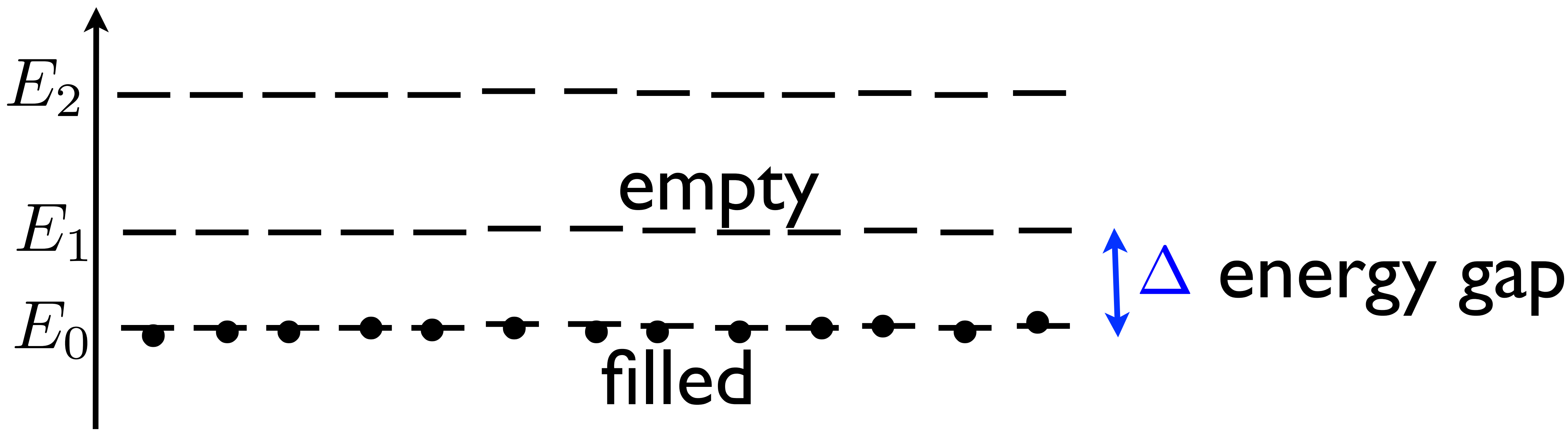


unlike atoms, the number of orbitals in each "Landau level" is <u>huge</u>!

number of orbitals is proportional to area of surface!

$$\text{degeneracy of Landau level} = \frac{\text{Total magnetic flux through surface}}{\text{(London) quantum of magnetic flux}} = \frac{B \times \text{area}}{h/e}$$

- For a fixed density of electrons let's choose the magnetic field B just right, so the lowest level is filled:

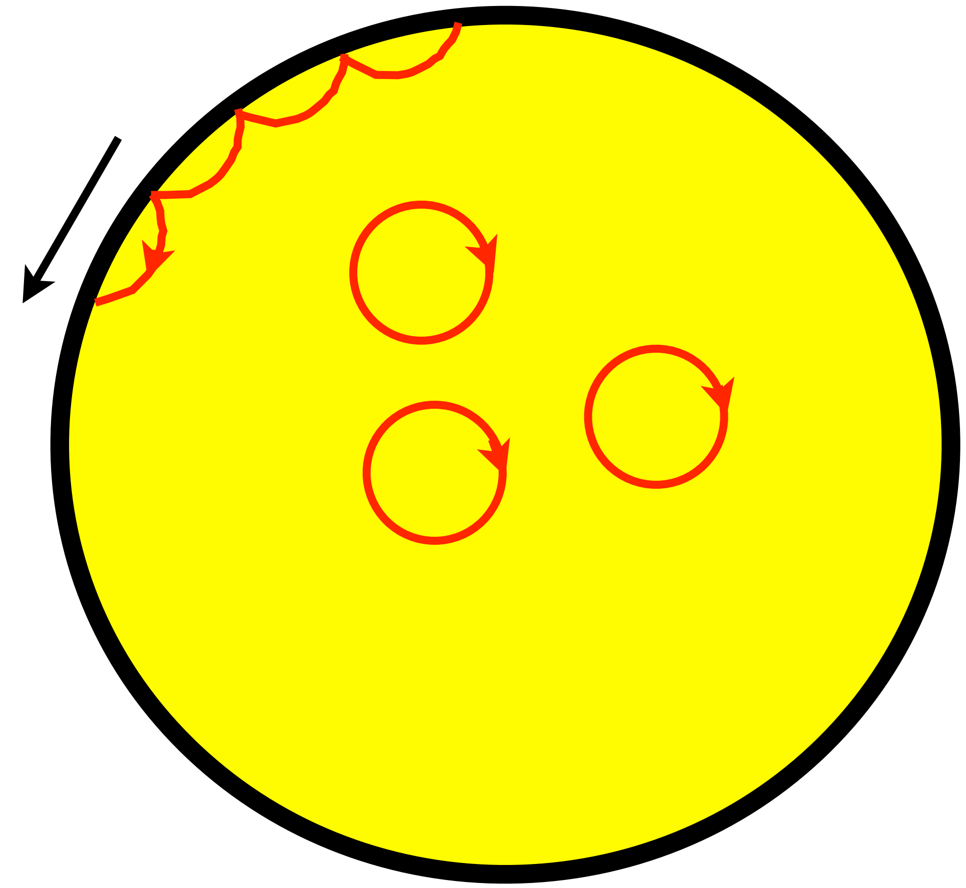


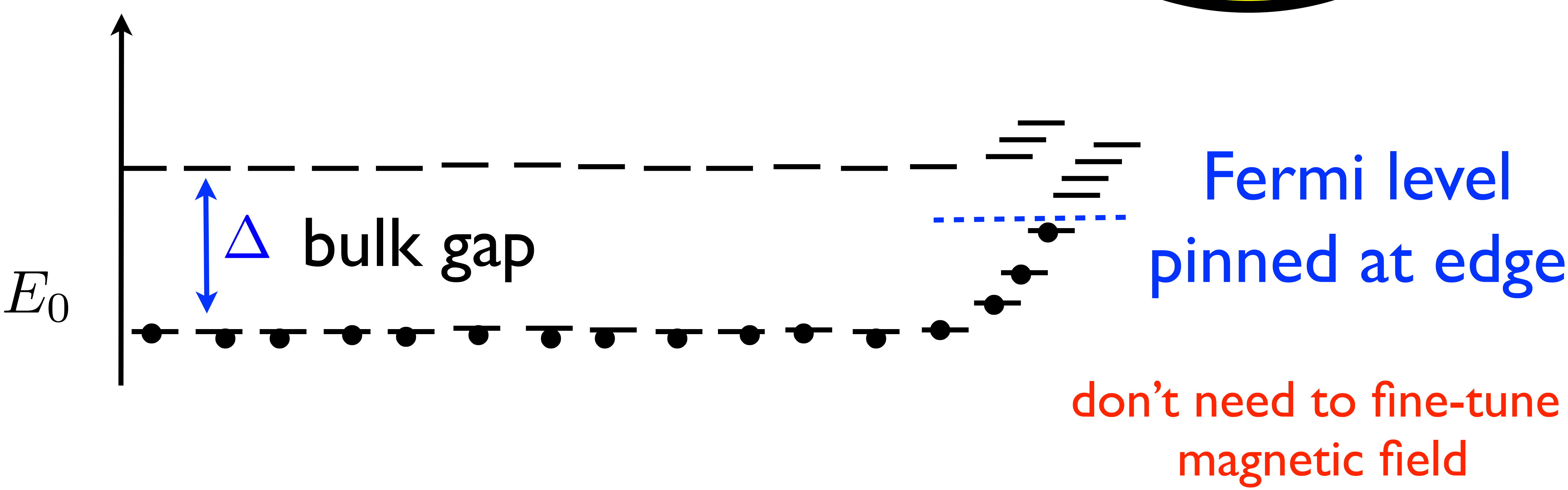
electron density if if n Landau levels are exactly filled $\dfrac{eB}{2\pi\hbar}$

independent of details

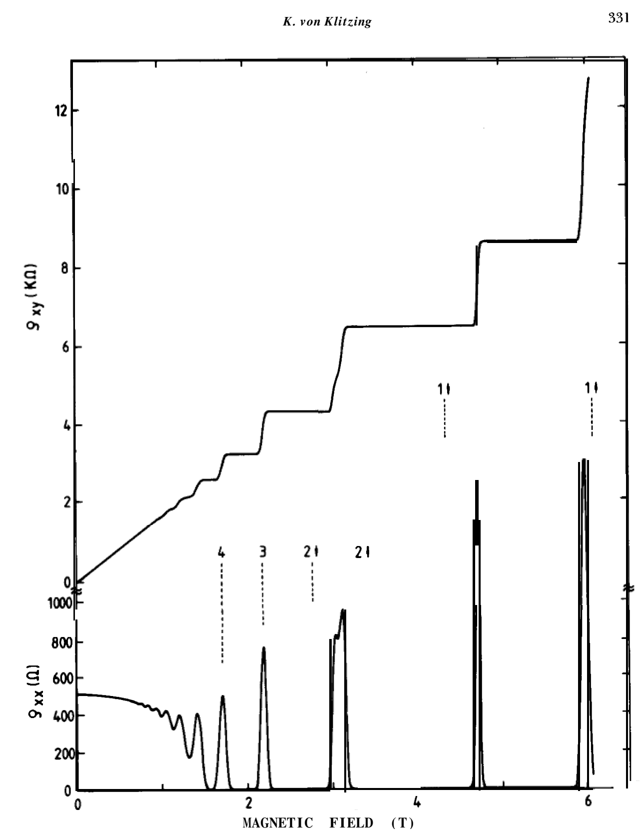
- This appears to describe the integer quantum Hall states discovered by Klaus von Klitzing (Nobel Laureate 1985)
- BUT: seems to need the magnetic field to be "fine-tuned".
- In fact, this is a "topological state" with extra physics at edges of the system that fix this problem

- counter-propagating "one-way" edge states (Halperin)
- confined system with edge must have edge states!





- The integer quantum Hall effect (1980) was the first "topological quantum state" to be experimentally discovered (Nobel Laureate 1985, Klaus von Klitzing)



- Hall conductance

$$j^x = \sigma_H E_y$$

$$\sigma_H = \nu \frac{e^2}{2\pi\hbar}$$

$$\nu = \text{integer}$$

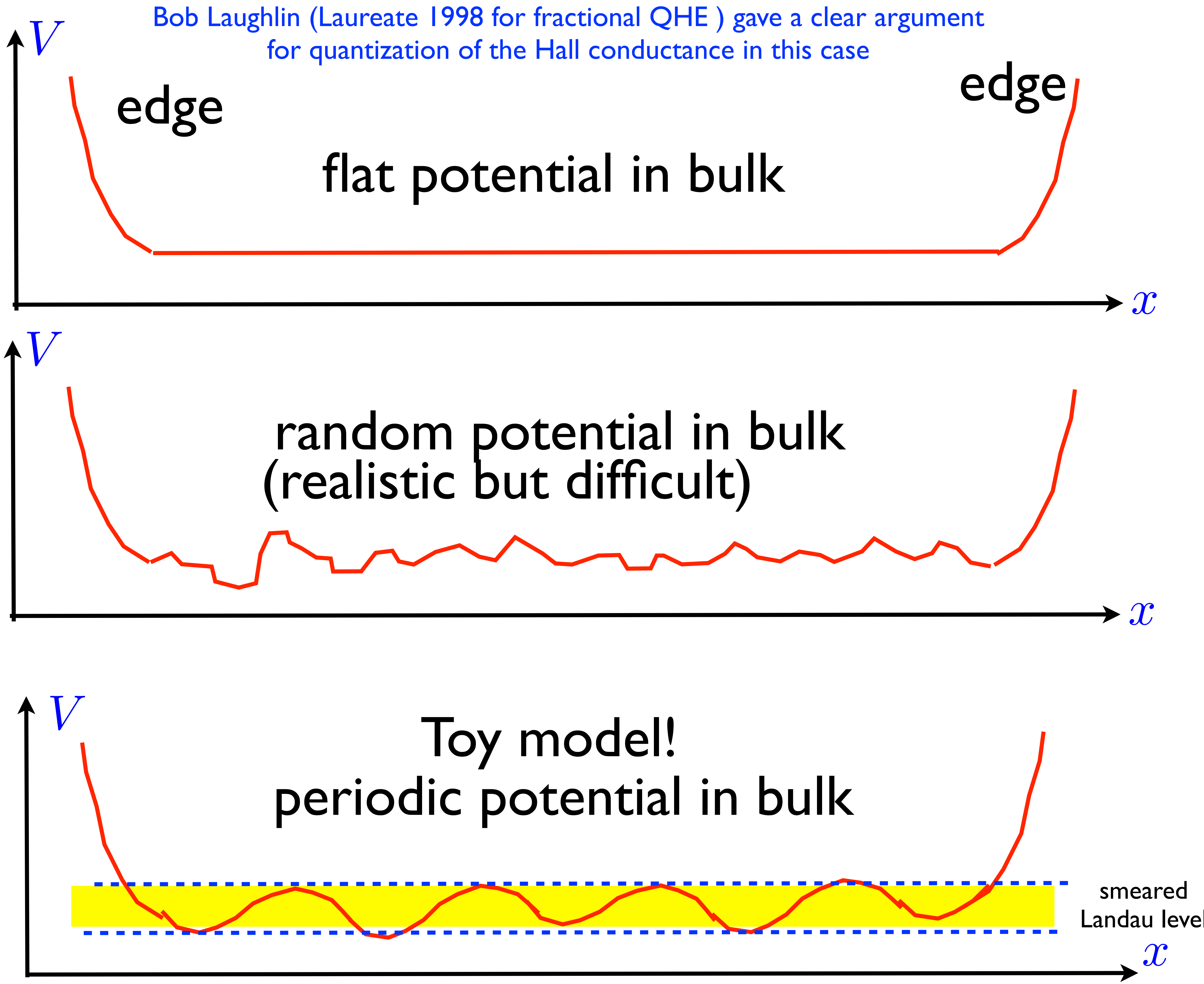
(number of filled Landau levels)

current

$\vec{E}$

dissipationless current
flows at right angles to electric field

- Von Klitzing’s system is much dirtier that the theoretical toy model and work in the early1980‘s focussed on difficult problems of disorder, random potentials and localized states
- David Thouless had the idea to study the effect of a <u>periodic potential</u> in perturbing the flat Landau levels of the integer quantum Hall states:


Bob Laughlin (Laureate 1998 for fractional QHE) gave a clear argument
for quantization of the Hall conductance in this case
V
edge
edge
flat potential in bulk
x
V
random potential in bulk
(realistic but difficult)
x
V
Toy model!
periodic potential in bulk
smeared
Landau level
x

The TKNN or TKN^2 paper

Quantized Conductance in a Two-Dimensional Periodic Potential

D. J. **T**houless, M. **K**ohmoto, M. P. **N**ightingale, and M. den **N**ijs

Physical Review Letters 49, 405 (1982)

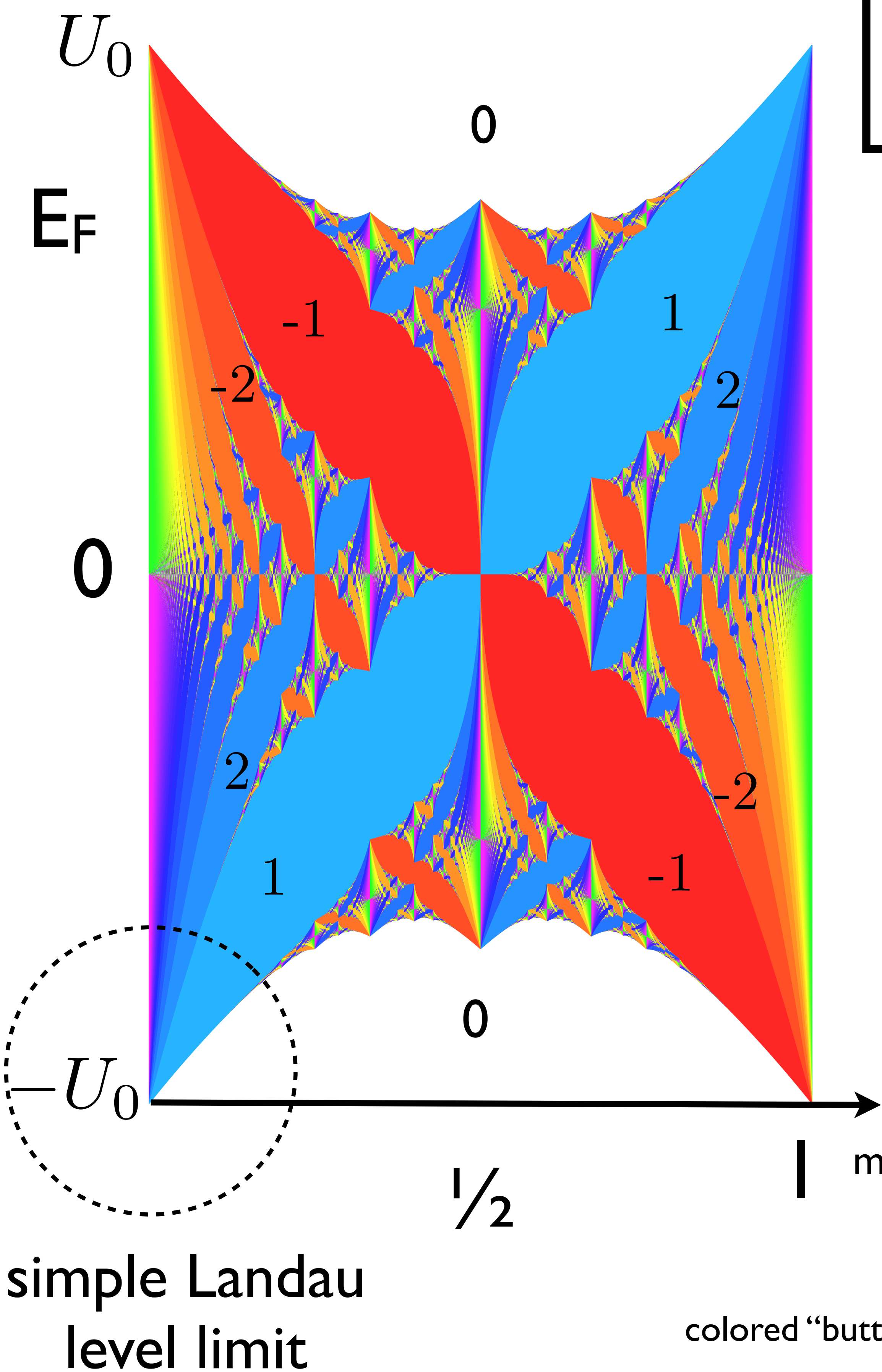
- In 1982 David Thouless with three postdoc collaborators (TKNN) asked how the presence of a periodic potential would affect the integer quantum Hall effect of an electron moving in a uniform magnetic field
- They found a remarkable formula .....

- David became particularly interested in an interesting "toy model", of a crystal in a magnetic field, a family of models including the "Hofstadter Butterfly"

$$H = \frac{1}{2m}|\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r})|^2 + U(\boldsymbol{r})$$

$$U(\boldsymbol{r}) = U_0(\cos(2\pi x/a) + \cos(2\pi y/a))$$

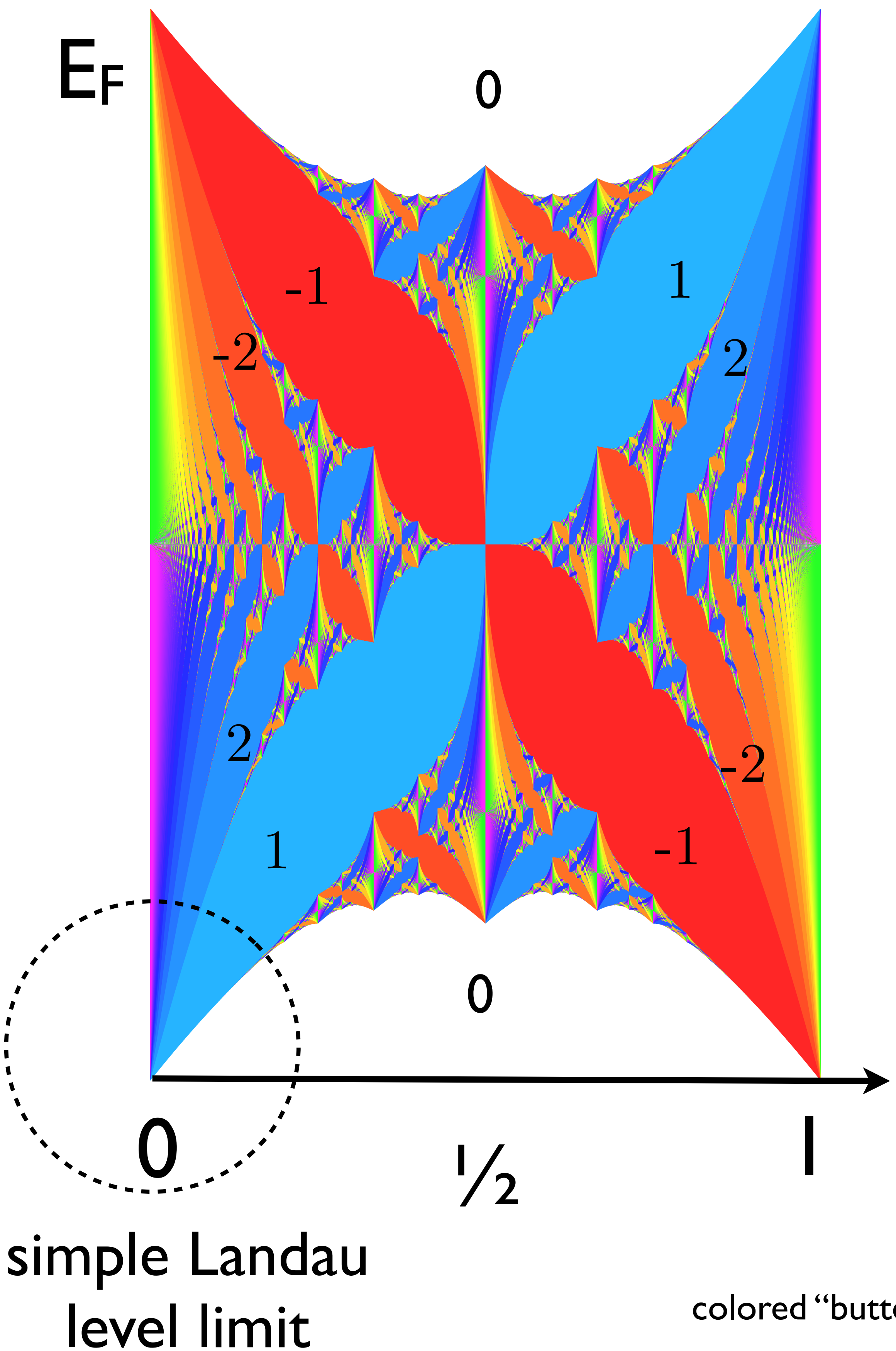
$U_0 \ll \hbar\omega_c$



- Harper's equation (square symmetry) or
- "Hofstadter's Butterfly" splits the lowest Landau level into bands separated by gaps.
- The band are very narrow, and the gaps wide, for low magnetic flux per cell (like Landau levels)

color-coded Hall conductance

colored "butterfly" courtesy of D. Osadchy and J. Avron



- TKNN pointed out that Laughlin's argument just required a bulk gap at the Fermi energy for the Hall conductance to be quantized as integers
- So it should work in gaps between bands of the "butterfly"
- so what was the integer?

colored "butterfly" courtesy of D. Osadchy and J. Avron

- Bloch's theorem for a particle in a periodic potential

$$\Psi_{\boldsymbol{k}n}(\boldsymbol{r}) = u_n(\boldsymbol{k},\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

periodic factor that varies over the unit cell of the potential

- Starting from the fundamental *Kubo formula* for electrical conductivity, TKNN obtained a remarkable formula that **does not depend in any way** on the energy bands, but just on the **Bloch wavefunctions**:

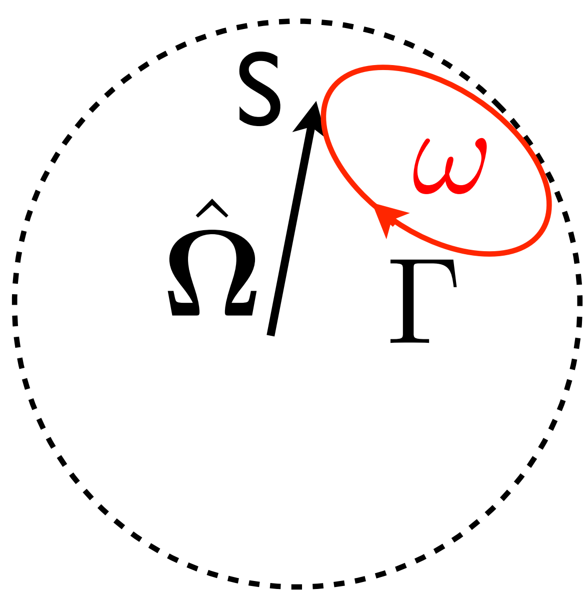
$$\boxed{\sigma_H = \frac{ie^2}{2\pi h}\sum_n \int_{\text{Brillouin zone}} d^2k \int_{\text{unit cell}} d^2r \left(\frac{\partial u_n^*}{\partial k_1}\frac{\partial u_n}{\partial k_2} - \frac{\partial u_n^*}{\partial k_2}\frac{\partial u_n}{\partial k_1}\right)}$$

TKNN first form

Sum over fully-occupied bands below the Fermi energy

- Shortly after the TKNN paper was published, Michael Berry (1983) (Lorentz Medal, 2014) discovered his famous geometric phase in adiabatic quantum mechanics.

- (The Berry phase is geometric, not topological, but many consider this extremely influential work a contender for a Nobel prize).



- Berry's example: a spin S aligned along an axis

direction of spin moves on closed path on unit sphere

$$\boxed{\underbrace{e^{i\Phi_\Gamma}}_{\text{Berry phase}} = e^{iS\omega}}$$

solid angle enclosed is ambiguous modulo 4π
so 2S must be an integer

- the mathematical physicist Barry Simon (1983) then recognized the TKNN expression as an integral over the (Berry) curvature associated with the Berry's phase, on a compact manifold: the Brillouin zone.

- This is mathematical extension of Carl Friedrich Gauss's* 1828 **Theorema Egregium**
  "remarkable theorem"

*foreign member of Royal Swedish Academy of Sciences

- **geometric** properties (such as curvature) are ***local*** properties
- but integrals over local geometric properties may characterize global topology!

Gauss-Bonnet (for a closed surface)

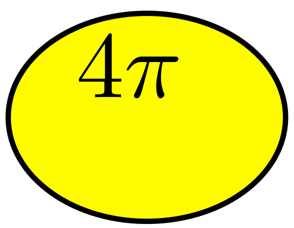
$$\int d^2\boldsymbol{r}(\text{Gaussian curvature}) = 4\pi(1 - \text{genus})$$

product of principal radii of cuvature $\dfrac{1}{R_1 R_2}$

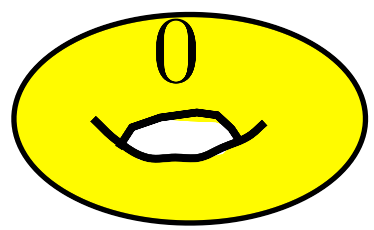
$$= 2\pi(\text{Euler characteristic})$$

$$4\pi r^2 \times \frac{1}{r^2} = 4\pi(1-0)$$

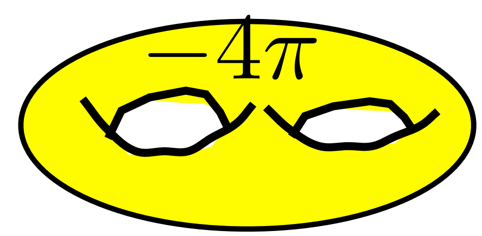
- trivially true for a sphere, but non-trivially true for any compact 2D manifold



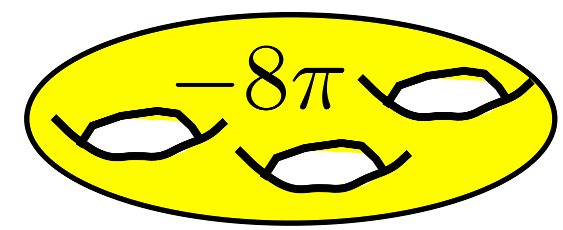
Ball



Bagel



Swedish Pretzel



German Pretzel

mug

coffee cup

“loving cup”

???

$$\mathcal{F}_n^{ab}(\boldsymbol{k}) = \frac{1}{2i}\int_{\text{unit cell}} d^d\boldsymbol{r}\,\left(\frac{\partial u_n^*}{\partial_{k_a}}\frac{\partial u_n}{\partial_{k_b}} - \frac{\partial u_n^*}{\partial_{k_a}}\frac{\partial u_n}{\partial_{k_b}}\right)$$

unit cell

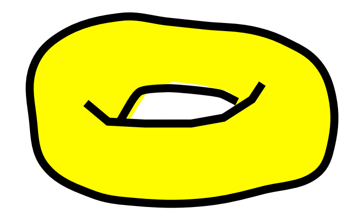
Berry curvature

an antisymmetric tensor in momentum space

- The two-dimensional 1982 TKNN formula

$$\sigma_H^{ab} = \frac{e^2}{\hbar}\sum_n \int_{\text{BZ}} \frac{d^2\boldsymbol{k}}{(2\pi)^2}\mathcal{F}_n^{ab}(\boldsymbol{k})$$

This is an integral over a "doughnut": the torus define by a complete electronic band in 2D



Interestingly It emerged in 1999 that a (non-topological) 3D version of this form applied to the anomalous Hall effect in ferromagetic metals can be found in a 1954 paper by Karplus and Luttinger that was unjustly denounced as wrong at the time!

- first form of the TKNN formula

$$\sigma_H^{ab} = \frac{e^2}{\hbar} \sum_n \int_{\mathrm{BZ}} \frac{d^2\boldsymbol{k}}{(2\pi)^2} \mathcal{F}_n^{ab}(\boldsymbol{k}) \qquad \mathcal{F}_n^{ab} = \frac{\partial}{\partial k_a} \mathcal{A}_{nb} - \frac{\partial}{\partial k_b} \mathcal{A}_{nb}$$

Like a magnetic flux but in k-space (the Brillouin zone)

Like a magnetic vector potential in k-space

Berry's phase (defined modulo 2π) is like a Bohm-Aharonov phase in k-space

$$e^{i\Phi_B(\Gamma)} = \exp\left(i \oint_\Gamma dk_a \mathcal{A}_n^a(\boldsymbol{k}) \right)$$

- because the Berry phase is only defined up to a multiple of 2π, $\displaystyle\int_{\mathrm{BZ}} d^2\boldsymbol{k}\, \mathcal{F}_n(\boldsymbol{k}) = 2\pi \times C_n$

TKNN formula form 2

Chern integer

- TKNN give the formula as

$$\sigma_H = \frac{ie^2}{4\pi\hbar} \sum_n \oint_{\mathrm{BZB}} dk_j \int d^2r \left(u_n^* \frac{\partial u_n}{\partial k_j} - \frac{\partial u_n^*}{\partial k_j} u_n^* \right)$$

I learned from Marcel den Nijs, and Peter Nightingale that their memory is that the inclusion of this explicit general formula (in a single paragraph) was an "afterthought" while writing the paper, which was focussed on the specific values of the integers for the Hofstadter model!

- Another quote from Marcel: "the genius of David Thouless to choose the periodic potential generalization[to split the Landau level] not the random potential one was the essential step"

- We finally arrive at the central TKNN result:

Integral of the (Berry) curvature over the 2D Brillouin zone = 2π times an integer C

Hall conductance: $\sigma_H = \frac{e^2}{h} \times C$

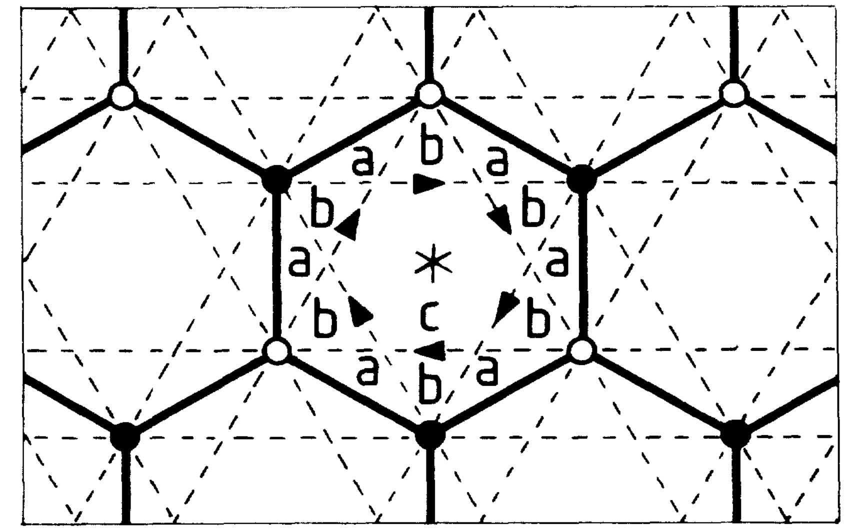
Chern number

QHE without Landau levels

- The 1982 TKNN paper considered the effect of a periodic potential on Landau Levels due to a strong magnetic field
- In 1988, I for reasons that are too long to describe here, I found that the Landau levels could be dispensed with altogether, provided some magnetism (broken time-reversal symmetry) was present.

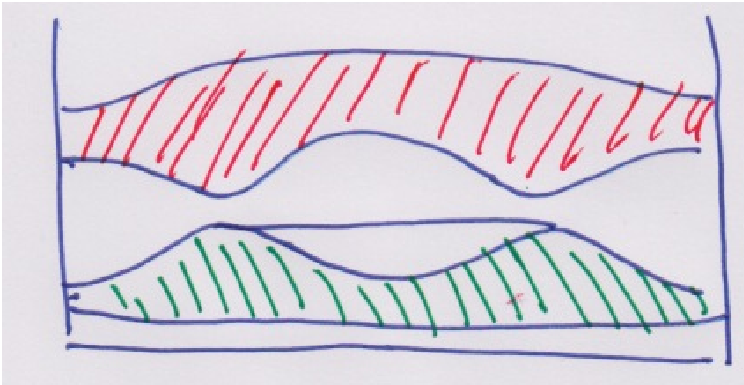
The 2D Chern insulator

- This was a model for a "quantum Hall effect without Landau levels" (FDMH 1988), now variously known as the "quantum anomalous Hall effect" or "Chern insulator".

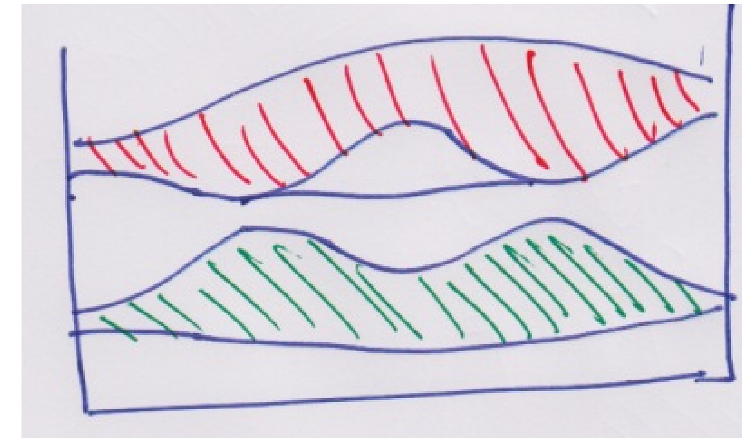


- It just involves particles hopping on a lattice (that looks like graphene) with some complex phases that break time reversal symmetry.

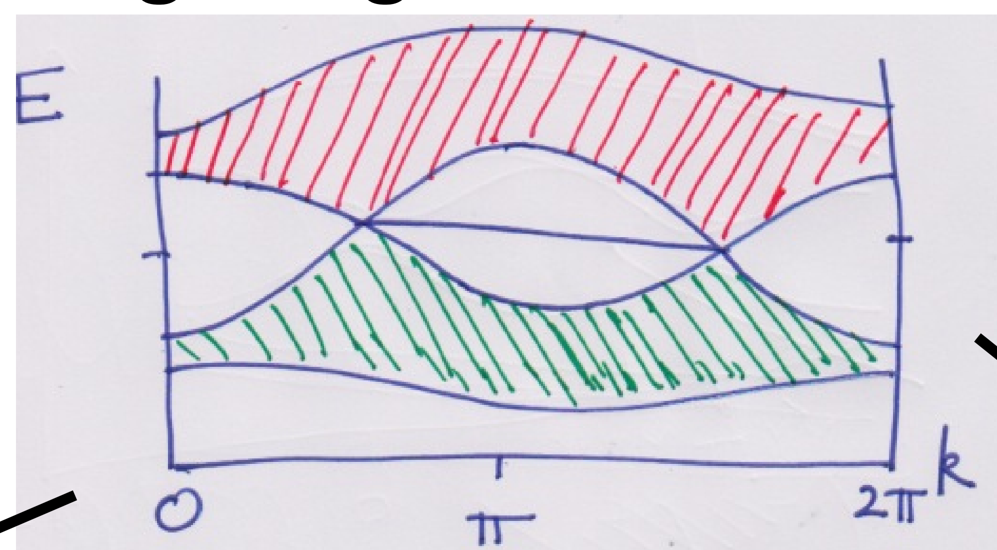
- By removing the Landau level ingredient, replacing it with a more standard crystalline model the "topological insulators" were born

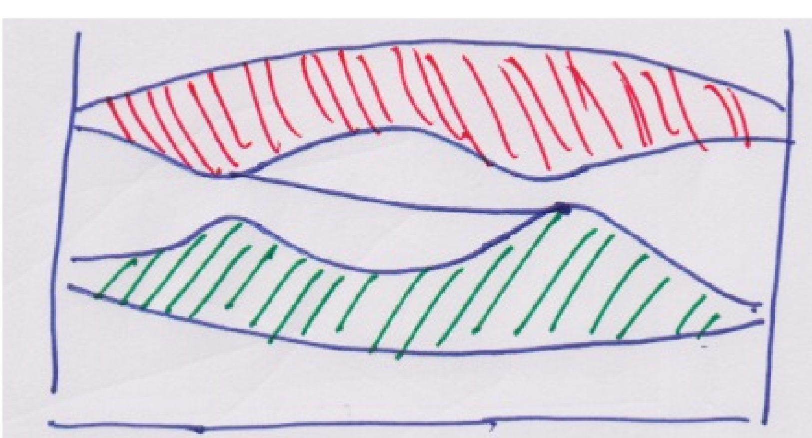


Broken
inversion

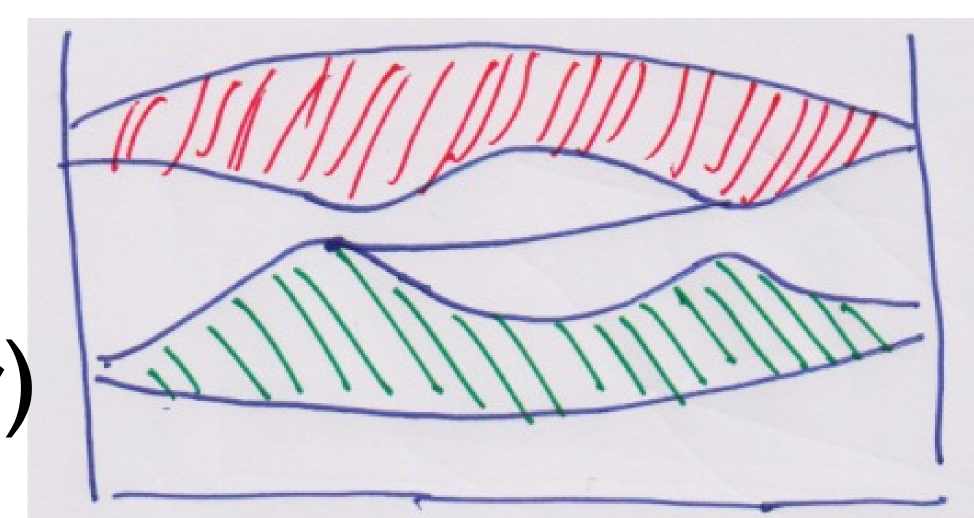


- gapless graphene "zig-zag" edge modes



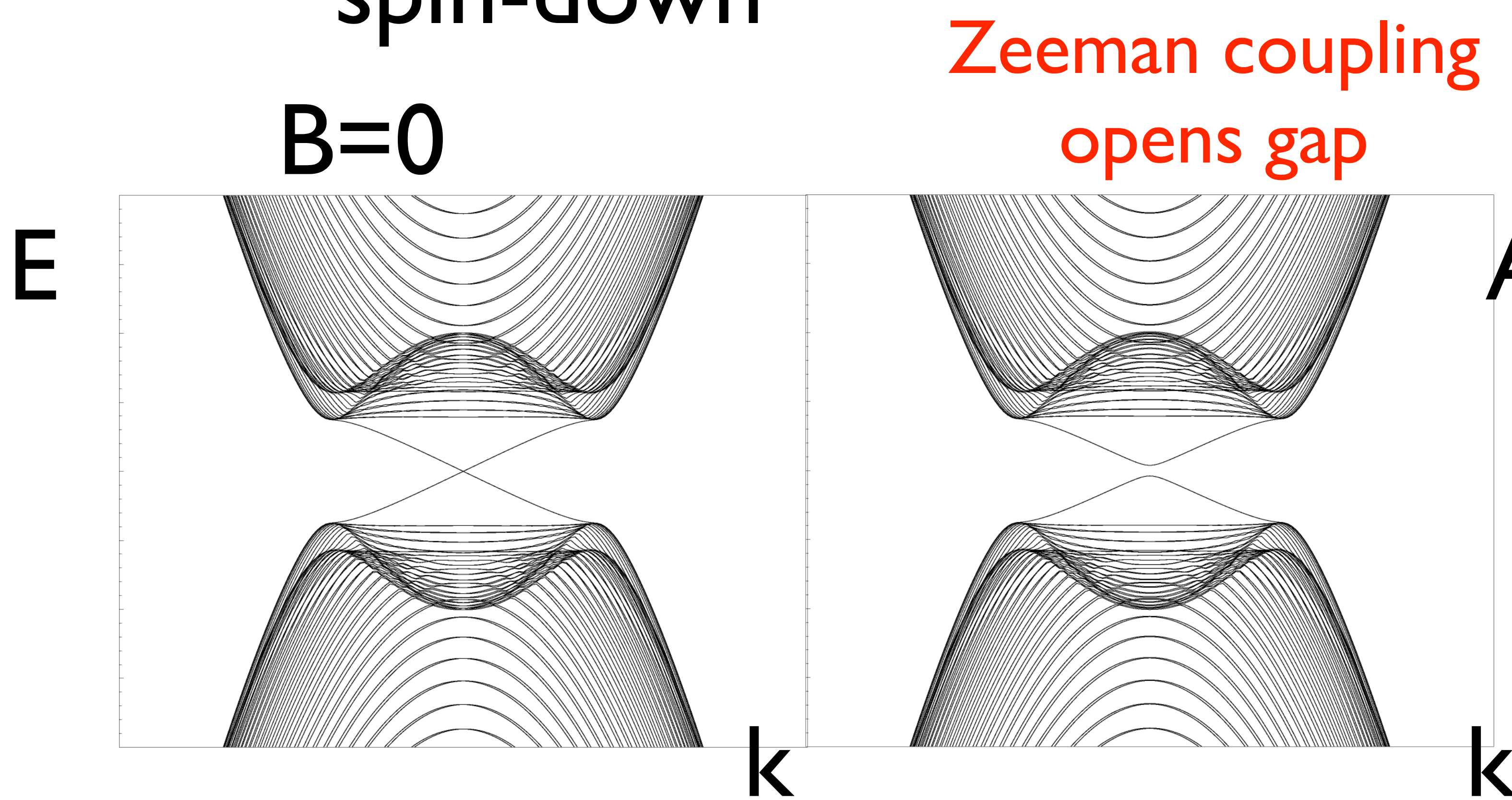


Broken
time-reversal
(Chern insulator)



Kane and Mele 2005

- Two conjugate copies of the 1988 spinless graphene model, one for spin-up, other for spin-down



At edge, spin-up moves one way, spin-down the other way

If the 2D plane is a plane of mirror symmetry, spin-orbit coupling preserves the two kind of spin. Occupied spin-up band has chern number +1, occupied spin-down band has chern-number -1.

From the account of Marcel Den Nijs, the TKNN formula was found unexpectly "by accident" because David picked just the right "toy model" to study

In 1981, I made a similar "unexpected discovery" that may be the simplest example of "topological matter

- Integer and half-integer quantum Antiferromagnetic Chains, "Quantum Kosterlitz-Thouless" and the "lost preprint".

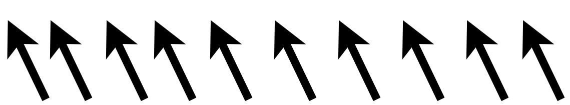
- ILL preprint SP81-95 (unpublished) (now available on arXiv)
- This original preprint was rejected by two journals and when the result was finally published, the connection to the Kosterlitz-Thouless work has been removed.
- The original preprint was lost, but now is found!

One dimensional quantum spin chains are currently the subject of much study. In this note, I outline some new results on axially-symmetric spin chains, without restriction on S, that confirm and extend earlier results[1,2] restricted to spin $S = \frac{1}{2}$, and lead to an unexpected conclusion: while half-integral spin isotropic antiferromagnets have a gapless linear spin wave spectrum and power-law decay of ground state correlations $\langle \vec{S}_n \cdot \vec{S}_0 \rangle \sim (-1)^n n^{-1}$, integral spin systems have a singlet ground state, with a gap for"massive" S = 1 elementary excitations, and exponential decay of ground state correlations:

- Conventional magnetic ground states have long-range order, without significant entanglement (modeled by product states)

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

Ferromagnet

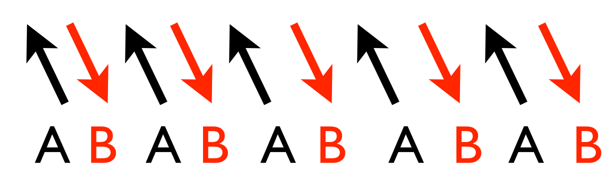


spin direction is arbitrary, but same for all spins

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

neighbors

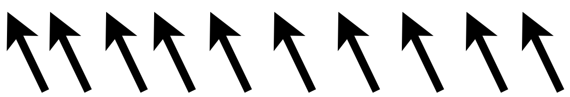
Antiferromagnet



spin direction is arbitrary, but same for all spins on same sublattice, opposite lattice spins are antiparallel

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

Ferromagnet

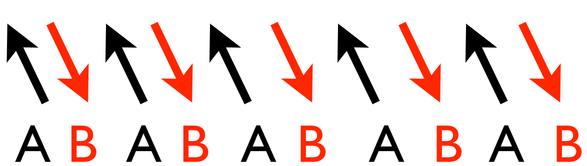


- Has a conserved order parameter direction (conserved total spin angular momentum)

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

neighbors

Antiferromagnet



- order parameter direction is NOT conserved (zero total spin angular momentum)
- quantum fluctuations destroy true long range order in one spatial direction

- For a long time the conventional wisdom assumed the one-dimensional antiferromagnetic systems behaved like the ordered 3D systems, with a harmonic-oscillator treatment of small fluctuations around the ordered state.
- This was partly due to a misinterpretation of a remarkable exact solution in 1931 of the S=1/2 chain by Hans Bethe* (before he moved on to nuclear physics!) The full understanding of Bethe's solution required almost fifty years!

* David Thouless's Thesis Advisor at Cornell!

- In the mid-1970's, another piece of work from the 1930's (the Jordan-Wigner transformation) provided another more standard way to analyze the spin-1/2 chain without Bethe's method.

spins:

$$S^+|\downarrow\rangle = |\uparrow\rangle$$
$$S^+|\uparrow\rangle = 0$$

(spinless) fermions:

$$c^\dagger|0\rangle = |1\rangle$$
$$c^\dagger|1\rangle = 0$$

fermion operators on different sites anticommute!

$$S_i^+ = \prod_{j<i}(-1)^{n_j} c_i^\dagger$$

needed so that $[S_i^+, S_j^+] = 0$

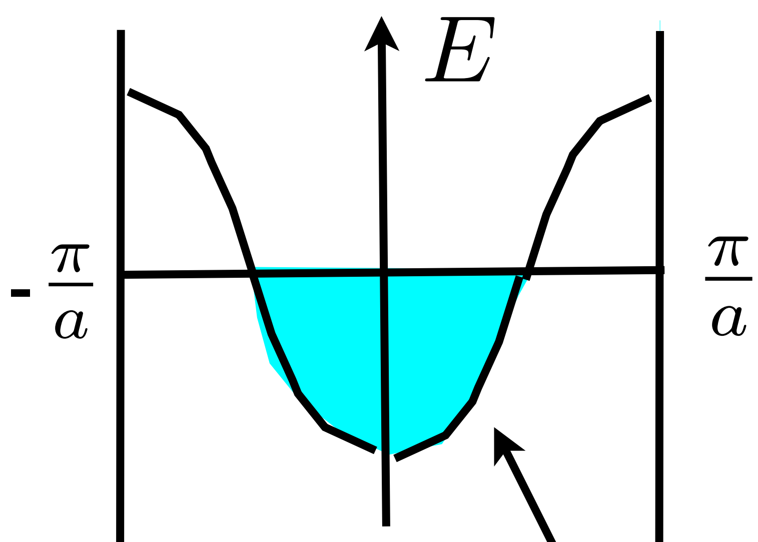
- This converts the spin-1/2 chain into a fermion problem

$$H = \sum_i \tfrac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \lambda S_i^z S_{i+1}^z$$

$\lambda < 1$ easy plane

$\lambda > 1$ easy axis

$$H = \sum_i \tfrac{1}{2}(c_i^+ c_{i+1} + c_{i+1}^\dagger c_i) + \lambda(n_i - \tfrac{1}{2})(n_{i+1} - \tfrac{1}{2})$$



$\lambda = 0$ free fermions

$4k_F = \frac{2\pi}{a}$ (Bragg vector)

"Umklapp processes"

Half-filled band (in zero magnetic field)

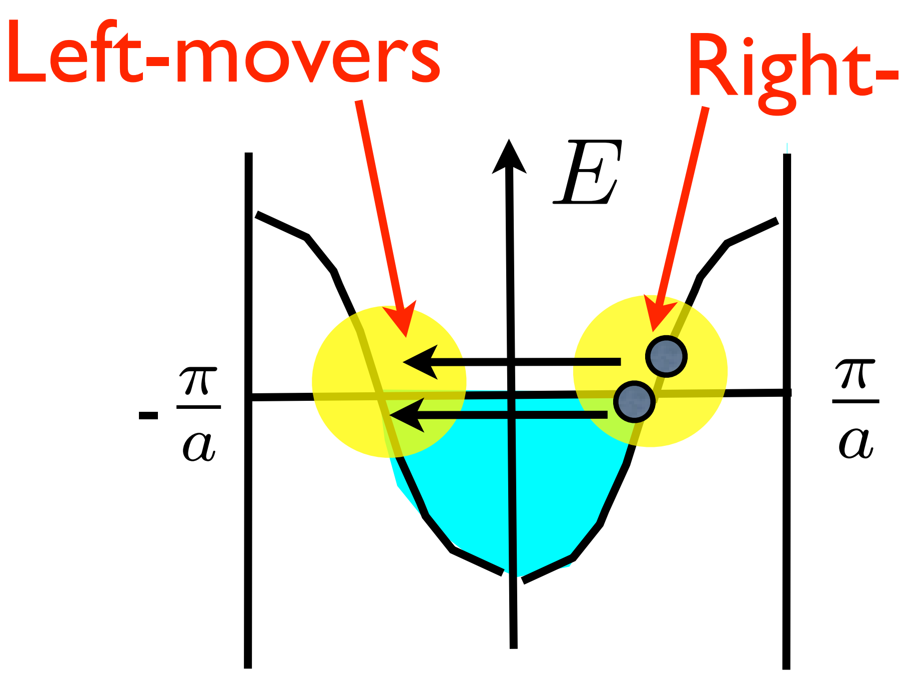
- Converting to a field theory (Luther and Peschel:)

$$H_0 = -i \int dx(\psi_R^\dagger \partial_x \psi_R - \psi_L^\dagger \partial_x \psi_L)$$

$$H = H_0 + \lambda \int dx(\psi_R^\dagger \psi_L - \psi_L^\dagger \psi_R)$$

4kF Umklapp?

$\psi_R^\dagger \psi_R^\dagger \psi_L \psi_L = 0$!



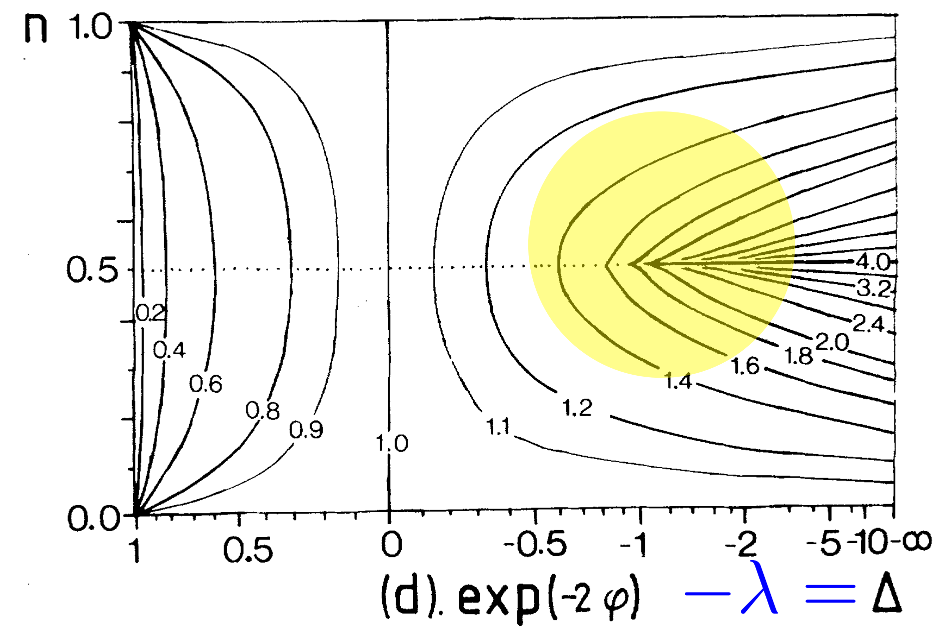
The forgotten Umklapp term!

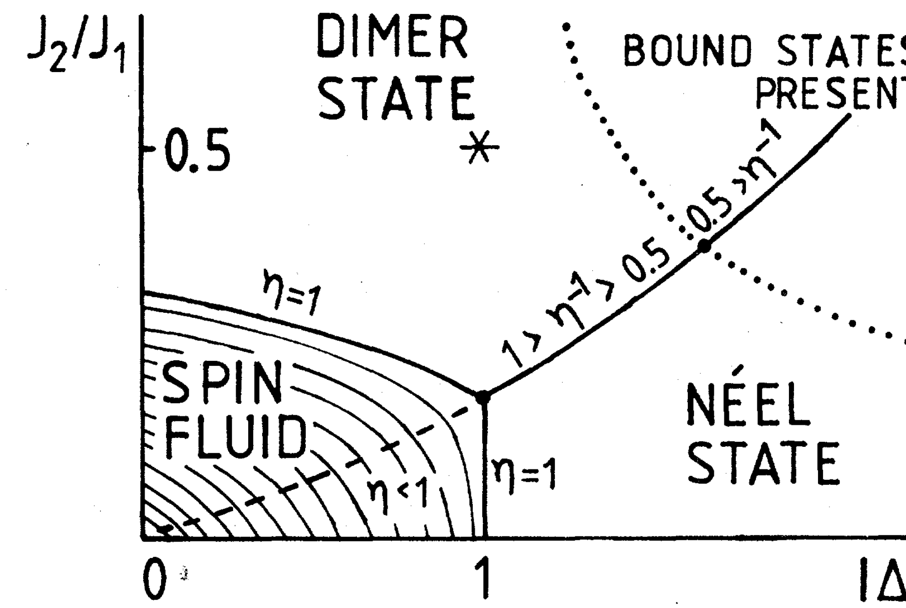
$$H' = \lambda \int dx(\psi_R^\dagger \partial_x \psi_R^\dagger \psi_L \partial_x \psi_L + h.c.$$

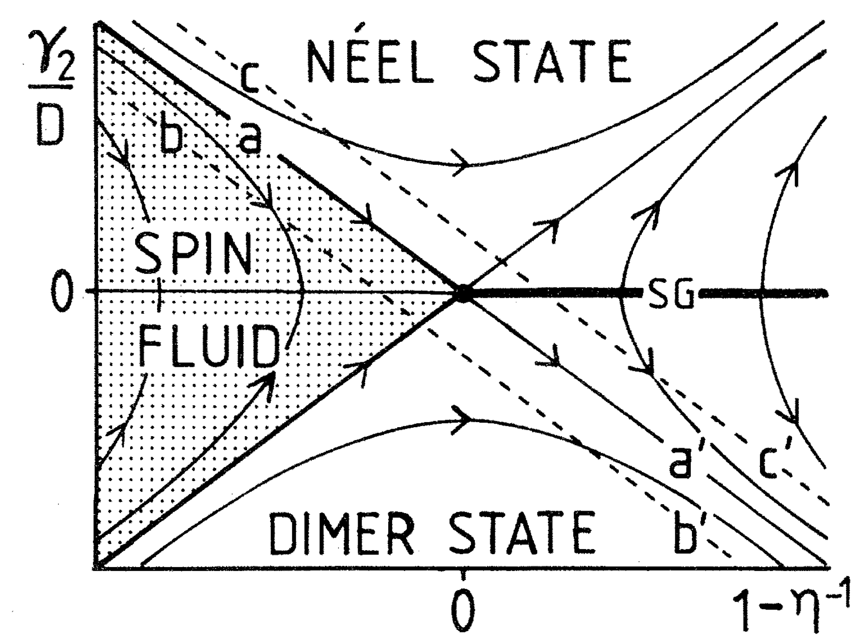
$4k_F = \frac{2\pi}{a}$ (Bragg vector)

- Around that time I developed the "Luttinger liquid theory" (a fit of microscopic models to an effective Tomonaga/Luttinger model), an Abelian precursor to the later-developed and more general conformal field theory, and applied it to this model:

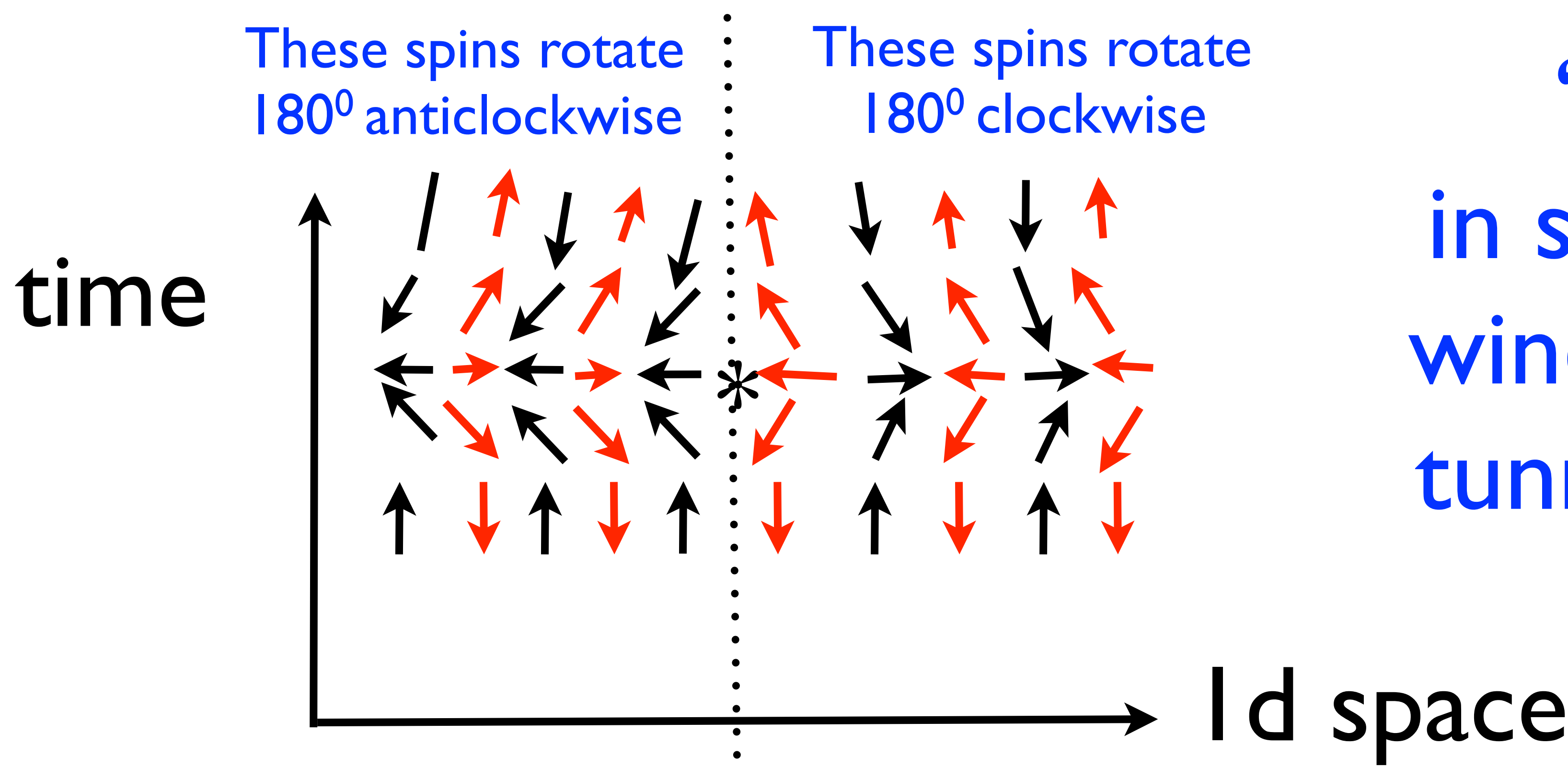
- From the numerical results using Bethe's methods it the presence of the till-then missed Umklapp term was obvious, and driving a quantum analog of the Kosterlitz-Thouless transition, but with a <u>"double vortex"</u> rather than a single vortex



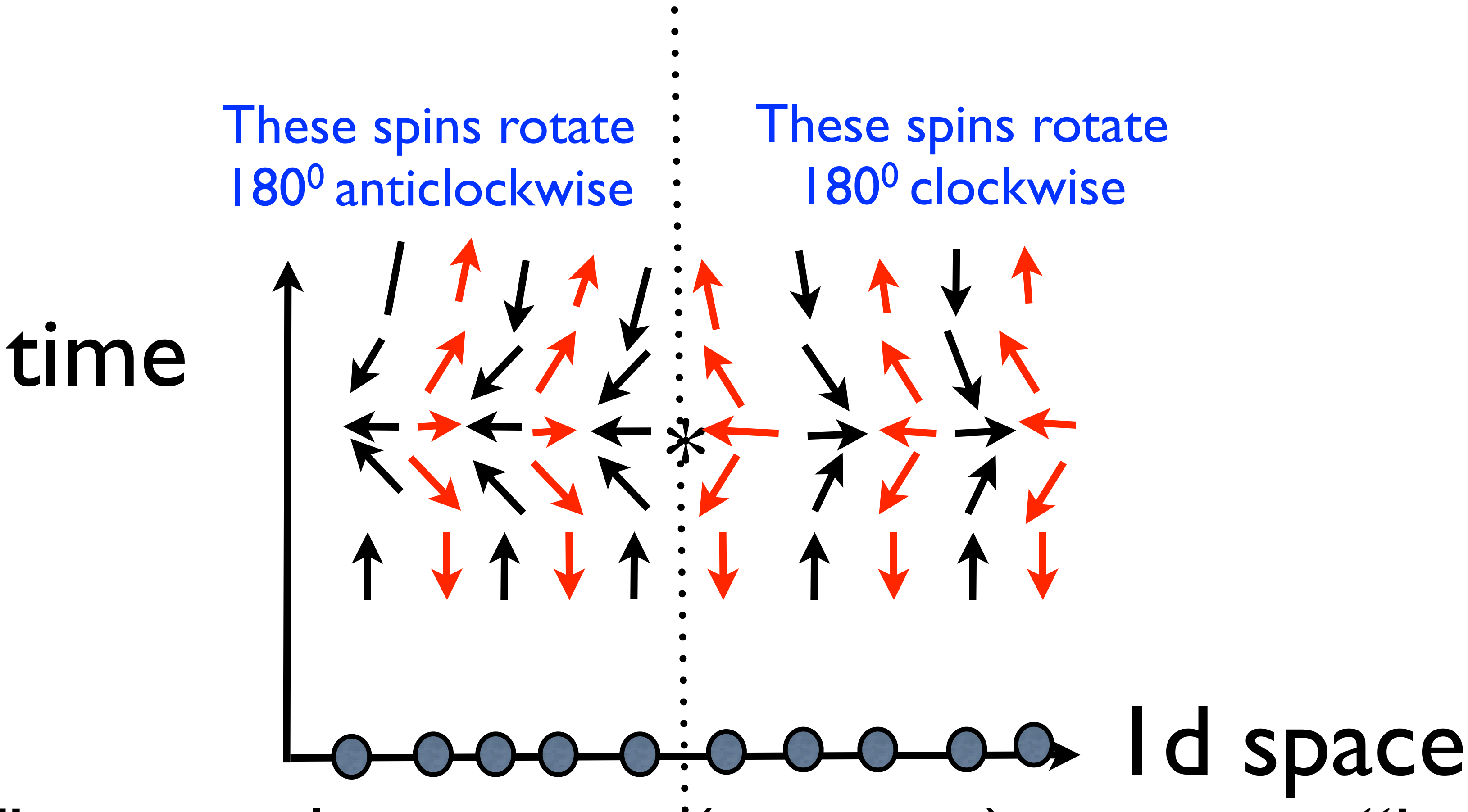




- The topological Kosterlitz-Thouless transition occurs in a "classical" system in two dimensions at finite temperature, but there is a well-know mapping from classical statistical mechanics in two spatial dimensions to quantum mechanics "(1+1) dimensions" (1D space + time)
- One difference is that in classical mechanics the Boltzmann probability is always positive, while the quantum amplitude can be positive, negative or complex giving rise to interference effects.

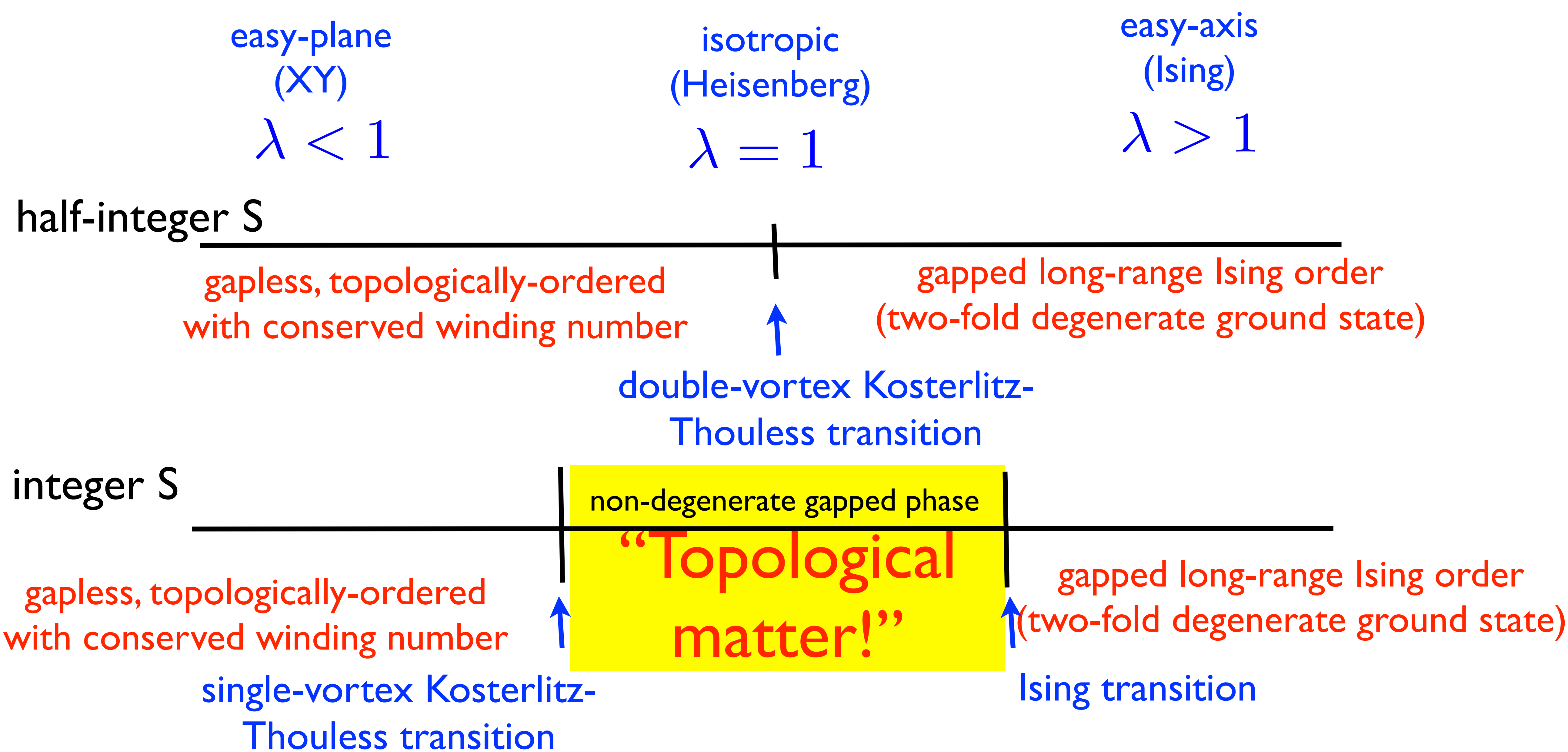


"vortex"
in space-time=
winding-number
tunneling event



- The tunneling events (vortices) occur on “bonds” that couple neighboring spins.
- If the bonds are equal strength, and the vortex is moved one bond to the right, one spin that formerly rotated 180^0 clockwise now rotates anticlockwise.
- The difference is a 360^0 rotation which gives phase factor of -1(and destructive quantum interference) if the spin is half-integral, $+1$ if not.

- From this, it became clear that the progression from easy plane to easy axis was different for integer and half-integer spin antiferromagnets



- The new gapped phase in a "window" containing the integer-spin isotropic Heisenberg point turned out to be the first example of what is now called "topological matter"
- The window is large for S=1, but gets very small for S =2, 3, ...
- The S=1 case is now classified as a "Symmetry-Protected Topological Phase" (the "protective symmetries" are time-reversal and spatial inversion)

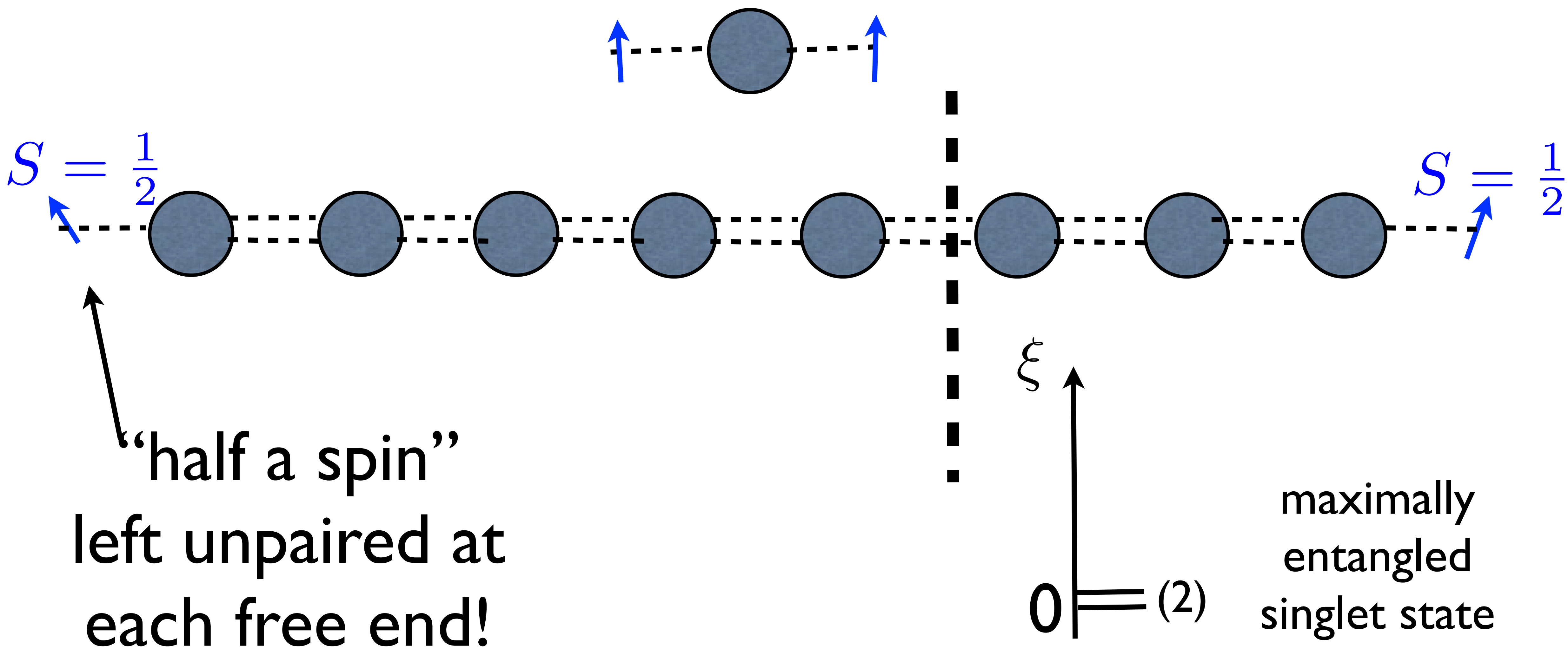
later developments were:

- the identification of a topological "theta" term in the effective field theory of the Heisenberg antiferromagnet that distinguishes integer and half-integer spins. This perhaps started to popularize Lagrangian actions to complement Hamiltonian descriptions in condensed matter theory.

- the identification (Affleck, Kennedy, Lieb, Tasaki) of the "AKLT model" that provides a very simple model state, which explicitly exhibits the remarkable topological edge states and entanglement of this phase

- AKLT state (Affleck, Kennedy, Lieb, Tasaki)

- regard a "spin-1" object as symmetrized product of two spin-$1/2$ spins, and pair one of these in a singlet state with "half" of the neighbor to the right, half with the neighbor to the left:



- The fragments of old work presented here may have seemed difficult for non-experts to understand, but mark the beginnings of what has turned into a completely now way to look at quantum properties of condensed matter
- A large experimental and theoretical effort is underway to find and characterise such new materials, study entanglement, and dream of new “quantum information technolgies”
- It has been a privilege to have contributed to these new ideas, and I thank the Royal Swedish Academy of Sciences for honoring us and our exciting field.