Topological Invariants in Quantum Systems

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Introduction

In order to reduce the sensitivity to errors of quantum states, Kitaev studied the behaviour of what is now known as the **Kitaev chain model** in his paper [**1**] which can have a phase where two unpaired Majorana fermions exist at the ends of quantum wires.
A topological invariant can be associated with the presence of Majorana modes, and this model can undergo a topological phase transition when the band gap closes.
The topological invariant can be studied by considering the **geometrical Berry phase** [**2**] when having infinite number of sites or applying periodic boundary condition to the Hamiltonian.

Geometric Berry phase

Write the Hamiltonian $H(\mathbf{R})$ of a system in terms of some parameter $\mathbf{R}(t)$ varying in time t.
If the parameter $\mathbf{R}(t)$ traces out a closed loop C in parameter space (i.e. $\mathbf{R}(0)=\mathbf{R}(T)$ for some $t=T$) with $H(\mathbf{R}(t))$ evolving adiabatically. A system initially prepared in one of the eigenstates $|\psi(0)\rangle = |n(\mathbf{R})\rangle$ of $H(\mathbf{R})$ with energies $E_n(\mathbf{R}(t))$ develops a total phase given by

$$|\psi(T)\rangle = exp\left\{\frac{-i}{\hbar}\int_0^T dt E_n(\mathbf{R}(t))\right\} exp(i\gamma_n(C))|\psi(0)\rangle$$

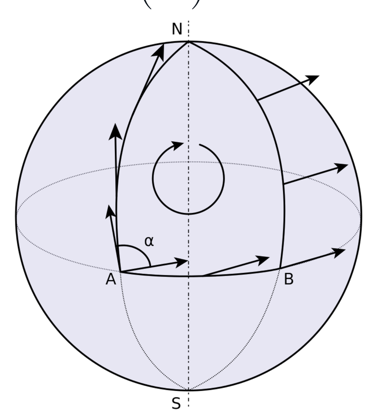
where the first exponential is the dynamical phase factor, and the second one corresponds to the **geometrical (Berry) phase change**

$$\gamma_n(C) = i\oint_C \langle n(\mathbf{R})|\nabla_{\mathbf{R}} n(\mathbf{R})\rangle \cdot d\mathbf{R}$$

which is independent of how the circuit is traversed. Just like the dynamical phase factor, the Berry phase factor is also observable by interference patterns.
In parallel transportation of a vecotr over a loop, the Berry phase is just the angle between the final and initial vectors.
For the two level Hamiltonian $H(\mathbf{R})$, expressed in terms of the Pauli matrices $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ as $H(\mathbf{R}) = \vec{n}(\mathbf{R})\cdot\vec{\sigma}$, it can be shown that the Berry phase can be calculated by the expression

$$\gamma(C) = -\frac{1}{2}\Omega(C)$$

with $\Omega(C)$ the **solid angle** swept out by $\vec{n}(\mathbf{R})$.



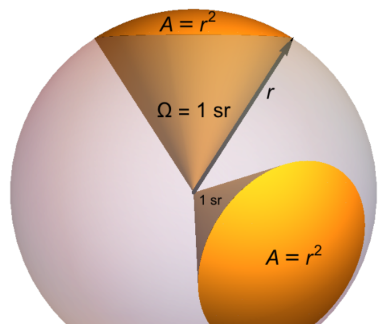


Figure 1: Graphic illustration of parallel transport [**3**] (left).
Figure 2: Graphic illustration of solid angle [**4**] (right).

Kitaev chain model

Assuming spinless fermions. Set up the Kitaev chain as:
A quantum wire with $L \gg 1$ fermionic sites sitting on the surface of a 3-dimensional superconductor. Each site can be either empty or occupied by an electron, described by a pair of annihilation and creation operators $a_j, a_j^\dagger$. The Hamiltonian is

$$H = \sum_{j=1}^{L}\left(-t(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) - \mu(a_j^\dagger a_j - \frac{1}{2}) + \Delta a_j a_{j+1} + \Delta^* a_{j+1}^\dagger a_j^\dagger\right)$$

where t is the hopping amplitude, μ the chemical potential, and $\Delta = |\Delta|e^{i\theta}$ the induced superconducting gap, all independent on site number.
The phase parameter θ can be hidden into the definition of two **Majorana operators** c_{2j-1} and c_{2j} for each site j:

$$c_{2j-1} = e^{i\frac{\theta}{2}}a_j + e^{-i\frac{\theta}{2}}a_j^\dagger, \qquad c_{2j} = -ie^{i\frac{\theta}{2}}a_j + ie^{-i\frac{\theta}{2}}a_j^\dagger \qquad (j = 1, ..., L)$$

which are hermitian operators and satisfy the anti-communication relatoin

$$\{c_l, c_m\} = 2\delta_{l,m} \qquad (l, m = 1, ..., 2L)$$

the Hamiltonian written in terms of these Majorana operators:

$$H = \frac{i}{2}\sum_{j=1}^{L}\Big(-\mu c_{2j-1}c_{2j} + (t + |\Delta|)c_{2j}c_{2j+1} + (-t + |\Delta|)c_{2j-1}c_{2j+2}\Big)$$

There are two special phases in the Kitaev chain model:

a) The tivial phase: $t = |\Delta| = 0$, $\mu < 0$.

$$H = -\mu\sum_{j=1}^{L}(a_j^\dagger a_j - \frac{1}{2}) = \frac{-i\mu}{2}\sum_{j=1}^{L}c_{2j-1}c_{2j}$$

with Majorana operators from the same site paired together, forming a ground state with occupation number 0.

b) The topological phase: $t = |\Delta| > 0, \mu = 0$.

$$H = it\sum_{j=1}^{L-1}c_{2j}c_{2j+1}$$

the Majorana operators from *different sites* paired together.

In case b), here are two Majorana operators c_1 and c_{2L} remaining unpaired at two ends of the chain thus two orthogonal ground states $|\psi_0\rangle$ and $|\psi_1\rangle$ satisfying

$$-ic_1c_{2L}|\psi_0\rangle = |\psi_0\rangle, \qquad -ic_1c_{2L}|\psi_1\rangle = -|\psi_1\rangle$$

with $|\psi_0\rangle$ having an even fermionic parity while $|\psi_1\rangle$ having an odd parity, measured by parity operator $P = \prod_{j=1}^{L}(-ic_{2j-1}c_{2j})$.

Figure 3: Graphic illustration of two special cases of pairing.

Hence we have a 1D system with zero energy states at the edges with which we can associate a topological invariant. This invariant is discussed in the final section.

References

[1] A. Kitaev. *Unpaired Majorana fermions in quantum wires. Physics Uspekhi* 44(2000), p.131.

[2] M. V. Berry. *Quantal Phase Factors Accompanying Adiabatic Changes. Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, 392(1802):45–57, 1984.

[3] Wikipedia. *Parallel transport.* https://en.wikipedia.org/wiki/Parallel_transport

[4] Wikipedia. *Solid angle.* https://en.wikipedia.org/wiki/Solid_angle

Band structure of the Kitaev model

For arbitrary values of t, μ and Δ with periodic boundary condition (i.e. $a_i = a_{i+L}$), the Hamiltonian can be expressed as

$$H = \Psi^\dagger H_{BdG}\Psi = \sum_k \Psi_k^\dagger H_k \Psi_k$$

where $\Psi_k = (a_k, a_{-k}^\dagger)^T$ is the Nambu spinor, and

$$H_k = \begin{bmatrix} -2t\cos k - \mu & 2i|\Delta|\sin k \\ -2i|\Delta|\sin k & 2t\cos k + \mu \end{bmatrix} = -2|\Delta|\sin k\sigma_y - (\mu + 2t\cos k)\sigma_z \qquad (\dagger)$$

with two energy bands:

$$E_\pm(k) = \pm\sqrt{(2t\cos k + \mu)^2 + 4|\Delta|^2\sin^2 k}$$

- gapped for all k as long as $|\mu| \neq |2t|$.
- bulk gap closes when $\mu = 2t$ and $\mu = -2t$ for $k = \pi$ and $k = 0$ respectively.

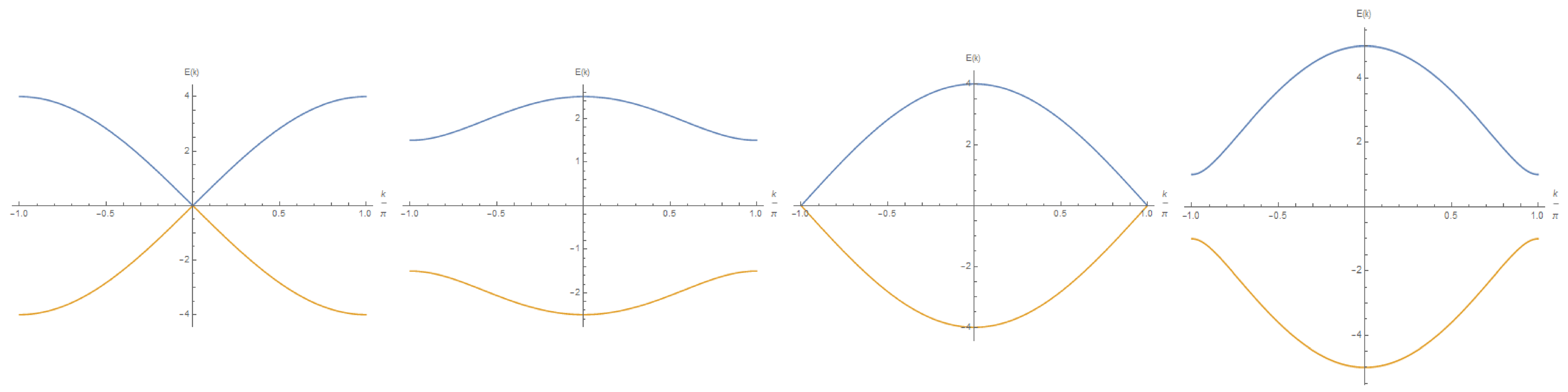


Figure 4: Energy spectra for $\mu = -2t$, $\mu = 0.5t$, $\mu = 2t$ and $\mu = 3t$ from left to right.

In an open chain with a finite number of sites and $|\mu| < |2t|$, there are two zero modes exponentially located near the edge of the chain, while they do not exist when $|\mu| > |2t|$.
At gap closing for $\mu = -2t$, linear approximation at $k = 0$ gives two eigenstates with energies given by

$$E = \pm 2|\Delta|k$$

corresponding to Majorana modes left-moving on the branch $E = -2|\Delta|k$ and right-moving on $E = 2|\Delta|k$, with the same speed $v = 2|\Delta|$.

Berry phase in Kitaev chain model

From ($\dagger$), we can write $H_k = -c\,\vec{n_k}\cdot\vec{\sigma}$, where $\vec{\sigma}$ is the Pauli matrices, c the normalization constant $c = 2\sqrt{|\Delta|^2\sin^2 k + (\frac{\mu}{2} + t\cos k)^2}$ and $\vec{n_k} = \frac{1}{c}(0,\ 2|\Delta|\sin k,\ \mu + 2t\cos k)$ a unit vector that lies in an equatorial plane of the Bloch sphere.
When $L \to \infty$, momentum moving around the Brillouin zone results in a Berry phase of π when $|\mu| < |2t|$, and a 0 Berry phase if $|\mu| > |2t|$.
These Berry phase factors 1 and -1 are topological $\mathbb{Z}_2$ invariants in the two phases.
Note that the same Berry phase can also be computed by applying a twisted boundary condition with factor $e^{i\theta}$ to a finite chain of L sites.

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