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Topological invariants of quantum systems

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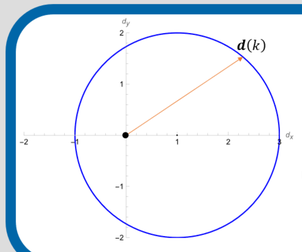

Fig. 3: A graph of the circle traced out by the endpoint of the vector $\boldsymbol{d}(k)$ in the x-y plane as the wavenumber runs through the first Brillouin zone for hopping amplitudes $t_\alpha = 1, t_\beta = 2$

Introduction

The physical properties exhibited by a quantum system often depend on external parameters which can be varied. Different configurations of these parameters in which different properties are exhibited by the system are said to be different physical phases. These phases can sometimes be distinguished by an associated topological invariant: an integer number which takes distinct values when the system is in distinct phases, and is invariant under adiabatic deformations. We begin this poster by investigating the geometric Berry phase associated with adiabatic deformations of a parameterised Hamiltonian. Then we analyse the SSH model - a simple 1-Dimensional quantum wire which acts as a topological insulator - and seek to compute a topological invariant for it, related to the Berry phase.

The Berry Phase

Consider a quantum system, with a Hamiltonian $\hat{H}(\mathbf{R})$ dependant on various parameters $\mathbf{R} = (X_1, X_2, ...)$, and suppose that these parameters are varied "slowly" around a circuit C in the Hamiltonian's parameter-space. This defines an adiabatic process, so the adiabatic theorem guarantees that the system will return to its initial state with the addition of a phase factor (There is a fundamental $U(1)$ gauge freedom over the choice of phase for quantum states, as the phase of a state has no bearing on the expectation values of its observable properties). On top of the dynamical phase factor that accompanies the time evolution of any state, there is also a geometric phase factor - the first explicit formula for which was derived in 1984 [1] - which is a geometric property of the circuit traversed in parameter space and has no dependence on the rate of traversal. This is called the Berry phase, which for a Hamiltonian with eigenstates $|n(t)\rangle$ has the form:

$$\gamma_n(C) = \iint_C \boldsymbol{\nabla} \times \mathbf{B}_n(\mathbf{R}) \bullet d\mathbf{R} \text{ where } B_n(\mathbf{R}) = i \langle n(\mathbf{R}) | \boldsymbol{\nabla} n(\mathbf{R}) \rangle$$

$B_n(\mathbf{R})$ is the Berry Connection, which acts as a vector potential for the quantity that is integrated to compute the Berry phase (analogous to the magnetic vector potential in electromagnetism).

A $U(1)$ gauge transformation is a transformation of the states by a phase factor:

$$|n\rangle \to \exp\{i\mu(\mathbf{R})\} |n\rangle \text{ and thus } B_n(\mathbf{R}) \to B_n(\mathbf{R}) + i\boldsymbol{\nabla}\mu(\mathbf{R})$$

Since the curl of a gradient is zero, one sees that the Berry phase itself is invariant under such a transformation, and is therefore $U(1)$ gauge invariant.

Acknowledgements and References

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[2] Lindsay, D. (2013) available here.
[3] Asboth, J., Oroszlany, L., Palyi, A (2015) A Short Course on Topological Insulators. Link
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The SSH Model

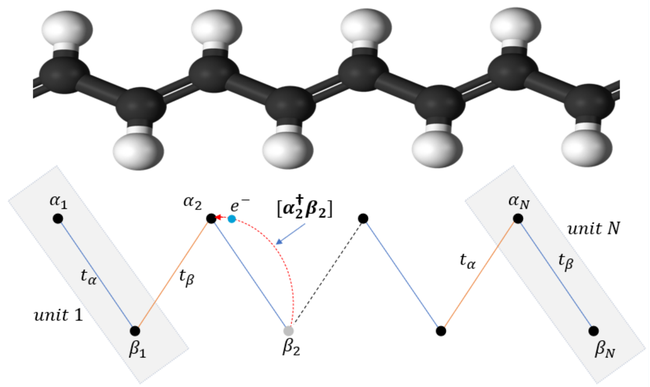


Fig. 1: Above: A stylised model of a polyacetylene molecule [2]. Below: A diagram of the edges of the SSH model.

The Su-Schrieffer–Heeger (SSH) model is a 1-dimensional model of a polyacetylene molecule, consisting of a 1D lattice of 2N sites (atoms) each of which can be occupied by a single spinless fermion. Due to the alternating identical bonds in the polyacetylene molecule, the lattice can be decomposed into N unit cells of two sites each α_i and β_i. The parameters t_α and t_β are the hopping amplitudes, which are related to the probabilities of an electron hopping between adjacent sites on the lattice, and μ_α and μ_β are the chemical potentials of the α and β sites. The second quantisation Hamiltonian for this system is:

$$\hat{H} = \sum_{j=1}^{N} t_\alpha(\beta_j^\dagger \alpha_j + \alpha_j^\dagger \beta_j) + t_\beta(\alpha_{j+1}^\dagger \beta_j + \beta_j^\dagger \alpha_{j+1}) + \mu_\alpha \alpha_j^\dagger \alpha_j + \mu_\beta \beta_j^\dagger \beta_j$$

Where α_i, β_i and $\alpha_i^\dagger, \beta_i^\dagger$ are fermionic annihilation and creation operators, and therefore must obey the canonical anti-commutation relations required of such operators by the Pauli exclusion principle. For example (as pictured in Fig. 1), the operator $\alpha_2^\dagger \beta_2$ annihilates a fermion at the 2nd cell's β site and then creates one at its α site when acting on a state in which such a "hop" is quantum mechanically permitted. This models the intracell hopping of an electron along a bond between sites in the second cell.

We can impose periodic (or twisted periodic) boundary conditions by linking the ends of the lattice together (with the addition of a phase factor in the twisted case) forming a ring, so that $\alpha_{N+1} = \alpha_1$. This Hamiltonian can be Fourier transformed and thus expressed in terms of the momentum space operators A_k and B_k for the α and β sublattices. This can be diagonalised, yielding the spectrum for the Hamiltonian:

$$\epsilon_\pm(k) = \frac{1}{2}(\mu_\alpha + \mu_\beta \pm \sqrt{(\mu_\alpha - \mu_\beta)^2 + 4(t_\alpha^2 + t_\beta^2 + t_\alpha t_\beta \cos\frac{2k\pi}{N}})$$

We can now plot the band structure of the SSH model for various values of the hopping amplitudes, to investigate its electronic properties.

Electronic Properties

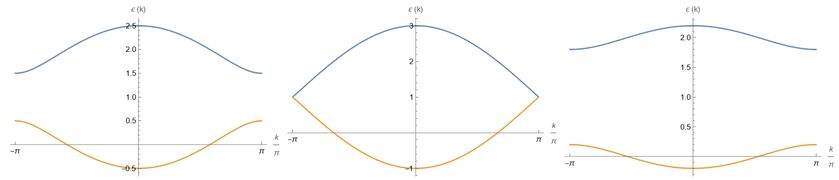
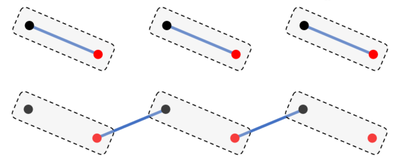


Fig. 2: Plots of the band structure of the SSH model's Hamiltonian for various values of the hopping amplitudes.
Left: $t_\alpha = 1,\ t_\beta = 0.5$ Middle: $t_\alpha = 1,\ t_\beta = 1$ Right: $t_\alpha = 0.2,\ t_\beta = 1$

There are 3 possible configurations of the hopping amplitudes that result in the SSH model exhibiting different physical properties at half-filling. The system is in the gapless **phase boundary** when $t_\alpha = t_\beta$. In this phase it behaves like a metal, since there is no band gap and hence eigenstates of arbitrarily small energy increments above the half-filled groundstate are free to be occupied and to carry fermions along the lattice. All other configurations behave as insulators, due to the non-zero band gap.
The system is in the **trivial phase** when $t_\alpha > t_\beta$, and the intracell hopping of fermions dominates the intercell hopping (as pictured in the top figure below). There are no zero-energy eigenstates at the edges in the trivial case.
The system is in the **topological phase** when $t_\alpha < t_\beta$, and the intercell hopping dominates. This results in there being an "isolated" site at both edges, for which a single zero energy eigenstate exists (see the bottom figure below).



These are distinct physical phases of the system, and you can not adiabatically deform a Hamiltonian corresponding to one phase into one corresponding to the other, since doing so would close the band-gap at the phase boundary where $t_\alpha = t_\beta$.

The Topological Invariant

Now consider the bulk Hamiltonian not as a whole, but parameterised by momenta and expressed in the basis of Pauli spin matrices (where $\mu := \mu_\alpha = \mu_\beta$):

$$\hat{H}(k) = d_0\sigma_0 + \mathbf{d}(k) \bullet \sigma \text{ where } \mathbf{d}(k) = \begin{bmatrix} t_\alpha + t_\beta \cos(k) \\ t_\beta \sin(k) \\ 0 \end{bmatrix} \text{ and } d_0 = \mu$$

The vector $\mathbf{d}(k)$ traces out a circle of radius t_β in the x-y plane of R^3 as momentum runs through the first Brillouin zone: $k = 0 \to 2\pi$ (See Fig. 3).
A topological invariant for the SSH model is the winding number ν of this closed curve around the origin. This can be calculated graphically by counting the intersections of the curve with an arbitrary "line of sight" from the origin to infinity, or it can be computed using the formula:

$$\nu = \frac{1}{2\pi}\int(\hat{\mathbf{d}}(k) \times \frac{d}{dk}\hat{\mathbf{d}}(k))_z dk \quad \text{where} \quad \hat{\mathbf{d}}(k) = \frac{\mathbf{d}(k)}{|\mathbf{d}(k)|}$$

In the trivial phase $\nu = 0$, on the phase boundary ν is undefined and in the topological phase $\nu = 1$. Explicit computation of the Berry phase associated with adiabatically transporting this parameterised Hamiltonian through the first Brillouin zone yields $\gamma = \nu\pi$. [4]