Topological Properties and Quantum Entanglement Features of Graphene with Vacancies

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I. Abstract

We consider topological and entanglement aspects of condensed matter systems, focusing on graphene with vacancies. Pristine (undoped) graphene does not have specific topological properties. We have shown that the removal of an atom (creating a vacancy) displays topological features. These features (e.g. a finite winding number) are directly measureable on the dislocation pattern of STM pictures. A direct method to calculate the winding number is presented. Other topological models are discussed, e.g. Kekule model. Entanglement properties of two distinguishable spins are studied by means of concurrence, and its' interplay with topological features e.g. Berry phase. These features are contrasted with intra-particle entanglement. Graphene with randomly distributed vacancies displays a new type of transport characterized by $\beta(g) = 0$, in contrast to other types of disorder e.g. adatoms. Here, the first order ($\propto 1/g$) correction is considered.

II. The Tenfold classification

Class	s	Θ	$\mathcal{C}$	S	$d=0$	1	2	3
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	1	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	0	+1	0	0	$\mathbb{Z}$	0	0	0
BDI	1	+1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
D	2	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
DIII	3	-1	+1	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	4	-1	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	5	-1	-1	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
C	6	0	-1	0	0	0	$2\mathbb{Z}$	0
CI	7	+1	-1	1	0	0	0	$2\mathbb{Z}$

The topological structure of the Hilbert space of quadratic Hamiltonians of fermions (describing weakly interacting systems) is based on two anti-unitary symmetries $(\Theta, \mathcal{C})$ and the (unitary) chiral symmetry (Π):

Time reversal	Particle hole	Chirality
$\Theta = 0, \pm$	$\mathcal{C} = 0, \pm$	$\Pi = 0, 1$

"±" conserves the symmetry
"0" breaks the symmetry

Dirac Hamiltonian representative

A Dirac Hamiltonian representative for each class can be defined using Dirac matrices and $\vec{k}, \vec{r}$ dependent coefficients:

$$H = \vec{A}(\vec{k},\vec{r}) \cdot \vec{\Gamma} + \vec{B}(\vec{k},\vec{r}) \cdot \vec{\gamma}$$

$$\vec{\Gamma} = (\Gamma_0, \ldots, \Gamma_p), \quad \vec{\gamma} = (\gamma_1, \ldots, \gamma_q), \quad s = p - q \mod 8$$

In this Clifford representation Γ_n and γ_m anti-commute:

$$\{\gamma_n, \gamma_m\} = \{\Gamma_n, \Gamma_m\} = \delta_{mn}, \quad \{\Gamma_n, \gamma_m\} = 0$$

Where $\vec{A}(\vec{k},\vec{r}) = \vec{A}(-\vec{k},\vec{r})$, $\vec{B}(\vec{k},\vec{r}) = -\vec{B}(-\vec{k},\vec{r})$.

Symmetry Relations

The symmetry relations are:

$$\Theta H\left(\vec{k},\vec{r}\right)\Theta^{-1} = H\left(-\vec{k},\vec{r}\right)$$

$$\mathcal{C} H\left(\vec{k},\vec{r}\right)\mathcal{C}^{-1} = -H\left(-\vec{k},\vec{r}\right)$$

$$\Pi H\left(\vec{k},\vec{r}\right)\Pi^{-1} = -H\left(\vec{k},\vec{r}\right)$$

For Dirac Hamiltonians this translates into:

$$\Theta\vec{\Gamma}\Theta^{-1} = \vec{\Gamma}, \quad \Theta\vec{\gamma}\Theta^{-1} = -\vec{\gamma}$$

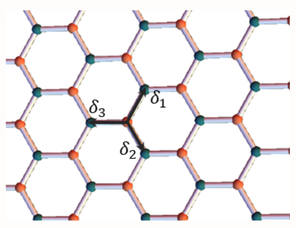
$$\mathcal{C}\vec{\Gamma}\mathcal{C}^{-1} = -\vec{\Gamma}, \quad \mathcal{C}\vec{\gamma}\mathcal{C}^{-1} = \vec{\gamma}$$

Spatial Dimension and Defects

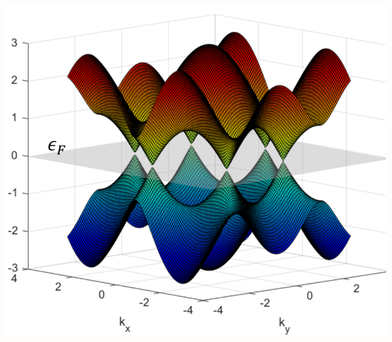
Kitaev and Schnyder et al extended the initial Altland-Zirnbauer classification to higher space dimension d. This is the dimension of the Brilouin zone T^d. The presence of defects is accounted for by introducing $\delta = d - D$, where D is the dimension of a sphere S^D surrounding the defect. The entries of the tenfold classification depend on the difference $s - \delta$.

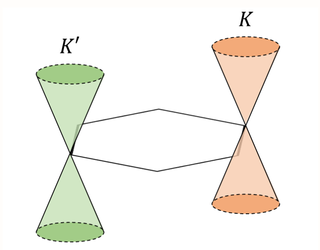
III. Graphene

Graphene is a 2-dimensional honeycomb lattice of Carbon atoms. It is bipartite with two atoms in a unit cell, i.e. composed of two triangular sublattices A and B. The tight binding Hamiltonian of graphene within the nearest neighbors approximation:



$$\mathcal{H}_0 = -t \sum_{\substack{i=0,1,2 \\ R\in A}} a_R^\dagger b_{R+\delta_i} + H.c.$$





At low energy H_0 admits a Dirac representation using 2×2 Pauli matrices around each valley K and K'.

$$H_0\left(\vec{k} = \vec{K} + \vec{q}\right) = v_F \vec{q} \cdot \vec{\sigma}, \quad v_F = \frac{3}{2}ta$$

Overall description using 2 pseudospins associated respectively to sublattice (A, B) and valleys (K, K'):

$$H_0 = v_F \begin{pmatrix} 0 & 0 & q_x - iq_y & 0 \\ 0 & 0 & 0 & -q_x - iq_y \\ q_x + iq_y & 0 & 0 & 0 \\ 0 & -q_x + iq_y & 0 & 0 \end{pmatrix}.$$

Equivalently $H_0 = v_F\left(q_x\sigma_x \otimes \sigma_z + q_y\sigma_y \otimes I\right)$, in the basis $\psi = \begin{pmatrix} \psi_A^K & \psi_A^{K'} & \psi_B^K & \psi_B^{K'} \end{pmatrix}^T$

Symmetry Class of Graphene

Graphene Hamiltonian is quadratic. In the Dirac representation we identify $q = 0$ and $p = 1$, which gives $s = 1$. Alternatively, we show that graphene is BDI using its anti-unitary symmetries and chirality:

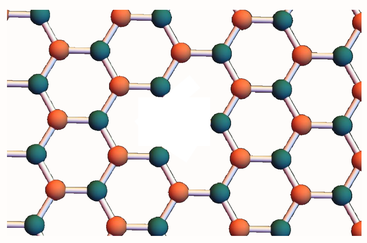
$$\Theta = \mathcal{K}, \quad \mathcal{C} = \sigma_x\mathcal{K}, \quad \Pi = \sigma_x$$

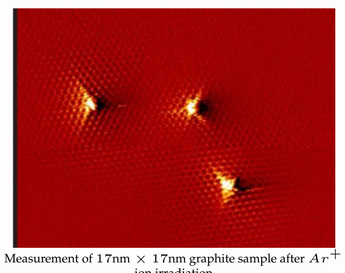
where K is the complex conjugate operator on the presented basis.

IV. Wavefront Dislocations

Vacancies in Graphene

A vacancy is defined as the removal of a single neutral atom from the lattice.





Measurement of 17nm × 17nm graphite sample after Ar^+ ion irradiation

According to the tenfold classification, graphene with a vacancy remains BDI. Since a vacancy is a point defect in 2d, $D = 1$ and $\delta = 2 - 1 = 1$. This system may have non-zero topological numbers.

Local density

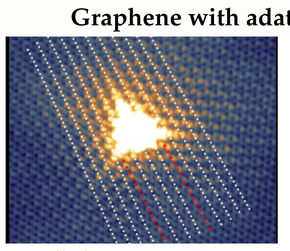
STM (scanning tunneling microscope) measures local density:

$$\rho(r) = \int dE\ \rho(r,E) = \int dE \sum_n |\psi_n(r)|^2 \delta(E - E_n)$$

Wavefront Dislocation

In graphene with a defect (vacancy or adatom), oscillations can be seen in $\rho(r)$. For graphene, the oscillation pattern contains dislocations: the number of maxima lines going in and out of the defect is different. The dislocation number is different for each defect type.

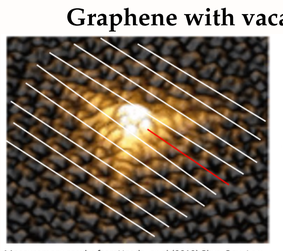
Graphene with adatom



Dutreix, et al (2019) Nature.

Two dislocations

Graphene with vacancy



Measurement results fromUgeda, et al (2010) Phys. Rev. Lett.

One dislocation

V. Model for Graphene Vacancy

Vacancy Potential in Tight Binding Model

We model the vacancy by destroying the three bonds with the neighbouring atoms. For a vacancy in located at R_0, in sublattice A:

$$V_A(r) = +t\left[a_{R_0}^\dagger b_{R_0} + a_{R_0}^\dagger b_{R_0+\delta_1} + a_{R_0}^\dagger b_{R_0+\delta_2}\right] + h.c.$$

Vacancy potential is localized (not periodic), i.e. it will not be diagonal in Fourier space $a_R = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} a_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}$. In the low-energy limit, $V_A(r)$ couples both $\vec{k}$ in the same valley (intravalley scattering) and $\vec{k}$ in different valleys (intervalley scattering).

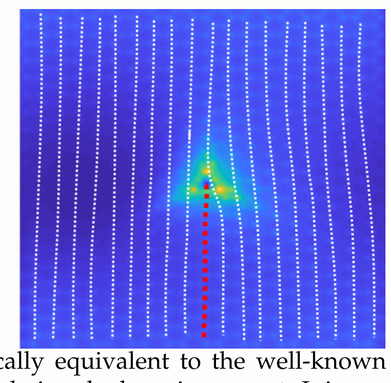
Vacancy Potential in the Continuum

In the basis $\psi = \begin{pmatrix} \psi_A^K & \psi_A^{K'} & \psi_B^K & \psi_B^{K'} \end{pmatrix}^T$, the vacancy potential contains intervalley and intravalley terms, dependent on $\vec{r}$, the distance from the vacancy. A generic form of such a potential is:

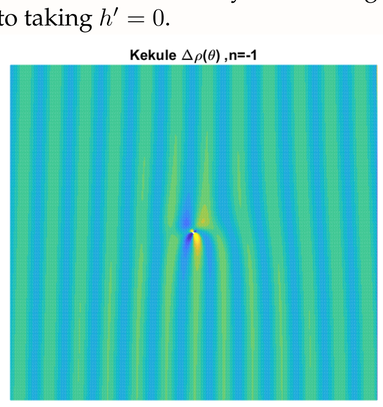
$$V_{\text{Vac}} = v_F \begin{pmatrix} 0 & 0 & h' & -ihe^{i\theta} \\ 0 & 0 & ihe^{-i\theta} & h' \\ h' & -ihe^{i\theta} & 0 & 0 \\ ihe^{-i\theta} & h' & 0 & 0 \end{pmatrix}$$

where h, h' are real functions of the distance r from the vacancy and θ is the angle of $\vec{r}$. A model for adatom also contains diagonal terms, which break BDI.
This potential creates new states at zero energy called zero modes. These states are localized near the vacancy, and as a result change the local density $\rho(\vec{r})$. We define: $\rho(\vec{r}) = \rho_0(\vec{r}) + f(r)\Delta\rho(\theta)$, where ρ_0 is the local density of graphene.

Numerical solution of the full model reproduces the dislocation pattern. $\Delta\rho(\theta)$ displays a line pattern (called wavefronts) which breaks near the vacancy. The difference between the number of line "entering" and "leaving" is 1, which means a single dislocation.



Our vacancy model is topologically equivalent to the well-known the Kekule model, obtained by modulating the hopping term t. It is equivalent to taking $h' = 0$.

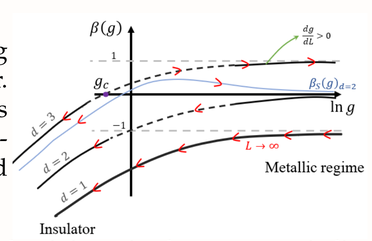


Numerical solution of the Kekule model gives exactly the same dislocation pattern. The analogy also shows that the non-trivial topology in the vacancy model comes from the intervalley scattering.

VI. Conductance β Function

Graphene is a 2d semi-metal, and as such the conductivity of pure graphene is: $\sigma_{xx} = 4e^2/h$.

Graphene with BDI-breaking disorder becomes an insulator. For a disorder that preserves the BDI symmetries, the conductivity remains constant and unchanged, i.e. $\beta(g) = 0$.



A perturbative expansion for the conductivity g in the mesoscopic limit may provide new physical insights for $\beta(g) = 0$.

VII. Entanglement and Geometric Phase

The Dirac Hamiltonian model for graphene with a vacancy is analogous to a two-qubit system. Is it possible to entangle the two pseudospins associated with the valley and sub-lattice? Is it related to the BDI topology?

Concurrence

Entanglement between two distinguishable qubits is measurable by the concurrence, $C \in [0,1]$, defined for pure states by:

$$C(|\psi\rangle) = |\langle\psi|\Theta|\psi\rangle| = |\langle\psi|(\sigma_y \otimes \sigma_y)\mathcal{K}|\psi\rangle|$$

where Θ is the antiunitary time reversal operator for 2 spin-1/2 particles.

Geometric phase

When a pure state density matrix undergoes cyclic evolution, the state may gather a gauge invariant phase, called the geometric or Berry phase. It is given by:

$$\gamma = i\int_0^T \left\langle\psi\left|\frac{\mathrm{d}}{\mathrm{dt}}\right|\psi\right\rangle dt + \arg\langle\psi(0)|\psi(T)\rangle$$

Geometric Phase for 2-Qubit Model

A 2-qubit pure state can be described using 6 angles:

$$|\psi\rangle = \cos\frac{\alpha}{2}|+\hat{n}_1\rangle \otimes |+\hat{n}_2\rangle + \sin\frac{\alpha}{2}e^{i\beta}|-\hat{n}_1\rangle \otimes |-\hat{n}_2\rangle$$

where $\hat{n}_{1,2}$ describe the Bloch vectors of qubit 1,2, and $\sin\alpha = C(|\psi\rangle)$, $\alpha \in [0,\pi)$. The geometric phase of a general path in the Hilbert space is:

$$\gamma = -\frac{1}{2}\oint \sqrt{1-C^2}\left(d\beta + \cos\theta_1 d\varphi_1 + \cos\theta_2 d\varphi_2\right)$$

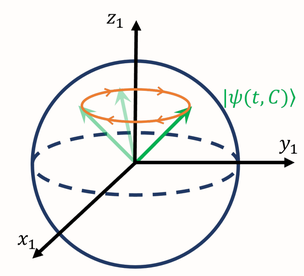
This establishes a relation between the concurrence and a topological property. We now show two examples.

Qubit 1 in a Magnetic Field

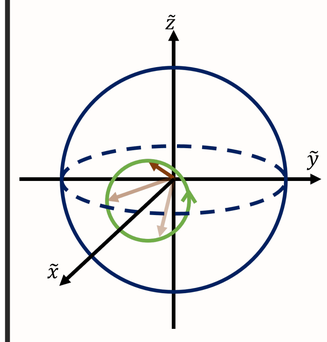
$$H = \vec{B}\cdot\vec{\sigma}\otimes I, \quad \vec{B} = B\hat{B}$$

The evolution of any $|\psi(t)\rangle$ is periodic. For $T = 2\pi/B$, the geometric phase is:

$$\gamma = 2\pi\sqrt{1-C^2}\hat{B}\cdot\hat{n}_1$$



Interactions Between Two Qubits



$$H = \lambda\vec{\sigma}_1\cdot\vec{\sigma}_2$$

We choose $|\psi(0)\rangle = \cos\frac{\alpha_0}{2}|+\hat{z}\rangle\otimes|-\hat{z}\rangle + \sin\frac{\alpha_0}{2}e^{i\beta_0}|-\hat{z}\rangle\otimes|+\hat{z}\rangle$ and for a single period:

$$\gamma = \pi C(t=0)\cos\beta_0.$$

This is the half the solid angle of a circular path in the sphere defined by α and β.

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