VACANCIES IN GRAPHENE: TOPOLOGICAL EDGE STATES, STM AND WAVEFUNCTION DISLOCATIONS

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I. ABSTRACT

We propose a way to systematically measure topological winding numbers in 2D materials with chiral symmetry. We consider the example of graphene with a vacancy, and model the vacancy potential in the continuum. The corresponding winding number indicates that graphene with vacancies is a topological material according to the tenfold classification generalised to defects by Teo and Kane. As a result of bulk-edge correspondence, topological edge states appear in the spectrum (zero modes) and are localised around the vacancy. These edge states and their topological winding number are measurable by the read-out of wavefront dislocations in STM data. Comparison with STM pictures of other (non topological) defects, e.g. adatoms, is discussed.

II. WAVEFRONT DISLOCATIONS

LOCAL DENSITY

STM (scanning tunneling microscope) measures local density:

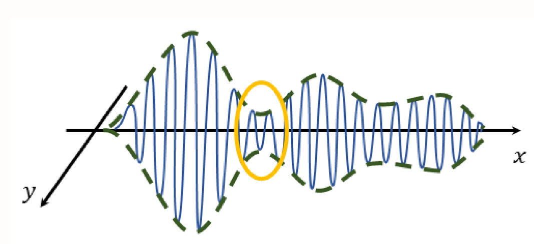
$$\rho(r) = \int dE\ \rho(r,E) = \int dE \sum_n |\psi_n(r)|^2 \delta(E-E_n)$$

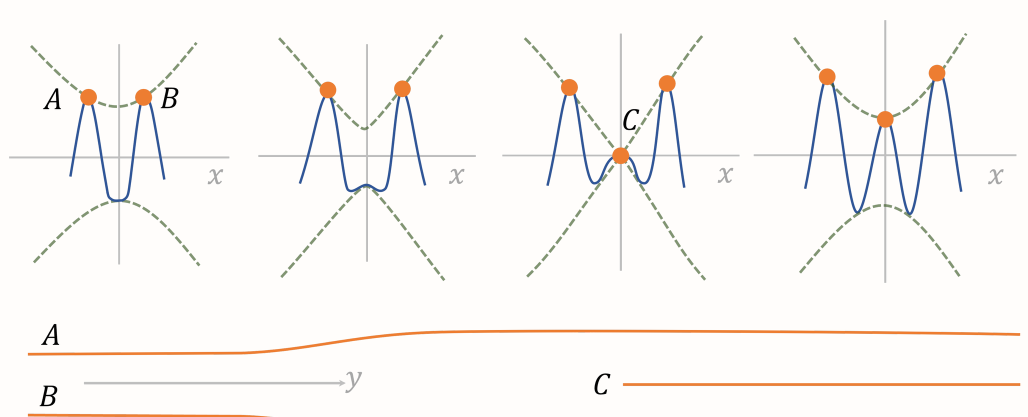
WAVEFRONT DISLOCATION

For a general function of the local density

$$\rho(\boldsymbol{r}) = \mathrm{Re} f(\boldsymbol{r})\, e^{i\chi(x,y)}$$

with amplitude $f(\boldsymbol{r})$, and oscillating term $\chi(x,y)$.





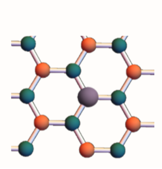
Dislocations can form where the amplitude of $\rho(r)$ vanishes, a point where a new wavefront may appear.

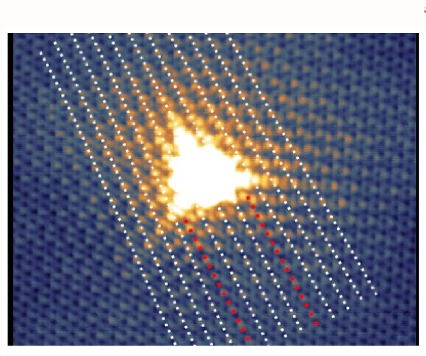
N_D - NUMBER OF DISLOCATIONS

In graphene with a defect (vacancy or adatom), oscillations can be seen in $\rho(r)$.

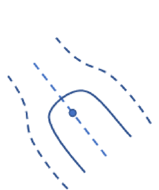
GRAPHENE WITH ADATOM

Adatom, an atom added to a lattice site





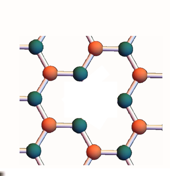
Dutreix, et al (2019) Nature.

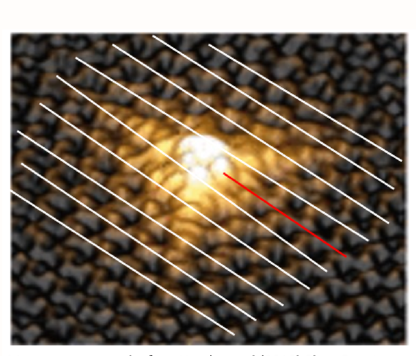


Two dislocations

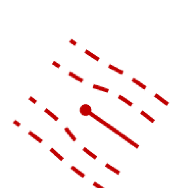
GRAPHENE WITH VACANCY

Vacancy, a neutral site removed from the lattice





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



One dislocation

III. THE TENFOLD CLASSIFICATION

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

The winding or Chern topological invariant is calculated using the Hamiltonian symbol, its classical counterpart, replacing operators with variables using a Weyl transform. For a Dirac symbol $\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) = \hat{\boldsymbol{h}}(\boldsymbol{k},\boldsymbol{r}) \cdot \vec{\gamma}$ the winding or Chern number is

$$\nu_{d+D} = \frac{1}{S_{d+D}} \int_{S^{d+D}} d^d k\, d^D r\, J(\boldsymbol{h},d,D)\,, \qquad J(\boldsymbol{h},d,D) = \begin{vmatrix} h_1 & \cdots & h_{d+D+1} \\ \partial_1 h_1 & \cdots & \partial_1 h_{d+D+1} \\ \vdots & \ddots & \vdots \\ \partial_{d+D} h_1 & \cdots & \partial_{d+D} h_{d+D+1} \end{vmatrix}$$

The topological structure 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
$\Theta = 0, \pm$	$\mathcal{C} = 0, \pm$	$\Pi = 0, 1$

"$\pm$" conserves the symmetry
"0" breaks the symmetry

This table has been generalised for the presence of defects, for a D dimensional sphere surrounding the defect, the spatial dimension d is replaced with

$$d \to \delta = d - D$$

The analytical index, Index$H$, for chiral Hamiltonian

$$H = \begin{pmatrix} 0 & Q \\ Q^\dagger & 0 \end{pmatrix}$$

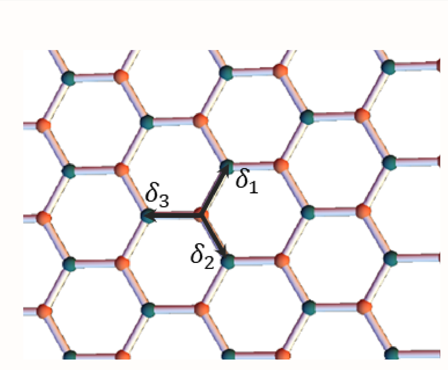
is equal to its symbol winding number

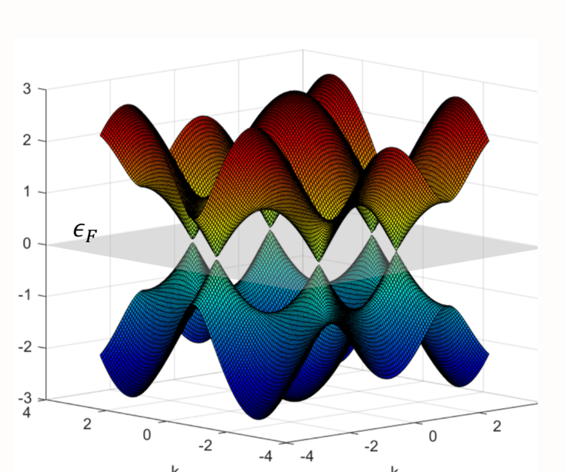
$$\nu_{d+D} = \ \text{Index } H = \dim\ker Q - \dim\ker Q^\dagger$$

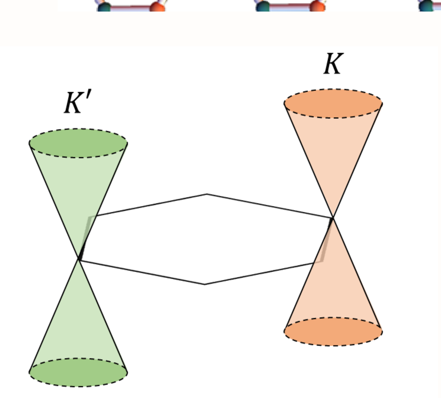
IV. GRAPHENE

Graphene is a single layer honeycomb lattice composed of two sublattices A and B. In the tight binding description, graphene Hamiltonian is bipartite $\{\sigma_3, H_0\} = 0$ under the nearest neighbors approximation

$$H_0 = -t \sum_{\substack{i=0,1,2 \\ R \in A}} a_R^\dagger b_{R+\delta_i} + H.c.$$







Close to the Fermi energy, set to be zero, graphene energy spectrum has a linear dispersion relation around two distinguished Dirac points K and K'. Graphene Hamiltonian can be described by effective massless and non interacting Dirac fermions,

$$H_0(\boldsymbol{k} = \boldsymbol{K} + \boldsymbol{q}) = v_F \boldsymbol{\sigma} \cdot \boldsymbol{q}$$

Therefore, the effective low energy Hamiltonian for graphene in the **continuum** limit describing the two valleys K and K' takes the form

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

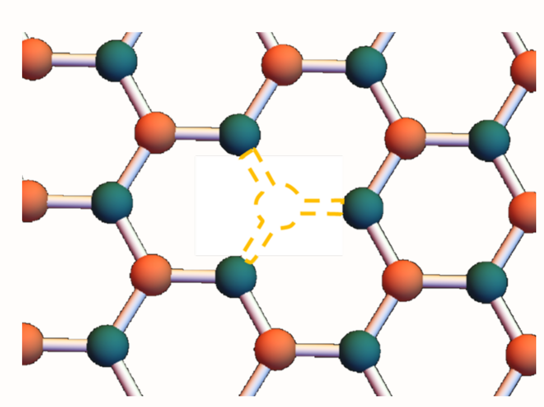
in the basis $\psi = \begin{pmatrix} \psi_A^K & \psi_A^{K'} & \psi_B^K & \psi_B^{K'} \end{pmatrix}^T$

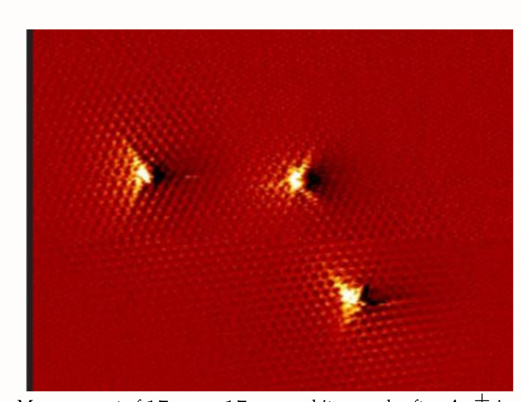
V. VACANCIES IN GRAPHENE

A **vacancy** is created by the removal of a single neutral atom in the lattice. It preserves the time reversal and particle-hole symmetries of graphene

$$\Theta = 1, \mathcal{C} = 1, \Pi = 1$$

The circle $D = 1$ surrounding the vacancy transforms the codimension into $\delta = 2 - 1 = 1$





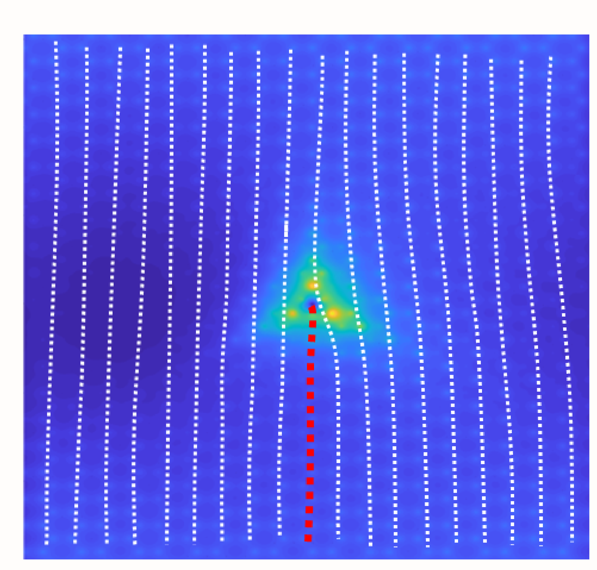
Measurement of 17nm $\times$ 17nm graphite sample after Ar^+ ion irradiation

VACANCY - TIGHT BINDING MODEL

We consider the vacancy as a destruction of the bonds connecting it site, R_0, to its neighbors, such that for a type A vacancy

$$V_{A,R_0} = t\left[a_{R_0}^\dagger b_{R_0} + a_{R_0}^\dagger b_{R_0+\delta_1} + a_{R_0}^\dagger b_{R_0+\delta_2}\right] + h.c.$$

Numeric results - a single wavefront dislocation in red of $\Delta\rho(\boldsymbol{r})$.

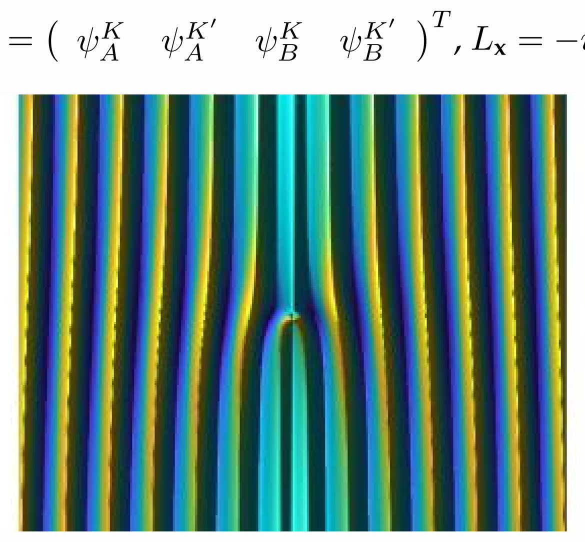


VACANCY - LOW ENERGY LIMIT

Vacancy potential in the low energy limit, $R_0 = 0$

$$V_A(\boldsymbol{r}) = a^2 v_F \begin{pmatrix} 0 & 0 & 0 & -\delta(\boldsymbol{r}) L_{\mathbf{x}}^\dagger \\ 0 & 0 & \delta(\boldsymbol{r}) L_{\mathbf{x}} & 0 \\ 0 & L_{\mathbf{x}}^\dagger \delta(\boldsymbol{r}) & 0 & 0 \\ -L_{\mathbf{x}} \delta(\boldsymbol{r}) & 0 & 0 & 0 \end{pmatrix}$$

$\psi = \begin{pmatrix} \psi_A^K & \psi_A^{K'} & \psi_B^K & \psi_B^{K'} \end{pmatrix}^T$, $L_{\mathbf{x}} = -i\partial_x - \partial_y$



The local density to first order

$$\Delta\rho^{(1)}(\boldsymbol{r}) = \frac{C}{r^2} \cos\theta \cos(\Delta\boldsymbol{K} \cdot \boldsymbol{r} + \theta)$$

C is a constant independent of the location and $\Delta K \equiv K - K'$

VI. KEKULE DISTORTION

The Kekule distortion model describes graphene with fluctuating hopping terms $t_{\boldsymbol{r}} = t + \delta t(\boldsymbol{r})$. For specific spatial fluctuations, connecting the two valleys with a 'twist' the Kekule Hamiltonain in Dirac notations is $H_{\text{Kekule}} = H_0 + V_{\text{Kek}}$

$$H_0 = iv_F \partial_x \sigma_x \otimes \tau_z - iv_F \partial_y \sigma_y \otimes I_\tau$$
$$V_{\text{Kek}} = -\Delta(r) \cos n\theta \sigma_x \otimes \tau_x - \Delta(r) \sin n\theta \sigma_x \otimes \tau_y.$$

where $\Delta(r)$ is a radial function, and σ_i (τ_i) represents the sublattice (valley).

The topological winding number equals n

VII. MEASURING TOPOLOGICAL NUMBER

GRAPHENE WITH VACANCY

The Hamiltonian H_V has a single zero mode.

The Hamiltonian's symbol $\mathcal{H}_V(\boldsymbol{r},\boldsymbol{k})$ produce $\nu_3 = 1$.

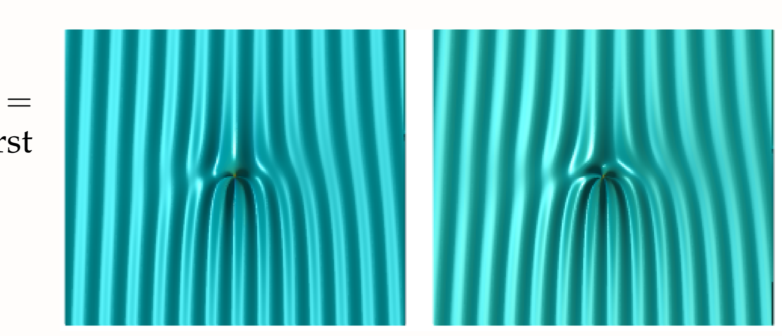
This **winding number** equals the number of **dislocations measured by the STM**.

$$\text{Index}H = \nu_3 = 1 \quad =$$

DISLOCATIONS FOR WINDING NUMBER $\nu = n$

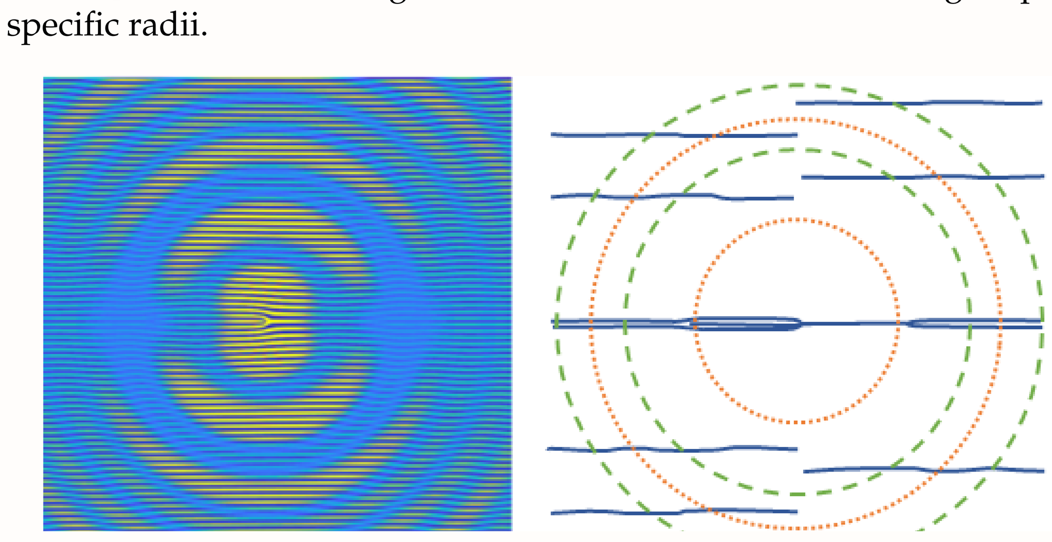
For Kekule distortion $\nu_3 = n$. The local density to first order provide

$$N_D = n = \nu_3$$



DISLOCATIONS FROM NON-TOPOLOGICAL DEFECTS

An adatom changes the chemical potential locally and breaks the particle-hole symmetry. Since $\mathcal{C} = 0$ the symmetry class is AI, with $\delta = 1$. This implies **no topology** .
Breaking the particle-hole symmetry enables Friedel oscillations, radial oscillations $\propto 2k_F$ which create rings around the adatom with vanishing amplitudes for specific radii.



The vanishing amplitude leads to different locations wherein the **number of dislocations vary with** r.

This is not the case for a vacancy, which preserved the particle-hole symmetry and does not exhibit Friedel oscillations. Such that for **any loop radius** there is a single dislocation.

VIII. CONCLUSION

We were able to show that the topological winding number equals to the number of the local density dislocations, thus can be measured through it. This was shown for a vacancy using the tight binding model to all orders, and calculated analytically to first order. This is also the case for the Kekule model, where the topological winding number is n. Non topological defect, adatom, was discussed wherein the number of dislocations change with the loop radius. Our results also agree with the index theorem relating the topological number to the number of zero energy modes. The number of zero modes is hard to measure since they overlap in STS measurments.

REFERENCES

[1] John Frederick Nye, Michael Victor Berry, and Frederick Charles Frank. Dislocations in wave trains. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, 336(1605):165–190, 1974.

[2] M. M. Ugeda, I. Brihuega, F. Guinea, and J. M. Gómez-Rodríguez. Missing atom as a source of carbon magnetism. *Phys. Rev. Lett.*, 104:096804, Mar 2010.

[3] Omrie Ovdat, Yaroslav Don, and Eric Akkermans. Vacancies in graphene : Dirac physics and fractional vacuum charges, 2018.

[4] R. Jackiw and C. Rebbi. Solitons with fermion number ½. *Phys. Rev. D*, 13:3398–3409, Jun 1976.

[5] W. P. Su, J. R. Schrieffer, and A. J. Heeger. Solitons in polyacetylene. *Phys. Rev. Lett.*, 42:1698–1701, Jun 1979.

[6] C. Dutreix, GonzÃ¡lez-Herrero H., I. Brihuega, M. I. Katsnelson, C. Chapelier, and V. T. Renard. Measuring the berry phase of graphene from wavefront dislocations in friedel oscillations. *Nature*, 574:219–222, Oct 2019.

[7] Jeffrey C. Y. Teo and C. L. Kane. Topological defects and gapless modes in insulators and superconductors. *Phys. Rev. B*, 82:115120, Sep 2010.