PHY552A Quantum Physics of Electrons in Solids, Day6







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We start then from the graphene Sessions (days) 4 and 5





Schrödinger equation in a periodic potential: $V(\vec{r} + \vec{R}) = V(\vec{r})$ $\begin{bmatrix} \hbar^2 & 7 \end{bmatrix}$ $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = \varepsilon\,\psi(\vec{r})$

Wave-functions take the following form:

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}.\vec{r}} u_{n\vec{k}}(\vec{r})$$

n: numbers the different eigenstates for same k. k ϵ 1. Brillouin zone ("1.BZ")

With u(r) a lattice-periodic function:

$$u(\vec{r} + \vec{R}) = u(\vec{r})$$



1st BZ = Wigner-Seitz cell of the reciprocal lattice = {k-points that are closer to K=0 than to any other point of the reciprocal lattice}

Special about honeycomb lattice



 $\mathbf{b}_1 = rac{a}{2}(3, -\sqrt{3})$ $\mathbf{b}_2 = -rac{a}{2}(3, \sqrt{3})$ $\mathbf{b}_3 = (0, \sqrt{3}a)$ 1 plane of graphene (3D graphite; present research 2 planes and Moire magic angles...)



2 Triangular lattices from Translation Operators in two dimensions defined through the Bravais lattice vectors **a**_i and equivalently **b**_i: `2 sublattices'

$$\overrightarrow{5_1} = \frac{\alpha}{2} \left(1_1 \sqrt{3} \right)_1 \quad \overrightarrow{5_2} = \frac{\alpha}{2} \left(1_1 - \sqrt{3} \right)_1 \quad \overrightarrow{5_3} = \left(-\alpha_1 \right)_1$$

Within these definitions:

<u>Reminder</u>

The restricted Bloch wave is

$$\psi_{j\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_m} e^{i\mathbf{k}\cdot\mathbf{R}_m} \Phi_j(\mathbf{r} - \mathbf{R}_m)$$

From Bloch theorem, $\psi(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$ with $u(\mathbf{r}) = \sum_j c_j \Phi_j(\mathbf{r})$. The functions Φ are centered at a site \mathbf{R}_m — meaning that $\Phi_j(\mathbf{r} - \mathbf{R}_m)$ refers to an electronic wave-function around the site \mathbf{R}_m — and periodic if we apply the translation operator of vector \mathbf{b}_j . From symmetries, the honeycomb lattice can be viewed as formed with two triangular lattices made of A and B sites respectively. In this description, N represents the number of A or B sites and a particle has equal probabilities to occupy a site such that $c_j = 1/\sqrt{N}$.

From the definitions, the Hamiltonian takes the form¹

$$H = -t \sum_{\mathbf{R}_m} \sum_{\delta_j} |\Phi(\mathbf{R}_m)\rangle \langle \Phi(\mathbf{R}_m + \delta_j)| + h.c.$$

After Fourier transform, the Hamiltonian takes the form $H = \sum_{\mathbf{k}} H(\mathbf{k})$ with

$$H_{\mathbf{k}} = -t \sum_{\delta_j} e^{-i\mathbf{k}\cdot\delta_j} |\psi_{A\mathbf{k}}\rangle \langle \psi_{B\mathbf{k}}| + h.c.$$

$$\psi_{j\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_m} e^{i\mathbf{k}\cdot\mathbf{R}_m} \Phi_j(\mathbf{r} - \mathbf{R}_m)$$

$$\int_{\mathbf{k}_1}^{\mathbf{k}_2} \int_{\mathbf{k}_2}^{\mathbf{k}_3} \int_{\mathbf{k}_4}^{\mathbf{k}_4} \int_{\mathbf{k}_4}^{\mathbf{k}_4} \int_{\mathbf{k}_4}^{\mathbf{k}_4} \int_{\mathbf{k}_4}^{\mathbf{k}_4} \int_{\mathbf{k}_5}^{\mathbf{k}_4} \int_{\mathbf{k}_5}^{\mathbf{k}_5} \int_{\mathbf{k}_5}^{$$

Close to the Dirac points \Box

$$E^2 = t^2 \left(\sum_{\delta_j} e^{i\mathbf{k}\cdot\delta_j} \right) \cdot \left(\sum_{\delta_j} e^{-i\mathbf{k}\cdot\delta_j} \right)$$

$$k_x = K_x + p_x = \frac{2\pi}{3a} + p_x$$
$$k_y = K_y + p_y = \frac{2\pi}{3\sqrt{3}a} + p_y$$

Wallace, 1947



$$E^2 \approx \frac{9}{4} (ta)^2 (p_x^2 + p_y^2)$$

implying







A. Bostwick et al.Nature Physics **3** 36 (2007)Photoemission

Similar Dirac points in high-Tc Superconductors

Linear energy dispersion



Useful Review:

Rev. Mod. Phys. 81, 109 (2009).

6 electrons in carbon: 2 in s1, 3 in sp2, 1 in p_z



<u>Question:</u> Where is E_F for graphene?

Answer:

E_F=0 Graphene is a semimetal

The <u>isospin</u> σ (helicity) acts on each branch (sublattice)

sp2 hybridization in graphene









Useful

For pencils For tennis Rackets For bicycles... For photo-synthesis





Within graphite, 2s and 2p orbitals undergo a sp2 hybridization

The geometry of the hybridized orbital is trigonal planar: 3 nearest neighbors



The last p-orbital forms the π -orbital

Diamond : sp3 hybridization

Yet be careful with "gas" emission For the planet

Eigenstates and Spin-1/2 quantum mechanics

$$H = \hbar v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$

$$H(\mathbf{p})|\psi(\mathbf{p})\rangle = \pm \hbar v_F |\mathbf{p}||\psi(\mathbf{p})\rangle$$

$$\boxed{\mathbf{f}x + i p_y} = |\mathbf{p}| e^{i\mathbf{f}}$$

$$\frac{\partial}{\partial \tilde{\varphi}} \psi_+ = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 \\ e^{i\tilde{\varphi}} \end{pmatrix}$$

$$\frac{\partial}{\partial \tilde{\varphi}} |\psi_+(\mathbf{K})| = \frac{1}{2},$$

$$\boxed{\gamma(\mathbf{K}) = \int_0^{2\pi} A_{\tilde{\varphi}} d\tilde{\varphi} = \pi = -\gamma(\mathbf{K}').}$$

$$\boxed{\psi_{\pm}(\mathbf{K}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{-i\tilde{\varphi}} \end{pmatrix}}$$

$$\boxed{\psi_{\pm}(\mathbf{K}') = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{-i\tilde{\varphi}} \end{pmatrix}}$$

$$\boxed{\psi_{\pm}(\mathbf{K}') = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{-i\tilde{\varphi}} \end{pmatrix}}$$

Berry phase (1984) encircling a Dirac point K

Lower and Upper bands described through an opposite phase

Klein Paradox for graphene:

Perfect transmission

Katnelson, Novoselov, Geim, Nature Physics 2006



A slowly varying barrier is more efficient: See Cheianov & Falko, PRB 2006 Dirac equation

$$-iv_F \boldsymbol{\sigma} \cdot \nabla \psi(\mathbf{r}) = E\psi(\mathbf{r})$$

た = 1

Nobel prize 2010

The transmission probability T is directionally-dependent. For high barriers ($V_0 >> E$)

$$T(\phi) \simeq \frac{\cos^2 \phi}{1 - \cos^2(Dq_x) \sin^2 \phi}$$

$$q_x = \sqrt{(V_0 - E)^2 / (v_F^2) - k_y^2}$$

If V's are different for different spin orientations (magnetic gates): spin-polarized currents

Topological Phases within the 2*2 Matrix approach

Personnel QUIZ: Find the associated years for prices?



1980 K-Von Klitzing, G. Dozola, M. Feyner 1981 R. Laughlin, D. Tsui, H. Stormer stion fractional case - Quantum Hall Effect, Mosfets Uniform magnetic field in z-direction

Analogy to Free particule in a unidimensional vector potential PHY430 Energy levels are related to the 1D harmonic oscillator



graphene? $E = \frac{1}{M_{c}(m + \frac{1}{2})}$

GaAs

Topology from the reciprocal space

How to induce a topological phase from the Bloch energy band formalism?

F. D. M Halolane



Quantum Hall effect on graphene



How to induce a topological phase from Bloch energy bands?

Magnetic field in k-space corresponds here to add a staggered potential on the lattice $H = M\sigma^{z}$

$$H(K) = \hbar v_F \begin{pmatrix} M & p_x - ip_y \\ p_x + ip_y & -M \end{pmatrix}$$

$$E = \pm \sqrt{(\hbar v_F |\mathbf{p}|)^2 + M^2}$$
Semenoff 1984
$$M = \frac{1}{2} M = \frac{1}{2}$$

If we look at energies such that $v_F p \gg M$, energies are unchanged and eigenstates are similar as before such that we can formulate the same arguments as before.

Route to Topological properties:

Corresponds to invert upper and lower bands at K': Additive Berry phases at K and K' Relation to Topological Chern number

Correspondence $(k_y, k_x) \rightarrow (\theta, \varphi)$

See PC Correspondence
$$(\mathsf{K}_{\gamma},\mathsf{K}_{\chi}) \rightarrow (\theta,\varphi)$$

$$\neg d(\cos\varphi\sin\theta,\sin\varphi\sin\theta,\cos\theta) = (v_{F}|\mathbf{p}|\cos\tilde{\varphi},v_{F}|\mathbf{p}|\sin(\zeta\tilde{\varphi}),-\zeta m).$$
Quantum Class I:
Quantum Class I:
 $\mathbf{u} \rightarrow \mathbf{k}$
 $\mathbf{u} \rightarrow \mathbf{u}$
 $\mathbf{u} \rightarrow \mathbf{u}$

Related to quest of Dirac monopoles and Skyrmions (P. Curie, 1894; P. Dirac 1931) Relation with physics of planets

Another way to apply (radial) magnetism:



$$B = B(n)$$

$$\mathbf{B} = \nabla \times \mathbf{A} = B\mathbf{e}_r$$

$$\frac{1}{r\sin\theta}\left(\frac{\partial}{\partial\theta}(A_{\varphi}\sin\theta) - \frac{\partial A_{\theta}}{\partial\varphi}\right) = B.$$

$$\frac{\partial}{\partial \theta} (A_{\varphi} \sin \theta) = Br \sin \theta.$$



To solve this equation, we can redefine

$$A'_{\varphi} = A_{\varphi} \sin \theta.$$
 $\partial A'_{\varphi} = Br \partial_{\theta} (\sin \theta).$

Requires at least 2 joint "domains"

T. Wu and C. N. Yang 1975 Book M. Nakahara: Geometry, Topology and Physics

$$A'_{\varphi}(\theta < \theta_c) = -Br(\cos \theta - 1) = 2Br \sin^2 \frac{\theta}{2}$$
$$A'_{\varphi}(\theta > \theta_c) = -Br(\cos \theta + 1) = -2Br \cos^2 \frac{\theta}{2}.$$

Review: K. Le Hur arXiv:2209.15381

Here, we precisely introduce $\tilde{A}_{\varphi}(\theta) = -Br\cos\theta$ such that on the two regions we have

$$A'_{\varphi}(\theta < \theta_c) = \tilde{A}_{\varphi}(\theta) - \tilde{A}_{\varphi}(0)$$
$$A'_{\varphi}(\theta > \theta_c) = \tilde{A}_{\varphi}(\theta) - \tilde{A}_{\varphi}(\pi),$$

and such that

$$=B\sin\theta \qquad \Phi = r^2 \left(\int_0^{2\pi} d\varphi\right) \left(\int_0^{\pi} F_{\theta\varphi} d\theta\right) = B(r)(4\pi r^2).$$

Definition similar to Plane or lattice: useful

 $F_{\theta\varphi} = \frac{1}{r} \partial_{\theta} A'_{\varphi}$

Simple Calculations!

$$\Phi = 2\pi r^2 \left(\int_0^{ heta_c^-} F_{ heta arphi} d heta + \int_{ heta_c^+}^{\pi} F_{ heta arphi} d heta
ight).$$

$$B = \frac{q_m}{2r^2} = B(r)$$

$$q_m = \frac{1}{2\pi}$$

q_m measures the topological charge

$$\Phi = 2\pi r \left(A'_{\varphi}(\theta_c^-) - A'_{\varphi}(\theta_c^+) \right) = 2\pi r (\tilde{A}_{\varphi}(\pi) - \tilde{A}_{\varphi}(0)).$$

Mathematics of Shapes and Table

Euler characteristic is defined as

 $\chi = V - E + F$

where V is the number of vertices (corners), E edges and F faces.

Take a cube. What is the Euler characteristic? Is this non-zero?

Sphere



- In the presence of a Dirac monopole or Topological charge, $\chi=2-2g=0$
- Agrees with Gauss-Bonnet theorem

on the surface and Poincare-Hopf Theorem; Similar to a cup or donut

- Equivalent to 2 circles from Stokes' theorem, can be measured at the poles

 $\chi = 2$

2





Quantum Correspondence & Topological Number:

Ã

B

Band Energy

-1

-2



Joel Hutchinson & Karyn Le Hur, Communications Physics 4, 144 (2021)

And this sphere can be real, adjustable

D. Schroer et al. PRL 2014 (Boulder, K. Lehnert)P. Roushan et al. Nature (John Martinis, Santa Barbara) 2014

Superconducting circuits And cavities





http://www.physics.rutgers.edu/pythtb/

Haldane Model 1988 PC

k_x

Realized in quantum materials, graphene, ultra-cold atoms, light systems

 $\mathcal{H}(\mathbf{k}) = -\mathbf{d} \cdot \boldsymbol{\sigma}$

$$\mathbf{d} = \left(t \sum_{\boldsymbol{\delta}_j} \cos(\mathbf{k} \cdot \boldsymbol{\delta}_i), t \sum_{\boldsymbol{\delta}_j} \sin(\mathbf{k} \cdot \boldsymbol{\delta}_i), \mathbf{+} t_2 \mathbf{\mathbf{\delta}}_{\mathbf{b}_j} \sin(\mathbf{k} \cdot \mathbf{b}_j)\right)$$

$$+d_z(\mathbf{K}) = 2t_2 \sum_{\mathbf{b}_j} \sin(\mathbf{K} \cdot \mathbf{b}_j) = 3\sqrt{3}t_2 = m$$
$$+d_z(\mathbf{K}') = 2t_2 \sum_{\mathbf{b}_j} \sin(\mathbf{K}' \cdot \mathbf{b}_j) = -3\sqrt{3}t_2 = -m.$$

The non-trivial topology of the Bloch bands translates to a nonzero winding number of the map $\hat{\mathbf{d}} = \mathbf{d}/|\mathbf{d}|$ from the torus (the first Brillouin zone) to the unit sphere.

F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988)

The phase $\phi = \frac{\pi}{2} can be realized$ with lasers, light-matter coupling: Control at the atomic scale!



Spin-1/2 analogy

$$\mathcal{H}_{\mathrm{H}}(\mathbf{k}) = -\mathbf{d}\left(\mathbf{k}\right) \cdot \hat{\sigma},$$

We have introduced the field $\psi(\mathbf{k}) = (b_A(\mathbf{k}), b_B(\mathbf{k}))^T$ of Fourier transforms of the annihilation operators for bosons on sublattices A and B. We wrote \mathcal{H}_{H} in the basis of Pauli matrices $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ in terms of

$$\mathbf{d}(\mathbf{k}) = \left(t_1 \sum_{i} \cos \mathbf{k} \, \mathbf{a}_i, t_1 \sum_{i} \sin \mathbf{k} \, \mathbf{a}_i, -2t_2 \sum_{i} \sin \mathbf{k} \, \mathbf{b}_i\right).$$

The non-trivial topology of the Bloch bands translates to a nonzero winding number of the map $\hat{\mathbf{d}} = \mathbf{d}/|\mathbf{d}|$ from the torus (the first Brillouin zone) to the unit sphere.

Light-induced anomalous Hall effect in graphene

J.W. McIver^{1*}, B. Schulte^{1*}, F.-U. Stein^{1*}, T. Matsuyama¹, G. Jotzu¹, G. Meier¹ and A. Cavalleri^{1,2}

Nature 2020



Fig. 1 | **Light-induced topological Floquet bands in graphene and device architecture used to detect ultrafast anomalous Hall currents. a**, A coherent interaction between graphene and circularly polarized light is predicted to open a topological band gap in the effective Floquet band

Light-Matter Coupling

D. Tran, A. Dauphin, A. G. Grushin, P. Zoller, N. Goldman Sciences Advances 2017

Philipp Klein, Adolfo Grushin, Karyn Le Hur, Phys. Rev. B 2021

Karyn Le Hur, arXiv: arXiv:2106.15665

 $A = A_0 e^{-i\omega t} (e_x \mp i e_y)$

 $\delta \mathcal{H}_{\pm} = A_0 e^{\pm i\omega t} |a\rangle \langle b| + h.c.$

Circular Dichroism Jones Polarizations



Realization in Hamburg in atoms (C. Weitenberg & K. Sengstock group): Luca Asteria et al. Nature Physics 2019

Photo-induced currents

Fermi golden's rule

$$\tilde{\Gamma}_{\pm} = \frac{2\pi}{\hbar} \frac{A_0^2}{2\hbar^2} \left| \left\langle \psi_- \left| \left(\frac{\partial H}{\partial p_x} + i \frac{\partial H}{\partial (\zeta p_y)} \right) \right| \psi_+ \right\rangle \right|^2 \delta(E_-(0) - E_+(0) - \hbar\omega).$$

$$\left|\Delta \tilde{\Gamma}\right| = \left|\frac{\Gamma_{+}(K) - \Gamma_{-}(K')}{2}\right| = \frac{2\pi}{\hbar} \frac{A_{0}^{2}}{4m^{2}}C$$

Stages 3A Joshua Benabou 2021 Han Yu Sit 2020





Relation to quantum Hall conductivity: D. Thouless (Nobel prize in physics 2016), M. Kohmoto, M. P. Nightingale, M. Den Nijs

Transport on the sphere

Joel Hutchinson, Karyn Le Hur, Communications Physics 4, 144 2021 Nature Journal, ArXiv: Feb 28 2020

$$H = \frac{(\hbar k_{\parallel})^2}{2m} + \frac{(\hbar k_{\perp})^2}{2m} + qV - \mathbf{d} \cdot \boldsymbol{\sigma}$$

Newton equation $ma_{\parallel} = \hbar k_{\parallel} = qE$

$$\theta(t) = k_{\parallel}(t) = \frac{q}{\hbar} E t.$$

Parseval-Plancherel Theorem (quantum mechanics)

 $\mathbf{E} = E\mathbf{e}_{x_{\parallel}} = -\nabla V$

 \mathbf{T}



Analogy Laughlin cylinder "Nobel Prize"

$$J_{\perp} = \frac{q}{T} \int_{0}^{T} dt \frac{d\langle x_{\perp} \rangle}{dt} = \frac{q}{T} \left(\langle x_{\perp} \rangle (T) - \langle x_{\perp} \rangle (0) \right) = \oint d\varphi \left(J_{\varphi}(\varphi, T) - J_{\varphi}(\varphi, 0) \right),$$

$$J_{\varphi}(\varphi, \theta) = \frac{iq}{4\pi T} \left(\psi^{*} \frac{\partial}{\partial \varphi} \psi - \frac{\partial \psi^{*}}{\partial \varphi} \psi \right) = \frac{iq}{2\pi T} \psi^{*} \frac{\partial}{\partial \varphi} \psi$$

$$q = -\varrho$$

$$J_{\perp}(\theta) = \frac{e}{2\pi T} \oint d\varphi A'_{N\varphi}(\varphi, \theta) = \frac{e}{T} A'_{\varphi}(\theta < \theta_{c}),$$

$$J_{\perp} = \frac{e}{4\pi T} \int d\varphi A'_{N\varphi}(\varphi, \theta) = \frac{e}{T} A'_{\varphi}(\theta < \theta_{c}),$$

Agrees with transport in the plane: Bloch bands (PC)

Topological States and Materials

The quantum Hall conductivity can be visualized as a Karplus-Luttinger velocity (1954) Applications in crystals: Ph. Nozieres and C. Lewiner, 1973; Review M. Nagaosa et al. 2010

Topological Insulators (Ti): Generalization with Spin-Orbit Coupling Theory Work of C. L. Kane & E. Mele and L. Fu starting in 2005 and also B. A. Bernevig, X. Qi, T. Hughes & S.-C. Zhang Realization in "Mercury" Materials in 2D (QSHE) and Bismuth Materials in 3D, ... Requires "Spin-Orbit Coupling" Characterization Through a Z₂ number Measures the number of "up" – "down" particles at the edges

Topological Superconductors and Majorana Fermions (1937) Electrons are bound in Cooper Pairs (Bosons, Superfluidity) Majorana Fermions are their own antiparticles, may be used For Topological quantum computing

Present research also includes Topological Semimetals

A Lot of questions here

Application for NanoElectronics, Spintronics, and Energy Photovoltaic Effect...



Review: J. Alicea, arXiv:1202.1293

 $\mathbf{v} = rac{e}{\hbar} \mathbf{E} imes \mathbf{F}.$

Topological states of matter: TRANSPORT AT THE EDGES



C. Z. Chang and M. Li, Topical Review, arXiv:1510.01754 From material science, to cold atoms and photons

REALIZED AT WURZBURG IN HGTE (Molenkamp) 3D MERCURY ANALOGUES, PRINCETON (Hasan)

Application spintronics: D. Pesin & A. H. Macdonald, Nature Materials 2012

Quantum Theory and Entangled Wave Function

Einstein-Poldosky-Rosen (EPR) Pair and Bell Tests of Quantum Mechanics (1964)

Our Logo at CPHT



$$| \downarrow \rangle = \frac{1}{\sqrt{2}} \left(| \uparrow \rangle \otimes | \downarrow \rangle \pm | \downarrow \rangle \otimes | \uparrow \rangle \right)$$

- Observation with Atoms : Serge Haroche (Nobel prize,) and Schrodinger Cats Applications in Rydberg Atoms and Quantum Circuits, cavities



- Applications with Photons (A. Aspect; Ph. Grangier; J. Dalibard) Nobel Prize 2022 (A. Aspect; J. Clauser; A. Zeilinger)! Quantum Security Protocols: BB84 Codes (Quantum Class I)
- New Applications in Quantum Information and Algorithms, New Interfaces: Everybody is welcome in Science



<u>Santa-Barbara:</u> P. Roushan et al. arXiv:1407.1585 Nature **515**, 241 (2014)



2 spheres



$$\mathcal{H}^{\pm} = -(\boldsymbol{H}_1 \cdot \boldsymbol{\sigma}^1 \pm \boldsymbol{H}_2 \cdot \boldsymbol{\sigma}^2) \pm \tilde{r} f(\theta) \sigma_z^1 \sigma_z^2$$

$$\boldsymbol{H}_i = (H\sin\theta\cos\phi, H\sin\theta\sin\phi, H\cos\theta + M_i)$$









Review: K. Le Hur arXiv:2209.15381