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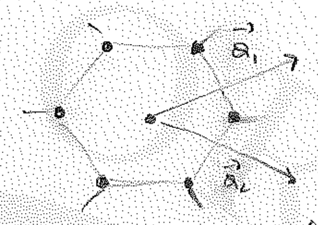
Symmetry and Dirac points in the spectrum of honeycomb Laplacian

Setting: Λ - lattice $\langle \vec{a}_1, \vec{a}_2; + \rangle$

$\mathbb{R}^2$



graphene crystal structure

H - s.-a. op invariant wrt Λ

Examples: * discrete infinite graphs (not necess. graphene)

* quantum graphs

* $H = -\Delta + q(\vec{x})$ on $\mathbb{R}^2$

$q(\vec{x} + \vec{a}_1) = q(\vec{x} + \vec{a}_2) = q(\vec{x})$, real

Floquet-Bloch: spectrum of a periodic operator

$$X(\vec{k}) = \{ \psi \in L^2_{loc} : \psi(\vec{x} + n_1\vec{a}_1 + n_2\vec{a}_2) = e^{i(k_1 n_1 + k_2 n_2)}\psi(\vec{x}),\ n_i \in \mathbb{Z} \}$$

$\vec{k} \in (-\pi, \pi]^2$ ← a Brillouin Zone

↖ quasi-momentum

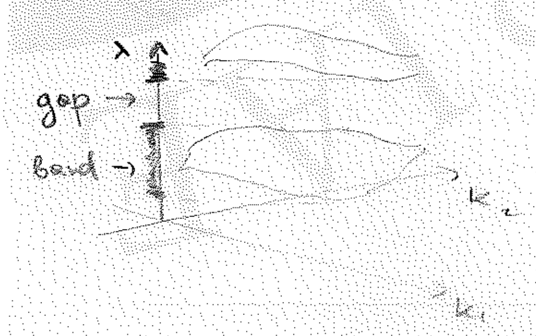
then $H = \bigoplus_{\vec{k} \in BZ} H(\vec{k})$ where $H(\vec{k}) = H\big|_{X(\vec{k})}$

$\Rightarrow \sigma(H) = \bigcup_{\vec{k}} \sigma\big(H(\vec{k})\big)$

(Better basis for BZ: $k_1 n_1 + k_2 n_2 = (\varkappa_1, \varkappa_2) \cdot (n_1\vec{a}_1 + n_2\vec{a}_2)$

$(k_1, k_2) = (\varkappa_1, \varkappa_2) A \qquad A = (\vec{a}_1 \mid \vec{a}_2)$)

$\sigma(H(\vec{k}))$ as a function of $\vec{k}$ is dispersion relation



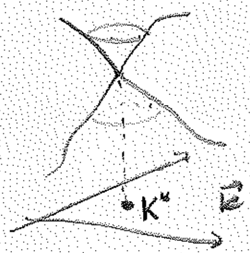
② Λ has symmetries that q may inherit:

D_6 $\begin{cases} R & \underline{\text{rot.}} \text{ by } \frac{2\pi}{3} \\ V & \underline{\text{inversion}} \quad \vec{x} \mapsto -\vec{x}, \text{ rot by } \pi \\ F & \text{horiz refl} \quad (x_1, x_2)^T \mapsto (-x_1, x_2), \ \underline{\text{flip}} \\ F_V = F \cdot V & \text{vert refl} \end{cases}$

If q has symmetries, they manifest in $\sigma(H(\vec{k}))$, better seen in $\vec{\varkappa}$ coords

<u>Fact</u>: Important physical properties of graphene are due to special structures in disp. rel.

conical or "Dirac" points



K^* indep of the precise nature of H!

Proofs of existence:

* tight-binding model: Wallace '49
* quantum graphs: Kuchment - Post '07
* Schröd. $\mathbb{R}^2$ Grushin (perturbative) '09

Fefferman - Weinstein '12

B. - Comech '14

Wave propagation governed by Dirac equation ; * error estimates F.-W. '12

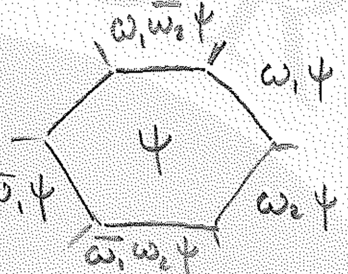
<u>Our results</u>: * Simpler proofs
* work for other H
* H has R symm and V <u>or</u> F
* In R+F case conical points move when symm. destroyed <u>but</u> along a known line

<u>Idea</u>: Use symmetry as much as possible!

Why k^*? When H has symmetry, $H(\vec{k}) = H|_{X(\vec{k})}$ may or may not inherit it, depends on $\vec{k}$

$X(\vec{k})$ must be invariant!

$$\omega_1 = e^{ik_1} \qquad \omega_2 = e^{ik_2}$$



$*$ $R\,X(\vec{k}) =: X(\hat{R}\vec{k})$

$$\hat{R} : \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix} \mapsto \begin{pmatrix} \overline{\omega_1}\,\omega_2 \\ \overline{\omega_1} \end{pmatrix}$$

$\tau = e^{\frac{2\pi}{3}i}$ Fixed point: $\begin{cases} \omega_1^3 = 1 \\ \omega_2 = \overline{\omega_1} \end{cases}$ $\begin{matrix} (1,1) \\ (\tau, \overline{\tau}) = k^* \\ (\overline{\tau}, \tau) \end{matrix}$

$*$ $\hat{V} : \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix} \mapsto \begin{pmatrix} \overline{\omega_1} \\ \overline{\omega_2} \end{pmatrix}$ F.P.: $(1,1)$

$*$ $\overline{V} = V +$ c.conjugation also a symmetry

$\hat{\overline{V}} : \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix} \mapsto \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix} \quad \Rightarrow \quad \overline{V}\,X(\vec{k}) = X(\vec{k}) \quad \forall \vec{k}$

Representation Theory

H - s.-a. operator, $\{S_1, S_2 \dots\}$ unitary symm. $HS_j = S_jH$

Rep. of G is $\{V, \rho\}$ $\quad g \mapsto \rho(g) : V \to V$

Irreducible if V has no inv. subspace $(\forall g \in G)$

If $H\psi = \lambda\psi$ then $HS_j\psi = S_jH\psi = \lambda S_j\psi$

E_λ is a representation of the group $\langle S_1, S_2 \dots \rangle$

④

Irreducible representation of degree $d = \dim V$ $\underset{\text{usually}}{\Longrightarrow}$ d-degenerate eigenvalues

Existence of deg

We are trying to prove $H(k^*)$ has double eigenvalues!

But... $\langle R, \bar{V} \rangle$ is abelian $R \cdot \bar{V} = \bar{V} \cdot R$

and all representations have degree 1 ?!

Over $\mathbb{C}$! And $\bar{V}$ is not $\mathbb{C}$-linear !

Wigner's Corepresentations

$$R : \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \to \begin{pmatrix} \tau z_1 \\ \bar{\tau} z_2 \end{pmatrix} \qquad \bar{V} : \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mapsto \begin{pmatrix} \bar{z}_2 \\ \bar{z}_1 \end{pmatrix}$$

is irreducible! $\Rightarrow$ $\sigma(H(k^*))$ have multiple eig.

Conical Shape

Dispersion rel is analytic $\Sigma(\lambda, \vec{\varkappa}) = 0$

expand to 2^{nd} order $\Rightarrow$ quadric surf (hyperboloid etc)

double root $\Rightarrow$ intersecting planes or cone

inv. wrt rot by $\frac{2\pi}{3}$ $\Rightarrow$ $\boxed{\text{circular cone}}$ (or horiz. planes)

OR

Perturbation Theory w/ Symmetry

$$\Sigma = \det\left(\varkappa_1 h_{\varkappa_1} + \varkappa_2 h_{\varkappa_2} - \lambda \right) + \text{h.o.t.}$$

$$h_{\vec{\varkappa}} = \Phi^* D_{\varkappa} H \, \Phi \qquad 2 \times 2 \text{ matrix}$$

$(\varphi_1 | \varphi_2) =: \Phi$ - basis for deg. eigenspace

$S : X(\vec{\varkappa}) \mapsto X(\hat{S}\vec{\varkappa})$ then $A_S h_{\varkappa} A_S^* = h_{\hat{S}\varkappa}$

where $A_S = \Phi^* S \Phi$ - rep of $\langle S_1, \dots \rangle$

we get $h_{\vec{\varkappa}} = \begin{pmatrix} 0 & (\varkappa_1 - i\varkappa_2)\alpha \\ (\varkappa_1 + i\varkappa_2)\bar{\alpha} & 0 \end{pmatrix}$

$\Rightarrow \quad \Sigma = |\alpha|^2 (\varkappa_1^2 + \varkappa_2^2) + \ldots$ - circular cone

<u>Time evolution</u> : $i\partial_t \psi = H\psi$

Wave packet $\psi_0(x) = \sum_{j=1}^{2} a_j \varphi_j \quad \notin L_2$

$= \sum_{j=1}^{2} \delta\, a_j(\delta\bar{x})\, \varphi_j(x)$

$$\psi(x,t) = e^{-i\lambda^* t}\left(\sum^{2} \delta\, a_j(\delta x, \delta t)\, \varphi_j + \eta^\delta(x,t)\right)$$

Careful estimates on η^δ : Fefferman - Weinstein

Set $\eta = 0$

Substitute into $i\partial_t \psi = (-\Delta + q(\bar{x}))\psi$

$$\cancel{\lambda^* \psi} + e^{-i\lambda^* t}\, i \sum \delta^2 \frac{\partial a_j}{\partial t} \varphi_j$$

$$= \cancel{\lambda^* \psi} + e^{-i\lambda^* t}\left(\cancel{\sum \delta^3 (-\Delta a_j)\varphi_j} - 2\sum \delta^2 \nabla a_j \cdot \nabla \varphi_j\right)$$

$$i\,\partial_t a_j = -2\, \varphi^* \sum_j \nabla a_j \cdot \nabla \varphi_j$$

$$H(\bar{\varkappa}) = -(\nabla + i\bar{\varkappa})^2 + q \quad \Rightarrow \quad -2i\,\vec{\varkappa}\cdot\nabla = D_{\vec{\varkappa}} H(\varkappa^*)$$

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$$i\partial_t \vec{a} = \frac{1}{i}\left(\Phi^* D_{\nabla a_1} H \Phi \begin{pmatrix}1\\0\end{pmatrix} + \Phi^* D_{\nabla a_2} H \Phi \begin{pmatrix}0\\1\end{pmatrix} \right)$$

$$= \frac{1}{i}\begin{pmatrix} (\partial_{x_1} a_1 + i\partial_{x_2} a_1)\,\bar{\alpha} \\ (\partial_{x_1} a_2 - i\partial_{x_2} a_2)\,\alpha \end{pmatrix}$$

$$i\partial_t \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{i}\begin{pmatrix} \bar{\alpha} & 0 \\ 0 & \alpha \end{pmatrix} \left(\sigma_1 \partial_{x_1} - \sigma_2 \partial_{x_2} \right) \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

<u>Stability of Conical Points</u>

~~K~~ + V

Berry phase β

rotation of eigenvector

Operator with C.C. symm $\Rightarrow \beta = 0$ or π

Contour contractable $\Rightarrow \beta = 0$

Contour encloses one conical point $\Rightarrow \beta = \pi$

$\therefore$ conical point cannot disappear