On dispersion of wave packets in Dirac materials

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arXiv:1604.00157

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Dirac materials

- systems (mostly in cond.mat.), where low-energy spectrum has linear dependence on the momentum - dynamics is well approximated by 2D or 1D Dirac equation!

2D stationary equation (for interactions changing smoothly on the interatomic distance and preserving spin)

$$\left[\begin{array}{cc} V(x,y)+M(x,y) & \Pi_x - i\Pi_y \\ \Pi_x + i\Pi_y & V(x,y)-M(x,y) \end{array}\right]\Psi = E\Psi$$

where

$$\Pi_x = -i\partial_x + A_x(x,y), \quad \Pi_y = -i\partial_y + A_y(x,y)$$

- interesting toy for mathematical physicists!

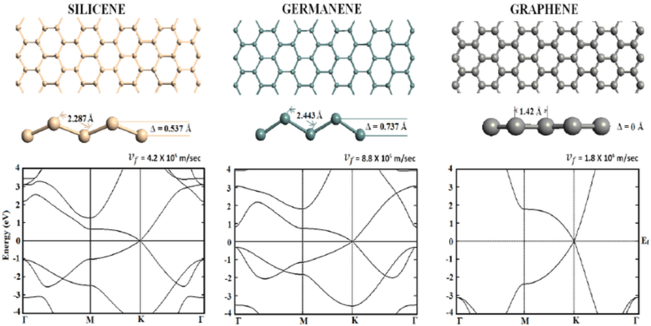
Relevant in description of surprising variety of physical systems

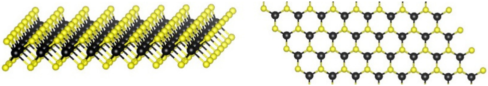
- Andreev approximation of BdG equations of superconductivity, high-temperature d-wave superconductors, superfluid phases of ^3He
- low-dimensional models in quantum field theory (GN,...)
- condensed matter systems where low-energy quasi-particles behave like massless Dirac fermions

Graphene and its cousins

- graphene, silicene, germanene, stanene, h-BN, dichalcogenides

Trivedi, J. Comp. Theor. NanoSci. 11, 1 (2014)



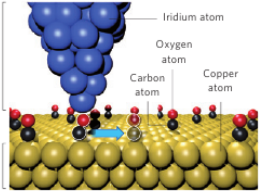


dichalcogenides

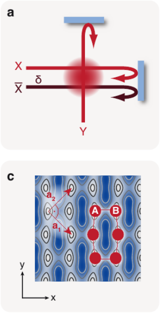
low-energy approximation of TBM of hexagonal lattice with nearest neighbor interaction, Hasegawa, PRB74, 033413

Artificial graphene

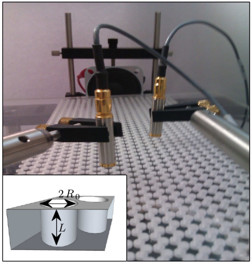
- artificial graphene - ultracold atoms in optical lattices, CO molecules assembled on copper surface, drilling holes in hexagonal pattern in plexiglass...



Manoharan, Nature 483, 306 (2012)



Tarruell, Nature 483, 302 (2012)



Torrent,PRL108,174301

Dirac materials - rapidly expanding ZOO of physical systems!

1D Dirac Hamiltonian - qualitative spectral analysis

Spectral properties of the Hamiltonian

$$h = (-i\sigma_1\partial_x + W(x)\sigma_2 + M\sigma_3)$$

with

$$\lim_{x\to\pm\infty} W(x) = W_\pm, \quad \lim_{x\to\pm\infty} W'(x) = 0, \quad |W_-| \leq |W_+|.$$

Sufficient conditions for existence of bound states in the spectrum (VJ,D.Krejčiřik Ann.Phys.349,268 (2014)), e.g.:

"When

$$\int_{-\infty}^{\infty}(W^2 - W_-^2) < 0,$$

then the Hamiltonian has at least one bound state with the energy $E \in \left(-\sqrt{W_-^2 + M^2}, \sqrt{W_-^2 + M^2}\right)$."

Question: What kind of observable phenomena can be attributed to the bound states? Let's make wave packets!

Absence of dispersion in the systems with translational invariance

Mathematical abstraction of the setting (forget about Dirac operator for now):

- *translational invariance*
  Let's have a (generic) Hamiltonian $H(x, y)$ that commutes with the generator of translations $\hat{k}_y = -i\hbar\partial_y$,
  $$[H(x, y), \hat{k}_y] = 0.$$
  After the partial Fourier transform $\mathcal{F}_{y\to k}$, the action of the Hamiltonian can be written as (direct integral decomposition)
  $$H(x, y)\psi(x, y) = (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} e^{\frac{i}{\hbar}ky} H(x, k)\psi(x, k)dk,$$
  where $H(x, k) = \mathcal{F}_{y\to k} H(x, y)\mathcal{F}^{-1}_{y\to k}$, and
  $$\psi(x, k) = \mathcal{F}_{y\to k}\psi(x, y) = (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} e^{-\frac{i}{\hbar}ky}\psi(x, y)dy.$$

- *discrete energies for fiber operators*
  Assume $H(x,k)$ has a non-empty set of discrete eigenvalues $E_n(k)$ for each $k \in J_n \subset \mathbb{R}$. The associated normalized bound states $F_n(x,k)$ satisfy

  $$(H(x,k) - E_n(k))F_n(x,k) = 0, \quad k \in J_n.$$

  We make a "linear combination" composed of $F_n(x,k)$ with fixed n

  $$\Psi_n(x,y) = (2\pi\hbar)^{-1/2} \int_{I_n} e^{\frac{i}{\hbar}ky} \beta_n(k) F_n(x,k) dk$$

  where $\beta_n(k) = 0$ for all $k \notin I_n \subset J_n$. Ψ_n is normalized as long as $\int_{I_n} |\beta_n(k)|^2 dk = 1$.

- Suppose that $E_n(k)$ is linear on I_n,

$$E_n(k) = e_n + v_n k, \quad k \in I_n.$$

Then Ψ_n evolves with a uniform speed without any dispersion,

$$e^{-\frac{i}{\hbar}H(x,y)t}\Psi_n(x,y) = c_n(t)\Psi_n(x, y - v_n t), \quad |c_n(t)| = 1.$$

Indeed, we have

$$\begin{aligned} e^{-\frac{i}{\hbar}H(x,y)t}\Psi_n(x,y) &= (2\pi\hbar)^{-1/2}\int_{I_n} e^{\frac{i}{\hbar}ky} e^{-\frac{i}{\hbar}H(x,k)t}(\beta_n(k)F_n(x,k)) \\ &= e^{-\frac{i}{\hbar}e_n t}(2\pi\hbar)^{-1/2}\int_{I_n} e^{\frac{i}{\hbar}k(y-v_n t)}\beta_n(k)F_n(x,k)dk \\ &= e^{-\frac{i}{\hbar}e_n t}\Psi_n(x, y - v_n t). \end{aligned}$$

  - independent on the actual form of $H(x,k)$
  - can be generalized to higher-dimensional systems with the translational symmetry
  - simple observation relevant for Dirac materials!

Realization of dispersionless wave packets

Linear dispersion relation - hard to get with Schrödinger operator, but available in Dirac systems

We fix the Hamiltonian in the following form

$$H(x,y) = v_F \tau_3 \otimes \left(-i\hbar\sigma_1\partial_x - i\hbar\sigma_2\partial_y + \frac{\gamma_0}{v_F} m(x)\sigma_3 \right),$$

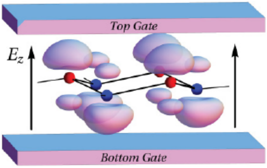
whose fiber operator reads

$H(x,k) = v_F \tau_3 \otimes \left(-i\hbar\sigma_1\partial_x + k\sigma_2 + \frac{\gamma_0}{v_F} m(x)\sigma_3 \right).$

Structure of bispinors: $\Psi = (\psi_{K,A}, \psi_{K,B}, \psi_{K',B}, \psi_{K',A})^T$

Topologically nontrivial mass term: $\lim_{x\to\pm\infty} m(x) = m_\pm$, $m_+ m_- < 0$

Mass term arises when sublattice symmetry is broken



Drummond et al, PRB 85, 075423 (2012)

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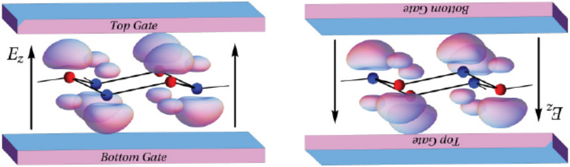


Drummond et al, PRB 85, 075423 (2012)

Then $H(x,k)$ has two nodeless bound states localized at the domain wall where the mass changes sign Semenoff, PRL 101,87204 (2008).

$$F_{+}(x) \equiv F_0(x,k) = (1,i,0,0)^T \, e^{-\frac{\gamma_0}{\hbar v_F}\int_0^x m(s)ds},$$
$$F_{-}(x) \equiv \tau_1 \otimes \sigma_2 \, F_{+}(x) = (0,0,1,i)^T \, e^{-\frac{\gamma_0}{\hbar v_F}\int_0^x m(s)ds}.$$

They satisfy

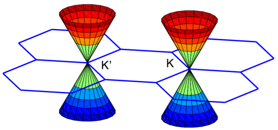
$$H(x,k)F_{\pm}(x) = \pm v_F k F_{\pm}(x).$$

As $F_{\pm}(x)$ do not depend on k, the nondispersive wave packet can be written as

$$\Psi_{\pm}(x,y) = F_{\pm}(x)G_{\pm}(y),$$

where $G_{\pm}(y)$ are arbitrary square integrable functions

- There are two counterpropagating dispersionless wave packets, one for each Dirac point (valleytronics)



Slowly dispersing wave packets

Assume the dispersion relation $E = E(k)$ is not linear. We define

$$B(k) = E_n(k) - (e + vk), \quad k \in I_n,$$

where e and v are free parameters so far.
We are interested in the transition probability

$$\begin{aligned} A(t) &= |\langle \Psi_n(x, y - vt), e^{-\frac{i}{\hbar}H(x,y)t}\Psi_n(x, y)\rangle|^2 \\ &= \int_{I_n \times I_n} dkds |\beta_n(k)|^2 |\beta_n(s)|^2 \cos\left((B(k) - B(s))\frac{t}{\hbar}\right) \end{aligned}$$

Let us find the lower bound of $A(t)$

$$\begin{aligned} A(t) &\geq \inf_{(k,s)\in I_n\times I_n} \cos\left((B(k) - B(s))\frac{t}{\hbar}\right) \\ &\geq 1 - \frac{t^2}{2\hbar^2} \sup_{(k,s)\in I_n\times I_n} (B(k) - B(s))^2 \geq 1 - \frac{2t^2}{\hbar^2} \sup_{k\in I_n} |B(k)|^2. \end{aligned}$$

We set average speed $v = \frac{\int_{I_n} E_n'(k)dk}{b-a} = \frac{E_n(b)-E_n(a)}{b-a}$, and e such that $\sup_{k\in I_n}(E_n(k) - vk - e) = -\inf_{k\in I_n}(E_n(k) - vk - e)$.

Example

The fiber Hamiltonian is

$$\tilde{H}_K(x,k) = -i\sigma_1\partial_x - \omega\alpha\tanh(\alpha x)\sigma_2 + k\sigma_3.$$

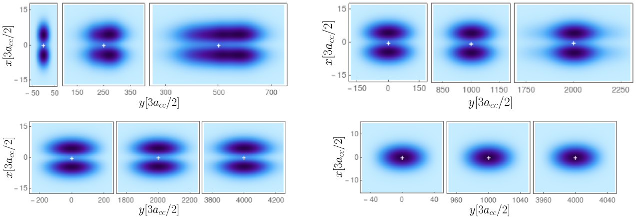
The solutions of stationary equation are

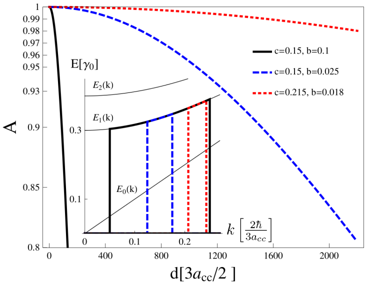
$$\begin{aligned}
\tilde{H}_K(x,k)\tilde{F}_n^{\pm}(x,k) &= \pm E_n(k)\tilde{F}_n^{\pm}(x,k), \\
\tilde{F}_n^{\pm}(x,k) &= \begin{pmatrix} 1 & 0 \\ 0 & \epsilon^{\pm}(k,n) \end{pmatrix} \left(\mathbf{1} + \frac{\tilde{H}_K(x,0)}{E_n(0)^2} \right) \begin{pmatrix} f_n(x) \\ 0 \end{pmatrix}, \\
E_n(k) &= \sqrt{n(-n+2\omega)\alpha^2 + k^2}
\end{aligned}$$

where we denoted $\epsilon^{\pm}(k,n) = \frac{E_n(0)}{\pm\sqrt{E_n(0)^2+k^2}+k}$ and

$$f_n(x) = \operatorname{sech}^{-n+\omega}(\alpha x)\,{}_2F_1\left(-n, 1-n+2\omega, 1-n+\omega, \frac{1}{1+e^{2\alpha x}}\right).$$

The zero modes are $(\tilde{H}(x,k) - k)\tilde{F}_+(x) = 0$, $\tilde{F}_+(x) = (\operatorname{sech}^{\omega}(\alpha x), 0)^T$.



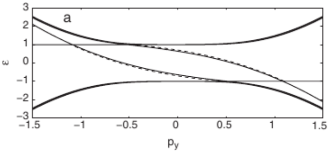


$$\beta_1(k) = C_b \exp\left(-\frac{1}{b^2-(k-c)^2}\right), \ \beta_1(k) = 0 \text{ for } k \neq (c-b, c+b).$$

$$\tilde{\Psi}_1 = \int_{I_1} e^{iky}\beta_1(k)\tilde{F}_1^{+}(x,k)\mathrm{d}k, \quad \tilde{\Psi}_+ = \tilde{F}_+(x)\int_{I_1} e^{iky}\beta_1(k)\mathrm{d}k,$$

Discussion and Outlook

- insight into experimental data (e.g. existence of slowly dispersing wave packets in bilayer graphene "highways")



Martin et al, PRL100,036804 (2008)

- realization of quantum states following classical trajectories seeked already by Schödinger (free particle Berry, Am. J. Phys. 47, 264 (1979), Trojan states for Rydberg atoms Bialnicki-Birula et al, PRL 73,1777 (1994))
- experimental preparation of the disperionless wave packets requires precise control of quantum states: achieved by laser pulses for Rydberg atoms (Weinacht, Nature 397 (1999), 233; Verlet, Phys. Rev. Lett. (2002) 89, 263004)

generalizations

- improvements of estimates for slowly dispersing wp (lower bound for transition amplitude, weighted group velocity of the packet)
- extension to other geometries
- (geometrically) imperfect systems, crossroads