Dispersionless wave packets in graphene and Dirac materials

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Low-dimensional Dirac equation

Relevant in description of surprising variety of physical systems

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

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


dichalcogenides

low-energy approximation of TBM of hexagonal lattice with nearest neighbor interaction, Hasegawa, PRB74, 033413
- artificial graphene - ultracold atoms in optical lattices, CO molecules assembled on copper surface, drilling holes in hexagonal pattern in plexiglass...

Manoharan Lab


Torrent, PRL108, 174301
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 (V.J.D.Krejčiřík 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?
Absence of dispersion in the systems with translational invariance

Hamiltonian $H(x, y)$ 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 $\mathcal{F}_{y \rightarrow k}$, the action of the Hamiltonian can be written as

$$H(x, y)\psi(x, y) = (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} e^{i\frac{ky}{\hbar}} H(x, k)\psi(x, k) dk,$$

where $H(x, k) = \mathcal{F}_{y \rightarrow k} H(x, y) \mathcal{F}_{y \rightarrow k}^{-1}$, and

$$\psi(x, k) = \mathcal{F}_{y \rightarrow k} \psi(x, y) = (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} e^{-i\frac{ky}{\hbar}} \psi(x, y) dy.$$
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 take a “linear combination” composed of $F_n(x, k)$ with fixed $n$

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

where $\beta_n(k) = 0$ for all $k \notin I_n \subset J_n$. $\Psi_n$ 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 $\Psi_n$ 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

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

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

- independent on the actual form of the fiber Hamiltonian
- also works for higher-dimensional systems with translational symmetry
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

\[ \lim_{x \to \pm \infty} m(x) = m_{\pm}, \quad m_- < 0, \quad m_+ > 0. \]
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

\[
H(x, k)F_\pm(x) = \pm v_F kF_\pm(x).
\]

The nondispersive wave packet

\[
\Psi_\pm(x, y) = F_\pm(x)G_\pm(y),
\]

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

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

where $e$ and $v$ are free parameters so far.

We are interested in the transition probability

$$A(t) = |\langle \Psi_n(x, y - vt), e^{-\frac{i}{\hbar}H(x,y)t}\Psi_n(x, y) \rangle|^2$$

$$= \int_{I_n \times I_n} dk ds |\beta_n(k)|^2 |\beta_n(s)|^2 \cos \left((B(k) - B(s))\frac{t}{\hbar}\right)$$

let us find the lower bound

$$\geq \inf_{(k,s) \in I_n \times I_n} \cos \left((B(k) - B(s))\frac{t}{\hbar}\right)$$

$$\geq 1 - \frac{t^2}{2\hbar^2} \sup_{(k,s) \in I_n \times I_n} (B(k) - B(s))^2 \geq 1 - \frac{2t^2}{\hbar^2} \sup_{k \in I_n} |B(k)|^2.$$ 

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 $\sup_{k \in I_n} (E_n(k) - vk - e) = -\inf_{k \in I_n} (E_n(k) - vk - e)$. 
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

$$\tilde{H}_K(x, k)\tilde{F}_n^\pm(x, k) = \pm E_n(k)\tilde{F}_n^\pm(x, k),$$

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

$$E_n(k) = \sqrt{n(-n + 2\omega)\alpha^2 + k^2}$$

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

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

The zero modes are $(\tilde{H}(x, k) - k)\tilde{F}_+(x) = 0$, $\tilde{F}_+(x) = (\text{sech}^\omega(\alpha x), 0)^T$. 
\[ \beta_1(k) = C_b \exp \left( -\frac{1}{b^2-(k-c)^2} \right), \beta_1(k) = 0 \text{ for } k \neq (c - b, c + b). \]

\[ \tilde{\Psi}_1 = \int_{l_1} e^{iky} \beta_1(k) \tilde{F}_1^+(x, k) dk, \quad \tilde{\Psi}_+ = \tilde{F}_+(x) \int_{l_1} e^{iky} \beta_1(k) dk, \]
Discussion and Outlook

- insight into experimental data (e.g. bilayer graphene "highways")


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 (long-living quasiparticles on the "highways" in bilayer graphene)