Effective Dirac equations in honeycomb structures

Young Researchers Seminar, CERMICS, Ecole des Ponts ParisTech

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The 2D Dirac operator

The 2D Dirac operator is defined as

$$\mathcal{D} = \mathcal{D}_0 + m\sigma_3 = -i(\sigma_1\partial_1 + \sigma_2\partial_2) + m\sigma_3. \tag{1}$$

where σ_k are the Pauli matrices and $m \geq 0$ is the mass of the particle. It acts on $\mathbb{C}^2$-valued spinors.

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It is self-adjoint on $L^2(\mathbb{R}^2, \mathbb{C}^2)$ and the spectrum is given by

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The domain of the operator and form domain are $H^1(\mathbb{R}^2, \mathbb{C}^2)$ and $H^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2)$, respectively.

Remark

The negative spectrum is associated with antiparticles, in relativistic theories.

Honeycomb structures

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Recently, new two dimensional materials possessing Dirac fermion low-energy excitations have been discovered. The most famous example is graphene, which can be modeled as 2D honeycomb lattice of carbon atoms:

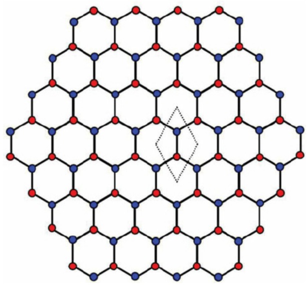

Figure: The hexagonal lattice H is a superposition of two copies of a triangular lattice Λ : $H = (A + \Lambda) \cup (B + \Lambda)$

Honeycomb potentials

Let $\Lambda := v_1\mathbb{Z} \oplus v_2\mathbb{Z}$ be a triangular lattice, and consider its dual $\Lambda^* := \{k \in \mathbb{R}^2 | k \cdot v \in 2\pi\mathbb{Z}, \forall v \in \Lambda\}$.
The dual lattice $H^* = (K + \Lambda^*) \cup (K' + \Lambda^*)$ is also hexagonal, and its primitive cell $\mathcal{B}$ is called the *Brillouin zone* of the lattice.

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Definition

A function $V \in C^\infty(\mathbb{R}^2, \mathbb{R})$ is called a *honeycomb potential* if there exists $x_0 \in \mathbb{R}^2$ such that $\tilde{V}(x) := V(x - x_0)$ satisfies:

- $\tilde{V}$ is Λ-periodic: $\tilde{V}(x + v) = \tilde{V}(x), \forall x \in \mathbb{R}^2, \forall v \in \Lambda$;
- $\tilde{V}$ is even: $\tilde{V}(-x) = \tilde{V}(x), \forall x \in \mathbb{R}^2$;
- $\tilde{V}$ is invariant by $\frac{2\pi}{3}$ rotations.

In the sequel V will denote a honeycomb potential.

The case of graphene

Graphene can be described by a periodic Schrödinger operator $-\Delta + V$, where $V \in C^\infty(\mathbb{R}^2, \mathbb{R})$ is a honeycomb potential.

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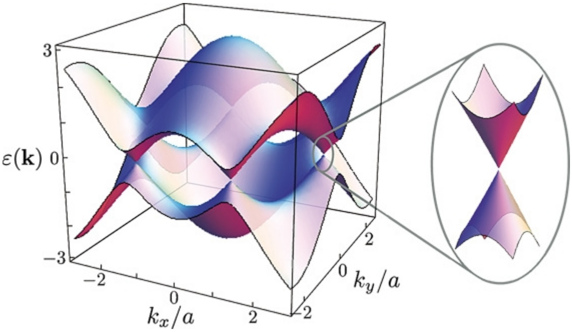
The spectrum has a band structure, possibly with gaps.
It exhibits conical intersections in the low-lying dispersion relations, around the so-called *Dirac points*:



The effective operator

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One expects the effective operator around a conical point to be the (massless) Dirac operator, acting on $\mathbb{C}^2$-valued spinors:

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Remark

In this case the vertex of the cone is the Fermi level, and there is no particles/antiparticles interpretation, but rather: positive energies = conduction electrons; negative energies = valence electrons.

Linear Dirac dynamics

Consider a wave packet spectrally concentrated around K_*:

$$u_0^\varepsilon(x) = \sqrt{\varepsilon}(\psi_{1,0}(\varepsilon x)\Phi_1(x) + \psi_{2,0}(\varepsilon x)\Phi_2(x)), \quad \varepsilon > 0 \qquad (2)$$

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Theorem (Fefferman, Weinstein '13)

Fix $\rho > 0, \delta > 0, N \in \mathbb{N}$. Then the linear Schrödinger equation $i\partial_t u = (-\Delta + V)u$ has a unique solution of the form

$$u^\varepsilon(t,x) = e^{-i\mu_* t}\left(\sum_{j=1}^{2} \sqrt{\varepsilon}\psi_j(\varepsilon t, \varepsilon x)\Phi_j(x) + \eta^\varepsilon(t,x)\right) \qquad (3)$$

with $u^\varepsilon(0,x) = u_0^\varepsilon(x), \eta^\varepsilon(0,x) = 0$. For any $|\beta| \leq N$ we have

$$\sup_{0 \leq t \leq \rho\varepsilon^{-2+\delta}} \|\partial_x^\beta \eta^\varepsilon(t,x)\|_{L_x^2(\mathbb{R}^2)} \xrightarrow{\varepsilon \to 0} 0$$

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The coefficients ψ_j form a global-in-time solution to the following Dirac equation

$$i\partial_t \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 & \overline{\lambda}(\partial_1 + i\partial_2) \\ \lambda(\partial_1 - i\partial_2) & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad 0 \neq \lambda \in \mathbb{C}$$

with initial data $\begin{pmatrix} \psi_1(0,x) \\ \psi_2(0,x) \end{pmatrix} = \begin{pmatrix} \psi_{1,0}(x) \\ \psi_{2,0}(x) \end{pmatrix} \in \left[\mathcal{S}(\mathbb{R}^2)\right]^2.$
The parameter $\lambda \in \mathbb{C}$ depends on the potential V.

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The parameter $\lambda \in \mathbb{C}$ depends on the potential V.

Remark

It is conceivable that the condition on the initial data can be weakened with additional work.

From NLS/GP to cubic Dirac

Consider the following *nonlinear Schrödinger/Gross-Pitaevskii equation*:

$$i\partial_t u = (-\Delta + V)u + \kappa|u|^2 u$$

where $\kappa \in \mathbb{R}$, and V is a honeycomb potential.

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$$i\partial_t u = (-\Delta + V)u + \kappa|u|^2 u$$

where $\kappa \in \mathbb{R}$, and V is a honeycomb potential.
The effective equation around a Dirac point is (Fefferman-Weinstein '12, formal derivation):

$$\begin{cases} \partial_t\psi_1 + \overline{\lambda}(\partial_1 + i\partial_2)\psi_2 = -i\kappa(\beta_1|\psi_1|^2 + 2\beta_2|\psi_2|^2)\psi_1 \\ \partial_t\psi_2 + \lambda(\partial_1 - i\partial_2)\psi_1 = -i\kappa(\beta_1|\psi_2|^2 + 2\beta_2|\psi_1|^2)\psi_2 \end{cases} \tag{4}$$

with $0 \neq \lambda \in \mathbb{C}$, $\beta_j > 0$ and $\psi = (\psi_1, \psi_2)^T$ is a $\mathbb{C}^2$-spinor.

Nonlinear Dirac dynamics

Let $u_0^\varepsilon(x) = \sqrt{\varepsilon}(\psi_{1,0}(\varepsilon x)\Phi_1(x) + \psi_{2,0}(\varepsilon x)\Phi_2(x)), \quad \varepsilon > 0.$

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Theorem (Arbunich,Sparber '16)

Consider the equation $i\partial_t u = (-\Delta + V)u + \kappa|u|^2 u$, and let $s > 1, S > 3$. There exists $T^\varepsilon \sim \varepsilon^{-1}$, s.t. the solution $u^\varepsilon \in C^0([0, T^\varepsilon), H^s(\mathbb{R}^2))$ of the equation with $u^\varepsilon(0,x) = u_0^\varepsilon(x)$ is of the form

$$u^\varepsilon(t,x) = e^{-i\mu_* t}\left(\sum_{j=1}^{2}\sqrt{\varepsilon}\psi_j(\varepsilon t, \varepsilon x)\Phi_j(x) + \eta^\varepsilon(t,x)\right),$$

provided that $\psi = (\psi_1, \psi_2)^T \in C^0([0, T^\varepsilon), H^S(\mathbb{R}^2, \mathbb{C}^2))$ is a solution of (4). In this case the approximation is valid on a time interval $\mathcal{O}(\varepsilon^{-1})$.

Towards Dirac solitons for NLS/GP

We are interested in stationary solutions of the focusing NLS/GP,

$$e^{-i\mu_* t}u(x)$$

where $\mu_* \in \sigma(-\Delta + V)$ is the energy of a Dirac point. Then u solves

$$(-\Delta + V - \mu_*)u = |u|^2 u.$$

In particular, we may look for solutions of the form
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- $\mu_* \in \sigma(-\Delta + V)$: generally speaking existence is not trivial,
- For the same reason, one expects $u \notin L^2(\mathbb{R}^2)$,
- μ_* correponds to $0 \in \sigma(\mathcal{D})$ for the effective operator.

Towards Dirac solitons for NLS/GP

Then one is lead to study the following effective equation for $\psi = (\psi_1, \psi_2)^T$:

$$\begin{cases} (\partial_1 + i\partial_2)\psi_2 = i(\beta_1|\psi_2|^2 + 2\beta_2|\psi_1|^2)\psi_1 \\ (\partial_1 - i\partial_2)\psi_1 = i(\beta_1|\psi_1|^2 + 2\beta_2|\psi_2|^2)\psi_2 \end{cases} \tag{5}$$

Theorem (W.B. '18)

The above equation $\mathcal{D}\psi = G_{\beta_1,\beta_2}(\psi)\psi$ admits infinitely many solutions $\psi \in C^\infty(\mathbb{R}^2, \mathbb{C}^2)$ of the form $\psi(r,\vartheta) = \begin{pmatrix} iu(r)e^{i\vartheta} \\ v(r) \end{pmatrix}$ with $u, v : [0, +\infty) \longrightarrow \mathbb{R}$, (r, ϑ) are polar coordinates. Moreover

$$|u(r)| \sim \frac{1}{r}, \quad |v(r)| \sim \frac{1}{r^2}, \text{as} \quad r \to +\infty.$$

In particular, $\psi \in L^p(\mathbb{R}^2, \mathbb{C}^2), \forall p > 2$, but $\psi \notin L^2(\mathbb{R}^2, \mathbb{C}^2)$.

Towards Dirac solitons for NLS/GP

Plugging the radial ansatz into the equation we get

$$\begin{cases} \dot{u} + \dfrac{u}{r} = (2\beta_2 u^2 + \beta_1 v^2)v, & u(0) = 0 \\ \dot{v} = -(2\beta_2 u^2 + \beta_1 v^2)u, & v(0) = \lambda \neq 0 \end{cases}$$

A solution of the ODE system $(v(r), u(r)) \to (0,0)$, as $r \to +\infty$, corresponds to a localized (non-trivial) solution of the PDE.

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A solution of the ODE system $(v(r), u(r)) \to (0, 0)$, as $r \to +\infty$, corresponds to a localized (non-trivial) solution of the PDE.

- The equation is scale-invariant and odd;
- For the above reason it suffices to prove the existence of only one solution;
- The solutions admit a variational characterization.
- No gap and conical degeneracy at the Dirac point: the rigorous justification of the effective equation is a challenging problem.

The massive case

Dirac points are stable w.r.t. small honeycomb perturbations.
Adding a suitable perturbation breaking *parity* opens a gap at a Dirac point (Fefferman-Weinstein '12).
This results in a mass term for the effective operator.

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Theorem (W.B. '17/'18)

For a fixed $\omega \in (-m, m)$, the equation

$$(\mathcal{D}_0 + m\sigma_3 - \omega)\psi = G_{\beta_1,\beta_2}(\psi)\psi$$

has a (non-trivial) smooth solution of the form $\psi(r,\vartheta) = \begin{pmatrix} iu(r)e^{i\vartheta} \\ v(r) \end{pmatrix}$, with exponential decay at infinity.

Some remarks

Plugging the radial ansatz into the equation we get

$$\begin{cases} \dot{u} + \dfrac{u}{r} = (2\beta_2 u^2 + \beta_1 v^2)v - (m - \omega)v, & u(0) = 0 \\ \dot{v} = -(2\beta_2 u^2 + \beta_1 v^2)u - (m + \omega)u, & v(0) = \lambda \neq 0 \end{cases}$$

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- In the massive case nonlinear bound states of arbitrary form have exponential decay (Boussaïd-Comech '16);
- Variational characterization not yet available;
- The equation is odd: actually two non-trivial solutions;
- The mass term breaks scale-invariance: multiplicity is an open problem.

Thank you