Behaviour of zero modes for a one-dimensional Dirac operator arising in models of graphene

Daniel M. Elton

Lancaster University

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PEP programme, Isaac Newton Institute

Joint work with Michael Levitin (Reading) and Iosif Polterovich (Montreal)

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- Operators: straightforward 2×2 systems of first order odes.
- Methods: largely classical (hope to mention some ideas).
- Properties: some show remarkably subtle dependence on properties of the potential.

Graphene

Graphene has a (2-dimensional hexagonal) periodic structure. Bloch analysis of the tight binding model leads to a dispersion relation with "Dirac cones". The Fermi level sits at the tips of these cones; this allows a massless Dirac operator

$$-\mathrm{i}\sigma_1\nabla_x - \mathrm{i}\sigma_2\nabla_y + U(x,y)$$

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$U(x,y)$ is an external (electric) potential (this can be easily realised with an electrostatic gate placed on top of the graphene layer).

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Zero energy bound states of $\mathrm{T}_{k,V}$, or *zero modes*, correspond to conduction modes along the waveguide; want to determine when $\mathrm{T}_{k,V}\boldsymbol{\psi} = 0$ has a non-trivial solution $\boldsymbol{\psi} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \in L^2$.

Two spectral problems

Dependence on k: fix V consider the k-*spectrum*

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Remark. Since

$$\mathrm{T}_{k,V} = \mathrm{T}_{0,V} + k\sigma_3 \quad \text{and} \quad \mathrm{T}_{k,\gamma V} = \mathrm{T}_{k,0} + \gamma V,$$

K_V and Σ_V are the spectra of the linear operator pencils $k \mapsto \mathrm{T}_{0,V} + k\sigma_3$ and $\gamma \mapsto \mathrm{T}_{k,0} + \gamma V$ respectively.

Definition of the operator

Case $V \equiv 0$: viewing $\mathrm{T}_{k,0}$ as a multiplication operator in Fourier space we get a closed unbounded operator with $\mathrm{dom}(\mathrm{T}_{k,0}) = H^1$ and ${\mathrm{T}_{k,0}}^* = \mathrm{T}_{\overline{k},0}$. The (usual) spectrum is

$$\mathrm{spec}(\mathrm{T}_{k,0}) = \mathrm{spec}_{\mathrm{ess}}(\mathrm{T}_{k,0}) = \{\pm\sqrt{\xi^2 + k^2} : \xi \in \mathbb{R}\}.$$

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Potential classes: let $c_0(L^2)$ denote those functions $V : \mathbb{R} \to \mathbb{R}$ which are locally L^2 and satisfy

$$\|V\|_{L^2((x-1,x+1))} \to 0 \quad \text{as } |x| \to \infty.$$

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Multiplication by $V \in c_0(L^2)$ defines a compact map $H^1 \to L^2$ and hence a relatively compact perturbation of $\mathrm{T}_{k,0}$; $\mathrm{T}_{k,\gamma V} = \mathrm{T}_{k,0} + \gamma V$ can then be defined as a closed operator with $\mathrm{dom}(\mathrm{T}_{k,\gamma V}) = H^1$ and ${\mathrm{T}_{k,\gamma V}}^* = \mathrm{T}_{\overline{k},\overline{\gamma} V}$.

Spectral type

Theorem

For $V \in c_0(L^2)$ *we have:*

- $K_V = \mathrm{i}\mathbb{R} \cup K_{V,d}$ *where* $K_{V,d}$ *is a discrete subset of* $\mathbb{C} \setminus \mathrm{i}\mathbb{R}$ *consisting of eigenvalues with geometric multiplicity* 1 *which can only accumulate along* $\mathrm{i}\mathbb{R}$*.*
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Proof uses the compactness of $V : H^1 \to L^2$ and the equivalences

- $k \in K_V \iff -k \in \mathrm{spec}(\sigma_3(\mathrm{T}_{0,0} + V))$.
- $\gamma \in \Sigma_V \iff -1/\gamma \in \mathrm{spec}(V{\mathrm{T}_{k,0}}^{-1})$.

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The bound on the geometric multiplicity follows from the fact that the eigenvalue equation is an ode.

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We will henceforth assume $k > 0$ when considering Σ_V.

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If V is single-signed we have

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Can be proved using a fairly direct argument based on symmetries.

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$$\#\big(\Sigma_V \cap \{z \in \mathbb{C} : |z| \leq R\}\big) \leq C_p \, \|V\|_{L^p}^p \, R^p$$

for any $R \geq 0$, where C_p depends only on p (can take $C_1 = 4\mathrm{e}/\pi$).

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Several other approaches are almost certainly possible!

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$$\#(\Sigma_V \cap [0, R]) \geq \frac{R}{\pi} \left| \int_{\mathbb{R}} V(x) \mathrm{d}x \right| + o(R)$$

as $R \to \infty$. *The same estimate holds for* $\#(\Sigma_V \cap [-R, 0])$.

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- If $\int_{\mathbb{R}} V(x)\mathrm{d}x \neq 0$ then $\Sigma_V \cap \mathbb{R}$ contains infinitely many points.
- There are limits to possible improvements for a general lower bound; for example, $\Sigma_V \cap \mathbb{R} = \emptyset$ for anti-symmetric potentials.

Asymptotics I

For any $V \in \ell^1(L^2)$ we have asymptotic upper and lower bounds on $\#(\Sigma_V \cap [0, R])$ of

$$C\frac{R}{\pi}\int_{\mathbb{R}}|V(x)|\mathrm{d}x \quad \text{and} \quad \frac{R}{\pi}\left|\int_{\mathbb{R}} V(x)\mathrm{d}x\right|$$

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Another class of potentials: let BV_0 denote functions of bounded variation with compact support. We say $V \in BV_0$ has *no gaps* if

$$\left|\left(\text{co}(\text{ess supp}(V))\right) \cap V^{-1}(0)\right| = 0.$$

Asymptotics II

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Suppose V *satisfies one of*

(i) $V \in \ell^1(L^2)$ *is single-signed.*

(ii) $V \in BV_0$ *has no-gaps.*

Then

$$\#(\Sigma_V \cap [0, R]) = \frac{R}{\pi} \left| \int_{\mathbb{R}} V(x) \mathrm{d}x \right| + o(R)$$

as $R \to \infty$*. The same asymptotics holds for* $\#(\Sigma_V \cap [-R, 0])$*.*

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We can equivalently express this result as an asymptotic formula for points in $\Sigma_V \cap \mathbb{R}$; if $0 < \gamma_1 < \gamma_2 < \dots$ denotes the sequence of positive points in Σ_V then

$$\gamma_n = \frac{\pi}{\|V\|_{L^1}} n + o(n) \quad \text{as } n \to \infty.$$

One gap potentials: preliminaries I

We say $V \in BV_0$ *has one gap* if $V = V_1 + V_2$ for non-zero $V_1, V_2 \in BV_0$ which have no gaps and disjoint supports.

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For $j = 1, 2$ set $\mathrm{supp}(V_j) = [a_j, b_j]$ and $v_j = \int_{\mathbb{R}} V_j(x)\mathrm{d}x$.
Assume $b_1 < a_2$ and $\int_{\mathbb{R}} V(x)\mathrm{d}x = v_1 + v_2 \neq 0$.

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$$\alpha = \tanh(k(a_2 - b_1)) \quad \text{and} \quad \beta = \left| \frac{v_1 - v_2}{v_1 + v_2} \right|.$$

- $\alpha \in (0, 1)$ gives a measure of the gap length.

One gap potentials: preliminaries I

We say $V \in BV_0$ *has one gap* if $V = V_1 + V_2$ for non-zero $V_1, V_2 \in BV_0$ which have no gaps and disjoint supports.

Theorem

If $V \in BV_0$ has one gap and satisfies $\int_{\mathbb{R}} V(x)\mathrm{d}x = 0$ then $\Sigma_V \cap \mathbb{R}$ contains only finitely many points.

For $j = 1, 2$ set $\mathrm{supp}(V_j) = [a_j, b_j]$ and $v_j = \int_{\mathbb{R}} V_j(x)\mathrm{d}x$.
Assume $b_1 < a_2$ and $\int_{\mathbb{R}} V(x)\mathrm{d}x = v_1 + v_2 \neq 0$. Set

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- $\alpha \in (0, 1)$ gives a measure of the gap length.
- $\beta \geq 0$ gives a measure of the relative sizes of v_1 and v_2. $\beta \in [0, 1)$ if $v_1 v_2 > 0$ and $\beta > 1$ if $v_1 v_2 < 0$.

One gap potentials: preliminaries II

When $\alpha\beta > 1$ define

$$\nu_{\alpha,\beta} = \frac{2}{\pi}\left[\beta \arcsin\frac{\sqrt{\alpha^2\beta^2-1}}{\sqrt{\beta^2-1}} + \arcsin\frac{\sqrt{1-\alpha^2}}{\alpha\sqrt{\beta^2-1}}\right].$$

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If β is positive and rational write $\beta = p/q$ where $p, q \in \mathbb{N}$ are coprime. If p and q are both odd set $p_\beta = p$ and $q_\beta = q$; if p and q have opposite parity set $p_\beta = 2p$ and $q_\beta = 2q$.

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Set

$$A(\alpha,\beta) = \begin{cases} 1 & \text{if } \alpha\beta < 1, \\ \nu_{\alpha,\beta} & \text{if } \alpha\beta > 1 \text{ and } \beta \notin \mathbb{Q}, \\ \dfrac{4}{q_\beta}\left\lfloor \dfrac{1}{4}(p_\beta + q_\beta \nu_{\alpha,\beta}) \right\rfloor - \dfrac{p_\beta}{q_\beta} + \dfrac{2}{q_\beta} & \text{if } \alpha\beta > 1 \text{ and } \beta \in \mathbb{Q}; \end{cases}$$

($\lfloor x \rfloor$ denotes the largest integer which is less than x)

One gap potentials: asymptotics I

Theorem

Let $V \in BV_0$ *be a one-gap potential with* $\int_{\mathbb{R}} V(x)\,\mathrm{d}x \neq 0$*. Suppose* $\alpha\beta \neq 1$*. If* $\alpha\beta > 1$ *and* $\beta \in \mathbb{Q}$ *suppose additionally that* $p_\beta + q_\beta \nu_{\alpha,\beta} \notin 4\mathbb{Z}$*. Then*

$$\#(\Sigma_V \cap [0, R]) = \frac{1}{\pi} A(\alpha, \beta)\, |v_1 + v_2|\, R + o(R)$$

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- When $\alpha\beta > 1$ and $\beta \in \mathbb{Q}$ we have

$$\nu_{\alpha,\beta} - \frac{2}{q_\beta} \leq A(\alpha, \beta) \leq \nu_{\alpha,\beta} + \frac{2}{q_\beta}.$$

One gap potentials: asymptotics II

For different V we can obtain an asymptotic formula

$$\#(\Sigma_V \cap [0, R]) = \frac{C}{\pi} R + o(R) \tag{1}$$

as $R \to \infty$, for any C (strictly) between $\left|\int_{\mathbb{R}} V(x)\,\mathrm{d}x\right|$ and $\|V\|_{L^1}$.

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Theorem

Let $0 < v < A < u$. Then there exists a piecewise constant one-gap potential V such that $\left|\int_{\mathbb{R}} V(x)\,\mathrm{d}x\right| = v$, $\|V\|_{L^1} = u$ and (1) holds with $C = A$.

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Define a differentiable function $\Delta_V : \mathbb{R} \to \mathbb{R}$ by

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- If V is single-signed then $\Delta_V(\gamma)$ is monotonic in γ, strictly increasing (resp., decreasing) if $V \geq 0$ (resp., $V \leq 0$).
- If $V \in BV_0$ has no gaps then, for $n = 0, 1, 2$,

$$\frac{\mathrm{d}^n}{\mathrm{d}\gamma^n}\left(\Delta_V(\gamma) - \gamma \int_{\mathbb{R}} V(x)\mathrm{d}x\right) = o(1) \quad \text{as } \gamma \to \infty.$$

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- Prove the result for $\phi \equiv 0$, then show the addition of ϕ only changes $N_0(R)$ by $o(R)$.

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Case $\beta \in \mathbb{Q}$: (easier!). Periodicity and condition $p_\beta + q_\beta \nu_{\alpha,\beta} \notin 4\mathbb{Z}$ ensures zeros of f_0 are uniformly transversal. Conditions on ϕ ($n = 0, 1$) then means number of zeros is unchanged for sufficiently large x.

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- A uniform lower bound on $|f_0(x)| + |f_0'(x)| + |f_0''(x)|$ and the conditions on ϕ ensures the number of zeros changes by at most 2 near each such turning point for sufficiently large x.

k-spectrum

As before:

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- For the potential γV these bounds scale as $O(\gamma)$ and $O(\gamma^2)$ when $\gamma \to \infty$; the former is optimal, the latter probably not.
- Current methods rely on compact support (or super-exponential decay); extension to general $V \in \ell^1(L^2)$ is unclear.

Estimates: upper bounds

Various bounds on the number of points in $K_{V,d}$ can be obtained.

Proposition

Suppose $V \in BV_0$ with $\text{supp}(V) \subseteq I$ for some bounded interval I. Then

(i) $\#(K_{V,d} \cap \mathbb{R}) \leq C\,|I|\,\|V\|_{L^\infty}$.

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- For the potential γV these bounds scale as $O(\gamma)$ and $O(\gamma^2)$ when $\gamma \to \infty$; the former is optimal, the latter probably not.
- Current methods rely on compact support (or super-exponential decay); extension to general $V \in \ell^1(L^2)$ is unclear.
- For $V \in \ell^1(L^2)$ can obtain bounds on $\#(K_{V,d} \cap (\epsilon, \infty))$ for a fixed $\epsilon > 0$ (these bounds diverge as $\epsilon \to 0^+$).

Central potentials

We say that $V \in \ell^1(L^2)$ is a *central* potential if there exists $x_0 \in \mathbb{R}$ such that V is increasing on $(-\infty, x_0]$ and decreasing on $[x_0, \infty)$.

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Theorem

Suppose $V \in \ell^1(L^2)$ is central. Then

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- If V is central is it the case that $K_{V,d} \subset \mathbb{R}$?
- Gaps (or dips) in a potential can alter the picture radically. For a potential consisting of two square steps separated by a gap of length g numerics give $\#K_{V_g,d} = O(g)$ as $g \to +\infty$ (however $\#(K_{V_g,d} \cap \mathbb{R})$ seems to remain bounded).