

Bound states in semi-Dirac semi-metals

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ABSTRACT

New insights into transport properties of nanostructures with a linear dispersion along one direction and a quadratic dispersion along another are obtained by analysing their spectral stability properties under small perturbations. Physically relevant sufficient and necessary conditions to guarantee the existence of discrete eigenvalues are derived under rather general assumptions on external fields. One of the most interesting features of the analysis is the evident spectral instability of the systems in the weakly coupled regime. The rigorous theoretical results are illustrated by numerical experiments and predictions for physical experiments are made.

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Semi-Dirac semi-metals have attracted a lot of attention in the last decade; see, e.g., [1–5] and references therein. The most striking feature of these recently discovered nanostructures is that they exhibit unprecedented band structure properties: (electron or hole) quasiparticles disperse linearly in one direction and quadratically in the orthogonal direction. The situation is neither conventional zero-gap semiconductor-like, nor graphene-like, but has in some sense aspects of both.

Using a tight-binding model of spinless fermions, it is commonly accepted that the Hamiltonian

$$H_0 := \begin{pmatrix} -i\partial_y & -\partial_x^2 + \delta \\ -\partial_x^2 + \delta & i\partial_y \end{pmatrix} \quad (1)$$

is the right low-energy description of the unperturbed system. Here we disregard all the physical constants of [2,3], for they can always be considered to be equal to 1 by suitably re-scaling the space variables $\mathbf{r} := (x, y) \in \mathbb{R}^2$, except for the gap parameter δ which we assume to be a positive constant.

We understand H_0 as the operator acting in the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^2)^2$ consisting of all \mathbb{C}^2 -valued functions

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \quad \text{such that} \quad \|\psi\|_{\mathcal{H}}^2 := \int_{\mathbb{R}^2} |\psi|^2 < \infty,$$

where $|\psi| := \sqrt{|\psi_1|^2 + |\psi_2|^2}$ is the usual Euclidean norm and $L^2(\mathbb{R}^2)$ is the Lebesgue space of square-integrable functions over \mathbb{R}^2 . For the operator domain, we take

$$\text{dom } H_0 := \left\{ \psi \in \mathcal{H} : \partial_x \psi, \partial_x^2 \psi, \partial_y \psi \in \mathcal{H} \right\},$$

which, in contrast to the conventional Dirac operator, is a proper subset of the Sobolev space $H^1(\mathbb{R}^2)^2$. Anyway, applying the Fourier transform in the spirit of [6, §V.5.4] or [7, §1.4], it is easily verified that H_0 is self-adjoint and that its spectrum is given by

$$\sigma(H_0) = (-\infty, -\delta] \cup [\delta, \infty). \quad (2)$$

Moreover, the total spectrum is purely absolutely continuous, which is traditionally interpreted (see [8] for a nice overview) as the existence of transport for the whole set of energies E satisfying $|E| \geq \delta$.

In this paper, we are concerned with spectral stability properties of H_0 . More specifically, we consider a general matrix multiplication operator

$$V := \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}, \quad (3)$$

whose coefficients are bounded complex-valued functions $V_{11}, V_{12}, V_{21}, V_{22} : \mathbb{R}^2 \rightarrow \mathbb{C}$, and study the spectrum of the perturbed operator

$$H_\varepsilon := H_0 + \varepsilon V, \quad \text{dom } H_\varepsilon = \text{dom } H_0,$$

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as the positive coupling parameter ε tends to zero. To make H_ε self-adjoint, we always assume that V_{11} and V_{22} are in fact real-valued, while V_{12} and V_{21} are allowed to be complex-valued but the Hermiticity relation $V_{21} = \overline{V_{12}}$ is postulated. In addition, we assume that V_{11}, V_{12}, V_{22} are vanishing at infinity, in order to have (cf. [7, § 4.3.4]) the stability of the essential spectrum

$$\sigma_{\text{ess}}(H_\varepsilon) = (-\infty, -\delta] \cup [\delta, \infty). \quad (4)$$

Recall that the essential spectrum is composed of accumulation points of the spectrum and possibly also of infinitely degenerate eigenvalues. For the stability issues, we are more interested in the discrete spectrum $\sigma_{\text{disc}}(H_\varepsilon)$, which consists of isolated eigenvalues of finite multiplicities in the essential spectral gap $(-\delta, \delta)$. Physically, the eigenvalues are energies of bound states of H_ε representing stationary solutions of the time-dependent Dirac equation. Our objective is to derive physically relevant sufficient and necessary conditions for the existence of the discrete eigenvalues. Contrary to the Schrödinger case, this is methodologically by no means evident, for no direct variational principles are available for the operator H_ε due to its unboundedness from below.

Our strategy to overcome this difficulty is to pass to the square H_ε^2 , which is a non-negative operator, apply the standard variational principle (see, e.g., [9, § 4.5]) to it and employ the spectral mapping equivalence

$$E \in \sigma(H_\varepsilon) \iff E^2 \in \sigma(H_\varepsilon^2) \quad (5)$$

valid for all real energies E . Consequently, in order to ensure that there exists a discrete eigenvalue $E \in (-\delta, \delta)$, it is enough to construct a test function $\psi \in \text{dom } H_0$ such that

$$Q_\varepsilon[\psi] := \|H_\varepsilon \psi\|_{\mathcal{H}}^2 - \delta^2 \|\psi\|_{\mathcal{H}}^2 < 0. \quad (6)$$

Motivated by the theory of quantum waveguides [10], we choose the test function as follows. Observing that, formally(!), $H_0 \psi^\pm \stackrel{!}{=} \delta^2 \psi^\pm$, where

$$\psi^+ := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \psi^- := \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (7)$$

we see that ψ^\pm are generalised eigenvectors of H_0^2 corresponding to the ionisation energy δ^2 . Therefore they are generalised minimisers of the functional Q_0 and it is admissible to expect them to be suitable building blocks for possible minimisers of Q_ε as well, at least if ε is small. Still formally(!), one easily computes

$$\begin{aligned} Q_\varepsilon[\psi^+] &\stackrel{!}{=} \int_{\mathbb{R}^2} (\varepsilon^2 |V_{11}|^2 + \varepsilon^2 |V_{12}|^2 + 2\delta\varepsilon \Re V_{12}) =: I_\varepsilon^+, \\ Q_\varepsilon[\psi^-] &\stackrel{!}{=} \int_{\mathbb{R}^2} (\varepsilon^2 |V_{22}|^2 + \varepsilon^2 |V_{12}|^2 + 2\delta\varepsilon \Re V_{12}) =: I_\varepsilon^-. \end{aligned} \quad (8)$$

To make sense of the integrals, we henceforth assume $V_{11}, V_{22} \in L^2(\mathbb{R}^2)$ and $V_{12} \in L^2(\mathbb{R}^2) \cap L^1(\mathbb{R}^2)$. We have thus obtained the following sufficient condition:

$$(I_\varepsilon^+ < 0 \quad \text{or} \quad I_\varepsilon^- < 0) \implies \sigma_{\text{disc}}(H_\varepsilon) \neq \emptyset, \quad (9)$$

meaning that H_ε possesses at least one isolated eigenvalue of finite multiplicity located in the interval $(-\delta, \delta)$. As a matter of fact, the variational principle implies that H_ε possesses at least two discrete eigenvalues (counting multiplicities) provided that $I_\varepsilon^+ < 0$ and $I_\varepsilon^- < 0$ hold, because the test functions ψ^\pm are mutually orthogonal.

To justify the formal computations above ($\psi^\pm \notin \mathcal{H}$!), we replace the inadmissible test functions (7) by their regularised versions $\psi_n^\pm := \phi_n \psi^\pm$ with $n > 1$. Here $\phi_n : \mathbb{R}^2 \rightarrow \mathbb{R}$ is a smooth

function of compact support such that $\phi_n = 1$ on the disk of radius n , $\phi_n = 0$ outside the disk of radius n^2 and $\phi_n(\mathbf{r}) := \xi(f(\mathbf{r}))$ elsewhere, where $f(\mathbf{r}) := \log_n(n^2/r)$ with $r := |\mathbf{r}|$ and $\xi : \mathbb{R} \rightarrow [0, 1]$ is any smooth function such that $\xi = 0$ in a right neighbourhood of 0 and $\xi = 1$ in a left neighbourhood of 1. Then the formal results (8) are indeed justified through the limits $Q_\varepsilon[\psi_n^\pm] \rightarrow I_\varepsilon^\pm$ as $n \rightarrow \infty$. Consequently, assuming $I_\varepsilon^+ < 0$ (respectively, $I_\varepsilon^- < 0$), then there exists a positive number n_0 such that $Q_\varepsilon[\psi_n^+] < 0$ (respectively, $Q_\varepsilon[\psi_n^-] < 0$) for all $n > n_0$. Hence (9) holds true as well as the remark about the existence of two discrete eigenvalues.

It is remarkable that the sufficient condition (9) is always satisfied in the weakly coupled regime provided that

$$\Re V_{12} < 0. \quad (10)$$

Indeed, under this condition, there obviously exists a positive number ε_0 such $I_\varepsilon^+ < 0$ and $I_\varepsilon^- < 0$ for all $\varepsilon < \varepsilon_0$. It follows that, for all sufficiently small ε , H_ε possesses at least two isolated eigenvalues of finite multiplicities located in the interval $(-\delta, \delta)$. We interpret the result as the *spectral instability* (or *criticality*) of H_0 , for there always exists an electromagnetic potential V such that the spectrum of H_ε with an arbitrarily small ε differs from that of H_0 given by (2).

A special situation in which the discrete spectrum exists is the potential V with vanishing diagonal components $V_{11} = 0 = V_{22}$ and the off-diagonal component V_{12} satisfying (10). In this case the critical coupling constant satisfies

$$\varepsilon_0 \geq \frac{-2\delta \langle \Re V_{12} \rangle}{\|V_{12}\|^2}, \quad (11)$$

where we abbreviate $\langle \Re V_{12} \rangle := \int_{\mathbb{R}^2} \Re V_{12}$ and $\|\cdot\|$ denotes the norm of $L^2(\mathbb{R}^2)$.

At least in this special setting and if V_{12} is real-valued, it is worth noticing that (10) represents also a necessary condition for the existence of discrete spectrum. To see it, let us now assume that $V_{11} = 0 = V_{22}$ and

$$V_{12} = V_{21} \geq 0. \quad (12)$$

From the first component of the eigenvalue equation $H_0 \psi = E \psi$, we get $\psi_2 = -R(-i\partial_y - E)\psi_1$, where the inverse $R := (-\partial_x^2 + \delta + \varepsilon V_{12})^{-1}$ is a well defined isomorphism on $L^2(\mathbb{R}^2)$ because of (12). Plugging this relationship between ψ_1 and ψ_2 into the second component of the eigenvalue equation, we arrive at the functional identity

$$(-\partial_x^2 + \delta + \varepsilon V_{21})\psi_1 - (i\partial_y - E)R(-i\partial_y - E)\psi_1 = 0.$$

Multiplying both sides by $\overline{\psi_1}$, integrating over \mathbb{R}^2 , taking the real part of the obtained scalar identity and using the self-adjointness of R , we get

$$\|\partial_x \psi_1\|^2 + \delta \|\psi_1\|^2 + (\psi_1, \varepsilon V_{21} \psi_1) + \|R^{1/2} \partial_y \psi_1\|^2 = E^2 \|R^{1/2} \psi_1\|^2, \quad (13)$$

where (\cdot, \cdot) denotes the inner product of $L^2(\mathbb{R}^2)$ associated with $\|\cdot\|$. Since V_{12} is assumed to be real-valued, $-\partial_x^2 + \delta + \varepsilon V_{12}(x, y)$ considered as an operator in $L^2(\mathbb{R})$ parametrically dependent on y is self-adjoint. Recalling in addition that $V_{12} \geq 0$ vanishes at infinity, so that the spectrum of the one-dimensional Schrödinger operator equals $[\delta, \infty)$, one has the estimate

$$\|R^{1/2} \psi_1\|^2 \leq \|R\| \|\psi_1\|^2 = \delta^{-1} \|\psi_1\|^2.$$

Using this bound in (13), we finally get $\delta^2 \leq E^2$, which proves that the discrete spectrum of H_ε is empty in view of (5) and (4).

Our last theoretical objective is to establish quantitative bounds for the discrete eigenvalues existing under the hypothesis (10) in the weakly coupled regime. To this aim, we henceforth assume that the bounded functions V_{11}, V_{12}, V_{22} are compactly supported. As in the beginning, we allow V_{12} to be complex-valued. By the variational principle, one has the bound

$$E^2 - \delta^2 \leq \frac{Q_\varepsilon[\psi_n^\pm]}{\|\psi_n^\pm\|_{\mathcal{H}}^2},$$

where the test functions ψ_n^\pm are the regularised versions of (7) as above.

Let us begin with the test function ψ_n^+ . One has

$$\begin{aligned} \|H_\varepsilon \psi_n^+\|_{\mathcal{H}}^2 &= \|(-\partial_x^2 + \delta + \varepsilon V_{21})\phi_n\|^2 + \|(-i\partial_y + \varepsilon V_{11})\phi_n\|^2 \\ &= \|\partial_x^2 \phi_n\|^2 + \delta^2 \|\phi_n\|^2 + 2\delta \|\partial_x \phi_n\|^2 + \|\partial_y \phi_n\|^2 + I_\varepsilon^+, \end{aligned}$$

where the second equality holds for all sufficiently large n when V_{12} and $\partial_x^2 \phi_n$ (and V_{11} and $\partial_y \phi_n$) have disjoint supports. Using the chain rule when differentiating ϕ_n , estimating the derivative of ξ by its maximal value $\|\xi'\|_\infty := \max_{[0,1]} |\xi'|$ and passing to polar coordinates, we have

$$\|\partial_x \phi_n\|^2 \leq \frac{\|\xi'\|_\infty^2}{\log^2 n} \int_{\{n < r < n^2\}} \frac{x^2}{r^4} dx dy = \frac{c_1}{\log n},$$

where $c_1 := \pi \|\xi'\|_\infty^2$. The same estimate holds for $\|\partial_y \phi_n\|$. Similarly,

$$\begin{aligned} \|\partial_x^2 \phi_n\|^2 &\leq \frac{2\|\xi''\|_\infty^2}{\log^4 n} \int_{\{n < r < n^2\}} \frac{x^4}{r^8} dx dy \\ &\quad + \frac{2\|\xi'\|_\infty^2}{\log^2 n} \int_{\{n < r < n^2\}} \frac{(x^2 - y^2)^2}{r^8} dx dy \\ &= \left(\frac{3\pi \|\xi''\|_\infty^2}{4\log^4 n} + \frac{\pi \|\xi'\|_\infty^2}{\log^2 n} \right) \left(\frac{1}{n^2} - \frac{1}{n^4} \right) \\ &\leq \left(\frac{3\pi \|\xi''\|_\infty^2}{4\log n} + \frac{\pi \|\xi'\|_\infty^2}{\log n} \right) \frac{1}{e^2} =: \frac{c_2}{\log n}, \end{aligned}$$

where e is the base of the natural logarithm \log and the last, crude estimate holds for all $n \geq e$.

Using these estimates, we observe that $Q_\varepsilon[\psi_n^+] \rightarrow I_\varepsilon^+$ as $n \rightarrow \infty$, in agreement with our claim above. Under the hypothesis (10), the limit I_ε^+ is negative for all sufficiently small ε ; in fact, whenever

$$\varepsilon < \frac{-2\delta \langle \Re V_{12} \rangle}{\|V_{11}\|^2 + \|V_{12}\|^2}.$$

Henceforth we therefore assume this inequality and then choose $n \geq e$ so large that $Q_\varepsilon[\psi_n^+]$ is negative. Finally, using

$$\|\psi_n^+\|_{\mathcal{H}}^2 = \|\phi_n\|^2 \leq \int_{\{r < n^2\}} 1 dx dy = \pi n^4,$$

it follows that

$$E^2 - \delta^2 \leq \frac{1}{\pi n^4} \left(\frac{c}{\log n} + I_\varepsilon^+ \right) =: g^+(\varepsilon, n),$$

where $c := c_1 + 2\delta c_1 + c_2$.

Using the test function ψ_n^- instead of ψ_n^+ , the proof follows analogously. In fact, it is enough to replace V_{11} by V_{22} (and

thus I_ε^+ by I_ε^-) in the formulae above. In particular, we have $E^2 - \delta^2 \leq g^-(\varepsilon, n)$, where g^- is defined as g^+ with I_ε^+ being replaced by I_ε^- .

The function $n \mapsto g^\pm(\varepsilon, n)$ achieves its negative minimum for the critical value n_ε^\pm satisfying

$$\frac{1}{\log n_\varepsilon^\pm} := \frac{-2I_\varepsilon^\pm}{c + \sqrt{c^2 - cI_\varepsilon^\pm}}$$

(notice that $n_\varepsilon^\pm \rightarrow \infty$ as $\varepsilon \rightarrow 0$). In summary, we have got an explicit quantitative bound for the discrete energies

$$E^2 - \delta^2 \leq g^\pm(\varepsilon, n_\varepsilon^\pm). \quad (14)$$

In the weakly coupled regime, one has

$$g^\pm(\varepsilon, n_\varepsilon^\pm) \approx -\frac{\delta^2 \langle \Re V_{12} \rangle^2 \varepsilon^2}{\pi c} \exp\left(\frac{2c}{\delta \langle \Re V_{12} \rangle \varepsilon}\right) \quad (15)$$

as $\varepsilon \rightarrow 0$.

Now we turn to numerical verifications of the established theoretical results. Our numerical scheme consists in expanding the components ψ_1, ψ_2 of an eigenvector $\psi \in \text{dom } H_0 \subset \mathcal{H}$ of H_ε corresponding to an eigenvalue E into a basis $\{\varphi_j\}_{j=1}^\infty$ of $L^2(\mathbb{R}^2)$:

$$\psi_1 = \sum_{j=1}^\infty a_j \varphi_j \quad \text{and} \quad \psi_2 = \sum_{j=1}^\infty b_j \varphi_j,$$

where $a_j := (\varphi_j, \psi_1)$ and $b_j := (\varphi_j, \psi_2)$. The eigenvalue problem $H_\varepsilon \psi = E \psi$ in \mathcal{H} is cast into a system of algebraic equations for the coefficients $\mathbf{a} := \{a_j\}_{j=1}^\infty$ and $\mathbf{b} := \{b_j\}_{j=1}^\infty$ in the sequence space ℓ^2 :

$$\begin{pmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{21} & \mathbf{C}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = E \begin{pmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{D} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix},$$

where

$$\begin{aligned} \mathbf{C}_{11} &:= \{(\varphi_k, -i\partial_y \varphi_j) + (\varphi_k, \varepsilon V_{11} \varphi_j)\}_{k,j=1}^\infty, \\ \mathbf{C}_{12} &:= \{(\varphi_k, (-\partial_x^2 + \delta)\varphi_j) + (\varphi_k, \varepsilon V_{12} \varphi_j)\}_{k,j=1}^\infty, \\ \mathbf{C}_{21} &:= \{(\varphi_k, (-\partial_x^2 + \delta)\varphi_j) + (\varphi_k, \varepsilon V_{21} \varphi_j)\}_{k,j=1}^\infty, \\ \mathbf{C}_{22} &:= \{(\varphi_k, i\partial_y \varphi_j) + (\varphi_k, \varepsilon V_{22} \varphi_j)\}_{k,j=1}^\infty, \\ \mathbf{D} &:= \{(\varphi_k, \varphi_j)\}_{k,j=1}^\infty. \end{aligned}$$

The numerical approximation consists in replacing the infinite matrices by finite ones. The obtained system can be then solved by standard tools of numerical linear algebra. Since no natural basis seems to be available for the problem, we choose the basis consisting of Gaussian radial basis function centered at a set of scattered nodes, in the line of the Radial Basis Function Method.

In our numerical experiments, we considered potentials V with coefficients being either piecewise-constant or fastly decaying functions. In both cases, we got the same qualitative behaviour of the eigenvalues and a quantitative verification of the spectral enclosure (14). Therefore it is expected that this bound is more universal.

The dependence of several eigenvalues (blue curves) on the coupling parameter ε in the gap $(-\delta, \delta)$ is depicted in Fig. 1 for two settings. In both cases, χ_D denotes the characteristic function of the disk D of radius 2 centered at the origin and $\delta = 5$. We also plot the bounds $\pm h$ (red curves) of the estimates

$$-h(\varepsilon) \leq E(\varepsilon) \leq h(\varepsilon) := \sqrt{\delta^2 + g^\pm(\varepsilon, n_\varepsilon^\pm)} \quad (16)$$

directly obtained from (14). It turns out that the bounds (16) become too crude for larger values of ε .

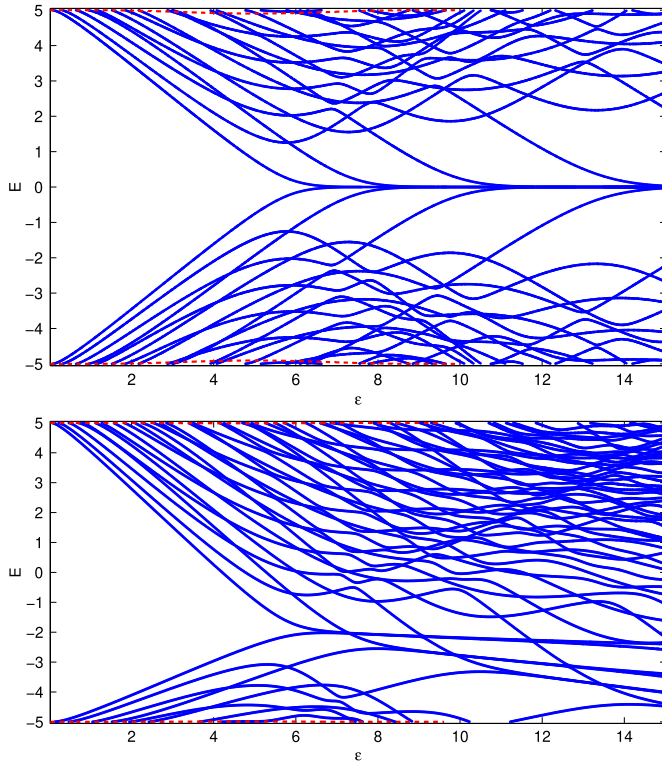


Fig. 1. Plots of eigencurves $E(\varepsilon)$ (in blue) and the bounds $h(\varepsilon)$ of (16) (in red) for $\delta = 5$. The apparently symmetric setting in the upper figure is due to the choice $V_{11} = 0 = V_{22}$ and $V_{21} = -\chi_D$, while the lower figure corresponds to $V_{21} = -\chi_D$, $V_{11} = 0.2\chi_D$, $V_{22} = -0.9\chi_D$. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

Fig. 2 visualises the ground and excited states.

In conclusion, we have derived sufficient and necessary conditions for the existence of discrete energies in semi-Dirac semi-metals perturbed by general local electromagnetic fields. The existence of bound states is particularly ensured in the regime of weak coupling provided that the off-diagonal component of the perturbation is attractive in the sense of (10). On the other hand, the discrete spectrum is empty in the opposite regime of real-valued repulsive off-diagonal component and absent diagonal components. We have also derived an explicit quantitative bound (14) for the discrete energies. Numerical experiments support our theoretical results and predict the existence of excited states as well.

Because of the tremendous progress in manipulation with materials whose low-energy excitations are described by semi-Dirac fermions, it is our belief that an experimental verification of our theoretical predictions is within the reach of contemporary physics. The simplest experimental setting should be considering an electromagnetic potential (3) with $V_{11} = 0 = V_{22}$ and $V_{12} = \overline{V_{21}}$ being a locally distributed perturbation (possibly piecewise constant). We predict that the transport properties of the material should significantly depend on the sign of $\Re V_{12}$. Is the estimate (11) on the critical coupling sharp? Do the bound state energies follow the theoretical estimate (14) with (15) in the weakly coupled regime?

The present model is challenging also from purely mathematical perspectives. Because of unavailability of an explicit form of the kernel of the resolvent operator of the unperturbed Hamiltonian H_0 , we have not been able to apply the traditional approach to weakly coupled bound states based on the Birman–Schwinger principle (see the classical reference [11] in the Schrödinger case).

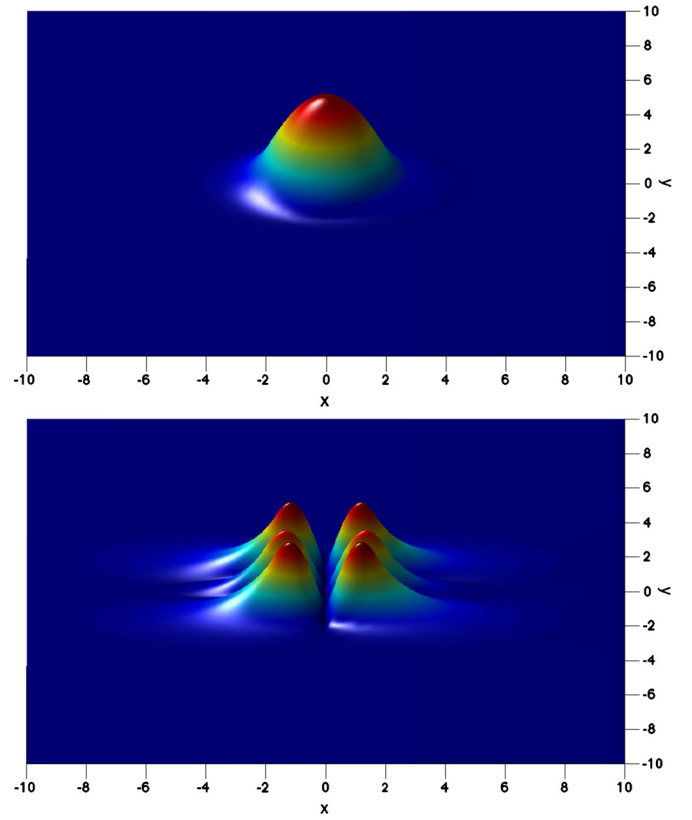


Fig. 2. Plots of the magnitude $|\psi|$ of eigenfunctions ψ corresponding to eigenvalues $E \approx 2.9893$ (up) and $E \approx 4.8284$ (down) of the symmetric setting of Fig. 1 for $\varepsilon = 2.5$.

In particular, we leave as an open problem how to establish a (good) lower bound for discrete energies complementing (14), without speaking about the exact asymptotics as $\varepsilon \rightarrow 0$. It is also challenging to study perturbations of the non-self-adjoint model recently introduced in [5].

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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