SPECTRAL GAPS IN GRAPHENE ANTIDOT LATTICES

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Abstract. We consider the gap creation problem in an antidot graphene lattice, i.e. a sheet of graphene with periodically distributed obstacles. We prove several spectral results concerning the size of the gap and its dependence on different natural parameters related to the antidot lattice.

1. Introduction

Graphene, a two-dimensional material made of carbon atoms arranged in a honeycomb structure, has risen a lot of attention due to its many unique properties. Remarkably, charge carriers close to the Fermi energy behave as massless Dirac fermions. This is due to its energy band structure which exhibits two bands crossing at the Fermi level making graphene a gapless semimetal [5]. Many efforts have been carried out for the possibility of tuning an energy gap in graphene [6].

The main physical motivation of our work is related to the so-called antidot graphene lattice [13], which consists of a regular sheet of graphene having a periodic array of obstacles well separated from each other. These obstacles can be thought, for instance, as actual holes in the graphene layer [13]. More generally, substrate induced obstacles [9] or those created by doping or by mechanical defects have also been considered in the literature (see e.g., [6] and references therein). It has been observed both experimentally and numerically that such an array causes a band gap to open up around the Fermi level, turning graphene from a semimetal into a gapped semiconductor (see e.g., [3], [9], and [6]).

In [7] and [4] there are given several proposals concerning the modelling of this phenomenon. In one of these proposals the authors replace the usual tight-binding lattice model by a two-dimensional massless Dirac operator, while a hole is modeled with the help of a periodic mass term. For a large mass term held fixed the authors numerically analyse how the gap appearing near the zero energy depends on the natural parameters of the antidot lattice, namely, the area occupied by one mass-insertion versus the area of the super unit-cell which contains only one such hole. For holes with armchair type of boundaries, this model is in very good agreement with tight-binding and density functional ab-initio calculations [4] (see also [3, 11, 12]). Moreover, the Dirac operator with a mass term varying in a superlattice has also been used to explain the gap appearing when a layer of graphene is placed on substrate of hexagonal boron nitride [9] (see also [15] for the inclusion of electronic interaction).

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In this article we consider the Dirac model with a periodic mass term and we estimate the size of the energy gap in terms of the strength and shape of the mass-insertion together with the natural parameters of the antidot lattice. Let us now formulate more precisely the problem we want to investigate.

1.1. Setting and main results. Let $\chi : \mathbb{R}^2 \to \mathbb{R}$ be a bounded function supported on a compact subset $S$ included in $\Omega := (-1/2, 1/2)^2$ satisfying
\[ \int_{\Omega} \chi(x) dx := \Phi \geq 0 \quad \text{and} \quad \int_{\Omega} |\chi(x)|^2 dx = 1. \tag{1.1} \]
We use the standard notation for the Pauli matrices
\[ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]
We define the massless free Dirac operator in $L^2(\mathbb{R}^2, \mathbb{C}^2)$ as
\[ H_0 := \frac{1}{i} \sigma \cdot \nabla = \begin{pmatrix} 0 & -i \partial_1 - \partial_2 \\ -i \partial_1 + \partial_2 & 0 \end{pmatrix}. \tag{1.2} \]
Let $\alpha \in (0, 1]$ be a dimensionless parameter and let $L > 0$ have dimensions of length. In physical units, the operator describing a mass-periodically perturbed graphene sheet is given by
\[ \tilde{H}(\alpha, \mu, L) = \hbar v_F H_0 + \sigma_3 \mu \sum_{\gamma \in \mathbb{Z}^2} \chi(x - \gamma L \alpha L). \tag{1.3} \]
where $\hbar$ is Plank’s constant divided by $2\pi$ and $v_F$ is the Fermi velocity in graphene. Here $\mu \geq 0$ has dimensions of energy and represents the strength of the mass-insertion which is $L\mathbb{Z}^2$-periodic. We note that in order for the continuum Dirac model to hold one needs $L$ to be much larger than the distance between the carbon atoms constituting graphene.

As it is well known, the spectrum of $H_0$ covers the whole real line. Our main interest in this paper is finding sufficient conditions that the function $\chi$ must satisfy in order to create a gap around zero in the spectrum of $\tilde{H}$ and to estimate its size in terms of $\alpha, \mu,$ and $L$. By making the scaling transformation $x \mapsto Lx$ one gets that
\[ \tilde{H}(\alpha, \mu, L) = \frac{\hbar v_F}{L} H_0 \left( \alpha, \frac{\mu L}{\hbar v_F} \right). \tag{1.4} \]
Note that $\frac{\mu L}{\hbar v_F}$ is a dimensionless parameter. Here, for $\beta > 0$, we define the operator in $L^2(\mathbb{R}^2, \mathbb{C}^2)$
\[ H(\alpha, \beta) := H_0 + \sigma_3 \beta \sum_{\gamma \in \mathbb{Z}^2} \chi(x - \gamma \alpha). \tag{1.5} \]
This new operator is clearly periodic with respect to $\mathbb{Z}^2$ and (just like $\tilde{H}$) it is self-adjoint on the first Sobolev space $H^1(\mathbb{R}^2, \mathbb{C}^2)$ (see [10]).

Given a self-adjoint operator $T$, we denote by $\rho(T)$ its resolvent set. Here is the first main result of our paper.
**Theorem 1.1.** Assume $\Phi \neq 0$. Then there exist two constants $C > 0$ and $\delta \in (0, 1)$ such that for all $\alpha \in (0, 1/2]$ and $\beta > 0$ obeying $\alpha \beta < \delta$ we have

$$[-\alpha^2 \beta (\Phi - C\alpha \beta), \alpha^2 \beta (\Phi - C\alpha \beta)] \subset \rho(H(\alpha, \beta)).$$

**Remark.** Let us comment on the consequences of this result regarding the energy gap, $E_g$, for the family $\tilde{H}$ defined in (1.3). Let us define the area of the supercell $A_t := L^2$ and $A_r := \alpha^2 L^2$ representing the area supporting one mass perturbation. In view of (1.4), Theorem 1.1 states that for $\alpha \frac{\mu L}{\hbar v_F}$ small enough and for $\Phi$ in (1.1) positive

$$E_g \gtrsim \mu \Phi \alpha^2 = \mu \Phi \frac{A_r}{A_t}. \quad (1.6)$$

Remarkably this estimate does not depend on the side $L$ of the supercell. This is to be contrasted with the regime of $\mu \to \infty$ considered in [13] and [4] where it was found that, for $\alpha$ small enough (see e.g., Equation A.8 of [4]),

$$E_g \sim \frac{\hbar v_F}{L} \sqrt{\frac{A_r}{A_t}}. \quad (1.7)$$

This latter regime can be mathematically investigated using the Dirac operator with infinite mass boundary conditions proposed in [2] (see [1] for its rigorous definition).

In the case $\Phi = 0$ it is still possible to prove the existence of a gap opening at zero. The next result needs some assumptions on $\chi$ in terms of its Fourier coefficients

$$\hat{\chi}(m) = \int_{\Omega} e^{-2\pi i m \cdot x} \chi(x) dx, \quad m \in \mathbb{Z}^2. \quad (1.8)$$

Note that $\Phi = 0$ means that $\hat{\chi}(0, 0) = 0$. In terms of the operator $H$ in (1.5), this time we keep $\alpha = 1$ and we make $\beta$ smaller than certain constant times the $L^\infty$-norm of $\chi$. Then the gap can still survive but it scales with $\beta^3$ instead of $\beta$. As a consequence, the gap for $\tilde{H}$ has the following behaviour, for $\alpha \frac{\mu L}{\hbar v_F}$ small enough,

$$E_g \gtrsim \mu \left( \frac{\mu L}{\hbar v_F} \right)^2. \quad (1.9)$$

**Theorem 1.2.** Assume $\Phi = \hat{\chi}(0, 0) = 0$, and at the same time:

$$\sum_{m \neq 0} \sum_{m' \neq 0} \frac{m \cdot m'}{|m|^2 |m'|^2} \bar{\chi}(m) \chi(m') \hat{\chi}(m - m') \neq 0. \quad (1.10)$$

Then there exist two positive numerical constants $\beta_0$ and $C$ such that for every $0 < \beta < \beta_0/\|\chi\|_\infty$ we have

$$[-C\beta^3, C\beta^3] \subset \rho(H(1, \beta)).$$
Let us describe a particular class of potentials where assumption (1.10) holds true. Assume that $\chi(x)$ is of the form

$$\chi(x) = \sum_{N-10 \leq |m| \leq N+10} 2 \cos(2\pi m \cdot x), \quad N \gg 1.$$ 

By construction, all the Fourier coefficients $\hat{\chi}(m) = \hat{\chi}(-m)$ equal either 1 or 0. The non-zero coefficients are those for which $m$ lies in an annulus with outer radius $N + 10$ and inner radius $N - 10$. When $N$ becomes large enough, the triples of vectors $m$, $m'$ and $m - m'$ for which the Fourier coefficients in (1.10) are simultaneously non-zero form a triangle which “almost” coincides with an equilateral triangle with side-length equal to $N$. Here “almost” means that the angle between $m$ and $m'$ is close to $\pi/3$ when $N$ is large enough. Thus the scalar product $m \cdot m'$ is positive whenever the Fourier coefficients are non-zero (provided $N$ is large enough) and the double sum in (1.10) is also positive.

In the rest of the paper we give the proof of the two theorems listed above.

2. Proof of Theorem 1.1

Throughout this work we use the notation

$$\|f\|_p = \left( \int_{\Omega} |f(x)|^p dx \right)^{1/p}, \quad p \in [1, \infty).$$

Note that our conditions on $\chi$ imply:

$$0 < \Phi \leq \|\chi\|_1 \leq \|\chi\|_2 = 1.$$ 

(2.11)

2.1. Bloch-Floquet representation and proof of Theorem 1.1

In this subsection we start by presenting the main strategy of the proof of Theorem 1.1. It consists of a suitable application of the Feshbach inversion formula to the Bloch-Floquet fiber of $H(\alpha, \beta)$. The main technical ingredients are Lemmas 2.2 and 2.3 whose proof can be found in the next subsection. At the end of this subsection we present the proof of Theorem 1.1.

Let $\mathcal{S}(\mathbb{R}^2, \mathbb{C})$ denote the Schwartz space of test functions. Consider the map

$$\tilde{U} : \mathcal{S}(\mathbb{R}^2, \mathbb{C}) \subset L^2(\mathbb{R}^2, \mathbb{C}) \longrightarrow L^2(\Omega, L^2(\Omega, \mathbb{C})),

(\tilde{U} \Psi)(x; k) := \sum_{\gamma \in \mathbb{Z}^2} e^{2\pi i k \cdot (x + \gamma)} \Psi(x + \gamma), \quad x, k \in \Omega.$$

It is well known (see [14]) that $\tilde{U}$ is an isometry in $L^2(\mathbb{R}^2, \mathbb{C})$ that can be extended to a unitary operator. We denote its unitary extension by the same symbol. We define the Bloch-Floquet transform as $U := \tilde{U} \otimes 1_{\mathbb{C}^2}$. Then we have that

$$U H(\alpha, \beta) U^* = \int_{\Omega} h_k(\alpha, \beta) dk, \quad h_k(\alpha, \beta) := (-i\nabla_{x}^{\text{PBC}} - 2\pi k) \cdot \sigma + \beta \chi_\alpha(x)\sigma_3,$$

where $\mathcal{P}^{\text{PBC}}$ is the periodic boundary condition.
where each fiber Hamiltonian \( h_k(\alpha, \beta) \) is defined in \( L^2(\Omega, \mathbb{C}^2) \). Here \( \nabla_x^{\text{PBC}} \) is the gradient operator with periodic boundary conditions and
\[
\chi_\alpha(x) := \chi(x/\alpha).
\]
The spectra of \( H(\alpha, \beta) \) and \( h_k(\alpha, \beta) \) are related through
\[
\sigma(H(\alpha, \beta)) = \bigcup_{k \in \Omega} \sigma(h_k(\alpha, \beta)). \tag{2.12}
\]
We will use the standard eigenbasis of \( \nabla_x^{\text{PBC}} \) given by
\[
\psi_m(x) := e^{2\pi i m \cdot x}, \quad m \in \mathbb{Z}^2, \ x \in \Omega,
\]
which is periodic and satisfies
\[
-i \nabla_x^{\text{PBC}} \psi_m = 2\pi m \psi_m.
\]
For \( m \in \mathbb{Z}^2 \) define the projections
\[
P_m := |\psi_m\rangle \langle \psi_m| \otimes 1_{\mathbb{C}^2} \quad \text{and} \quad Q_0 := \text{Id} - P_0. \tag{2.13}
\]

**Lemma 2.1.** Let \( \alpha \in (0, 1) \) and \( \beta > 0 \). Then, for every \( k \in \Omega \) and \( \psi \in P_0L^2(\Omega, \mathbb{C}^2) \), we have that
\[
\|P_0 h_k(\alpha, \beta) P_0 \psi\| \geq \beta \alpha^2 \Phi \|\psi\|.
\]

**Proof.** For every \( k \in \Omega \) we have:
\[
P_0 h_k(\alpha, \beta) P_0 = (-2\pi \sigma \cdot k + \alpha^2 \beta \Phi \sigma_3)P_0.
\]
Using the anticommutation relations of the Pauli matrices we get for any \( \psi \in P_0L^2(\Omega, \mathbb{C}^2) \) that
\[
\|P_0 h_k(\alpha, \beta) P_0 \psi\|^2 = ((2\pi k)^2 + (\alpha^2 \beta \Phi)^2) \|\psi\|^2 \geq (\alpha^2 \beta \Phi)^2 \|\psi\|^2.
\]

The previous lemma shows that \( h_k(\alpha, \beta) \) has a spectral gap of order \( \beta \alpha^2 \) on the range of \( P_0 \). In order to investigate whether that is still the case on the full Hilbert space we use the Feshbach inversion formula (see Equations (6.1) and (6.2) in [10]). The latter states in this case that \( z \in \rho(h_k(\alpha, \beta)) \) if the Feshbach operator
\[
\mathcal{F}_{P_0}(z) := P_0(h_k(\alpha, \beta) - z)P_0 - \beta^2 P_0 \chi_\alpha \sigma_3 Q_0 (Q_0(h_k(\alpha, \beta) - z)Q_0)^{-1} Q_0 \chi_\alpha \sigma_3 P_0,
\]
is invertible on \( P_0L^2(\Omega, \mathbb{C}^2) \). Here we used that \( P_0 h_k(\alpha, \beta) Q_0 = \beta P_0 \chi_\alpha \sigma_3 Q_0 \).

The next lemma shows that the inverse of \( Q_0(h_k(\alpha, \beta) - z)Q_0 \) is well defined on the range of \( Q_0 \).

**Lemma 2.2.** There exists a constant \( \delta \in (0, 1) \) such that for all \( \alpha \in (0, 1/2) \) and \( \beta > 0 \) with \( \alpha \beta < \delta \), we have that \( Q_0(h_k(\alpha, \beta) - z)Q_0 \) is invertible on the range of \( Q_0 \), for any \( z \in [-\pi/2, \pi/2] \) and \( k \in \Omega \).
The following lemma controls the second term of the Feshbach operator $\mathcal{F}_{P_0}(z)$

$$\mathcal{B}_{P_0}(z) := \beta^2 P_0 \chi_\alpha \sigma_3 Q_0 (Q_0 (h_k(\alpha, \beta) - z) Q_0)^{-1} Q_0 \chi_\alpha \sigma_3 P_0.$$  

**Lemma 2.3.** There exist two constants $\delta \in (0, 1)$ and $C > 0$ such that for all $\alpha \in (0, 1/2)$ and $\beta > 0$ with $\alpha \beta < \delta$ we have

$$\|\mathcal{B}_{P_0}(z)\psi\| \leq C \beta^2 \alpha^3 \|\psi\|,$$

for any $z \in [-\pi/2, \pi/2]$, $k \in \Omega$, and $\psi \in P_0 L^2(\Omega, \mathbb{C}^2)$.

Having stated all the above ingredients we can proceed to the proof of our first main result.

**Proof of Theorem 1.1.** In view of (2.12) it is enough to show the invertibility of the Feshbach operator uniformly in $k \in \Omega$. Using Lemmas 2.1 and 2.3 we get that for any $\psi \in P_0 L^2(\Omega, \mathbb{C}^2)$

$$\|\mathcal{F}_{P_0}(z)\psi\| \geq \|(P_0(h_k(\alpha, \beta) - z) P_0)\psi\| - \|\mathcal{B}_{P_0}(z)\psi\| \geq (\beta\alpha^2\Phi - |z| - c_0^2 \beta^2) \|\psi\|.$$

This concludes the proof by picking $\alpha \beta$ so small that $\Phi > C \alpha \beta$. \hfill $\square$

### 2.2. Analysis of the Feshbach operator.

In this section we provide the proofs of Lemmas 2.2 and 2.3 from the previous section. For that sake, let us first state some preliminary estimates. Let

$$h_k^{(0)} := (-i \nabla_{x}^\text{PBC} - 2\pi k) \cdot \sigma$$

**Lemma 2.4.** There exists a constant $C > 0$, independent of $\alpha \in (0, 1)$, such that for all $k \in \Omega$

$$\|\sqrt{\chi_\alpha} P_0\| \leq \alpha$$

$$\||\chi_\alpha|^{1/2} (h_k^{(0)} \pm i)^{-1} |\chi_\alpha|^{1/2}\| \leq C(\alpha + \frac{\alpha^2}{1 - \alpha})$$

$$\||\chi_\alpha|^{1/2} (h_k^{(0)} \pm i)^{-1}\| \leq C(\sqrt{\alpha} + \frac{\alpha}{1 - \alpha}).$$

**Proof.** In order to show (2.15) we compute for $f, g \in L^2(\Omega, \mathbb{C}^2)$ (see also (2.11)):

$$|\langle f, \sqrt{|\chi_\alpha|} P_0 g \rangle| \leq |\langle f, \sqrt{|\chi_\alpha|} \psi_0 | \langle \psi_0, g \rangle | \leq \| \chi_\alpha \|^1/2 \| f \| \| g \| \leq \alpha \| f \| \| g \|.$$  

We now turn to the proof of equations (2.16) and (2.17). Denote the integral kernels of $(H_0 - i)^{-1}$ and $(h_k^{(0)} \pm i)^{-1}$ by $(H_0 - i)^{-1}(x, x')$ and $(h_k^{(0)} \pm i)^{-1}(x, x')$. In the proof we will use the identity for $x \neq x'$

$$(h_k^{(0)} - i)^{-1}(x, x') = \sum_{\gamma \in \mathbb{Z}^2} e^{2\pi i k \cdot (x + \gamma - x')}(H_0 - i)^{-1}(x + \gamma, x'), \quad x, x' \in \Omega.$$
Let us first estimate the quadratic form of \((h_{k_0}^{(0)} - i)^{-1}\) for any \(\phi, \psi \in L^2(\Omega, \mathbb{C}^2)\). According to Lemma A.1, we have
\[
|\langle \phi, (h_{k_0}^{(0)} - i)^{-1}\psi \rangle| \leq C \sum_{\gamma \in \mathbb{Z}^2} \int_{\Omega \times \Omega} |\phi(x)||\psi(x')| dxdx'
\]
\[
\leq Ce^{\sqrt{2}} \sum_{\gamma \in \mathbb{Z}^2} e^{-|\gamma|} \int_{\Omega \times \Omega} |\phi(x)||\psi(x')| dxdx',
\]
where in the last step we bound the exponential using that \(|x - x' - \gamma| \geq |\gamma| - |x - x'| \geq |\gamma| - \sqrt{2}.

Now assume that the support of \(\phi\) lies in \(\Omega_\alpha := (-\alpha/2, \alpha/2)^2\), i.e., \(\phi \in \Omega_\alpha\) above. Then it is easy to check that if \(\gamma \neq 0\) then \(|x - x' + \gamma| \geq (1 - \alpha)\). Therefore, we find for such a case that
\[
|\langle \phi, (h_{k_0}^{(0)} - i)^{-1}\psi \rangle| \leq Ce^{\sqrt{2}} \left( \int_{\Omega \times \Omega} \frac{|\phi(x)||\psi(x')|}{|x - x'|} dxdx' + \frac{1}{1 - \alpha} \left( \sum_{\gamma \neq 0} e^{-|\gamma|} \right) \|\phi\|_1 \|\psi\|_1 \right).
\]

Using the Hardy-Littlewood-Sobolev inequality for \(p = r = 4/3\) (see Lieb and Loss Theorem 4.3) we get
\[
\int_{\Omega \times \Omega} \frac{|\phi(x)||\psi(x')|}{|x - x'|} dxdx' \leq C\|\phi\|_{4/3}\|\psi\|_{4/3}.
\] (2.19)

Thus, denoting the universal constants by \(C\) we obtain, for any \(\phi, \psi \in L^2(\Omega, \mathbb{C}^2)\) with \(\text{supp}(\phi) \subset \Omega_\alpha\),
\[
|\langle \phi, (h_{k_0}^{(0)} - i)^{-1}\psi \rangle| \leq C \left( \|\phi\|_{4/3}\|\psi\|_{4/3} + (1 - \alpha)^{-1}\|\phi\|_1\|\psi\|_1 \right).
\] (2.20)

For some \(f \in L^2(\Omega, \mathbb{C}^2)\) we observe that (see Remark 2.11)
\[
\|\|\chi_\alpha\|^{1/2} f\|_1 \leq \|\|\chi_\alpha\|^{1/2}\|f\|_2 \leq \alpha\|f\|_2.
\] (2.21)

Moreover, Hölder’s inequality yields
\[
\|\|\chi_\alpha\|^{1/2} f\|_{4/3} \leq \left( \|\|\chi_\alpha\|^{2/3}\|f\|^{4/3}\|\|3/2 \right)^{3/4}
\]
\[
= \|\|\chi_\alpha\|^{1/2}\|f\|_2 \leq \sqrt{2}\|f\|_2.
\] (2.22)

In order to get the desired bounds we recall that the norm of an operator \(T\) is given by \(\|T\| = \sup_{f,g \neq 0} \|\langle f, Tg \rangle\|/\|\|f\|\|g\|\|\). Hence we find (2.16) by using (2.20) with \(\phi = \|\chi_\alpha\|^{1/2} f\) and \(\psi = \|\chi_\alpha\|^{1/2} g\) together with the bounds (2.21) and (2.22). Analogously, we obtain (2.17) using again (2.20) with \(\phi = \|\chi_\alpha\|^{1/2} f\) and \(\psi = g\). \(\square\)

**Lemma 2.5.** For any \(f \in \mathcal{D}(h_{k_0}^{(0)})\) we have
\[
\|h_{k_0}^{(0)} f\| \geq \pi\|f\|.
\] (2.23)
Proof. For all $m \in \mathbb{Z}^2$ and $k \in \Omega$, we have the identity
\[ P_m h_k^{(0)} P_m = 2\pi \sigma \cdot (m - k) P_m. \]
Thus, we obtain for all $f \in Q_0 D(h_k^{(0)})$,
\[ \| h_k^{(0)} Q_0 f \|^2 = (2\pi)^2 \sum_{m \neq 0} \| \sigma \cdot (m - k) P_m f \|^2 \geq \pi^2 \sum_{m \neq 0} \| P_m f \|^2. \]
\[ \square \]

Let us introduce some notation: For a self-adjoint operator $T$ and an orthogonal projection $Q$, we define
\[ \rho_Q(T) := \{ z \in \mathbb{C} \text{ such that } Q(T - z)Q : \text{Ran}Q \to \text{Ran}Q \text{ is invertible} \}. \]
We set
\[ R_0(z) := \left( Q_0(h_k^{(0)} - z)Q_0 |_{\text{Ran}Q_0} \right)^{-1}, \quad z \in \rho_Q(h_k^{(0)}), \]
\[ R(z) := \left( Q_0(h_k^{(0)} - z)Q_0 |_{\text{Ran}Q_0} \right)^{-1}, \quad z \in \rho_Q(h_k^{(0)}). \]
Let $U : L^2(\Omega, \mathbb{C}^2) \to \text{Ran}Q_0$ and $W : \text{Ran}Q_0 \to L^2(\Omega, \mathbb{C}^2)$ be defined as
\[ W := \sqrt{\beta} \left( \sqrt{|\chi_0|} \sigma_3 \right) Q_0, \]
\[ U := \sqrt{\beta} Q_0 \left( \text{sgn}(\chi_0) \sqrt{|\chi_0|} \right). \]

Lemma 2.6. There exists $C > 0$, independent of $\alpha \in (0, 1/2]$ and $\beta > 0$, such that for all $|z| \leq \pi/2$,
\[ \| WR_0(z)U \| < C\alpha \beta. \]
Proof. Note that due to Lemma 2.5 we have for $|z| \leq \pi/2$
\[ \| R_0(z) \| \leq \frac{2}{\pi}. \] (2.24)
Using the first resolvent identity
\[ WR_0(z)U = WR_0(i)U + (z - i)WR_0(i)^2U + (z - i)^2WR_0(i)R_0(z)R_0(i)U. \] (2.25)
We shall estimate separately each term on the right hand side of (2.25).
Since $h_k^{(0)}$ commutes separately each term on the right hand side of (2.25) we have
\[ R_0(i) = \left( h_k^{(0)} - i \right)^{-1} - \left( P_0(h_k^{(0)} - i)P_0 |_{\text{Ran}P_0} \right)^{-1}. \] (2.26)
Thus, using (2.15), we obtain the estimate
\[ \| W(P_0(h_k^{(0)} - i)P_0 |_{\text{Ran}P_0})^{-1}U \| \leq \beta \| \sqrt{|\chi_0|} P_0 \| \| (h_k^{(0)} - i)^{-1} \| \| \sqrt{P_0 |\chi_0|} \| \leq \beta \alpha^2. \] (2.27)
Lemma 2.7. For any $z \in S$ we have that $z \in \rho_{Q_0}(h_k(\alpha, \beta))$ and

$$R(z) = R_0(z) - R_0(z)U(1 + WR_0(z)U)^{-1}WR_0(z).$$

Proof. For $z \in S$ we define for short

$$B(z) := R_0(z) - R_0(z)U(1 + WR_0(z)U)^{-1}WR_0(z).$$

The identity (2.26) together with the inequalities (2.16) and (2.27), imply that there are universal constants $c, C > 0$, such that for $|\alpha| < 1/2$

$$\|WR_0(i)U\| \leq \|W(h_k(0) - i)^{-1}U\| + \|W(P_0(h_k(0) - i)P_0|_{\text{Ran}P_0})^{-1}U\| \leq c\beta\alpha + \beta\alpha^2 \leq C\beta\alpha.$$  (2.28)

This bounds the first term on the right hand side of (2.25). To estimate the second one we first notice that

$$(h_k(0) - i)^{-2} = (Q_0(h_k(0) - i)Q_0|_{\text{Ran}Q_0})^{-2} + (P_0(h_k(0) - i)P_0|_{\text{Ran}P_0})^{-2}$$

Therefore, using the same strategy as in (2.27), there exists $C > 0$ independent of $\alpha$ and $\beta$ such that

$$\|(z - i)WR_0(i)^2U\| = \|(z - i)W((h_k(0) - i)^{-2} - (P_0(h_k(0) - i)P_0|_{\text{Ran}P_0})^{-2})U\| \leq \|(z - i)W((h_k(0) - i)^{-2}U\| + |z - i|\beta\alpha^2 \leq \pi\beta\|\sqrt{|\chi_\alpha|}(h_k(0) - i)^{-1}\|\|\text{Ran}P_0(h_k - i)P_0^{-1}\| + \pi\beta\alpha^2 \leq C\beta\alpha,$$  (2.29)

where we used (2.17) in the last inequality.

Finally, we bound the last term on the right hand side of (2.25). Observe that from Lemma 2.4 and inequality (2.15), we obtain that there exists $c > 0$ such that for all $\alpha \leq 1/2$

$$\|\sqrt{|\chi_\alpha|}R_0(i)\| \leq \|\sqrt{|\chi_\alpha|}(h_k(0) - i)^{-1}\| + \|\sqrt{|\chi_\alpha|}P_0(h_k - i)P_0^{-1}\| \leq c\sqrt{\alpha}.$$  (2.27)

Therefore, using (2.24) and (2.17)

$$\|(z - i)^2WR_0(i)R_0(z)R_0(i)U\| \leq \beta|z - i|^2\|\sqrt{|\chi_\alpha|}R_0(i)\|\|R_0(z)\|\|R_0(i)\sqrt{|\chi_\alpha|}\| \leq C\beta|z - i|^2\alpha.$$  (2.25)

In view of (2.25), the latter bound together with (2.28) and (2.29) concludes the proof. $\square$

Before stating the next lemma we define the set

$$S := \{z \in \rho_{Q_0}(h_k(0)) : \|WR_0(z)U\| < 1\}.$$  (2.26)
Since \( \|WR_0(z)U\| < 1 \) we may use Neumann series to get
\[
B(z) = R_0(z) - R_0(z)U \left( \sum_{n \geq 0} (-1)^n(WR_0(z)U)^n \right)WR_0(z)
\]
\[
= R_0(z) \left[ 1 - \sum_{n \geq 0} (-1)^n(UWR_0(z)U)^nWR_0(z) \right] = R_0(z) \sum_{n \geq 0} (-1)^n(UWR_0(z))^n,
\]
where the absolute convergence of the last expression is a consequence of the identity:
\[
(UWR_0(z))^n = U(WR_0(z)U)^{n-1}WR_0(z), \quad n \geq 1,
\]
and the boundedness of \( U \) and \( W \).

For \( z \in \mathcal{S} \cap \mathbb{R} \) we define \( z_\varepsilon := z + i\varepsilon \). Since \( \mathcal{S} \) is an open set we may choose \( \varepsilon > 0 \) so small that \( z_\varepsilon \in \mathcal{S} \). We first prove that the claim holds for \( z_\varepsilon \). A simple iteration of the second resolvent identity gives
\[
R(z_\varepsilon) = R_0(z_\varepsilon) \sum_{n \geq 0} (-1)^n(UWR_0(z_\varepsilon))^n + T_{N+1},
\]
where
\[
T_{N+1} = (-1)^{N+1}(UWR_0(z_\varepsilon))^NW = (-1)^{N+1}U[WR_0(z_\varepsilon)U]^NW(z_\varepsilon).
\]
Hence \( \|T_{N+1}\| \) converges to zero and \( R(z_\varepsilon) = B(z_\varepsilon) \). Taking the limit \( \varepsilon \to 0 \) on the right hand side of this identity finishes the proof. \( \Box \)

**Proof of Lemmas 2.2 and 2.3.** Notice that the proof of Lemma 2.2 follows from Lemma 2.7 since \( z \in \mathcal{S} \) provided \( \alpha \beta \) is small enough (see Lemma 2.6).

In order to show Lemma 2.3 observe that
\[
\beta^2 \|P_0\chi_\alpha R_0(z)X_\alpha P_0\| \leq \beta \|P_0|\chi_\alpha^{1/2}\|WR_0(z)U\|\|X_\alpha^{1/2}P_0\| \leq c\beta^2\alpha^3,
\]
where we used Lemma 2.6 and (2.15). Moreover, assuming \( \alpha \beta \) is so small that \( \|WR_0(z)U\| < 1/2 \) we have
\[
\beta^2 \|P_0\chi_\alpha R_0(z)(1 + WR_0(z)U)^{-1}WR_0(z)X_\alpha P_0\|
\leq \beta \|P_0|\chi_\alpha^{1/2}\|WR_0(z)U\|\|1 + WR_0(z)U\|^{-1}\|WR_0(z)U\|\|X_\alpha^{1/2}P_0\|
\leq c\beta^3\alpha^4.
\]
The latter inequality together with (2.32) finishes the proof of Lemma 2.3 in view of the resolvent identity of Lemma 2.7. \( \Box \)

### 3. Proof of Theorem 1.2

In this section we remind that we fix \( \alpha = 1 \) in the definition of \( h_k(\alpha, \beta) \). Let us redenote the Feshbach operator \( F_{P_0}(z) \) by \( F_k(z) \) to emphasize its dependence on the vector \( k \in \Omega \):
\[
F_k(z) := P_0(h_k(1, \beta) - z)P_0 - \beta^2P_0X_3Q_0(Q_0(h_k(1, \beta) - z)Q_0)^{-1}Q_0X_3P_0.
\]
We shall later on prove that \( \mathcal{F}_k(0) \) is invertible for all \( k \in \Omega \), with an inverse uniformly bounded in \( k \). We now show that this information is enough for the existence of a gap near zero for the original operator \( H(1, \beta) \).

**Lemma 3.1.** Assume that there exists a constant \( C > 0 \) such that

\[
\sup_{k \in \Omega} \| \mathcal{F}_k(0)^{-1} \| \leq C/\beta^3. \tag{3.33}
\]

Then there exists a constant \( \tilde{C} > 0 \) such that for all \( |z| \leq \tilde{C} \beta^3 \), we have \( z \in \rho(H(1, \beta)) \).

**Proof.** There exists \( C' \) such that

\[
\sup_{k \in \Omega} \| \mathcal{F}_k(z) - \mathcal{F}_k(0) \| \leq C'|z|.
\]

Using (3.33) yields

\[
\sup_{k \in \Omega} \| (\mathcal{F}_k(z) - \mathcal{F}_k(0))\mathcal{F}_k(0)^{-1} \| \leq C'|z| \frac{C}{\beta^3}.
\]

Hence, \( \mathcal{F}_k(z) = [1 + (\mathcal{F}_k(z) - \mathcal{F}_k(0))\mathcal{F}_k(0)^{-1}] \mathcal{F}_k(0) \) is invertible for \( |z| \leq \frac{\beta^3}{2CC'} \) uniformly in \( k \in \Omega \). This implies that \( z \in \rho(H(1, \beta)) \). \( \square \)

Now we focus on proving the estimate (3.33). For that sake we consider two regimes in \( k \).

**Lemma 3.2.** Let \( \beta \in (0, \pi/(2\|\chi\|_{\infty})) \) and let \( k \in \Omega \) such that \( |k| > 2\beta^2/\pi^2 \). Then \( \mathcal{F}_k(0) \) is invertible and

\[
\sup_{k \in \Omega, |k| > 2\beta^2/\pi^2} \| \mathcal{F}_k(0)^{-1} \| \leq \frac{\pi}{2\beta^2}. \tag{3.34}
\]

**Proof.** From Lemma 2.5 we have \( \| h_k(1,0)f \| \geq \pi\|f\| \) for all \( f \in Q_0D(h_k(1,0)) \). Thus for \( \beta \in (0, \pi/(2\|\chi\|_{\infty})) \):

\[
\|Q_0h_k(1,\beta)f\| = \|h_k(1,0)f + Q_0\beta\chi\sigma_3f\| \geq \pi\|f\| - \beta\|\chi\|_{\infty}\|f\| \geq \frac{\pi}{2}\|f\|.
\]

Thus using \( \|\chi\|_2 = 1 \):

\[
\| \mathcal{F}_k(0) + 2\pi\sigma \cdot kP_0 \| = \beta^2\| \sigma_3P_0\chiQ_0[Q_0h_k(1,\beta)Q_0]^{-1}Q_0\chiP_0\sigma_3 \|
\leq \beta^2\| [Q_0h_k(1,\beta)Q_0]^{-1} \| \leq \frac{2}{\pi}\beta^2.
\]

We have the identity

\[
(P_02\pi\sigma \cdot kP_0)^{-1} = P_0 \frac{1}{2\pi k^2}\sigma \cdot k, \tag{3.36}
\]

hence under our assumption on \( k \) we get that the operator \( 1 - (\mathcal{F}_k(0) + 2\pi\sigma \cdot kP_0)(P_02\pi\sigma \cdot kP_0)^{-1} \) is invertible, and

\[
\| \mathcal{F}_k(0)^{-1} \| = \left\| P_0 \frac{1}{2\pi k^2}\sigma \cdot k \left( 1 - (\mathcal{F}_k(0) + 2\pi\sigma \cdot kP_0)P_0 \frac{1}{2\pi k^2}\sigma \cdot k \right)^{-1} \right\| \leq \frac{\pi}{2\beta^2}
\]

which proves (3.34). \( \square \)
Now we focus on the case $|k| \leq 2\beta^2/\pi^2$. Applying the resolvent formula to the operator $\mathcal{F}_k(0)$ yields
\begin{equation}
\mathcal{F}_k(0) = -2\pi \sigma \cdot k P_0 - \beta^2 \sigma_3 P_0 \chi Q_0 (Q_0 h_0(1, \beta)Q_0)^{-1} Q_0 \chi P_0 \sigma_3 + \beta^2 \sigma_3 P_0 \chi Q_0 (Q_0 h_0(1, \beta)Q_0)^{-1} 2\pi \sigma \cdot k (Q_0 h_0(1, \beta)Q_0)^{-1} Q_0 \chi P_0 \sigma_3 \tag{3.37}
\end{equation}
where we used $\beta$ to prove that the third term on the right hand side of the first equality is $O(\beta^2|k|)$. The operator $M_k(\beta)$ has the structure $P_0 \otimes m_k(\beta)$ where its matrix part $m_k(\beta)$ is acting on $\mathbb{C}^2$.

**Lemma 3.3.** The matrix $m_k(\beta)$ is traceless, i.e. $\text{Tr}(m_k(\beta)) = 0$. In particular, defining the three dimensional vector
\[ W_k(\beta) := (\text{Tr}(\sigma_1 m_k(\beta)), \text{Tr}(\sigma_2 m_k(\beta)), \text{Tr}(\sigma_3 m_k(\beta))) \in \mathbb{R}^3, \]
we have
\[ m_k(\beta) = W_k(\beta) \cdot \sigma. \tag{3.38} \]

**Proof.** Consider the anti-unitary charge conjugation operator $U_c$ defined by $U_c \psi = \sigma_1 \bar{\psi}$. Then a straightforward computation yields $U_c^2 = 1$ and
\[ U_c P_0 = P_0 U_c, \quad U_c \sigma_3 = -\sigma_3 U_c, \quad U_c h_0(1, \beta) = -h_0(1, \beta) U_c. \]
Also:
\[ U_c \left[ \sigma_3 P_0 \chi Q_0 (Q_0 h_0(1, \beta)Q_0)^{-1} Q_0 \chi P_0 \sigma_3 \right] U_c = -\sigma_3 P_0 \chi Q_0 (Q_0 h_0(1, \beta)Q_0)^{-1} Q_0 \chi P_0 \sigma_3. \]
Since $\text{Tr}(U_c A U_c) = \text{Tr}(A)$ if $A$ is self-adjoint, we must have $\text{Tr}(m_k(\beta) + 2\pi \sigma \cdot k) = 0$. Since $\text{Tr}(\sigma \cdot k) = 0$, we conclude that $\text{Tr}(m_k(\beta)) = 0$ and the lemma is proved. \qed

**Lemma 3.4.** Assume that hypothesis (1.10) of Theorem 1.2 holds. Then there exists $\beta_0 > 0$ and $C > 0$ such that for all $\beta \in (0, \beta_0)$, and all $k \in \Omega$ such that $|k| \leq 2\beta^2/\pi^2$, $M_k(\beta)$ is invertible and
\[ \|M_k(\beta)^{-1}\| \leq C/\beta^3. \tag{3.39} \]

**Proof.** Due to (3.38), we have
\[ M_k(\beta)^{-1} = \frac{1}{|W_k(\beta)|^2} M_k(\beta), \]

hence
\[ \|M_k(\beta)^{-1}\| = \frac{1}{|W_k(\beta)|^2} \leq \frac{1}{|\text{Tr}(\sigma_3 M_k(\beta))|}. \tag{3.40} \]

Let us now compute (remember that the "third" component of $k$ is by definition equal to zero):
\[ \text{Tr}(\sigma_3 M_k(\beta)) = \text{Tr} \left( \sigma_3 \left( -2\pi \sigma \cdot k P_0 - \beta^2 \sigma_3 P_0 \chi Q_0 (Q_0 h_0(1, \beta)Q_0)^{-1} Q_0 \chi P_0 \sigma_3 \right) \right) \]
\[ = -\beta^2 \text{Tr} \left( P_0 \chi Q_0 (Q_0 h_0(1, \beta)Q_0)^{-1} Q_0 \chi P_0 \sigma_3 \right) =: -\beta^2 w(\beta), \tag{3.41} \]
which is independent of \( k \). Using \((2.13)\) we get
\[
(Q_0 h_0 (1, 0) Q_0)^{-1} = \sum_{m \neq 0} \frac{1}{2\pi |m|^2} P_m \sigma \cdot m = \sum_{m \neq 0} \frac{1}{2\pi |m|^2} P_m (m_1 \sigma_1 + m_2 \sigma_2).
\]
Hence we obtain \( w(0) = 0 \) because
\[
\text{Tr} \left( P_0 \chi Q_0 (Q_0 h_0 (1, 0) Q_0)^{-1} Q_0 \chi P_0 \sigma_3 \right) = 0.
\]
Moreover
\[
w'(0) = \text{Tr} \left( P_0 \chi Q_0 (Q_0 h_0 (1, 0) Q_0)^{-1} \chi \sigma_3 (Q_0 h_0 (1, 0) Q_0)^{-1} Q_0 \chi P_0 \sigma_3 \right)
= \sum_{m \neq 0} \sum_{m' \neq 0} \frac{\hat{\chi}(m)}{2\pi |m|^2} \hat{\chi}(m') \frac{\hat{\chi}(m)}{2\pi |m'|^2} \Tr((m \cdot \sigma) \sigma_3 (m' \cdot \sigma) \sigma_3)
\]
\[
= - \sum_{m \neq 0} \sum_{m' \neq 0} \frac{\hat{\chi}(m)}{2\pi |m|^2} \hat{\chi}(m) \hat{\chi}(m') \frac{\hat{\chi}(m)}{2\pi |m'|^2} m \cdot m'.
\]
With equations \((3.41)-(3.43)\) we get
\[
\text{Tr}(\sigma_3 M_k(\beta)) = \frac{\beta^3}{4\pi^2} \sum_{m \neq 0} \sum_{m' \neq 0} \frac{m \cdot m'}{|m|^2 |m'|^2} \hat{\chi}(m) \hat{\chi}(m') \hat{\chi}(m - m') + O(\beta^4),
\]
which together with \((3.40)\) concludes the proof of the lemma since we assumed hypothesis \((1.10)\).

\textit{Proof of Theorem 1.2.} Equation \((3.37)\) together with \((3.39)\) implies that for \( \beta \in (0, \beta_0) \) and \( |k| \leq 2\beta^2 / \pi^2 \), the operator \( \mathcal{F}_k(0) \) is invertible and
\[
\sup_{k \in \Omega, |k| \leq 2\beta^2 / \pi^2} \| \mathcal{F}_k(0)^{-1} \| \leq C / \beta^3
\]
for some constant \( C > 0 \) independent of \( \beta \). Using in addition the estimate \((3.34)\) of Lemma 3.2 it implies that there exists a constant \( C > 0 \) independent of \( \beta \) such that
\[
\sup_{k \in \Omega} \| \mathcal{F}_k(0)^{-1} \| \leq C / \beta^3.
\]
Together with Lemma 3.1, this concludes the proof of Theorem 1.2.

\textbf{Appendix A. Estimate for the resolvent kernel}

\textbf{Lemma A.1.} There exists a constant \( C > 0 \) such that the following kernel estimate holds for all \( x \neq x' \in \mathbb{R}^2 \)
\[
| (H_0 \pm i)^{-1} (x, x') | \leq C e^{-|x - x'| / |x - x'|}.
\]
\textit{Proof.} The relation \((H_0 + i)(H_0 - i) = (-\Delta + 1)\) implies that
\[
(H_0 - i)^{-1} = (H_0 + i)(-\Delta + 1)^{-1}.
\]
In order to obtain the kernel for the Laplacian we recall the well-known formula for its heat kernel in dimension $n \geq 1$

$$e^{t \Delta}(x, x') = \frac{1}{(4\pi t)^{n/2}} e^{-\frac{|x-x'|^2}{4t}}.$$

Thus, by the usual integral representation of the resolvent in terms of the heat kernel we get

$$(-\Delta + 1)^{-1}(x, x') = \frac{1}{4\pi} \int_0^\infty e^{-\frac{|x-x'|^2}{4t}} e^{-\frac{t}{t}} dt = \frac{1}{2\pi} K_0(|x - x'|),$$

where $K_0$ is a modified Bessel function (see Formula 8.432(6) in [8]). Using this in (A.44) and that $K'_0(z) = -K_1(z)$ (see Formula 8.486(18) in [8]) we get that

$$(H_0 \pm i)^{-1}(x, x') = \frac{i}{2\pi} (K_1(|x - x'|) \sigma \cdot \nabla_x |x - x'| + K_0(|x - x'|)).$$

Thus $|(H_0 \pm i)^{-1}(x, x')| \leq \frac{1}{2\pi} (|K_0(|x - x'|)| + |K_1(|x - x'|)|)$ the claim now follows by the asymptotic behavior of the Bessel functions $K_0$ and $K_1$ at zero and infinity (see Formulas 8.447(3), 8.446 and 8.451(6) in [8]). □

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