Dipoles in Graphene Have Infinitely Many Bound States

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We show that in graphene, modelled by the two-dimensional Dirac operator, charge distributions with non-vanishing dipole moment have infinitely many bound states. The corresponding eigenvalues accumulate at the edges of the gap faster than any power.

CONTENTS

I. INTRODUCTION

Graphene close to the Fermi surface is often described by two-dimensional massless Dirac operators. Strained graphene, though develops a mass gap (Vozmediano et al[18]). These materials together with an electric dipole recently attracted attention by De Martino et al[4]. They predicted that the corresponding Hamiltonian would have infinitely many bound states inside the spectral gap regardless of the strength of the dipole moment. These bound states should be supported at long distances and small momenta where the non-relativistic behavior of the operator – due to the mass gap – is dominant. It is thus plausible that their result agrees with the prediction of Connolly and Griffiths[3] for the two-dimensional Schrödinger operator. In contrast, for the three-dimensional Schrödinger operator there is a critical dipole moment below which no bound states exist, see Abramov and Komarov[1].

The argument of De Martino et al is based on replacing the electric potential by the pure dipole part whose singularity is cut off at small distances; the problem is then explicitly solvable in terms of Mathieu functions and McDonald functions. The dipole approximation is – physically – justified, since – as pointed out above – almost all the bound states are supported at large distances. Since those bound states have energies close to zero, the standard approximation for graphene by a Dirac operator is physically justified.

In this paper we will show that the predictions of De Martino and al based on non-rigorous arguments can indeed to a large extend be proven and – in fact – be generalized – up to technical constraints – to arbitrary charge distributions of total vanishing charge.

Indeed, the non-vanishing of either the total charge or the dipole moment is necessary and sufficient for the existence of infinitely many bound states.

De Martino et al also predicted exponential clustering of those eigenvalues E_n as they approach edges of the gap $(-m, m)$. We show – in the same vein – that all the moments of the distance to the nearest gap edge, i.e., $\sum_n (m - |E_n|)^\delta$, converge for all positive δ.

We will use the following notation. Let $x_0 \in \mathbb{R}^2 \setminus \{0\}$. The two-dimensional Dirac operator D is initially given on the dense domain $\mathcal{D}_0 := C_0^\infty(\mathbb{R}^2 \setminus \{-x_0, x_0\})$ as

$$\begin{aligned} D &= D_0 + \gamma V, \\ D_0 &= -\mathrm{i}\sigma \cdot \nabla + m\sigma_3 \\ V(x) &= |x - x_0|^{-1} - |x + x_0|^{-1}, \end{aligned} \tag{1}$$

where $\sigma = (\sigma_1, \sigma_2)$ and $\sigma_1, \sigma_2, \sigma_3$ are the standard Pauli matrices. We may assume without loss of generality that the coupling constant γ (which plays the role of the dipole moment in the present case) is positive; otherwise, we could just replace x_0 by $-x_0$. Note D is symmetric but not essentially self-adjoint. We will find a distinguished self-adjoint extension with the property that the kinetic energy remains finite. The punctured plane $\mathbb{R}^2 \setminus \{-x_0, x_0\}$ is chosen here because of the Coulomb singularities of the potential could be replaced by $\mathbb{R}^2$ for regular V.

We write $\mathcal{B}(\mathcal{H}, \mathcal{K})$ for the bounded operators from a Hilbert space $\mathcal{H}$ to a Hilbert space $\mathcal{K}$. If $\mathcal{K} = \mathcal{H}$, we just write $\mathcal{B}(\mathcal{H})$. The identity in $\mathcal{K}$ is denoted by$I_{\mathcal{K}}$. In the following, we shall set $\mathcal{H} = L^2(\mathbb{R}^2, \mathbb{C}^2)$ and denote its scalar product (linear in the second argument) and norm by $(\cdot, \cdot)$ and $\|\cdot\|$, respectively. Moreover, we use $\mathfrak{S}_p$ for the Schatten ideal of order p in $\mathcal{H}$ and $R_0(z) = (D_0 - z)^{-1}$ for the free resolvent.

II. SELF-ADJOINT EXTENSION

Since the potential has Coulomb singularities, the extension of the above symmetric operator is not entirely straightforward. In particular, in the absence of a Hardy inequality in two dimensions it is – contrary to the three dimensional case – not even possible for small coupling constant to define the operator as an operator sum by means of the perturbation theory of Kato and Rellich. Instead, we resort to a resolvent type equation, in the spirit of Kato[7] and Nenciu[12]. We emphasize at this point that we choose a particular self-adjoint extension only for definiteness of our model; the existence of infinitely many bound states (Theorem 2) does not depend on this choice, since the most bound states are supported far away from the singularities.

Theorem 1 (Existence of a distinguished self-adjoint extension) *Assume that $\gamma < 1/2$. Then there exists a unique self-adjoint extension D_{ex} of D with the property $\mathcal{D}(D_{\mathrm{ex}}) \subset H^{1/2}(\mathbb{R}^2, \mathbb{C}^2)$.*

Proof: Step 1: We claim that for any $a \in \mathbb{R}^2$, $\eta \in \mathbb{R}$ and $\psi \in C_0^\infty(\mathbb{R}^2, \mathbb{C}^2)$,

$$\| |x-a|^{1/2} (D_0 - \mathrm{i}\eta) |x-a|^{1/2} \psi \|^2 \geq \frac{1}{4} \|\psi\|^2 \tag{2}$$

By translation invariance of D_0 it is sufficient to prove (2) for $a = 0$. We write D_0 in polar coordinates (r, θ),

$$D_0 = \begin{pmatrix} m & \mathrm{e}^{-\mathrm{i}\theta}\left(-\mathrm{i}\partial_r - \frac{1}{r}\partial_\theta\right) \\ \mathrm{e}^{\mathrm{i}\theta}\left(-\mathrm{i}\partial_r + \frac{1}{r}\partial_\theta\right) & -m \end{pmatrix}.$$

Then, for $\psi \in C_0^\infty(\mathbb{R}^2)$,

$$\begin{aligned} \|r^{1/2}(D_0 - \mathrm{i}\eta) r^{1/2}\psi\|^2 &= (m^2 + \eta^2)\|r\psi\|^2 + \|r^{1/2}\partial_r r^{1/2}\psi\|^2 + \|\partial_\theta \psi\|^2 \\ &\geq \|r^{1/2}\partial_r r^{1/2}\psi\|^2. \end{aligned}$$

Setting $\chi = r\psi$, and integrating by parts, we obtain

$$\|r^{1/2}\partial_r r^{1/2}\psi\|^2 = \int_0^{2\pi}\int_0^\infty |\partial_r \chi|^2 r \,\mathrm{d}r\,\mathrm{d}\theta + \frac{1}{4}\int_0^{2\pi}\int_0^\infty \frac{|\chi|^2}{r^2} r\,\mathrm{d}r\,\mathrm{d}\theta \geq \frac{1}{4}\|\psi\|^2,$$

which proves (2). Incidentally, the constant $1/4$ in (2) is sharp. This fact becomes apparent in the invariant subspace decomposition of D_0 with respect to the total angular momentum $J = -\mathrm{i}\partial_\theta + \frac{1}{2}\sigma_3$, and is related to the sharp one-dimensional Hardy inequality.

Step 2: We first consider the case of one Coulomb singularity. We introduce the scale of spaces

$$\mathcal{H}^+ \subset \mathcal{H} \subset \mathcal{H}^-, \quad \mathcal{H}^\pm := H^{\pm 1/2}(\mathbb{R}^2, \mathbb{C}^2),$$

where the embeddings are dense and continuous. As is customary, we shall denote the duality pairing in $\mathcal{H}^+ \times \mathcal{H}^-$ by $(\cdot, \cdot)$ as well. Obviously,

$$D_0 \in \mathcal{B}(\mathcal{H}^+, \mathcal{H}^-), \quad R_0(\mathrm{i}\eta) \in \mathcal{B}(\mathcal{H}^-, \mathcal{H}^+). \tag{3}$$

Following the method of Kato[9] we show that

$$\begin{aligned} \mathcal{D}(D_a) &:= \{\psi \in \mathcal{H}^+ : (D_0 + \gamma|x-a|^{-1})\psi \in \mathcal{H}\}, \\ D_a\psi &:= (D_0 + \gamma|x-a|^{-1})\psi, \end{aligned} \tag{4}$$

is a self-adjoint operator. By the basic criterion for self-adjointness[15] (Thm. VIII.3), it is sufficient to show that D_a is symmetric and that $\mathrm{Ran}(D_a \pm \mathrm{i}) = \mathcal{H}$. Since $\mathcal{D}_0 \subset \mathcal{D}(D_a)$, the operator D_a is densely defined. To prove that D_a is symmetric, it remains to show that

$$(D_a\phi, \psi) = (\phi, D_a\psi), \quad \phi, \psi \in \mathcal{D}(D_a). \tag{5}$$

For later use, we recall the following generalized Hardy inequality (see Herbst[6]). Let $0 < \alpha < n$. Then on $H^{\alpha/2}(\mathbb{R}^n)$,

$$|\sqrt{-\Delta}|^\alpha - 2^\alpha \left[\frac{\Gamma\left(\frac{n+\alpha}{4}\right)}{\Gamma\left(\frac{n-\alpha}{4}\right)}\right]^2 |x|^{-\alpha} > 0, \tag{6}$$

and the inequality continues to hold (with the same sharp constant) if $\sqrt{-\Delta}$ is replaced by $\sqrt{-\Delta + m^2}$ and/or $|x|$ is replaced by $|x-a|$ (by translation invariance). In particular, (6) (with $n = 2$, $\alpha = 1/2$) implies that

$$|x-a|^{-1/2} \in \mathcal{B}(\mathcal{H}^+, \mathcal{H}) \cap \mathcal{B}(\mathcal{H}, \mathcal{H}^-), \tag{7}$$

which, together with (3), implies that

$$|x-a|^{-1} \in \mathcal{B}(\mathcal{H}^+, \mathcal{H}^-), \quad D_0 + \gamma|x-a|^{-1} \in \mathcal{B}(\mathcal{H}^+, \mathcal{H}^-). \tag{8}$$

Let $\phi, \psi \in \mathcal{D}(D_a) \subset \mathcal{H}^+$. By[10] (Thm. 7.14), there exist $(\psi_n)_n \subset C_0^\infty(\mathbb{R}^2)$ such that $\psi_n \to \psi$ in $\mathcal{H}^+$. By the definition of the weak derivative and (8),

$$\begin{aligned} (D_a\phi, \psi) &= ((D_0 + \gamma|x-a|^{-1})\phi, \psi) = \lim_{n\to\infty} \big((D_0\phi, \psi_n) + (\gamma|x-a|^{-1}\phi, \psi_n)\big) \\ &= \lim_{n\to\infty} \big((\phi, D_0\psi_n) + (\phi, \gamma|x-a|^{-1}\psi_n)\big) = \lim_{n\to\infty} (\phi, (D_0 + \gamma|x-a|^{-1})\psi_n) \\ &= (\phi, (D_0 + \gamma|x-a|^{-1})\psi) = (\phi, D_a\psi). \end{aligned}$$

This proves (5).

To show that $\mathrm{Ran}(D_a \pm \mathrm{i}) = \mathcal{H}$, observe that by (3), (7)

$$Q(\mathrm{i}\eta) := |x-a|^{-1/2} R_0(\mathrm{i}\eta) |x-a|^{-1/2} \in \mathcal{B}(\mathcal{H}). \tag{9}$$

Moreover, (2) implies $\|Q(\mathrm{i}\eta)\|_{\mathcal{B}(\mathcal{H})} \le 2$. By the Neumann series, for $\gamma < 1/2$, the operator

$$R(\mathrm{i}\eta) := R_0(\mathrm{i}\eta) - \gamma R_0(\mathrm{i}\eta)|x-a|^{-1/2}\left(I + \gamma Q(\mathrm{i}\eta)\right)^{-1}|x-a|^{-1/2}R_0(\mathrm{i}\eta) \tag{10}$$

is in $\mathcal{B}(\mathcal{H}^-, \mathcal{H}^+)$. A straightforward computation (compare Kato[9]) shows that

$$\begin{aligned} R(\mathrm{i}\eta)(D_0 + \gamma|x-a|^{-1} - \mathrm{i}\eta) &= I_{\mathcal{H}^+}, \\ (D_0 + \gamma|x-a|^{-1} - \mathrm{i}\eta)R(\mathrm{i}\eta)) &= I_{\mathcal{H}^-}, \end{aligned} \tag{11}$$

Let $\psi \in \mathcal{H} \subset \mathcal{H}^-$. Then $\phi = R_0(\mathrm{i}\eta)\psi \in \mathcal{H}^+$, and by the second identity in (11), $(D_0 + \gamma|x-a|^{-1})\phi = \psi \in \mathcal{H}$, so that $\phi \in \mathcal{D}(D_a)$, and $D_a\phi = \psi$. This completes the proof of $\mathrm{Ran}(D_a \pm \mathrm{i}) = \mathcal{H}$.

Step 3: Following Nenciu[13], we extend the above proof to the two-center potential $V = V_1 - V_2$, where

$$V_1(x) = \frac{1}{|x-x_0|}, \quad V_2(x) = \frac{1}{|x+x_0|}.$$

Let $\chi \in C_0^\infty(\mathbb{R}_+)$ be a nonnegative function such that $\chi(r) = 1$ for $r \le |x_0|/4$ and $\chi(r) = 0$ for $r \ge |x_0|/2$, and let

$$\widetilde{V}_1(x) := \chi^2(|x-x_0|)V_1(x), \quad \widetilde{V}_2(x) := \chi^2(|x+x_0|)V_2(x).$$

We split V into a singular and a regular part, $V = \widetilde{V} + (V - \widetilde{V})$, where $\widetilde{V} := \widetilde{V}_1 - \widetilde{V}_2$. Note that the analogues of (7)–(8) hold for $\widetilde{V}$, $\widetilde{V}_i$, $i = 1, 2$, while $V - \widetilde{V} \in \mathcal{B}(\mathcal{H})$. We will use (2) to show that for any $\varepsilon > 0$ there exists $\eta_0 > 0$ such that

$$\||\widetilde{V}|^{1/2}R_0(\mathrm{i}\eta)|\widetilde{V}|^{1/2}\|_{\mathcal{B}(\mathcal{H})} \le (2+\varepsilon), \quad |\eta| > \eta_0. \tag{12}$$

Repeating the arguments of the last step, one then sees that the operator $\widetilde{D}$, defined as in (4), but with $|x-a|^{-1}$ replaced by $\widetilde{V}$, is a self-adjoint operator for $\gamma < 1/2$. Self-adjointness of $D_{\mathrm{ex}} := \widetilde{D} + \gamma(V - \widetilde{V})$ then follows from the Kato-Rellich theorem[15]. Indeed, upon substituting $|x-a|^{-1/2}$ in (9)–(10) by $|V|^{1/2}$ and $V^{1/2}$ in the first, respectively in the second occurrence, one checks that $R(\mathrm{i}\eta) \in \mathcal{B}(\mathcal{H}^-, \mathcal{H}^+)$ is the inverse of $D_0 + \gamma\widetilde{V} - \mathrm{i}\eta \in \mathcal{B}(\mathcal{H}^+, \mathcal{H}^-)$. Here, $V^{1/2} := |V|^{1/2}U$ where U is the partial isometry in the polar decomposition of V. Note that, by the support properties of χ, we have

$$|\widetilde{V}|^{1/2} = |\widetilde{V}_1|^{1/2} - |\widetilde{V}_2|^{1/2}, \tag{13}$$

so that by the triangle inequality, we have for $\psi \in \mathcal{H}$,

$$\||\widetilde{V}|^{1/2}R_0(\mathrm{i}\eta)|\widetilde{V}|^{1/2}\psi\|^2 \leq A_1^2 + A_2^2 + 2B(A_1+A_2) + B^2,$$

with

$$A_i := \||\widetilde{V}_i|^{1/2}R_0(\mathrm{i}\eta)|\widetilde{V}_i|^{1/2}\psi\|^2, \quad B := \sum_{i\neq j}\||\widetilde{V}_i|^{1/2}R_0(\mathrm{i}\eta)|\widetilde{V}_j|^{1/2}\psi\|^2 \quad i,j=1,2.$$

By (2),

$$\begin{aligned}
A_1^2 &= \|\chi(|x-x_0|)|V_1|^{1/2}R_0(\mathrm{i}\eta)\chi(|x-x_0|)|V_1|^{1/2}\psi\|^2 \\
&\leq \||V_1|^{1/2}R_0(\mathrm{i}\eta)\chi(|x-x_0|)|V_1|^{1/2}\psi\|^2 \\
&\leq 4\|\chi(|x-x_0|)\psi\|^2,
\end{aligned}$$

and similarly for A_2^2. Therefore,

$$A_1^2 + A_2^2 \leq 4\left(\|\chi(|x-x_0|)\psi\|^2 + \|\chi(|x+x_0|)\psi\|^2\right) \leq 4\|\psi\|^2.$$

To finish the proof of (12), we claim that

$$\lim_{|\eta|\to\infty}\frac{\||\widetilde{V}_i|^{1/2}R_0(\mathrm{i}\eta)|\widetilde{V}_j|^{1/2}\psi\|^2}{\|\psi\|^2} = 0, \quad i \neq j. \tag{14}$$

This follows from the following estimate for the free resolvent kernel. For $k,l=1,2$, $|x-y| \geq |x_0|$ and $|\eta| \geq \eta_0$,

$$|R_0(\mathrm{i}\eta)_{kl}(x-y)| \leq C(x_0,\eta_0)\mathrm{e}^{-\frac{1}{4}\sqrt{m^2+\eta^2}|x-y|}. \tag{15}$$

Indeed, assuming (15) for the moment, it follows that

$$\||\widetilde{V}_i|^{1/2}R_0(\mathrm{i}\eta)|\widetilde{V}_j|^{1/2}\|_{\mathfrak{S}_2} \leq 4C(x_0,\eta_0)\mathrm{e}^{-\frac{1}{4}\sqrt{m^2+\eta^2}|x_0|}\|\widetilde{V}_i\|_{L^1(\mathbb{R}^2)}\|\widetilde{V}_j\|_{L^1(\mathbb{R}^2)},$$

and this converges to zero as $|\eta| \to \infty$. Since the operator norm is bounded by the Hilbert-Schmidt norm, (14) follows. It remains to prove (15). Noticing that

$$R_0(\mathrm{i}\eta) = (D_0 + \mathrm{i}\eta)(-\Delta + k^2)^{-1}, \quad \kappa^2 := m^2 + \eta^2,$$

and using the explicit formula for the heat kernel of $-\Delta$, we arrive at

$$\begin{aligned}
|R_0(\mathrm{i}\eta)_{kl}(x-y)| &= \left|\frac{1}{4\pi}\int_0^\infty (D_0+\mathrm{i}\eta)_{kl}\,\mathrm{e}^{-\kappa^2 t}\mathrm{e}^{-\frac{|x-y|^2}{4t}}\,\frac{\mathrm{d}t}{t}\right| \\
&\leq \frac{1}{4\pi}\int_0^\infty\left(\frac{|x-y|}{2t}+\kappa\right)\mathrm{e}^{-\kappa^2 t}\mathrm{e}^{-\frac{|x-y|^2}{4t}}\,\frac{\mathrm{d}t}{t} \\
&\leq C(x_0,\eta_0)\mathrm{e}^{-\frac{1}{4}\kappa|x-y|},
\end{aligned}$$

for $|x-y| \geq |x_0|$, $|\eta| \geq \eta_0$ and $k,l = 1,2$; the constant can be taken e.g. as

$$C(x_0,\eta_0) := \frac{1}{4\pi}\left(\frac{4}{|x_0|} + \frac{16}{|x_0|^2\sqrt{m^2+\eta_0^2}}\right).$$

Step 4: To prove the uniqueness statement of the Theorem, suppose that there is another self-adjoint extension $H \supset D$ such that $\mathcal{D}(H) \subset \mathcal{H}^+$. Let $\phi \in \mathcal{D}(H) \subset \mathcal{H}^+$ and $\psi \in \mathcal{D}(D) = \mathcal{D}_0$. Regarding $D_0 + \gamma V$ as an operator in $\mathcal{B}(\mathcal{H}^+,\mathcal{H}^-)$ again and repeating the integration by parts argument in the proof of (5), we obtain

$$(H\phi,\psi) = (\phi, H\psi) = (\phi, D\psi) = (\phi,(D_0+\gamma V)\psi) = ((D_0+\gamma V)\phi,\psi).$$

Since $\mathcal{D}_0$ is dense in $\mathcal{H}$, this implies $(D_0+\gamma V)\phi = H\phi \in \mathcal{H}$. Hence, $\phi \in \mathcal{D}(D_{\mathrm{ex}})$, and $H\phi = D_{\mathrm{ex}}\phi$. This proves that $H \subset D_{\mathrm{ex}}$. The reverse inclusion is proved similarly. ∎

Remark 1 *The proof can easily be extended to cover the case of N Coulomb singularities, see Nenciu*[13] *for the three-dimensional case.*

Proposition 1 *The essential spectrum of D_{ex} is*

$$\sigma_{\mathrm{ess}}(D_{\mathrm{ex}}) = \sigma_{\mathrm{ess}}(D_0) = (-\infty,-m] \cup [m,\infty).$$

Proof: We show that the resolvent difference of D_{ex} and D_0 is compact. The claim then follows from Weyl's essential spectrum theorem[16] (Thm. XIII.14). As in the proof of Theorem 1 let $\widetilde{D}$ be the self-adjoint operator corresponding to the singular part of V, and denote its resolvent by $\widetilde{R}(\mathrm{i}\eta)$. By the Kato-Seiler-Simon inequality[17] (Thm. 4.1),

$$\||\widetilde{V}_i|^{1/2}R_0(\mathrm{i}\eta)\|_{\mathfrak{S}_p} \leq C\||\widetilde{V}_i|^{1/2}\|_p\|(|\cdot|^2+m^2)^{-1/2}\|_p, \tag{16}$$

and the right hand side is finite for all $p \in (2,4)$. By (13) and the triangle inequality, (16) continues to hold (with $2C$) if $\widetilde{V}_i$ is replaced by $\widetilde{V}$. The analogue of the resolvent formula (10) for $\widetilde{D}$ and the trace ideal property of $\mathfrak{S}_p$ then imply that $\widetilde{R}(\mathrm{i}\eta) - R_0(\mathrm{i}\eta) \in \mathfrak{S}_p$ for all $p > 1$, in particular it is compact. Denoting by $R(\mathrm{i}\eta)$ the resolvent of $D_{\mathrm{ex}} = \widetilde{D} + \gamma(V - \widetilde{V})$, we have

$$R(\mathrm{i}\eta) - R_0(\mathrm{i}\eta) = -\gamma R(\mathrm{i}\eta)(V-\widetilde{V})\widetilde{R}(\mathrm{i}\eta) + (\widetilde{R}(\mathrm{i}\eta) - R_0(\mathrm{i}\eta)).$$

It remains to be shown that first summand is compact. Indeed, its $\mathfrak{S}_p$-norm is bounded by

$$\gamma\|R(\mathrm{i}\eta)\|\|(V-\widetilde{V})(I-\Delta)^{-1/4}\|_{\mathfrak{S}_p}\|(I-\Delta)^{1/4}\widetilde{R}(\mathrm{i}\eta)(I-\Delta)^{1/4}\|\|(I-\Delta)^{-1/4}\|,$$

which is finite for $p > 4$ by the Kato-Seiler-Simon inequality. ∎

III. EXISTENCE OF INFINITELY MANY EIGENVALUES

Theorem 2 *Any self-adjoint extension of D (defined in (1)) has infinitely many eigenvalues in $(-m, m)$.*

Proof: Let H be a self-adjoint extension of D. Then H^2, defined by the spectral theorem, is the unique operator associated to the nonnegative symmetric form

$$q(\phi, \psi) := (H\phi, H\psi), \quad \psi \in \mathcal{D}(q) := \mathcal{D}(H)$$

by the first representation theorem[8] (Thm. 2.1). Indeed, the form q is closed since H is (self-adjoint and hence) closed. Let T be the self-adjoint operator associated to the form q by the first representation theorem. Since $(H\phi, H\psi) = (T\phi, \psi)$ for all $\phi \in \mathcal{D}(T)$ and $\psi \in \mathcal{D}(H)$, it follows that $T \subset H^2$. Since T is self-adjoint, we have $T = H^2$.

Let q_0 be the nonnegative symmetric form

$$q_0(\phi, \psi) := (D\phi, D\psi), \quad \psi \in \mathcal{D}(q) := \mathcal{D}(D) = \mathcal{D}_0.$$

We use the Cauchy-Schwarz inequality to obtain

$$\begin{aligned} q_0[\psi] &= \|\nabla\psi\|^2 + \gamma^2\|V\psi\|^2 + 2\gamma \mathrm{Re}\,(-\mathrm{i}\sigma \cdot \nabla\psi, V\psi) + 2m\gamma(\sigma_3 V\psi, \psi) \\ &\leq 2\|\nabla\psi\|^2 + 2\gamma^2\|V\psi\|^2 + 2m\gamma(\sigma_3 V\psi, \psi) =: s_+[\psi_+] + s_-[\psi_-], \end{aligned}$$

with $\psi = (\psi_+, \psi_-)^T$ and

$$s_\pm[\psi_\pm] := \|\nabla\psi_\pm\|^2 + \gamma^2\|V\psi_\pm\|^2 \pm \gamma m(V\psi_\pm, \psi_\pm), \quad \mathcal{D}(s_\pm) = \mathcal{D}_0.$$

Clearly, $q_0 \subset q$, which (by the variational principle) implies that

$$\begin{aligned} N(H \in (-m, m)) = N(H^2 - m < 0) &= \sup_{M \subset \mathcal{D}(q)} \{\dim M : q[\psi] < 0,\, \psi \in M\} \\ &\geq \sup_{M \subset \mathcal{D}(q_0)} \{\dim M : q_0[\psi] < 0,\, \psi \in M\} \\ &= \sup_{M \subset \mathcal{D}(s_+)} \{\dim M : s_+[\psi] < 0,\, \psi \in M\} \\ &+ \sup_{M \subset \mathcal{D}(s_-)} \{\dim M : s_-[\psi] < 0,\, \psi \in M\}. \end{aligned}$$

It is thus sufficient to show that there exist infinitely many orthonormal functions $\varphi_n \in \mathcal{D}_0$ such that $s_-[\varphi_n] < 0$. Note that we could as well have chosen s_+ because of the symmetry $s_+[U\psi] = s_-[\psi]$, where $U\psi(x) := \psi(x - 2x \cdot x_0/|x_0|)$ is a unitary transformation.

Without loss of generality, we may assume that $x_0 = e_1$. In polar coordinates (by Taylor's theorem) we then have

$$V(r,\theta) = -2\frac{\cos\theta}{r^2} + O(r^{-3}).$$

For $k > 1$ define the radially symmetric function

$$\chi(r) := \begin{cases} 0 & r \le k, \\ \frac{r-k}{k^2-k} & k \le r \le k^2, \\ 1 & k^2 \le r \le k^3, \\ \frac{k^4-r}{k^4-k^3} & k^3 \le r \le k^4, \\ 0 & k^4 \le r. \end{cases} \tag{17}$$

We set $\chi_R(r) := R^{-1}\chi(r/R)$. Moreover, let $Y_0(q;\cdot)$ be the normalized eigenfunction corresponding to the lowest eigenvalue $\lambda_0(q)$ of the Mathieu operator

$$M(q) = -\partial_\theta^2 + 2q\cos\theta \tag{18}$$

on $L^2(S^1)$. It is known that $\lambda_0(q) < 0$ for any $q > 0$, see McLachlan[11], Section 2.150, Formula (7). Setting

$$\psi_R(r,\theta) := \chi_R(r)Y_0(m\gamma;\theta), \tag{19}$$

we obtain

$$\begin{aligned} s_-[\psi_R] &= R^{-2}\|\partial_r\chi\|^2_{L^2(\mathbb{R}_+, r\,\mathrm{d}r)} + R^{-2}\lambda_0(m\gamma)\|r^{-1}\chi\|^2_{L^2(\mathbb{R}_+, r\,\mathrm{d}r)} + O(k^{-1}) \\ &\le R^{-2}\left(\frac{k^2+k}{k^2-k} + \frac{k^4+k^3}{k^4-k^3}\right) + R^{-2}\lambda_0(m\gamma)\ln k + O(k^{-1}), \end{aligned}$$

and this is negative for sufficiently large k. Hence, the functions $\varphi_n := \psi_{2^n}/\|\psi_{2^n}\|$ with $2^n > k^3$, are orthonormal and satisfy $s_\pm[\varphi_n] < 0$ for all such n. ∎

Remark 2 *The existence of infinitely many eigenvalues for arbitrarily small dipole moment γ is a consequence of the fact that the Mathieu operator* (18) *always has a negative eigenvalue for any $q > 0$. Moreover, as the dipole moment (and hence $q = m\gamma$) increases, additional negative eigenvalues may emerge. Each time such a threshold is crossed, another infinite sequence of trial functions (with Y_0 in* (19) *replaced by any eigenfunction of the Mathieu operator corresponding to a negative eigenvalue) can be constructed. These infinite sequences, labeled by the negative eigenvalues of the Mathieu operator, were called "towers" by De Martino et al.*[4].

IV. CLUSTERING OF EIGENVALUES AT THE EDGES OF THE GAP

In the following theorem, we denote by C_H the constant in (6) for $n = 2$, $\alpha = 1$,

$$C_H := \frac{4\pi^2}{\Gamma(1/4)^4} \approx 0.229.$$

Theorem 3 *Let $\delta > 0$ and $\gamma < C_H$. Then the eigenvalues E_n of D_{ex} satisfy*

$$\sum_n (m - |E_n|)^\delta \leq \frac{L m^{1+\delta-\delta_0} \gamma^{1+\delta_0} |x_0|^{1-\delta_0}}{(1-\gamma/C_H)^{2+\delta_0}} \frac{1}{\delta_0(1-\delta_0)} \tag{20}$$

for any $\delta_0 \in (0,1)$ such that $\delta_0 \leq \delta$; here, L is some universal constant.

Proof: We follow the lines of the proof of Frank and Simon[5] (Thm. 7.1) for the one-dimensional Dirac operator. The main tool in their proof, Theorem 1.4 in their article, is stated for relatively compact perturbations, but still applies if the resolvent difference of the perturbed and unperturbed operator is compact; this is the case here, by Proposition 1. Proceeding as in Thm. 7.2 of Ref.[5], one can then show that

$$\sum_n (m - |E_n|)^\delta \leq 2 \left[\operatorname{tr}(H_0 - \gamma V_-)_-^\delta + \operatorname{tr}(H_0 - \gamma V_+)_-^\delta \right],$$

where $H_0 := \sqrt{|p|^2 + m^2} - m$ and $V_\pm$ are the positive and negative parts of V, respectively. By decomposing H_0 into a part with small momentum and a part with large momentum, one can estimate

$$\operatorname{tr}(H_0 - \gamma V_\pm)_-^\delta \leq \operatorname{tr}\left(\frac{c_1 |p|^2}{m} - \theta^{-1}\gamma V_\pm\right)_-^\delta + \operatorname{tr}\left(c_2 |p| - (1-\theta)^{-1}\gamma V_\pm\right)_-^\delta \tag{21}$$

where $c_1 = (\sqrt{\rho^2 + 1} - 1)\rho^{-2}$, $c_2 = (\sqrt{\rho^2+1} - 1)\rho^{-1}$, and where $\rho > 0$ and $0 < \theta < 1$ are arbitrary parameters (see (7.9)–(7.12) in Ref.[5]). Since $V_\pm$ decay like $|x|^{-2}$ at infinity,

$$\operatorname{tr}\left(\frac{c_1 |p|^2}{m} - \theta^{-1}\gamma V_\pm\right)_-^\delta \leq c_1^{-1} \theta^{-1-\delta} m L_{\delta,2}^{\text{LT}} \int_{\mathbb{R}^2} (\gamma V_\pm)^{1+\delta} \, \mathrm{d}x < \infty \tag{22}$$

for all $\delta \in (0,1)$, where $L_{\delta,2}^{\text{LT}}$ is the best constant in the Lieb-Thirring inequality. The case $\delta \geq 1$ is prohibited by the singularities of $V_\pm$ at $\pm x_0$; however, the left hand side of (20) is clearly finite for all $\delta \geq \delta_0$ if it is finite for δ_0 since

$$\sum_n (m - |E_n|)^\delta \leq m^{\delta-\delta_0} \sum_n (m - |E_n|)^{\delta_0}. \tag{23}$$

We now show that the second term in (21) is in fact zero. We may assume that $x_0 = |x_0|e_1$. Then

$$V_+(x) = V(x)\chi\{x_1 \geq 0\} \leq |x - x_0|^{-1},$$
$$V_-(x) = -V(x)\chi\{x_1 \leq 0\} \leq |x + x_0|^{-1}.$$

Hence, by Hardy's generalized inequality (6),

$$c_2|p| - (1-\theta)^{-1}\gamma V_\pm \geq c_2|p| - (1-\theta)^{-1}\gamma|x \mp x_0|^{-1} > 0,$$

provided $\gamma \leq c_2(1-\theta)C_H$. We will choose θ such that equality holds. Moreover, we pick ρ such that $c_2 = (1+\gamma/C_H)/2$ and evaluate the bound (22). For $\delta \in (0,1)$, we estimate the integral in (22) in the regions $|x| \leq 2|x_0|$ and $|x| \geq 2|x_0|$, for $\delta \geq 1$, we use (23). ∎

V. GENERAL CHARGE DISTRIBUTIONS

Let μ be a signed Borel measure on $\mathbb{R}^3$. The corresponding potential is

$$V(x) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{\mathrm{d}\mu(y)}{|x-y|}. \tag{24}$$

The physically relevant potential is the restriction of V to the hyperplane $x_3 = 0$.

If we assume that μ has compact support, $\mathrm{supp}(\mu) \subset B(0,R)$, then the multipole expansion of V is given by

$$V(x) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \frac{1}{2l+1} q_{lm} \frac{Y_{lm}(x/|x|)}{|x|^{l+1}}, \quad |x| \geq 2R, \tag{25}$$

with the multipole moments

$$q_{lm} = \int_{\mathbb{R}^3} Y_{lm}(y/|y|)|y|^l \,\mathrm{d}\mu(y).$$

Note that (25) converges absolutely and uniformly. Denote

$$e = q_{00} = \int_{\mathbb{R}^3} \mathrm{d}\mu(y), \quad \text{(total charge)},$$
$$p_i = q_{1i} = \int_{\mathbb{R}^3} y_i \,\mathrm{d}\mu(y), \quad i = -1, 0, 1, \quad \text{(dipole moment)}$$

and $p = (p_{-1}, p_0, p_1)$. In the next theorem, we show that the condition $e = p = 0$ is necessary and sufficient for the finiteness of the number of eigenvalues (at least for absolutely continuous measures).

Theorem 4 *Let μ be absolutely continuous with respect to (three-dimensional) Lebesgue measure, with compactly supported density ρ. Then the number of eigenvalues of $D_0 + V$ in $(-m, m)$ is finite if and only if $e = p = 0$.*

Remark 3 *Under the assumptions on the density ρ, the potential* (24) *is a bounded function, and hence $D_0 + V$ is self-adjoint on $\mathcal{D}(D_0) = H^1(\mathbb{R}^2, \mathbb{C}^2)$ by the Kato-Rellich theorem.*

Proof of Theorem 4: If $e \neq 0$ or $p \neq 0$, a straightforward adaptation of the proof of Theorem 2, using the multipole expansion (25), shows that the there are infinitely many eigenvalues in $(-m, m)$. In the former case, we just replace the test functions ψ_R by the radial functions χ_R.

Let $e = p = 0$, and let $l \geq 2$ be the least integer for which not all q_{lm} are zero. Then (25) and the boundedness of V imply that $|V(r\mathrm{e}^{\mathrm{i}\phi}, 0)| \leq C_l q_l W_l(r)$, where $W_l(r) := (1 + r)^{-l-1}$, $q_l = \max_{-l \leq m \leq l} |q_{lm}|$, and $C_l > 0$ is a constant. Hence,

$$\begin{aligned}
\|(D_0 + V)\psi\|^2 &\geq \frac{1}{2}\|\nabla\psi\|^2 - \|V\psi\|^2 - m(|V|\psi, \psi) \\
&\geq \frac{1}{2}\|\nabla\psi\|^2 - C_l^2 q_l^2 \|W_l\psi\|^2 - mC_l q_l (W_l\psi, \psi)
\end{aligned}$$

and

$$\begin{aligned}
N(D_0 + V \in (-m, m)) &= N((D_0 + V)^2 - m < 0) \\
&\leq N(-\Delta - C_l^2 q_l^2 W_l^2 - mC_l q_l W_l < 0).
\end{aligned} \tag{26}$$

Since

$$\int_0^\infty r(W_l(r) + W_l(r)^2)\,\mathrm{d}r < \infty,$$

Bargmann-type bounds[14] imply that the rightmost quantity in (26) is bounded by $1 + C_l'(mq_l + q_l^2)$ for some constant C_l'. Note that an upper bound to the right hand side in inequality (2) in Ref.[14] is easily obtained by replacing the logarithm by a small power. ∎

We have seen that the moments $\sum_j (m - |E_j|)^\delta$ for the pure dipole potential V in (1) are finite for all $\delta > 0$, while for $e = p = 0$ they are finite for all $\delta \geq 0$. Under rather general assumptions on the density (in particular, the monopole moment e is not assumed to be zero), the following theorem asserts that the moments exist at least for $\delta > 1$.

Theorem 5 *Let* $\delta > 1$ *and* $\rho \in L^{\frac{3(2+\delta)}{2(3+\delta)}}(\mathbb{R}^3) \cap L^{\frac{3(2+\delta)}{2(3+\delta)}}(\mathbb{R}^3)$. *Then, the eigenvalues* E_n *of* $D_0 + V$ *satisfy*

$$\sum_n (m - |E_n|)^\delta \leq C_\delta \left(m\|\rho\|^{1+\delta}_{L^{\frac{3(1+\delta)}{2(2+\delta)}}(\mathbb{R}^3)} + \|\rho\|^{2+\delta}_{L^{\frac{3(2+\delta)}{2(3+\delta)}}(\mathbb{R}^3)} \right).$$

Proof: The claim follows from (21) and the (relativistic and non-relativistic) Lieb-Thirring inequalities, upon estimating the corresponding Lebesgue norms of V in terms of ρ by means of the sharp trace inequality by Adams[2] (Thm. 2). Note also that in view of Sobolev embedding, V is relatively bounded with respect to D_0, with relative bound zero; in particular, $D_0 + V$ is self-adjoint. ∎

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