Eigenvalue inequalities for Klein-Gordon Operators

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Abstract

We consider the pseudodifferential operators $H_{m,\Omega}$ associated by the prescriptions of quantum mechanics to the Klein-Gordon Hamiltonian $\sqrt{|P|^2 + m^2}$ when restricted to a compact domain $\Omega$ in $\mathbb{R}^d$. When the mass $m$ is 0 the operator $H_{0,\Omega}$ coincides with the generator of the Cauchy stochastic process with a killing condition on $\partial\Omega$. (The operator $H_{0,\Omega}$ is sometimes called the fractional Laplacian with power $\frac{1}{2}$, cf. [19].) We prove several universal inequalities for the eigenvalues $0 < \beta_1 < \beta_2 \leq \cdots$ of $H_{m,\Omega}$ and their means $\overline{\beta}_k := \frac{1}{k} \sum_{\ell=1}^{k} \beta_\ell$.

Among the inequalities proved are:

$$\overline{\beta}_k \geq \text{cst.} \left( \frac{k}{|\Omega|} \right)^{1/d}$$

for an explicit, optimal “semiclassical” constant, and, for any dimension $d \geq 2$ and any $k$:

$$\beta_{k+1} \leq \frac{d+1}{d-1} \overline{\beta}_k.$$ 

Furthermore, when $d \geq 2$ and $k \geq 2j$,

$$\frac{\overline{\beta}_k}{\overline{\beta}_j} \leq \frac{d}{2^{1/d} (d-1)} \left( \frac{k}{j} \right)^{\frac{d}{2}}.$$ 

Finally, we present some analogous estimates allowing for an external potential energy field, i.e, $H_{m,\Omega} + V(x)$, for $V(x)$ in certain function classes.

Key words: Fractional Laplacian, Weyl law, Dirichlet problem, Riesz means, universal bounds, Cauchy process, Dirac equation, Klein-Gordon equation, semiclassical, relativistic particle.

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1 Introduction

The quantum-mechanical operator corresponding to the Klein-Gordon Hamiltonian is a first-order pseudodifferential operator used to model relativistic particles in quantum mechanics. On unrestricted space the part representing kinetic energy $\sqrt{|P|^2 + m^2}$ can be defined as the square root of $-\Delta + m^2$, where $m$ is a nonnegative constant corresponding to the mass, in units where the speed of light is set to 1. We restrict it to a compact domain in $\mathbb{R}^d$ and designate the quantum version of $\sqrt{|P|^2 + m^2}$ as $H_{m,\Omega}$. (A full definition of $H_{m,\Omega}$ is provided below.) The operator $H_{m,\Omega}$ is positive definite with compact inverse and hence it has purely discrete spectrum consisting of positive eigenvalues $0 < \beta_1 < \beta_2 \leq \ldots$. When $m = 0$ the operator $H_{0,\Omega}$ reduces to the generator of the Cauchy stochastic process [49, 5], and because

$$H_{0,\Omega} \leq H_{m,\Omega} \leq H_{0,\Omega} + m,$$ \hfill (1.1)

we shall sometimes be able to restrict to this case without of generality.

Our aim is to find analogues for $H_{m,\Omega}$ of some familiar inequalities of a general nature that apply to the eigenvalues $0 < \lambda_1 < \lambda_2 \leq \ldots$ of the Dirichlet problem for the Laplacian on a bounded domain $\Omega \subset \mathbb{R}^d$. In some of these the spectrum is constrained by the shape and size of $\Omega$; for example the volume of $\Omega$ appears in both the Faber-Krahn lower bound for $\lambda_1$ and in the Weyl estimate of $\lambda_k$ as $k \to \infty$. In addition, there are universal bounds, whereby either $\lambda_k$ individually, or else some quantity involving many eigenvalues such as an average, a gap, or a ratio, is controlled by a different spectral quantity, independently of the geometry of $\Omega$. Various aspects of the well-developed subjects of geometric and universal bounds are treated, for instance, in [114, 19, 28]. One way to generate geometric and universal bounds for the Laplacian is based on identities for traces of commutators of operators [21, 25, 26, 33, 2], and with the benefit of hindsight these algebraic methods can be perceived implicitly in most of the classic universal spectral bounds for Laplacians [44, 29, 58]. Moreover, comparable universal bounds have been obtained with the same strategy for Schrödinger operators on Euclidean spaces [26], and both Laplacians and Schrödinger operators on embedded manifolds [34, 59, 25, 37, 12, 13, 17, 21, 22]. In many cases examples can be identified in which the inequalities are saturated.

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The plan of attack is to use trace identities to derive universal spectral bounds and geometric spectral bounds for $H_{m,\Omega}$. The generator of the Cauchy process, corresponding to the case $m = 0$, is often referred to as the fractional Laplacian and designated $\sqrt{-\Delta}$. The latter is, unfortunately, ambiguous notation, since this operator is distinct from the operator $\sqrt{-\Delta_\Omega}$ as defined by the functional calculus for the Dirichlet Laplacian $-\Delta_\Omega$, except when $\Omega$ is all of $\mathbb{R}^d$. For this reason we shall avoid the ambiguous notation when speaking of compact $\Omega$. (For the spectral theorem and the functional calculus, see, e.g., [47].)

Whereas several universal eigenvalue bounds, mostly of unknown or indifferent sharpness, have been obtained for higher-order partial differential operators such as the bilaplacian (e.g., [32,25,14,54,57]), and for some first-order Dirac operators [11], universal bounds for pseudodifferential operators appear not to have been studied before.

In a final section we study interacting Klein-Gordon operators of the form

$$H = H_{m,\Omega} + V(x),$$

allowing an external force field. An additional contemporary motivation for (1.2) comes from nanophysics, because when a nonrelativistic particle travels in a two-dimensional hexagonal structure like carbon graphene, the effective Hamiltonian operator is relativistic in form, albeit with a characteristic speed smaller than the speed of light [53].

Klein-Gordon operators can be conveniently defined using the Fourier transform on the dense subspace of test functions $C_\infty^c(\mathbb{R}^d)$. With the normalization

$$\hat{\varphi}(\xi) = \mathcal{F}[\varphi] := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \exp(-i\xi \cdot x)\varphi(x)d\mathbf{x},$$

the Laplacian is given by $-\Delta \varphi := \mathcal{F}^{-1}|\xi|^2\hat{\varphi}(\xi)$, and therefore

$$\sqrt{-\Delta + m^2} \varphi := \mathcal{F}^{-1}\sqrt{|\xi|^2 + m^2}\hat{\varphi}(\xi).$$

(1.3)

The semigroup generated on $L^2(\mathbb{R}^d)$ is known explicitly, so that, for instance with $m = 0$,

$$\exp(-\sqrt{-\Delta}t) [\varphi](x) = p_0(t,\cdot) \ast \varphi,$$

(1.4)

where for $t > 0$ the transition density (= convolution kernel) is

$$p_0(t,x) := \frac{c_d t}{(t^2 + |x|^2)^{d+1}},$$

(1.5)
with \( c_d := \frac{d!}{(4\pi)^{d/2}\Gamma(1+d/2)} \). (Cf. [5]. We note that \( c_d \) is the same “semiclassical” constant that appears in the Weyl estimate for the eigenvalues of the Laplacian. It is given in [5] and some other sources as \( \pi^{\frac{d+1}{2}} \Gamma\left(\frac{d+1}{2}\right) \), which is equal to \( c_d \) by an application of the duplication formula of the gamma function.)

If \( \Omega \) is a non-empty, bounded, open subset of \( \mathbb{R}^d \), then we define \( H_{m,\Omega} \) as follows. Consider the quadratic form on \( C^\infty_c(\Omega) \) given by

\[
\varphi \rightarrow \int_\Omega \nabla \sqrt{-\Delta + m^2} \varphi
\]

(Here \( \sqrt{-\Delta + m^2} \) is calculated for \( \mathbb{R}^d \).) Since this quadratic form is positive and defined on a dense set, it extends to a unique minimal positive operator (the Friedrichs extension) on \( L^2(\Omega) \), which we designate \( H_{m,\Omega} \). The semigroup \( e^{-tH_{m,\Omega}} \) has an integral kernel \( p_{m,\Omega}(t, x, y) \), the form of which is typically not known explicitly.

We remark that the Fourier transform can be more directly applied to \( H_{m,\Omega} \) than to the square root of the Dirichlet Laplacian according to the functional calculus, which dominates it in the following sense:

Suppose that \( \varphi \in C^\infty_c(\Omega) \subset C^\infty_c(\mathbb{R}^d) \). Then

\[
\langle \varphi, H^2_{m,\Omega}\varphi \rangle = \|H_{m,\Omega}\varphi\|^2 = \int_\Omega \left| \mathcal{F}^{-1}\left( \sqrt{|\xi|^2 + m^2}\hat{\varphi}\right) \right|^2 \\
= \int_{\mathbb{R}^d} \chi_\Omega \mathcal{F}^{-1}\left( \sqrt{|\xi|^2 + m^2}\hat{\varphi}\right)^2 \\
\leq \int_{\mathbb{R}^d} \mathcal{F}^{-1}\left( \sqrt{|\xi|^2 + m^2}\hat{\varphi}\right)^2 \\
= \int_{\mathbb{R}^d} \nabla(-\Delta + m^2)\varphi \\
= \int_\Omega \nabla(-\Delta + m^2)\varphi,
\]

because \( \text{supp}(\varphi) \in \Omega \) and \( -\Delta \) is a local operator. Therefore, if \( \beta_k \) denotes the \( k^{th} \) eigenvalue of \( H_{m,\Omega} \), and \( \lambda_k \) is the \( k^{th} \) eigenvalue of \( -\Delta \),

\[
\beta_k \leq \sqrt{\lambda_k + m^2}.
\]
2 Trace formulae and inequalities for spectra of $H_{m,\Omega}$

In [23] universal bounds for spectra of Laplacians were found as consequences of differential inequalities for Riesz means defined on the sequence of eigenvalues. The strategy here is the same, as adapted to the eigenvalues $\beta_j$, $j = 1, \ldots$ of the first-order pseudodifferential operator $H_{m,\Omega}$. However, as the earlier article made heavy use of the fact that the Laplacian is of second order and acts locally, neither of which circumstance applies here, the results we obtain here and the details of the argument are quite different.

An essential lemma is an adaptation of a result of [26,27].

**Lemma 2.1** (Harrell-Stubbe) Let $H$ be a self-adjoint operator on $L^2(\Omega)$, $\Omega \in \mathbb{R}^d$, with discrete spectrum $\beta_1 \leq \beta_2 \leq \ldots$. Denoting the corresponding normalized eigenfunctions $\{u_j\}$, assume that for a Cartesian coordinate $x_\alpha$, the functions $x_\alpha u_j$ and $x_\alpha^2 u_j$ are in the domain of definition of $H$. Then

$$\sum_{j: \beta_j \leq z} (z - \beta_j) \langle u_j, [x_\alpha, [H, x_\alpha]] u_j \rangle - 2 \| [H, x_\alpha] u_j \|^2 \leq 0, \quad (2.1)$$

and

$$\sum_{j: \beta_j \leq z} (z - \beta_j)^2 \langle u_j, [x_\alpha, [H, x_\alpha]] u_j \rangle - 2(z - \beta_j) \| [H, x_\alpha] u_j \|^2 \leq 0. \quad (2.2)$$

So that this article is self-contained, we provide a proof of the lemma.

**Proof.** Elementary calculations show that, subject to the domain assumptions made in the statement of the theorem,

$$[H, x_\alpha] u_j = (H - \beta_j) x_\alpha u_j,$$

and

$$\langle u_j, [x_\alpha, [H, x_\alpha]] u_j \rangle = 2\langle x_\alpha u_j, (H - \beta_j) x_\alpha u_j \rangle.$$

These two identities can be combined and slightly rearranged to yield:

$$\begin{align*}
(z - \beta_j) \langle u_j, [x_\alpha, [H, x_\alpha]] u_j \rangle &- 2 \| [H, x_\alpha] u_j \|^2 \\
&= 2\langle ((z - \beta_j) - (H - \beta_j)) x_\alpha u_j, (H - \beta_j) x_\alpha u_j \rangle \\
&= 2\langle (z - H) x_\alpha u_j, (H - \beta_j) x_\alpha u_j \rangle. \quad (2.3)
\end{align*}$$

Using the completeness of the eigenfunctions of $H$,

$$(H - \beta_j) x_\alpha u_j = \sum_k (\beta_k - \beta_j) \langle x_\alpha u_j, u_k \rangle u_k,$$
so the right side of (2.3) can be rewritten as

\[ 2 \sum_k (z - \beta_k) \langle u_k, x_\alpha u_j \rangle (\beta_k - \beta_j) \langle x_\alpha u_j, u_k \rangle = 2 \sum_k (z - \beta_k) (\beta_k - \beta_j) |\langle u_k, x_\alpha u_j \rangle|^2 \]

\[ \leq 2 \sum_{k: \beta_k < z} (z - \beta_k) (\beta_k - \beta_j) |\langle u_k, x_\alpha u_j \rangle|^2, \]  

(2.4)

provided that \( \beta_j \leq z \). If we now sum (2.3) over \( j \) with \( \beta_j \leq z \), i.e., the same values of \( j \) as for \( k \) in (2.4), then after symmetrizing in \( j, k \),

\[ \sum_{j: \beta_j \leq z} (z - \beta_j) \langle u_j, [x_\alpha, [H, x_\alpha]] u_j \rangle - 2 \| [H, x_\alpha] u_j \|^2 \]

\[ \leq \sum_{j,k: \beta_k, \beta_j < z} ((z - \beta_k) - (z - \beta_j)) (\beta_k - \beta_j) |\langle u_k, x_\alpha u_j \rangle|^2, \]

which simplifies to

\[ - \sum_{j,k: \beta_k, \beta_j < z} (\beta_k - \beta_j)^2 |\langle u_k, x_\alpha u_j \rangle|^2 \leq 0, \]

as claimed in (2.1). In order to establish (2.2), multiply (2.4) by \( (z - \beta_j) \) and then sum on \( j \) for \( \beta_j < z \). The summand on the right side is odd in the exchange of \( j \) and \( k \), and thus the right side equates to 0. \( \square \)

Some consequences of more general forms of the lemma are worked out in [27]. Before deriving a differential inequality that will be useful to control the spectrum, we first follow the strategy of [26] to obtain a universal bound on \( \beta_{n+1} \) in terms of the statistical distribution of the lower eigenvalues. For this purpose we introduce notation for the normalized moments of the eigenvalues:

**Definition.** For a real number \( r \) and an integer \( k > 0 \), \( \overline{\beta}_k^r := \frac{1}{k} \sum_{j=1}^k \beta_j^r \). When \( r = 1 \) we simply write \( \overline{\beta}_k = \overline{\beta}_k^1 \).

**Theorem 2.1** If \( d \geq 2 \), then for each \( k \), the eigenvalues \( \beta_k \) of \( H_{m, \Omega} \) satisfy

\[ \beta_{k+1} \leq \frac{1}{(d-1)\overline{\beta}_k} \left( d + \sqrt{d^2 - (d^2 - 1)\overline{\beta}_k \overline{\beta}_k^{-1}} \right). \]  

(2.5)

Before giving the proof we note two slightly weaker but more appealing variants of (2.5) using the Cauchy-Schwarz inequality, \( 1 \leq \overline{\beta}_k \overline{\beta}_k^{-1} \), with the aid of which the universal bound simplifies to

\[ \beta_{k+1} \leq \frac{d+1}{(d-1)\overline{\beta}_k} \leq \frac{d+1}{d-1} \overline{\beta}_k. \]  

(2.6)
In particular, 
\[
\frac{\beta_2}{\beta_1} \leq \frac{d + 1}{d - 1},
\] 
(2.7)

regardless of any property of the domain other than compactness.

In this connection, recall that R. Bañuelos and T. Kulczycki have proved in [6] that the fundamental gap of the Cauchy process is controlled by the inradius in the case of a bounded convex domain \(\Omega\) of inradius \(\text{Inr}(\Omega)\), viz., for \(m = 0\),

\[
\beta_2 - \beta_1 \leq \sqrt{\lambda_2 - (1/2)\sqrt{\lambda_1}} \frac{1}{\text{Inr}(\Omega)}.
\]

where \(\lambda_1\) and \(\lambda_2\) are the first and second eigenvalues for the Dirichlet Laplacian for the unit ball, \(B_1\) in \(\mathbb{R}^d\). (Recall that the inradius \(\text{Inr}(\Omega)\) of a region \(\Omega\) is defined by

\[
\text{Inr}(\Omega) = \sup \{d(x) : x \in \Omega\},
\]

where \(d(x) = \min\{|x - y| : y \notin \Omega\}\).)

Since a ratio bound like (2.7) is algebraically equivalent to a gap bound, (2.7) provides an independent upper bound on the gap \(\beta_2 - \beta_1\). Continuing to set \(m = 0\), (1.6) and (2.7) in the form \(\beta_2 - \beta_1 \leq \frac{2}{d-1} \beta_1\) imply:

**Corollary 2.2** If \(\beta_1^*\) and \(\lambda_1^*\) denote the fundamental eigenvalues of \(H_{0,\Omega}\) and \(-\Delta\), respectively, on the unit ball of \(\mathbb{R}^d\), then

\[
\beta_2 - \beta_1 \leq \left(\frac{2}{d-1}\right) \frac{\beta_1^*}{\text{Inr}(\Omega)} \leq \left(\frac{2}{d-1}\right) \frac{\sqrt{\lambda_1^*}}{\text{Inr}(\Omega)}.
\]

(2.8)

**Proof of Corollary 2.2.** Since \(H_{0,\Omega}\) is defined by closure from a core of functions in \(C_0^\infty\), its fundamental eigenvalue satisfies the principle of domain monotonicity. That is, if \(\Omega_1 \supset \Omega_2\), then \(\beta_1(\Omega_1) \leq \beta_1(\Omega_2)\). In particular, if \(\Omega\) is a ball of radius \(r\), then \(\beta_1(\Omega) \leq \frac{\beta_1^*}{r}\), which is the fundamental eigenvalue of the unit ball \(B_1\) by scaling. The first inequality follows from (2.7), and the second one by (1.6). \(\square\)

**Proof of Theorem 2.1.** We make the special choice \(H = H_{m,\Omega}\) and calculate the first and second commutators with the aid of the Fourier transform:

Writing \(H_{m,\Omega} = \chi_\Omega \mathcal{F}^{-1} \sqrt{|\xi|^2 + m^2} \mathcal{F},\)
\[ [H_{m,\Omega}, x_\alpha] \varphi = (H_{m,\Omega} x_\alpha - x_\alpha H_{m,\Omega}) \varphi \]
\[ = \chi_\Omega \mathcal{F}^{-1} \sqrt{|\xi|^2 + m^2} \mathcal{F}[x_\alpha \varphi] - \chi_\Omega x_\alpha \mathcal{F}^{-1}[\sqrt{|\xi|^2 + m^2} \dot{\varphi}] \]
\[ = \chi_\Omega \mathcal{F}^{-1} \left[ \sqrt{|\xi|^2 + m^2} \frac{\partial \dot{\varphi}}{\partial \xi_\alpha} - \frac{\partial}{\partial \xi_\alpha} (\sqrt{|\xi|^2 + m^2} \dot{\varphi}) \right] \]
\[ = -i \chi_\Omega \mathcal{F}^{-1} \frac{\xi_\alpha}{\sqrt{|\xi|^2 + m^2}} \dot{\varphi}. \quad (2.9) \]

Similarly,

\[ [x_\alpha, [H_{m,\Omega}, x_\alpha]] \varphi = \chi_\Omega \mathcal{F}^{-1} \left[ \left( \frac{1}{\sqrt{|\xi|^2 + m^2}} - \frac{\xi_\alpha^2}{(|\xi|^2 + m^2)^{3/2}} \right) \dot{\varphi} \right]. \quad (2.10) \]

Due to (2.9) and (2.10), there are simplifications when we sum over \( \alpha \):

\[ \sum_{\alpha=1}^{d} \| [H_{m,\Omega}, x_\alpha] \varphi \|^2 \leq \left\langle \dot{\varphi}, \frac{|\xi|^2}{|\xi|^2 + m^2} \dot{\varphi} \right\rangle \leq 1, \]

and

\[ \sum_{\alpha=1}^{d} \left( \frac{1}{\sqrt{|\xi|^2 + m^2}} - \frac{\xi_\alpha^2}{(|\xi|^2 + m^2)^{3/2}} \right) = \frac{(d - 1)|\xi|^2 + dm^2}{(|\xi|^2 + m^2)^{3/2}} \geq \frac{d - 1}{\sqrt{|\xi|^2 + m^2}}. \]

In consequence, (2.2) implies that

\[ (d - 1) \sum_{j=1}^{n} (z - \beta_j)^2 (u_j, H_{m,\Omega}^{-1} u_j) - 2 \sum_{j} (z - \beta_j) \leq 0, \quad (2.11) \]

provided \( z \in [\beta_n, \beta_{n+1}] \). Because

\[ H_{m,\Omega}^{-1} u_j = \frac{1}{\beta_j} u_j, \]

and

\[ (z - \beta_j) = -\frac{(z - \beta_j)(z - \beta_j - z)}{\beta_j}, \]

Eq. (2.11) can be rewritten as

\[ (d + 1) \sum_{j=1}^{n} \frac{(z - \beta_j)^2}{\beta_j} - 2z \sum_{j=1}^{n} \frac{(z - \beta_j)}{\beta_j} \leq 0, \quad (2.12) \]

or, equivalently,

\[ (d - 1) \beta_n^{-1} z^2 - 2dz + (d + 1) \beta_n \leq 0. \quad (2.13) \]

Setting \( z = \beta_{n+1} \), we see that \( \beta_{n+1} \) must be less than the larger root of (2.13), which is the conclusion of the theorem. \( \square \)
For future purposes we note that this theorem extends with small modifications to semirelativistic Hamiltonians of the form $H_{m,\Omega} + V(x)$. More specifically, (2.11) is valid when \( \{u_k\} \) and \( \{\beta_k\} \) are the eigenfunctions and eigenvalues of $H_{m,\Omega} + V(x)$.

We next apply similar reasoning to a function related to Riesz means. With 
\[
a_+ := \max(0, a),
\]
let
\[
U(z) := \sum_k \frac{(z - \beta_k)^2}{\beta_k},
\]
where $z$ is a real variable. Note that if $z \in [\beta_j, \beta_{j+1}]$, then
\[
U(z) = \beta_j^{-1}z^2 - 2z + \beta_j.
\]

**Theorem 2.3** The function $z^{-(d+1)}U(z)$ is nondecreasing in the variable $z$. Moreover, for $d \geq 2$ and any $j \geq 1$, the “Riesz mean” $R_1(z) := \sum_k (z - \beta_k)_+$ satisfies
\[
R_1(z) \geq \frac{2j(d-1)^d}{(d+1)^{d+1}\beta_j^d} z^{d+1}
\]
for all $z \geq (\frac{d+1}{d-1})\beta_j$.

**Proof.** In notation that suppresses $n$, Eq. (2.12) can be written
\[
(d + 1) \sum_k \frac{(z - \beta_k)^2}{\beta_k} - 2z \sum_k \frac{(z - \beta_k)_+}{\beta_k} \leq 0,
\]
which for the function $U$ reads
\[
(d + 1)U(z) - zU'(z) \leq 0,
\]
or, equivalently,
\[
\frac{d}{dz} \left\{ \frac{U(z)}{z^{d+1}} \right\} \geq 0,
\]
proving the claim about $U$.

Eq. (2.11) tells us that
\[
R_1(z) \geq \frac{d - 1}{2} U(z).
\]

Since $U(z)$ is nondecreasing, when $z \geq z_j^* \geq \beta_j$,
\[
U(z) \geq \left( \frac{z}{z_j^*} \right)^{d+1} U(z_j^*).
\]
From (2.15) with the Cauchy-Schwarz inequality we get
\[
\frac{U(z)}{j} \geq \frac{1}{\beta_j} (z - \bar{\beta_j})^2,
\] (2.21)
so that with (2.19) and (2.20) we obtain
\[
R_1(z) \geq (d-1)j \left( \frac{z}{z_j^*} \right)^{d+1} \left( z_j^* - \bar{\beta_j} \right)^2.
\] (2.22)

We now choose an optimized value of \(z_j^*\) to maximize the coefficient of \(z^{d+1}\), viz., \(z_j^* = \frac{d+1}{d-1} \beta_j\). Substituting this into (2.22), we get (2.16), as claimed. □

The Legendre transform of \(R_1(z)\) is a straightforward calculation, to be found explicitly for example in [23,31]. The result for \(k-1 < w < k\) is
\[
R_1^*(w) = (w - [w])\beta_{[w]+1} + [w]\beta_{[w]},
\] (2.23)
where \([w]\) denotes the greatest integer \(\leq w\), and when \(w\) takes an integer value \(k\) from below, \(R_1^*(k) = k\beta_k\).

With the Legendre transform of the right side of (2.16), we get
\[
k \beta_k \leq \frac{d \beta_j}{2^{1/d} j^{1/d} (d-1)} k^{d+1}.
\] (2.24)

This leads us to the following upper bound for ratios of averages of eigenvalues of \(H_{m,\Omega}\):

**Corollary 2.4** For \(k > 2j\), Eq. (2.24) implies
\[
\frac{\beta_k}{\beta_j} \leq \frac{d}{2^{1/d} j^{1/d} (d-1)} \left( \frac{k}{j} \right)^{\frac{d+1}{2}}.
\] (2.25)

**Remark 2.5** The reason for the restriction on \(k, j\) is that in Theorem 2.3, we assumed that \(z \geq \left( \frac{d+1}{d-1} \right) \beta_j\). Since there is a monotonic relationship between \(w\) and the maximizing value of \(z^*_+\) in the calculation of the Legendre transform of the right side of (2.16), we get
\[
w = 2j \left( \frac{(d-1)z^*_+}{(d+1)\beta_j} \right)^d.
\] (2.26)

Thus the inequality is valid under the assumption that \(k > w \geq 2j\).
In this section we consider the eigenvalues $\beta_k$ of $H_{m,\Omega}$ as $k \to \infty$. In view of the elementary inequalities \[ \frac{1}{|\xi|} \leq \frac{\sqrt{|\xi|^2 + m^2}}{|\xi|} = 1, \] it suffices to consider the case $m = 0$.

We begin with the analogue of the Weyl formula for the Laplacian, adapting one of the standard proofs of the latter, which relies on an estimate of the partition function $Z(t) := \sum e^{-\beta_j t}$ for $t > 0$. Recall that the function $Z(t)$ can be written as
\[ Z(t) = \int e^{-\beta t} dN(\beta), \tag{3.1} \]
where $N(\beta) := \sum_{\beta_i \leq \beta} 1$ is the usual counting function. Another standard formula for the partition function is
\[ Z(t) = \int_{\Omega} p_{\Omega}(x, x, t) dx. \tag{3.2} \]

If we accept that $H_{m,\Omega}$ is well approximated by $\sqrt{-\Delta_{\Omega}}$ in the “semiclassical limit,” then the analogue for $N(\beta)$ of the Weyl asymptotic formula for the Laplacian should be identical to the usual Weyl formula, with the identification of $\beta_k$ with $\sqrt{\lambda_k}$. This intuition is confirmed by the following:

**Proposition 3.1** As $\beta \to \infty$,
\[ N(\beta) \sim \frac{|\Omega|}{(4\pi)^{d/2} \Gamma(1 + d/2)} \beta^d. \tag{3.3} \]

Equivalently, as $k \to \infty$,
\[ \beta_k \sim \sqrt{4\pi} \left( \frac{\Gamma(1 + d/2)k}{|\Omega|} \right)^{1/d}. \tag{3.4} \]

Moreover, the function $U$ of (2.14) satisfies
\[ U(z) \sim \frac{|\Omega|}{2\pi^{d/2}(d^2 - 1)\Gamma(1 + d/2)} z^{d+1}. \]

**Proof.** By Karamata’s Tauberian theorem \[51\], if we can show that for $t \to 0$,
\[ t^d Z(t) \to c_d |\Omega|, \]
then the first claim follows from (3.1). The further claims for \( \beta_k \) and \( U(z) \) are easy consequences of (3.3).

By a standard comparison,

\[
p_\Omega(x, y, t) < p_0(x - y, t)
\]

(3.5)
on \( \Omega \), where \( p_\Omega \) is the integral kernel of the semigroup \( e^{-tH_{0, \Omega}} \). Define

\[
r_\Omega := p_0(x - y, t) - p_\Omega(x, y, t),
\]

and let \( \delta_\Omega(x) := \text{dist}(x, \partial \Omega) \). According to [5],

\[
0 \leq r_\Omega \leq \frac{t}{\delta^{d+1}_\Omega(x)} c_d \mathcal{P}^y(\tau_\Omega < t),
\]

where \( \mathcal{P}^y(\tau_\Omega < t) \) is the probability that a path originating at \( y \) exits \( \Omega \) before time \( t \). Thus,

\[
\int_\Omega p_\Omega(x, x, t) \, dx = \int_\Omega p_0(0, t) \, dx - \int_\Omega r_\Omega \, dx 
\geq c_d \frac{|\Omega|}{t^d} - (o(1_t)) \cdot \left\{ \int_{\{x: \delta(x) < \sqrt{t}\}} \frac{t}{\delta^{d+1}_\Omega(x)} \right\}.
\]

(3.6)

The first integral on the right side of (3.6) becomes

\[
\int_{\{x: \delta(x) < \sqrt{t}\}} r_\Omega \, dx = \int_{\{x: \delta(x) < \sqrt{t}\}} \frac{t}{\delta^{d+1}_\Omega(x)} \, dx 
\leq C \int_{\Omega - \Omega_{\sqrt{t}}} \frac{t}{(t^2)(d+1)/2} \, dx 
= C t^{-d} \, |\Omega - \Omega_{\sqrt{t}}|.
\]

(3.7)

As for the second integral,

\[
\int_{\{x: \delta(x) > \sqrt{t}\}} r_\Omega \, dx = \int_{\{x: \delta(x) > \sqrt{t}\}} \frac{t}{\delta^{d+1}_\Omega(x)} \, dx 
\leq \frac{t}{(t^2)(d+1)/2} \left|\Omega\right| 
= O(t^{1-d}/2) << t^{-d}.
\]

(3.8)
With (3.7) we thus validate the condition allowing the application of Karamata’s Tauberian Theorem.

An easy corollary of Theorem 2.3 is a counterpart for $H_{0,\Omega}$ to the Li-Yau inequality for the Laplacian [35]. (As noted in [31], the Li-Yau inequality is equivalent to an earlier inequality by Berezin [8] through the Legendre transform. See also [36].)

Since we know that $z^{-(d+1)}U(z) \uparrow \frac{2c_d|\Omega|}{d!(d^2-1)}$, and that because of (2.6), a choice of $z$ safely guaranteed to exceed $\beta_k$ is $z = \frac{d+1}{d-1}\beta_k$, with the aid of (2.21) we obtain

$$\frac{2c_d|\Omega|}{d!(d^2-1)} \geq k\beta_k^2 \left(\frac{d-1}{d}\beta_k\right)^2 \left(\frac{d+1}{d}\beta_k\right)^{-d}. $$

This leads directly to the semiclassical estimate:

$$\beta_k \geq \frac{(d-1)2^{1/d}\sqrt{4\pi}}{d+1} \left(\frac{\Gamma(1+d/2)k}{|\Omega|}\right)^{1/d}. \quad (3.9)$$

However, a better estimate, improving $(d-1)2^{1/d}$ to $d$, can be derived by following the argument of Li and Yau [35] more closely. As a first step we slightly generalize the lemma attributed in [35] to Hörmander:

**Lemma 3.1** Let $f: \mathbb{R}^d \to \mathbb{R}$ satisfy $0 \leq f(\xi) \leq M_1$ and

$$\int_{\mathbb{R}^d} f(\xi)w(|\xi|)d\xi \leq M_2, \quad (3.10)$$

where the weight function $w$ is nonnegative and nondecreasing. Define $R = R(M_1, M_2)$ by the condition that

$$\int_{B_R} w(|\xi|)d\xi = \omega_{d-1} \int_0^R w(r)r^{d-1}dr = \frac{M_2}{M_1}, \quad (3.11)$$

where $\omega_{d-1} := |S^{d-1}| = \frac{2\pi^{d/2}}{\Gamma(d/2)}$. Then

$$\int_{\mathbb{R}^d} f(\xi)d\xi \leq \frac{\pi^{d/2}M_1}{\Gamma(1+d/2)}R^d. \quad (3.12)$$

As a special case, if $w(\xi) = |\xi|^p$, then $R = \left[\frac{M_2(d+p)}{M_1w_{d-1}}\right]^\frac{1}{d+p}$, and so

$$\int_{\mathbb{R}^d} f(\xi)d\xi \leq \frac{1}{d}((d+p)M_2)\frac{\pi^{d/2}}{d+p}(w_{d-1}M_1)^\frac{p}{d+p}$$

$$= \left(\frac{d+p}{d}M_2\right)^\frac{d}{d+p} \left(\frac{\pi^{d/2}M_1}{\Gamma(1+d/2)}\right)^\frac{p}{d+p}. $$

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Proof. Let \( g(\xi) := M_1 \chi_{\{|\xi| \leq R\}} \) and note that according to the definition of \( R, \int w(|\xi|)g(\xi)d\xi = M_2 \). We observe that \( (w(|\xi|) - w(R))(f(\xi) - g(\xi)) \geq 0 \) for all \( \xi \). (Check \(|\xi| \leq R \) and \(|\xi| > R \) separately.) Hence

\[
w(R) \int (f(\xi) - g(\xi))d\xi \leq \int w(|\xi|)(f(\xi) - g(\xi)) = 0,
\]

and, consequently,

\[
\int f(\xi)d\xi \leq \int g(\xi)d\xi = |B_R|M_1 = \frac{\pi^{d/2}M_1}{\Gamma(1 + d/2)}R^d.
\]

For the application to \( H_{0,\Omega} \), note that

\[
\beta_\ell = \langle u_\ell, H_{0,\Omega}u_\ell \rangle = \int |\xi||\hat{u}_\ell(\xi)|^2 d\xi
\]

Choosing \( w(|\xi|) = |\xi| \) in the lemma, with \( f(\xi) = \sum_{\ell=1}^k |\hat{u}_\ell(\xi)|^2 \), we find

\[
k = \int f(\xi)d\xi \leq \left( \|f\|_\infty \frac{\pi^{d/2}}{\Gamma(1 + d/2)} \right)^{\frac{1}{d+1}} \left( \sum_{\ell=1}^k \beta_\ell \right)^{\frac{d}{d+1}} \left( \frac{d+1}{d} \right)^{\frac{1}{d+1}},
\]

or

\[
\sum_{\ell=1}^k \beta_\ell \geq \frac{d}{d+1} \left( \frac{\Gamma(1 + d/2)}{\pi^{d/2}\|f\|_\infty} \right)^{1/d} k^{1 + \frac{1}{d}}.
\]

As for \( \|f\|_\infty \),

\[
\sum_{\ell=1}^k |\hat{u}_\ell(\xi)|^2 = \sum_{\ell=1}^k \frac{1}{(2\pi)^d} \left| \int \Omega e^{ix \cdot \xi} u_\ell(x) dx \right|^2 = \frac{1}{(2\pi)^d} \sum_{\ell=1}^k \left| \langle e^{ix \cdot \xi}, u_\ell \rangle \right|^2 \leq \frac{|\Omega|}{(2\pi)^d}
\]

by Bessel’s inequality, as \( \|e^{ix \cdot \xi}\|_2^2 = |\Omega| \). In conclusion, we have an analogue of the Li-Yau inequality [35]:

**Theorem 3.2** For all \( k = 1, \ldots, \), the eigenvalues \( \beta_k \) of \( |P|_\Omega \) satisfy

\[
\beta_k \geq \frac{\sqrt{4\pi d}}{d+1} \left( \frac{\Gamma(1 + d/2)k}{|\Omega|} \right)^{1/d}.
\]

We observe that, just like the Li-Yau inequality for the Laplacian, (3.18) has the best possible coefficient consistent with the Weyl-type law of Proposition 3.1. Moreover, in view of (1.6), Theorem 3.2 has a corollary for the Dirichlet
Laplacian:
\[ \frac{1}{k} \sum_{\ell=1}^{k} \sqrt{\lambda_{\ell}} \geq \frac{\sqrt{4\pi d}}{d + 1} \left( \frac{\Gamma(1 + d/2)k}{|\Omega|} \right)^{1/d}, \] (3.19)
which is comparable to the Li-Yau inequality, but neither implies it nor is directly implied by it. (For an alternative route to (3.19) see Theorem 5.1 of [27].)

4 Universal bounds for \( H_{m,\Omega} + V(x) \)

We turn now to the Klein-Gordon Hamiltonian with an external interaction,
\[ H = H_{m,\Omega} + V(x). \] (4.1)

In a semi-relativistic approximation this Hamiltonian models the motion of a spinless particle in an external force field. As mentioned above, Hamiltonian operators similar to (4.1) have also recently been of interest as models of nonrelativistic charge carriers traveling in a two-dimensional hexagonal structure like carbon graphene. (What distinguishes graphene from the common material graphite is that graphene sheets are only one atom thick.) This material has been the subject of intense study recently because of its remarkable electronic properties. Due to the special symmetry of the hexagonal lattice, standard approximations in condensed-matter theory do not lead to the usual effective mass approximation for charge carriers, but rather, they behave like relativistic particles with a reduced “speed of light.” On the theoretical side this has been known since 1947 when the (unintegrated) density of states at low energies was calculated in a tight-binding approximation and found to be proportional to \( |E - E_0| \) as a function of energy \( E \), as is the case for a two-dimensional relativistic particle [53]. Confirming experiments date from the past decade (e.g., [42,48,16]), where the charge carriers are electrons. A calculation of the density of states does not in fact allow an unambiguous determination of the effective Hamiltonian of particles moving in graphene, so the details of models used in the physical literature vary. Furthermore, although the standard effective-mass approximation for periodic Schrödinger Hamiltonians has had a rigorous mathematical basis since the work of Odeh and Keller [43] (see also [9,20,41,18]), we are unaware of comparably convincing analysis of the effective Hamiltonian for materials like graphene that offer a clear prescription for treating boundaries. The practice in the physical literature has been to propose relativistic Hamiltonians with ad hoc modifications to account for the effect of the boundary geometry, the effects of have become accessible to experiment quite recently (e.g., [38,40,45,43]). For a sampling of the different graphene-related models and calculations, see [53,52,50,30,46]. Because the usual charge carrier is an electron, which is a spin \( \frac{1}{2} \) particle, more often than not the Hamiltonian is chosen as a Dirac operator acting on
the set of two-component spinors. We hope to elaborate the spectral theory of Hamiltonians with spin in future work, but in the present work we content ourselves with the study of (4.1), and we also continue to restrict the Hamiltonian to a finite domain in order to achieve a discrete spectrum. Our point of departure to derive useful spectral bounds for (4.1) is (2.11), which remains valid for interacting operators $H$.

**Theorem 4.1** Let $\beta_k$ denote the eigenvalues of (4.1), and set

$$U(z) := \sum_k \frac{(z - \beta_k)^2}{\beta_k} \quad \text{as in } (2.14).$$

Assume that the measurable function $V = V_+ - V_-$ with $V_+ \geq 0$ and $V_- \in L^s$ for some $2 \leq d < s < \infty$. If

$$\|V_+\|_s < \frac{\sqrt{\pi} 2^{-\frac{(d-1)^2}{d}} \Gamma \left(\frac{d}{2}\right)^{\frac{1-2d}{d}} (d|\Omega|)^{\frac{s-d}{s}} (s-d)^{\frac{s-1}{s}}}{(d-2)! (s-1)^{\frac{s-1}{s}}},$$

then let us define $\alpha < 1$ by

$$\alpha := \frac{\|V_+\|_s (d-2)! (s-1)^{\frac{s-1}{s}}}{\sqrt{\pi} 2^{-\frac{(d-1)^2}{d}} \Gamma \left(\frac{d}{2}\right)^{\frac{1-2d}{d}} (d|\Omega|)^{\frac{s-d}{s}} (s-d)^{\frac{s-1}{s}}}. $$

Then for each $k$, the eigenvalues $\beta_k$ satisfy

$$\frac{\beta_{k+1}}{\beta_k} \leq \frac{\beta_k^{-1} \beta_{k+1} \leq 1 + \frac{2}{(d-1)(1-\alpha)}}.$$

Moreover, $\frac{U(z)}{z((d+1)\alpha - 1)}$ is a nondecreasing function of $z \in \mathbb{R}$, and for $k > 2j$,

$$\frac{\beta_k}{\beta_j} \leq \frac{\frac{d - \alpha(d-1)}{(d-1)(1-\alpha)^{2/(d-\alpha(d-1))}} \left(\frac{k}{j}\right)^{(d-\alpha(d-1))}}{1}. $$

**Proof.** From (2.11),

$$(d - 1) \sum_{j=1}^n (z - \beta_j)^2 \langle u_j, H_{m,\Omega}^{-1} u_j \rangle - 2 \sum_j (z - \beta_j) \leq 0. \quad (4.5)$$

Since $V_+ \geq 0$,

$$H_{m,\Omega} + V > H_{m,\Omega} - V_-, $$

and so

$$(H_{m,\Omega} + V)^{-1} \leq (H_{m,\Omega} - V_-)^{-1}. $$

Hence,
\[
\frac{1}{\beta_j} = \langle u_j, (H_{m,\Omega} + V)^{-1}u_j \rangle \leq \langle u_j, (H_{m,\Omega} - V_{-})^{-1}u_j \rangle \\
\leq \langle u_j, (H_{m,\Omega} - V_{-})^{-1}u_j \rangle \\
= \langle u_j, H_{m,\Omega}^{-1}u_j \rangle + \langle u_j, (H_{m,\Omega} - V_{-})^{-1}V_{-}H_{m,\Omega}^{-1}u_j \rangle,
\]
according to the resolvent formula.

If \(2 \leq d \leq s < \infty\), we now claim that

\[
\|V_{-}H_{m,\Omega}^{-1}\varphi\|_2 \leq \alpha \|\varphi\|_2 \quad (4.6)
\]

for any \(\varphi \in L^2\). Granting the claim, with \(\varphi = u_j\) in (4.6), we get

\[
\frac{1 - \alpha}{\beta_j} \leq \langle u_j, H_{m,\Omega}^{-1}u_j \rangle. \quad (4.8)
\]

To establish (4.7) begin by noting that by Hölder’s inequality,

\[
\|V_{-}H_{m,\Omega}^{-1}\varphi\|_2 \leq \|V_{-}\|_s \|H_{m,\Omega}^{-1}\varphi\|_s. \quad (4.9)
\]

Because \(H_{m,\Omega} \geq H_{0,\Omega}\),

\[
\|H_{m,\Omega}^{-1}\varphi\|_s \leq \|H_{0,\Omega}^{-1}\varphi\|_s. \quad (4.10)
\]

Inequality (3.5) for the transition density implies

\[
e^{-tH_{0,\Omega}}(x, y, t) \leq p_0(x - y, t) = \frac{-cd}{d - 1} \frac{\partial}{\partial t} \left( t^2 + |x - y|^2 \right)^{-\left(\frac{d-1}{2}\right)}.
\]

Applying the Laplace transform, the kernel of \(H_{0,\Omega}^{-1}\) is less than

\[
\int_0^\infty \left( \frac{-cd}{d - 1} \frac{\partial}{\partial t} \left( t^2 + |x - y|^2 \right)^{-\left(\frac{d-1}{2}\right)} \right) dt = \frac{cd}{d - 1} |x - y|^{-(d-1)}.
\]

Together with (4.9) and (4.10) we get

\[
\|V_{-}H_{m,\Omega}^{-1}\varphi\|_2 \leq \frac{cd}{d - 1} \|V_{-}\|_s \|x|^{-(d-1)} \ast \varphi\|_s.
\]

According to Young’s convolution inequality,

\[
\|x|^{-(d-1)} \ast \varphi\|_s \leq \|x|^{-(d-1)}\|_s \|\varphi\|_2,
\]

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so
\[ \left\| V - H^{-1}_{m,\Omega} \varphi \right\|_2 \leq \frac{\Gamma \left( \frac{d+1}{2} \right)}{\pi^{(d+1)/2}(d-1)} \left\| V_{-} \right\| \| x \|^{-(d-1)} \left\| \varphi \right\|_2. \]  

(4.11)

For an upper bound to \[ \left\| x \right\|^{-(d-1)} \right\|_2 \], choose \( R^* \) as the radius of the ball \( B_{R^*} \) centered at the origin having the same volume as \( \Omega \). Since by rearrangement,
\[ \parallel x \parallel_{L^s}^{-(d-1)}(\Omega) \leq \parallel x \parallel_{L^s}^{-(d-1)}(B_{R^*}) = \left( \frac{\omega_{d-1}(R^*)^{d-1}(s-1)}{s-d} \right)^{\frac{s-1}{s}}, \]

we get the estimate
\[ \left\| x \right\|^{-(d-1)} \left\| x \right\|_{L^s}^{-(d-1)} \left( \frac{s-1}{s} \right)^{\frac{s-1}{s}}, \]

(4.12)

With (4.11) and (4.2) this implies (4.7) and consequently (4.8). Because \( \alpha < 1 \) by assumption, (4.5) together with (4.8) yield
\[ (d-1) \sum_{j=1}^{n} \frac{1-\alpha}{\beta_j} (z - \beta_j)^2 - 2 \sum_{j=1}^{n} (z - \beta_j) \leq 0, \]

(4.13)

or, equivalently,
\[ (d-1)(1-\alpha)\beta_k^{-1} z^2 - 2[d-\alpha(d-1)]z + [d+1-\alpha(d-1)] \beta_k \leq 0. \]

(4.14)

By setting \( z = \beta_{k+1} \), we see that \( \beta_{k+1} \) must be smaller than the larger root of (4.14), i.e., after some algebra,
\[ \beta_{k+1} \leq \frac{(d-1)(1-\alpha) + 1 + \sqrt{1 - ((d+\alpha-\alpha d)^2 - 1)(\overline{\beta k}^{-1})}}{(d-1)(1-\alpha)\beta_k^{-1}}. \]

(4.15)

As was the case for (2.6), with the Cauchy-Schwarz inequality in the form \( 1 \leq \overline{\beta_k}^{-1} \), (4.15) implies the simpler but slightly weaker inequalities (4.13).

Now observe that (4.13) differs from (2.12) only in the extra factor \( 1 - \alpha > 0 \), and therefore all of the consequences of that inequality can be recovered with suitable changes of some constants. In particular, the function \( U(z) \) is nonincreasing, and therefore,
\[ U(z) \geq \left( \frac{z}{z_j^*} \right)^{(d+1)-\alpha(d-1)} \] 

(4.16)
when \( z \geq z_j^* \geq \beta_j \).

At the same time, by (4.13) we have

\[
\frac{(d - 1)(1 - \alpha)}{2} U(z) \leq R_1(z). \tag{4.17}
\]

By (4.17) and the fact that \( U(z) \geq \frac{1}{\beta_j}(z - \beta_j)^2 \), we obtain

\[
R_1(z) \geq \frac{(d - 1)(1 - \alpha)j}{2\beta_j} \left( \frac{z}{z_j^*} \right)^{(d+1)-\alpha(d-1)} (z_j^* - \beta_j)^2. \tag{4.18}
\]

To maximize the coefficient of \( z^{d+1-\alpha(d-1)} \) we optimize \( z_j^* \) and get

\[
z_j^* = \frac{(d + 1) - \alpha(d - 1)}{(d - 1)(1 - \alpha)} \beta_j.
\]

Substituting this into (4.18) gives

\[
R_1(z) \geq \frac{2j[(d - 1)(1 - \alpha)]^{d-\alpha(d-1)}}{[(d + 1) - \alpha(d - 1)](d+1)-\alpha(d-1)\beta_j^{d-\alpha(d-1)} z^{(d+1)-\alpha(d-1)}} \tag{4.19}
\]

for all \( z \geq \frac{(d + 1) - \alpha(d - 1)}{(d - 1)(1 - \alpha)} \beta_j \).

With the Legendre transform of the right hand side of (4.19), we obtain

\[
k/\beta_k \leq \frac{[d - \alpha(d - 1)]\beta_j}{[(d - 1)(1 - \alpha)]2^{1/(d-\alpha(d-1))} \beta_j^{1/(d-\alpha(d-1))} k^{1+1/(d-\alpha(d-1))}}. \tag{4.20}
\]

Therefore,

\[
\frac{\beta_k}{\beta_j} \leq \frac{d - \alpha(d - 1)}{[(d - 1)(1 - \alpha)]2^{1/(d-\alpha(d-1))} \left( \frac{k}{j} \right)^{1/(d-\alpha(d-1))}} \tag{4.21}
\]

as claimed. \[\square\]

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