Perturbation of eigenvalues of the Klein Gordon operators II

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Abstract

We give estimates for the changes of the eigenvalues of the Klein Gordon operator under the change of the potential. In some relevant situations we improve the existing estimates. We test our results on some exactly solvable models (Coulomb potential, Klein-Gordon oscillator).

1 Introduction and preliminaries

The abstract time independent Klein-Gordon equation reads formally

$$(U^2 - (\lambda - V)^2)\psi = 0 \tag{1.1}$$

where U, (U^2 usually meaning the kinetic plus mass energy) is selfadjoint and positive definite operator in a Hilbert space $\mathcal{X}$ and V (the potential) symmetric and in some sense dominated by U and λ is the eigenvalue parameter. The most interesting application is the standard Klein-Gordon equation with $\mathcal{X} = L_2(\mathbb{R}^3)$ and

$$U^2 = c^2p^2 + mc^2, \quad p = (-ih\nabla - \frac{e}{c}A(x))^2, \quad V = V(x), \quad x \in \mathbb{R}^3 \tag{1.2}$$

where h, c are the common physical constants whereas the mass term m and the magnetic potential A may be position-dependent. Or else, U^2 may be some other elliptic differential operator.

Typically there is a spectral gap around zero, then isolated eigenvalues of finite multiplicity appear which may either be bounded by the spectral continuum reaching to $\pm\infty$ or else the whole spectrum is discrete again approaching $\pm\infty$. Of some interest could be also the case where U, V are finite matrices. The most interesting eigenvalues are those around zero.

The aim of this paper is to prove sharp perturbation estimates for discrete eigenvalues λ under the change of V and U. The main technical tool is the monotonic dependence of the eigenvalues as functions of the potential. In fact, once one has

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monotonicity, then for the perturbed potential $\tilde{V} = V + \delta V$ (with δV bounded) we would have

$$V - \inf \sigma(\delta V) \leq \tilde{V} \leq V - \sup \sigma(\delta V) \tag{1.3}$$

which immediately implies the perturbation bound

$$\lambda - \inf \sigma(\delta V) \leq \tilde{\lambda} \leq \lambda + \sup \sigma(\delta V) \tag{1.4}$$

where $\lambda, \tilde{\lambda}$ is the corresponding eigenvalue, respectively. In particular,

$$\lambda - \|\delta V\| \leq \tilde{\lambda} \leq \lambda + \|\delta V\|$$

While such monotonicities are plausible for the Schroedinger and Dirac operators, the Klein-Gordon case is less simple, because the potential V enters (1.1) as a quadratic polynomial. To explain this we give a simple heuristic derivation. Let $V = V_t$ be real analytic and produce t-dependent eigenvalue λ_t and eigenvector ψ_t then by differentiating (1.1) we obtain

$$\lambda_t' = \frac{(V_t^2{}'\psi_t, \psi_t) - 2\lambda_t (V_t'\psi_t, \psi_t)}{2((V_t - \lambda_t)\psi_t, \psi_t)} \tag{1.5}$$

(here $'$ stays for the derivative). Supposing λ_t to be, say, positive (1.5) will yield monotonicity, if V_t is negative semidefinite — which is a notable restriction. Note also that growing V_t will produce falling V_t^2 only if V_t all commute (which is secured with multiplicative potentials, but not generally).

A derivation to this effect was produced in [5].[1] Here we will make this result rigorous and more precise. We will also enlarge its validity and then apply it to obtain eigenvalue perturbation bounds. More specifically we will

(i) prove that analytic dependence of V on a parameter implies the same for the eigenvalues and eigenvectors, not just locally, but such as to produce eigenvalue bounds. In fact, analysing quadratic eigenvalue equation (1.1) involves unbounded non-selfadjoint phase space Hamiltonians which are symmetric with respect to an indefinite scalar product so some extra care has to be taken,

(ii) make sure that the desired monotonicity, as well as the bounds of the type (1.4) hold for increasingly ordered eigenvalues with their multiplicities, just as is obtained by standard minimax arguments, (this is not quite trivial even with common selfadjoint operators if one considers the discrete eigenvalues in gaps of the essential spectrum, see [20])

(iii) weaken the condition of positivity of the considered eigenvalues into the more natural, so-called *plus* property (which will, roughly speaking, cover all eigenvalues coming from the upper continuum as long as they do not clash with those coming from below). Unfortunately we were able to do this only partially, as yet, for instance for potentials of the form tV.

[1] This kind of monotonicity seems to be observed first in [12]. The result in [12] was stated under similar restrictive conditions, but it seems to us that the proof offered there has some gaps we were unable to fill.

(iv) also weaken the non-positivity of the potential V because even for non-positive potentials the two-sided inclusion (1.3) requires monotonicity for slightly indefinite potentials.

(v) give a collection of mostly exactly solvable examples illustrating the estimates. A particularly interesting case will be that of perturbed Coulomb potential, where the local deformation δV with

$$|\delta V(x)| \leq \beta \frac{1}{|x|}, \quad \beta < 1$$

leads to particularly tiny bound for the perturbed eigenvalue λ'

$$\lambda(1+\beta) \leq \lambda' \leq \lambda(1+\beta) \tag{1.6}$$

where $\lambda(t)$ is the corresponding eigenvalue corresponding to the potential $-t/|x|$ and is given by an explicit formula. We will also make comparison with the bounds obtained recently in [14] and show that our bounds complement the ones from [14].

Another example will be that of the Klein-Gordon oscillator in $L_2(\mathbb{R}^n)$ with $U^2 = -\Delta + x^2$ and $V = 0$ and then the bounds (1.4) will actually hold for both sides of the spectrum.

The plan of the paper is as follows. In Section 1. we give definitions and fundamental properties of the Hamiltonians considered, in Section 2. we derive the mononotonicity and in Section 3. give the resulting sharp eigenvalue bounds of the type (1.4), (4.22) together with illustrating examples.

2 The Hamiltonian formulation and analyticity

The eigenvalue analysis necessitates rewriting a quadratic eigenvalue problem as a linear one with 'doubled dimension'. By setting

$$\psi_1 = \psi, \quad \psi_1 = (\lambda I - V)\psi$$

we arrive at the eigenvalue equation $K\psi = \mu\psi$ with

$$K = \begin{bmatrix} V & I \\ U^2 & V \end{bmatrix}. \tag{2.7}$$

that is, $K = JL$ where L

$$L = JK = \begin{bmatrix} U^2 & V \\ V & I \end{bmatrix} \tag{2.8}$$

is again formally Hermitian. So, K is J-Hermitian. Our general assumption is

$$\|(V - \mu I)U^{-1}\| < 1, \tag{2.9}$$

for some real μ. This commonly used condition insures reasonable spectral properties of the operator K, see e.g. [14] and the literature cited there.[2] The set $\mathcal{I}$ of all such μ is obviously an open interval and we shall call it *the definiteness interval.* Under this condition L is rigorously defined by means of quadratic forms in the factorisation

$$L - \mu J = \begin{bmatrix} U & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & \overline{U^{-1}(V - \mu I)} \\ (V - \mu I)U^{-1} & I \end{bmatrix} \begin{bmatrix} U & 0 \\ 0 & I \end{bmatrix} \tag{2.10}$$

which is selfadjoint positive definite (being a symmetric product of three such factors). Thus we obtain a J-selfadjoint operator

$$K = JL, \quad J = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \tag{2.11}$$

that is, a selfadjoint operator with respect to the indefinite scalar product

$$[\psi, \phi] = (J\psi, \phi).$$

These operators have real spectrum and a rich spectral calculus, see [8]. By our condition (2.9) we have

$$\sigma(K) = \sigma_-(K) \cup \sigma_+(K), \quad \sigma_-(K) < \mathcal{I} < \sigma_+(K).$$

Moreover, as it is readily seen the eigenvalues on the right/left from μ have $[\cdot, \cdot]$-positive/negative eigenvactors, and will be called *plus/minus-eigenvalues*, respectively. Also obvious is the fact that all eigenvalues are semisimple.

The spectra of the operators H, K are connected with those of the quadratic families like (1.1).

The following Facts were shown in [19], Thms 2.4 and 4.2.

1. The sesquilinear form

$$q_\mu(\psi, \phi) = (U\psi, U\phi) - ((V - \mu I)\psi, (V - \mu I)\phi) \tag{2.12}$$

is closed and sectorial for every $\mu \in \mathbb{C}$ as defined on $\mathcal{D}(U)$ and it generates a closed sectorial operator Q_μ whose domain $\mathcal{D}(Q_\mu)$ is independent of μ.

2.

$$Q_\mu = Q_\lambda + 2(\mu - \lambda)V + (\mu^2 - \lambda^2)I \tag{2.13}$$

for any μ, λ.

3. Denoting by ρ the set of μ-s for which Q_μ^{-1} is everywhere defined and bounded and by σ its complement we have

$$\rho = \rho(K), \quad \sigma = \sigma(K).$$

[2]The Hamiltonian considered there is not the one from the present paper but the eigenvalues and their multiplicities are the same.

4.

$$\psi \in \mathcal{D}(Q_\mu), \quad Q_\mu \psi = 0$$

is equivalent to

$$\begin{bmatrix} \psi \\ \phi \end{bmatrix} \in \mathcal{D}(H)$$

for some ϕ and

$$H \begin{bmatrix} \psi \\ \phi \end{bmatrix} = \mu \begin{bmatrix} \psi \\ \phi \end{bmatrix}.$$

3 Monotonicity

We will show that the eigenvalues depend monotonically on the potential.

In order to compare the eigenvalues by means of analytic perturbations we will linearly connect them as

$$V_t = tV_1 + (1-t)V_0 = V_0 + t\delta V, \quad \delta V = V_1 - V_0 \geq 0 \tag{3.14}$$

$$0 \leq t \leq 1.$$

Lemma 3.1. *Let V_0, V_1 be symmetric and $\|(V_0 - \mu I)U^{-1}\|, \|(V_1 - \mu I)U^{-1}\| \leq \beta < 1$ for some real μ. Then*

$$\|(V_t - \mu I)U^{-1}\| \leq \beta.$$

Proof. It is sufficient to consider $\mu = 0$. We have

$$(\|V_t\psi\|^2 = t^2(V_1\psi, V_1\psi) + t(1-t)(V_1\psi, V_0\psi) + t(1-t)(V_0\psi, V_1\psi) + (1-t)^2(V_0\psi, V_0\psi)$$

$$\leq t^2\|V_1\psi\|^2 + 2t(1-t)\|V_1\psi\|\|V_0\psi\| + (1-t)^2\|V_0\psi\|^2$$

$$\leq t^2\beta\|U\psi\|^2 + 2\beta t(1-t)\|U\psi\|\|U\psi\| + (1-t)^2\beta\|U\psi\|^2 = \beta(t^2 + 2t(1-t) + (1-t)^2)\|U\psi\|^2$$

$$= \beta\|U\psi\|^2.$$

Q.E.D.

By the preceding lemma the operator K_t constructed with V_t via (2.10), (2.11) has the same properties as K. In particular

$$-\frac{\|U^{-1}\|^{-1}}{1-\beta} \leq \sigma(K_t) - \mu \leq \frac{\|U^{-1}\|^{-1}}{1-\beta}. \tag{3.15}$$

Theorem 3.2. *Let $V_0, V_1, \delta V$ be as in (3.14) and let V_0, V_1 commute, satisfy $\|(V_0 - \mu I)U^{-1}\|, \|(V_1 - \mu I)U^{-1}\| \leq \beta < 1$ and be ordered as*

$$(V_1\psi, \psi) \geq (V_0\psi, \psi) \geq -M(\psi, \psi) \tag{3.16}$$

where M is the right hand side of (3.15).

Suppose also that δV^2 and $\delta V V_0$ are defined on $\mathcal{D}(U)$. Denote by K_0, K_1 the corresponding operators from (2.10), (2.11). Assume that the top of the minus-spectrum of K_0 consists of discrete eigenvalues, counted with their (finite) multiplicities

$$\lambda_1^{(0)} \geq \cdots \geq \lambda_n^{(0)} > \tilde{\lambda}$$

such that the negative part of $\sigma_{ess}(K_t)$ stays left from $\tilde{\lambda}$ for $t \in [0,1]$, where the operator K_t belongs to the potential V_t from (3.14). Then the top of the minus-spectrum of K_1 also consists of discrete eigenvalues

$$\lambda_1^{(1)} \cdots \geq \lambda_n^{(1)} \geq \ldots$$

and we have

$$\lambda_i^{(1)} \geq \lambda_i^{(0)}.$$

Note that the last assumption in the preceding theorem is automatically fulfilled if the essential spectrum does not move at all with $V + t\delta V$, for instance, if both V and δV are either U-compact or U^2-compact (see [12] or [10]).

Proof. By the preceding lemma the operator K_t constructed with V_t via (2.7) has the same properties as K and it is analytic in t on a region containing the closed interval $[0,1]$. This is best seen in computing the inverse of L_μ factorised as in (2.10), replacing V by V_t and using the obvious Neumann expansion for the inverse of the middle term in (2.10). Now, as it was shown in [16] the analyticity properties of the isolated eigenvalues are similar as with standard selfadjoint analytic families. More precisely, let $\lambda \geq \tilde{\lambda}$ be any discrete minus-eigenvalue of K_t for some $0 \leq t_0 \leq 1$. Then the spectrum of K_t in a neighbourhood of t_0 is represented by one or several — according to the multiplicity of $\lambda(t_0)$ — analytic functions which, together with their J-orthonormal eigenvectors, can be analytically continued as long as

- they are separated from the continuous spectrum and
- they do not meet a plus-eigenvalue.

(The analyticity is not destroyed even at the places where the eigenvalues cross.) Both conditions are fullfilled by our assumptions. Indeed, the second condition is insured by the global estimate $\|V_t U^{-1}\| < 1$. This estimate together with the non-intruding insures the first condition by the assumed condition

$$\lambda_n^{(1)} \geq \tilde{\lambda}$$

for some λ. Consider any such analytic eigenpair $\lambda(t), \Psi(t)$:

$$K_t \Psi(t) = \lambda(t)\Psi(t). \tag{3.17}$$

This equation is equivalent to

$$Q_{\lambda,t}\psi(t) = 0 \tag{3.18}$$

where

$$\psi(t) = \psi_1(t), \quad \Psi(t) = \begin{bmatrix} \psi_1(t) \\ \psi_2(t) \end{bmatrix}$$

and $q_{\lambda,t}$, $Q_{\lambda,t}$ are defined by (2.12) with V replaced by V_t from (3.14) — see Fact 4 above. Looking for monotonicity we will have to differentiate the eigenvalue equation (3.18) with respect to t. This is certainly possible because by Fact 4 $\psi = \psi(t)$ appearing there is just the first component of $\Psi(t)$. In order to do this it will be convenient to know that the domain $\mathcal{D}_t$ does not depend on t either and to have an explicit operator expression for $Q_{\lambda,t}$.

Now replace in (2.12), (2.13) V by $V_t = V_0 + t\delta V$ thus obtaining

$$q_{\lambda,t}(\psi,\phi) = (U\psi, U\phi) - ((\lambda - V_0 - t\delta V)\psi, (\lambda - V_0 - t\delta V)\phi) \quad \psi,\phi \in \mathcal{D}(U). \tag{3.19}$$

and analogously for $Q_{\lambda,t}$. Let now $\psi \in \mathcal{D}(Q_{0,0})$ then

$$(U\psi, U\phi) - (V_0\psi, V_0\phi) = (Q_{0,0}\psi, \phi)$$

and

$$q_{\lambda,t}(\psi,\phi) = (Q_{0,0}\psi,\phi) -$$
$$-\lambda^2(\psi,\phi) - t^2(\delta V\psi, \delta V\phi) + 2\lambda(V_0\psi,\phi) + 2\lambda t(\delta V\psi,\phi) - t(\delta V\psi, V_0\phi) - t(V_0\psi, \delta V\phi).$$

Using the fact that V_0, δV are commuting and that the products $V_0\delta V$ and δV^2 are defined on $\mathcal{D}(U)$ we may write

$$q_{\lambda,t}(\psi,\phi) = (Q_{0,0}\psi,\phi) - \lambda^2(\psi,\phi) - t^2(\delta V^2\psi,\phi) + 2\lambda(V_0\psi,\phi) + 2\lambda t(\delta V\psi,\phi) - 2t(V_0\delta V\psi,\phi).$$

Since this is valid for any ϕ from $\mathcal{D}(U)$ on which $q_{\mu,t}$ is known to be closed the first representation theorem of Kato ([6]) implies $\psi \in \mathcal{D}(Q_{\lambda,t})$ and

$$Q_{\lambda,t}\psi = Q_{0,0}\psi - \lambda^2\psi - t^2\delta V^2\psi + 2\lambda V_0\psi + 2\lambda t\delta V\psi - 2tV_0\delta V\psi.$$

and by switching the roles of $Q_{\lambda,t}$ and $Q_{0,0}$ we have $\mathcal{D}(Q_{\lambda,t}) = \mathcal{D}(Q_{0,0})$ and the operator identity

$$Q_{\lambda,t} = Q_{0,0} - \lambda^2 - t^2\delta V^2 + 2\lambda V_0 + 2\lambda t\delta V - 2tV_0\delta V \tag{3.20}$$

on $\mathcal{D}(Q_{0,0})$.

In other words, as a function of t, $Q_{\lambda,t}$ is holomorphic of type (A) as defined in [6]. Thus, the domain $\mathcal{D} = \mathcal{D}_t = \mathcal{D}(Q_{\lambda,t})$ is independent of both λ and t.

We are now in a position to differentiate the quadratic eigenvalue equation (3.18) written in the form

$$(\psi, Q_{\lambda,t}\phi) = 0$$

where $\psi = \psi(t) \in \mathcal{D}$, $\lambda = \lambda(t)$, and ϕ is any vector from $\mathcal{D}$ independent of t and $Q_{\lambda,t}$ is given by (3.20) (note that for real λ the operator $Q_{\lambda,t}$ is selfadjoint). By differentiating this using the Leibniz rule we obtain

$$(\psi', Q_{\lambda,t}\phi) + (\psi, Q_{\lambda,t}\phi)') = 0$$

and by (3.20)

$$(\psi', Q_{\lambda,t}\phi) =$$

$$-2\lambda\lambda'(\psi,\phi)-2t(\psi,\delta V^2\phi)+2\lambda'(\psi,V_0\phi)+2\lambda' t(\psi,\delta V\phi)+2\lambda(\psi,\delta V\phi)-2(\psi,V_0\delta V\phi) = 0.$$

Now set $\phi = \psi$. Using $Q_{\lambda,t}\psi = 0$ we obtain

$$\lambda'(\psi,(V_0-\lambda+2t\delta V)\psi) + (\psi,(V_0-\lambda+2t\delta V)\delta V\psi) = 0.$$

Hence

$$\lambda' = \frac{(\psi,(V_0-\lambda+t\delta V)\delta V\psi)}{(\psi,(V_0-\lambda+t\delta V)\psi)} = \frac{(\psi,(V_t-\lambda I)\delta V\psi)}{(\psi,(V_t-\lambda I)\psi)} \tag{3.21}$$

which is in accordance with the heuristic formula (1.5). Using that $V_t - \lambda I$ and δV are positive semidefinite and commuting we infer that λ' is non-negative. The positive definiteness of the former follows from $\lambda < -M$ and our assumption (3.16).

We have thus obtained n functions

$$\lambda_1(t) \geq \cdots \geq \lambda_n(t)$$

non decreasing in t and representing discrete eigenvalues of K_t together with their multiplicities and such that

$$\lambda_1(0) = \lambda_1^{(0)} \geq \cdots \lambda_n(0) = \lambda_n^{(0)}$$

However this non-increasing ordering need not be kept by $\lambda_i(t)$ for all t because some other isolated (but also non-increasing in t) eigenvalues may be crossing so that from some t onwards we may have more than n eigenvalues larger than $\tilde{\lambda}$. To overcome this inconvenience we sort the eigenvalues $\lambda_i(t)$ non-increasigly in i for any t thus obtaining the n top eigenvalues

$$\tilde{\lambda}_1(t) \geq \cdots \geq \tilde{\lambda}_n(t)$$

which are still continuous and non-decreasing in t (but possibly only piecewise differentiable) This situation is illustrated on Figure 1.

Now

$$\lambda_i^{(1)} = \tilde{\lambda}_i(1)$$

are the top eigenvalues of K_1 as asserted in the statement. Q.E.D.

Of course, a completely symmetric estimate holds for *plus* eigenvalues (just turn V into $-V$) which is the common situation in Relativistic Quantum Mechanics.

The positive eigenvalues need not be monotone. The following example will show that.

Example 3.3. Set

$$U^2 = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, \quad V = t\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

with $0 \leq t \leq 2$. Note that here different tV 's commute.

The non-monotone behaviour of λ_1^+ is shown on Figure 2.

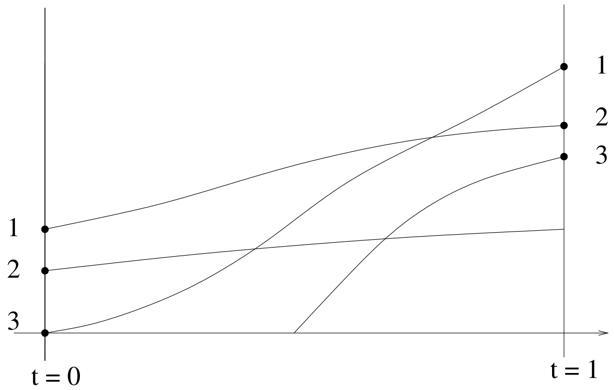

Figure 1: Ordering ascending eigenvalues

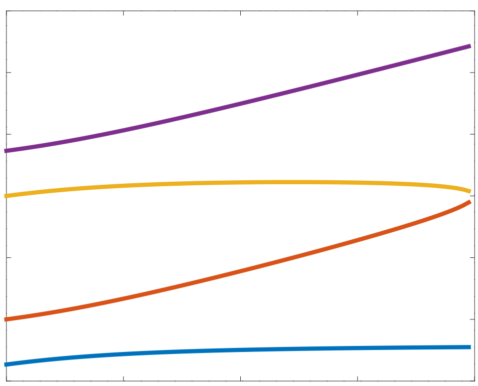

Figure 2: Eigenvalues as functions of $t \in [0, 2]$

In fact, as the figure indicates, at $t = 2$ both λ_1^- and λ_1^+ are equal to -1 and for $t > 2$ they will become non-real. However, it should be noted that the non-monotonicity appears only after a good while, as is also observed in [13].

There can well be cases, however, in which the unperturbed potential vanishes, or is lumped together with the free Hamiltonian. Then the mononicity will hold for both positive and negative part of the spectrum in opposite directions, respectively — as in the perturbation of the Klein-Gordon oscillator below.

4 The eigenvalue bounds

Take the perturbation δV as bounded and commuting with V, then set $\tilde{V} = V + \delta V$. Then

$$(\psi, (V - \|\delta V\| I)\psi) \leq (\psi, \tilde{V}\psi) \leq (\psi, (V + \|\delta V\| I)\psi).$$

Now use the fact that the potential and the eigenvalue enter (3.18) only as a difference. Since $V \pm \|\delta V\| I$ produces the eigenvalues $\lambda_j \pm \|\delta V\|$ the monotonicity Theorem 3.2 is applicable and it implies

$$\lambda_j - \|\delta V\| \leq \tilde{\lambda}_j \leq \lambda_j + \|\delta V\|. \tag{4.22}$$

Here, of course, to insure monotonicity we must assume that δV is sufficiently small as to have

$$V - \|\delta V\| I \geq -M. \tag{4.23}$$

In the most interesting case of a positive potential this is insured, if

$$\|\delta V\| \leq M \tag{4.24}$$

which leaves ample a margin for any practical purpose. More precisely, if

$$\delta_\pm = \begin{matrix} \sup_\psi \\ \inf_\psi \end{matrix} \frac{(\psi, \delta V \psi)}{(\psi, \psi)}$$

then (4.22) is strengthened into

$$\lambda_j - \delta_- \leq \tilde{\lambda}_j \leq \lambda_j + \delta_+. \tag{4.25}$$

This estimate can not be improved in general, just take V bounded and δV a scalar multiple of V.

We will compare our bound with the one obtained in [14] which reads[3]

$$|\tilde{\lambda} - \lambda| \leq \text{NVbound} := \frac{|\lambda| \|\delta V U^{-1}\|}{1 - \|V U^{-1}\|} \leq \zeta \|\delta V\|. \tag{4.26}$$

[3]For simplicity in the following we drop the indices of the eigenvalues and also — to prevent moving of the essential spectrum — we will assume all perturbations δV to have compact support thus insuring relative compactness.

with the penalty

$$\zeta = \frac{|\lambda| \|U^{-1}\|}{1 - \|VU^{-1}\|}. \tag{4.27}$$

We will now compare this bound with the bound (4.22) which is just $\|\delta V\|$ on a concrete example. We evaluate the penalty ζ for the case of the ground state of the *Coulomb relativistic Hamiltonian* given by

$$U^2 = -h^2 c^2 \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) + m^2 c^4, \quad V = -\frac{Ze^2}{|x|}, \tag{4.28}$$

where m, h, c, e, Z are the common physical constants, in particular, Z is the atomic number. The ground state energy is given as

$$\lambda_0 = mc^2 \left[1 + \frac{Z^2 \alpha^2}{(0.5 + \sqrt{.25 - Z^2 \alpha^2})^2} \right]^{-1/2} \tag{4.29}$$

where $\alpha = \frac{e^2}{hc} \approx 1/137$ is the fine structure constant. Note that the ground state is always positive and so of plus type. Obviously $\|U^{-1}\| = 1/(mc^2)$ whereas by the known estimate (see e.g. [6] , Ch. V, (5.30)) we have

$$\|VU^{-1}\| = 2Z\alpha$$

and, by inserting in (4.27) we obtain

$$\zeta = \left[1 + \frac{Z^2 \alpha^2}{(0.5 + \sqrt{.25 - Z^2 \alpha^2})^2} \right]^{-1/2} /(1 - 2Z\alpha).$$

The behaviour of this penalty as a function of the atomic number Z is shown on Figure 3.

Thus our present bound outdoes the one from [14] significantly for larger atomic numbers.

There are, hovewer, examples where our theory is void and (4.26) still valid because the latter has no restriction to positive eigenvalues only. Such is the case of deep potential well which may have negative plus-eigenvalues.

While the value $\|\delta V U^{-1}\|$ is not easy to evaluate with U^2 Laplacian and δV a multiplication operator, we can do with another relative estimate (we keep with non-positive V)

$$-\gamma_-(V\psi, \psi) \leq (\delta V\psi, \psi) \leq -\gamma_+(V\psi, \psi) \tag{4.30}$$

which is easily verifiable, being a consequence of

$$-\gamma_- V(x) \leq \delta V(x) \leq -\gamma_+ V(x). \tag{4.31}$$

This gives

$$(1 - \gamma_-)(V\psi, \psi) \leq ((V + \delta V)\psi, \psi) \leq (1 - \gamma_+)(V\psi, \psi).$$

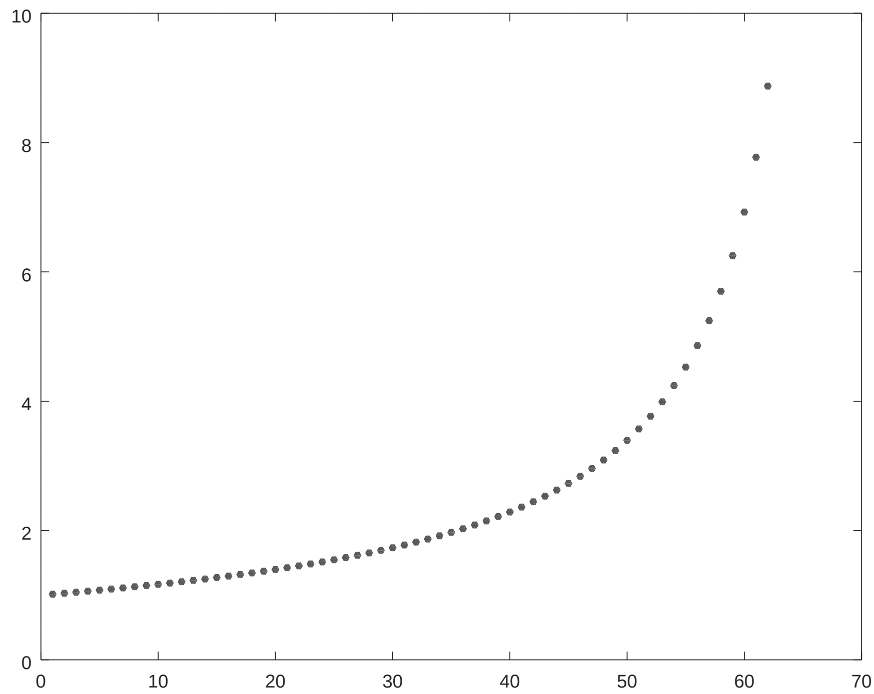

Figure 3: Penalty as function of the atomic number

This leads to an interesting bound which uses not only the unperturbed eigenvalue λ and the perturbation δV but the eigenvalues $\lambda(\varepsilon)$ belonging to the potential εV as follows

$$\lambda(1-\gamma_+) \le \tilde{\lambda} \le \lambda(1-\gamma_-) \tag{4.32}$$

where $\lambda = \lambda(1)$. So, the perturbed eigenvalue $\tilde{\lambda}$ is contained in the interval

$$\mathcal{I} = [\lambda(1-\gamma_-), \lambda(1-\gamma_+)] \tag{4.33}$$

(note that $\lambda(\varepsilon)$ is falling with ε).

The obtained bound is also sharp as is seen by taking δV proportional to V in which case $\gamma_\pm$ are just equal.

The knowledge of the whole family $\lambda(\varepsilon)$ is seldom available explicitly but just in the Coulomb case we have the explicit formula (4.29). Thus, if the perturbing potential satisfies (4.30) with V from (4.28) then for the ground state the perturbed eigenvalue $\tilde{\lambda}$ satisfies (4.32) where by (4.29)

$$\lambda(\varepsilon) = mc^2 \left[1 + \frac{\varepsilon^2 Z^2 \alpha^2}{(0.5 + \sqrt{.25 - \varepsilon^2 Z^2 \alpha^2})^2}\right]^{-1/2}.$$

To illustrate the power of this kind of estimate we take as the perturbation

$$\delta V(x) = \tau \begin{cases} \frac{Ze^2}{|x|}, & |x| > l \\ \\ \frac{Ze^2}{l}, & |x| \geq l, \end{cases} \qquad 0 < \tau < 1. \tag{4.34}$$

This perturbation has certain physical appeal, so we will go in some detail. We have here

$$\delta_- = 0, \quad \delta_+ = \frac{Ze^2}{l}$$

with

$$\lambda \leq \tilde{\lambda} \leq \frac{Ze^2}{l}$$

and

$$\gamma_- = 0, \quad \gamma_+ = \tau$$

with

$$\lambda \leq \tilde{\lambda} \leq \lambda(Z(1-\tau)).$$

For $Z = 40$ the behaviour of both bounds as functions of l is shown on Figure 4

The new bound (represented by crosses) is independent of the radius l and is clearly better as the norm bound (starred line) except for very large radii (from some 400 classical electron radii onwards). Besides, the value of the new bound is some 0.01. That is, 1% change of the potential produces 0.1% change of the eigenvalue. Thus the relative perturbation (4.31) produces very small changes of the eigenvalue. There is no reason to believe that this property holds only for the few potentials for which the dependence $\lambda(\varepsilon)$ is explicitly known.

Of course the two bounds (4.25) and (4.32) can be combined into one: if

$$\delta_- - \gamma_- V(x) - \leq \delta V(x) \leq \delta_+ - \gamma_+ V(x)$$

then

$$\delta_- + \lambda(1-\gamma_+) \leq \tilde{\lambda} \leq \delta_+ + \lambda(1-\gamma_-). \tag{4.35}$$

Remarks 4.1. 1. Note that our key results, notably Theorem 3.2 and the bounds (4.22), (4.25, (4.32) give not merely relations between existing eigenvalues, they rather include the *existence statements*, so for instance, in (4.32) between each pair $\lambda(1-\gamma_-), \lambda(1-\gamma_-)$ there is a perturbed $\tilde{\lambda}$ (including multiplicities).

2. Note the remarkable fact: under *just any* perturbation δV satisfying (4.31) no eigenvalue can cross the boundary mc^2 of the continuous spectrum, what is more, *the perturbed eigenvalues will be infinitely many and also accumulate at this boundary.* This is a general property of locally deformed Coulomb potentials.

3. The estimates of the type (4.32) will obviously hold for other quantum mechanical Hamiltonians (Schroedinger, Dirac...) where the eigenvalues are known to depend monotonically on the potential.

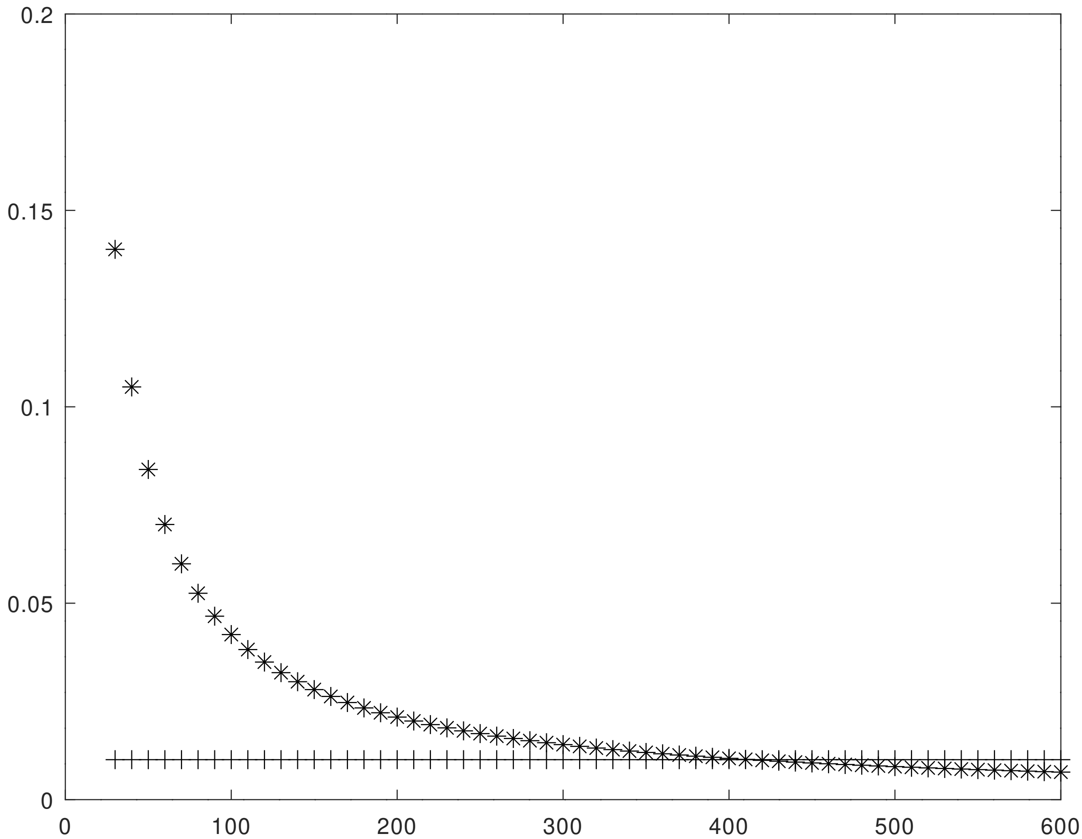

Figure 4: Absolute (*) and relative bound (+)

Our next example will the Klein-Gordon oscillator.Here we have

$$U = m^2c^4 + m^2c^2\omega^2|x|^2), \quad V(x) = \alpha x_1 \tag{4.36}$$

with

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^n, \quad p = -ih\nabla.$$

Here $\omega > 0$ is the classical oscillator frequency. The model is explicitly solvable and is readily seen that in this case

$$a = \|VU^{-1}\| = \frac{|\alpha|}{mc\omega},$$

whereas the spectrum is discrete and given by the eigenvalues

$$\lambda_k^\pm = \pm\sqrt{(2mc^2h\omega\nu_k(a) + m^2c^4)(1-a^2)}, \quad k = [k_0, \dots, k_n], \quad k_i = 0, 1, 2, \dots \tag{4.37}$$

with

$$\nu_k(a) = (1-a^2)^{1/2}\left(k_1 + \frac{1}{2}\right) + k_2 + \frac{1}{2} + \cdots + k_n + \frac{1}{2}, \quad k_1, \dots, k_n \geq 0$$

which are simple for $n = 1$. We see that the case $a \neq 0$ is completely out of reach of our theory because the homogeneous field $V = \alpha x_1$ is deeply indefinite. In contrast, the case $a = 0$ — this is the pure Klein-Gordon oscillator — we have non-trivial in fact, quite strong results. Then in the key formula (3.21) we have $V_0 = 0$ and it reads

$$\lambda' = \frac{(\psi, (-\lambda + t\delta V)\delta V\psi)}{(\psi, (-\lambda + t\delta V)\psi)}. \tag{4.38}$$

So, the condition (3.16) is automatically fulfilled if $V_1 = \delta V$ is positive semidefinite. Consequently, *plus and minus eigenvalues are monotone (in opposite directions) and our eigenvalue bounds (4.22) and (4.25) hold without any restriction.*

We can again compare this with the bound (4.26) where $V = 0$ gives

$$|\tilde{\lambda} - \lambda| \leq \frac{|\lambda|\|\delta V\|}{M}$$

which is as good as ours for the ground state $\lambda = \lambda_0^- = -M$. For higher energies the new bound gets better and better.

The estimate (4.32) can be used here, too. Perturbations, satisfying (4.31) will yield potentials $V + \delta V$ whose eigenvalues will have *the same spectral asymptotics as the Klein-Gordon oscillator*. Combined bounds (4.35) will hold, as well.

In trying to relax the conditions of Theorem 3.2 we will use the minimax formula obtained in [10]. We set

$$p_\pm(\psi) = (\psi, V\psi) \pm \sqrt{(\psi, V\psi)^2 + (U\psi, U\psi) - (V\psi, V\psi)}, \quad \|\psi\| = 1, \quad \psi\mathcal{D}(U). \tag{4.39}$$

Then, as is readily seen

$$\min \sigma_+(K) = \inf p_+(\psi), \quad \max \sigma_-(K) = \sup p_+(\psi)$$

and, as proved in [10]

$$\lambda_k^+ = \min_{S_k} \max_{\psi \in S_k, \|\psi\|=1} p_+(\psi), \quad \lambda_k^- = \max_{S_k} \min_{\psi \in S_k, \|\psi\|=1} p_-(\psi). \tag{4.40}$$

where S_k is any k-dimensional subspace of $\mathcal{D}(U)$ and $\lambda_i^\pm$ are the inner discrete eigenvalues with multiplicities ordered as

$$\cdots \le \lambda_2^- \le \lambda_1^- < \lambda_1^+ \le \lambda_2^+ \le \cdots \qquad \mathcal{I} = (\lambda_1^-, \lambda_1^+).$$

This time our conditions should accomodate the fact that, while working with positive potentials V_0, V_1 we will be considering *minus eigenvalues* which can well become positive if the potentials are deep enough (e.g. deep potential wells). So, the assumption $\|V_0\psi\| \le \|V_1\psi\| < 1$ would not do and we have to use (2.9). In order to prove the monotonicity we will have to investigate the dependence of $p_\pm$ on V, so we shall write

$$p_\pm(\psi) = p_\pm(\psi, V).$$

If we prove the monotonicity of $V \mapsto p_+(\psi, V)$ for any fixed unit ψ then the minimax formula (4.40) immediately implies the same for the plus eigenvalues. By setting

$$v = (\psi, V\psi), \quad w = (V\psi, V\psi), \quad \chi = (U\psi, U\psi)$$

we have to study the behaviour of the function

$$v, w \mapsto f(v, w) = p_-(\psi, V) = v - \sqrt{v^2 + \chi - w}$$

on the domain $v \ge 0, \quad 0 \le w < \chi$. We have

$$\frac{\partial f}{\partial v} = 1 - \frac{v}{\sqrt{v^2 + \chi - w}} > 0,$$

$$\frac{\partial f}{\partial w} = \frac{1}{2(\sqrt{v^2 + \chi - w})} > 0.$$

So, if V^2 is growing, then both v and w will be growing, hence f is growing for any fixed ψ that is, if $V_0, V_1 \ge 0$ and $V_0^2 \le V_1^2$ then

$$p_-(\psi, V_0) \le p_-(\psi, V_1).$$

Thereby this growing goes over to the minimax quantities from (4.40).

Now go into the proof of Theorem 3.2. There for any $t \in [0, 1]$ we have the top eigenvalues, counting multiplicities

$$\tilde{\lambda}_1(t) \ge \cdots \ge \tilde{\lambda}_n(t)$$

of $\sigma_-(K)$, piecewise differentiable in t. By the minimax formula we infer to the waxing in t as well. Altogether we have

Theorem 4.2. *Let V_0, V_1 be symmetric and and positive semidefinite with* $(V_1\psi, \psi) \leq (V_1\psi, \psi), \quad \psi \in \mathcal{D}(U)$ *and and let*

$$\|(V_0 - \mu)\psi\| < 1, \quad \|(V_1 - \mu)\psi\| < 1, \quad \psi \in \mathcal{D}(U) \tag{4.41}$$

for some real μ. Then the assertions of Theorem 3.2 hold true.

It is instructive to compare the conditions and also the results of this theorem with those of Theorem 3.2. The commutativity is dropped, and the clumsy assumptions on products of V_1, V_2 is replaced by (4.41). If V_1 (and then also V_0) is bounded, then (4.41) is implied by the single inequality

$$\|V_1\| < 2\|U^{-1}\|^{-1}. \tag{4.42}$$

However interesting in its own sake this theorem is by itself not sufficient to produce two-sided eigenvalue bounds (4.22), (4.25) and (4.32). (The last one will still hold under additional assumption that *both* V and $V + \delta V$ are non-negative.) This calls for some further research.

On the other hand Theorem 3.2 appears to be a special case of Theorem 4.2. But a closer look at the proof of the former shows that it in fact holds in *any* gap of the essential spectrum and not only in that around $\mathcal{I}$ which Theorem 3.2 does not. Also one might ask why in proving Theorem 4.2 we did not use minimax formulae alone without recurring to analytic perturbation theory. The reason is that as far as yet it is only the latter that guarantees the existence of the perturbed eigenvalues – at least with the present state of minimax theory as presented in [10].

A much stronger, in fact, the maximal result follows for the important special case of

$$V_t = tV.$$

We have

Corollary 4.3. *If V is positive semidefinite then with the potential tV, $t > 0$ the minus eigenvalues are monotone (as functions of t) in the sense of Theorem 4.2. This state of affairs carries on as long as $\|(tV - \mu I)U^{-1}\| < 1$ for some μ.*

Proof. We have

$$p_-(\psi) = p_-(\psi, t) = t(\psi, V\psi) - \sqrt{t^2(\psi, V\psi)^2 + (U\psi, U\psi) - t^2(V\psi, V\psi)}$$

and hence

$$p_(\psi, t)' = (\psi, V\psi) - t\frac{(\psi, V\psi)^2 - (V\psi, V\psi)}{\sqrt{t^2(\psi, V\psi)^2 - t^2(V\psi, V\psi) + (U\psi, U\psi)}}$$

$$= (\psi, V\psi) + t\frac{(\|(V - (\psi, V\psi)I)\psi\|^2}{\sqrt{t^2(\psi, V\psi)^2 - t^2(V\psi, V\psi) + (U\psi, U\psi)}} \geq 0$$

which holds as long as the radicand above is positive that is, if $\|(tV - \mu I)U^{-1}\| < 1$ for some μ.

The rest of the proof is as in Theorems 3.2, 4.2 respectively. Q.E.D.

Finite matrices. All our results above naturally comprise the case of finite matrices U, V. This is, however, of limited use in a computational environment where by various approximations and errors the commutativity of different V-s is easily lost. And without commutativity there is no way to convert the Loewner's theorem – monotonicity of positive operators does not generally extend to their squares – and this is needed to infer to the monotonicity of μ in (1.5).

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