Spectral perturbation bounds in gaps.

Krešimir Veselić, Fernuniversität Hagen

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- Construction of operators (pseudo-Friedrichs-like)

- Spectral bounds for $T = H + A$ of the type

$$|(A\psi,\psi)| \le a\|\psi\|^2 + b(|H|\psi,\psi), \quad \Longrightarrow |\mu - \lambda| \le a|\lambda| + b.$$

  - for both discrete eigenvalues and the essential spectrum
  - including monotonicity & eigenvalue multiplicity
  - eigenvalues in spectral gaps included

- Illustrations on Schroedinger and Dirac operators, some open problems.

Construction of the form sum

Theorem. Assume $H = H^*$, A symmetric and

$$|(A\psi,\psi)| \leq a\|\psi\|^2 + b(|H|\psi,\psi),\ \ a,b > 0,$$

$$H_1 = a + b|H|,\ \ (C\psi,\phi) = (AH_1^{1/2}\psi, H_1^{1/2}\phi).$$

$$C_\lambda = (H-\lambda)H_1^{-1} + C,$$

boundedly invertible for some λ. Then the form sum $H + A$ generates a 'unique' $T = T^*$:

$$T - \lambda = H_1^{1/2} C_\lambda H_1^{1/2},$$

(Here and further on A may be just a quadratic form.) Traditionally but not necessarily, $b < 1$. An instance

Quasidefinite matrix (formally)

$$H = \begin{bmatrix} H_+ & 0 \\ 0 & H_- \end{bmatrix}, \ A = \begin{bmatrix} 0 & A_{12} \\ A_{12}^* & 0 \end{bmatrix}, \quad H_\pm \text{ pos/neg. def.}$$

Schur decomposition

$$T = \begin{bmatrix} H_+ & A_{12} \\ A_{12}^* & H_- \end{bmatrix} =$$

$$\begin{bmatrix} 1 & 0 \\ H_+^{-1} A_{12}^* & 1 \end{bmatrix} \begin{bmatrix} H_+ & 0 \\ 0 & H_- - A_{12} H_- A_{12}^* \end{bmatrix} \begin{bmatrix} 1 & A_{12} H_+^{-1} \\ 0 & 1 \end{bmatrix}$$

— invertible. For general

$$H = \begin{bmatrix} H_+ & 0 \\ 0 & H_- \end{bmatrix}, \quad \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{bmatrix}$$

lump diag. blocks to H, the rest gratis.

Theorem. Let $0 \in (\lambda_-, \lambda_+) \subseteq \rho(H)$ and $|(A\psi, \psi)| \leq const\| |H|\psi\|^2$.

$$(A\psi, \psi) \leq a_+\|\psi\|^2 + b_+\| |H|^{1/2}\psi\|^2, \;\; P_-\psi = \psi, \tag{1}$$
$$(A\psi, \psi) \geq a_-\|\psi\|^2 + b_-\| |H|^{1/2}\psi\|^2, \;\; P_+\psi = \psi, \tag{2}$$

$P_\pm = P_\pm(H)$ projections to the $\pm$ subspaces and $|b_\pm| < 1$

$$\hat{\lambda}_- = a_+ + \lambda_-(1 - b_+) < \hat{\lambda}_+ = a_- + \lambda_+(1 - b_+). \tag{3}$$

Then $H + A$ naturally extends to $T = T^*$ with $\mathcal{D}(T)$ a core for $|H|^{1/2}$ and

$$(\hat{\lambda}_-, \hat{\lambda}_+) \subseteq \rho(T). \tag{4}$$

(KV. 2007, 2008. Partially contains/contained in Langer-Tretter 1998 and Cuenin 2012)

Sketch of proof. With $(C\psi,\phi) = (A|H|^{-1/2}\psi, |H|^{-1/2}\phi)$ and

$$H = \begin{bmatrix} H_+ & 0 \\ 0 & H_- \end{bmatrix}$$

factorise as

$$T-\lambda = |H|^{1/2} \begin{bmatrix} (H_+ - \lambda)H_+^{-1} + C_{11} & C_{12} \\ C_{12}^* & (H_- - \lambda)|H_-|^{-1} + C_{22} \end{bmatrix} |H|^{1/2}$$

Our conditions on A expressed as

$$C_{11} + a_- H_+^{-1} + b_- \geq 0, \quad C_{22} + a_+ |H_-|^{-1} + b_+ \leq 0.$$

$$(H_+ - \lambda)H_+^{-1} + C_{11} \geq I - \lambda H_+^{-1} + a_- H_+^{-1} - b_- \geq 1 - b_- - \frac{\lambda - a_+}{\lambda_+}$$

which is positive, if $\lambda < \hat{\lambda}_+ \implies$ positive definiteness.
(C_{22} similar).

$\Longrightarrow$ bdd. invertibility of the whole middle term $\Longrightarrow$ $T - \lambda$ bd. invertible.

– constructs the operator, gives an estimate of perturbed gap, includes monotonicity.

– offdiagonals of A need not be relatively small, just relatively bounded.

Essential spectrum. Same assumptions as above.

Essential spectral gap larger:

$$(\Lambda_-, \Lambda_+) \supseteq (\lambda_-, \lambda_+) \quad (\ni 0)$$

With

$$\hat{\Lambda}_- = a_+ + \Lambda_-(1 - b_+) < \hat{\Lambda}_+ = a_- + \Lambda_+(1 - b_+)$$

$\Longrightarrow (\hat{\Lambda}_-, \hat{\Lambda}_+) \subseteq \rho_{ess}(T)$.

To prove map $(\hat{\ })$ the relation $(T - \lambda)^{-1} =$

$$|H|^{-1/2} \begin{bmatrix} (H_+ - \lambda)H_+^{-1} + C_{11} & C_{12} \\ C_{12}^* & (H_- - \lambda)|H_-|^{-1} + C_{22} \end{bmatrix}^{-1} |H|^{-1/2}$$

into the Calkin algebra

$$\mathcal{A} = \mathcal{B}(\mathcal{X})/\mathcal{C}(\mathcal{X})$$

With $h_1 = \widehat{(H^{-1})}$, $p_\pm = \widehat{P_\pm}$ and

$$b = \widehat{\left[\begin{array}{cc} (H_+ - \lambda)H_+^{-1} + C_{11} & 0 \\ 0 & (H_- - \lambda)|H_-|^{-1} + C_{22} \end{array}\right]}$$

and

$$c = \widehat{\left[\begin{array}{cc} 0 & C_{12} \\ C_{12}^* & 0 \end{array}\right]}$$

$$\sigma(h_1) = \sigma_{ess}(|H|^{-1}) = \left[1/\widehat{\Lambda}_-, 1/\widehat{\Lambda}_+\right].$$

The map $\widehat{}$ decreases norms, $\Longrightarrow$ under our conditions b will be invertible with $p_+b = bp_+ \geq 0$, $p_-b = bp_- \leq 0$ provided $(\lambda \in \widehat{\Lambda}_-, \widehat{\Lambda}_+)$. Also $p_+cp_- = p_-cp_+ = 0$.

Proposition. Under the above conditions $b + c$ 'quasidefinite' hence invertible. (Proof mimics Schur decomposition.)

Finally $\widehat{(T-\lambda)}^{-1}$ is analytically continued to $(\hat{\Lambda}_-, \hat{\Lambda}_+) \Longrightarrow$

$$\sigma_{ess}(T) = 1/\sigma(\hat{T}^{-1}) \subseteq (\hat{\Lambda}_-, \hat{\Lambda}_+).$$

Instead of

$$C_{11} + a_- H_+^{-1} + b_- \geq 0, \quad C_{22} + a_+ |H_-|^{-1} + b_+ \leq 0.$$

$$\sigma_{ess}(C_{11} + a_- H_+^{-1} + b_-) \geq 0, \quad \sigma_{ess}(C_{22} + a_- |H_-|^{-1} + b_+) \leq 0.$$

works as well.

Extract a relatively compact part out of A beforehand. Or find (and dispose of) extremal discrete eigenvalues of $C_{11} + a_- H_+^{-1} + b_-$. Solve the eigenvalue equation

$$(A + a_- + b_- H_+)\psi = \nu H_+ \psi$$

for extremal discrete eigenvalues and discard them.

Illustration: The Dirac Coulomb Hamiltonian in $\mathcal{X} = L^2(\mathbf{R}^3)^4$:

$$H = c\alpha p + \beta mc^2, \quad p = -i\hbar\nabla$$

$$A\psi(x) = -Ze^2\psi(x)/|x|,$$

Z atomic charge. Absolute limit $Z < 137$

- Kato tinyness $\|A\psi\| \leq b\|H\psi\|$ Uses Hardy-norm

$$\int |x|^{-2}|\psi|^2 dx \leq 4 \int |\nabla\psi|^2 dx$$

  – selfadjointness for $Z < 68$.

- Kato form tinyness $|(A\psi, \psi)| \leq b(|H|\psi, \psi)$, $b < 1$. Uses the Hardy inequality

$$\int |x|^{-1}|\psi|^2 dx \leq \frac{\pi}{2} \int |\nabla\psi|^2 dx$$

— standard pseudo-Friedrichs selfadjointness $Z < 87$.

- Our diagonal tinyness. Uses the Hardy form inequality on Dirac spinors (Evans, Perry, Siedentop 1996)

$$\int |x|^{-1}|\psi|^2 dx \leq \frac{1}{2}\left(\frac{\pi}{2}+\frac{2}{\pi}\right)\int(|\nabla\psi|^2+|\psi|^2)dx, \qquad \text{for } \psi = P_\pm(H)\psi.$$

— selfadjointness for $Z < 124$. (Originally means that the Bethe-Salpeter cut operator $P_\pm(H)TP_\pm(H)$ is s.a. and bounded from below. Our quasidefinite construction naturally extends it to the *whole* of T and includes monotonicity (no movement of the negative spectrum).

- Nenciu 1976, specially tailored for Dirac Coulomb case $Z < 137$ (optimal).

Other gaps, not so 'privileged'. Have to require

$$(A\psi,\psi) \le a_+\|\psi\|^2 + b_+\||H|^{1/2}\psi\|^2, \tag{5}$$
$$(A\psi,\psi) \ge a_-\|\psi\|^2 + b_-\||H|^{1/2}\psi\|^2, \tag{6}$$

not just for $P_\mp\psi = \psi$ but on all of $\mathcal{D}(|H|^{1/2})$.

Theorem. Let H be positive definite with a spectral gap λ_-, λ_+ and (5,6). Then

$$(a_+ + \lambda_-(1 - b_+),\ a_- + \lambda_+(1 - b_+)) \subseteq \rho(T).$$

If H is merely bounded from below then with $H - d_0$ pos. definite

$$(a_- + \lambda_+ + b_-(\lambda_+ - d_0), a_+ + \lambda_- + b_+(\lambda_- - d_0)) \subseteq \rho(T).$$

This gets poor if d_0 large negative. Except for $b_\pm = 0$ i.e. the perturbation A is bounded and

$$a_- = \min \sigma(A), \quad a_+ = \max \sigma(A).$$

Then again

$$(a_- + \lambda_+, a_+ + \lambda_-) \subseteq \rho(T).$$

Typically, but not necessarily $a_-, b_- \leq 0$, $a_+, b_+ \geq 0$. The case $a_- > 0$ can be 'purged' by subtracting a constant.

(If H not bounded from below the formulae a bit less simple.)

Essential spectrum analogous.

Discrete eigenvalues. Desired are *two sided bounds* for $T = H + A$

$$a_- + b_-|H| \le A \le a_+ + b_+|H|$$

$\Longrightarrow$

$$a_- + b_-|\lambda_i| \le \mu_i - \lambda_i \le a_+ + b_+|\lambda_i|$$

– counted with their multiplicities. Not merely inclusions! Each inclusion interval contains 'its own' eigenvalue.

Method: analytic perturbations & monotonicity.

Monotonicity: Let $T_t = H + A_t$, $H_1 = a + b|H|$ pos. definite,

$$(C_t\psi, \psi) = (A_t H_1^{-1/2}\psi, H_1^{-1/2}\psi)$$

be analytic and non decreasing in $t \in [t_0, t_1]$. Let $(d, d_1) \cap \sigma_{ess}(T_t) = \emptyset$, $d \notin \sigma(T_t)$ Let

$$\lambda_1^1 \leq \lambda_2^1 \leq \cdots$$

be the eigenvalues in (d, d_1) of T_{t_1} Then $\sigma(T_{t_0})$ in (d, d_1) consists of the eigenvalues

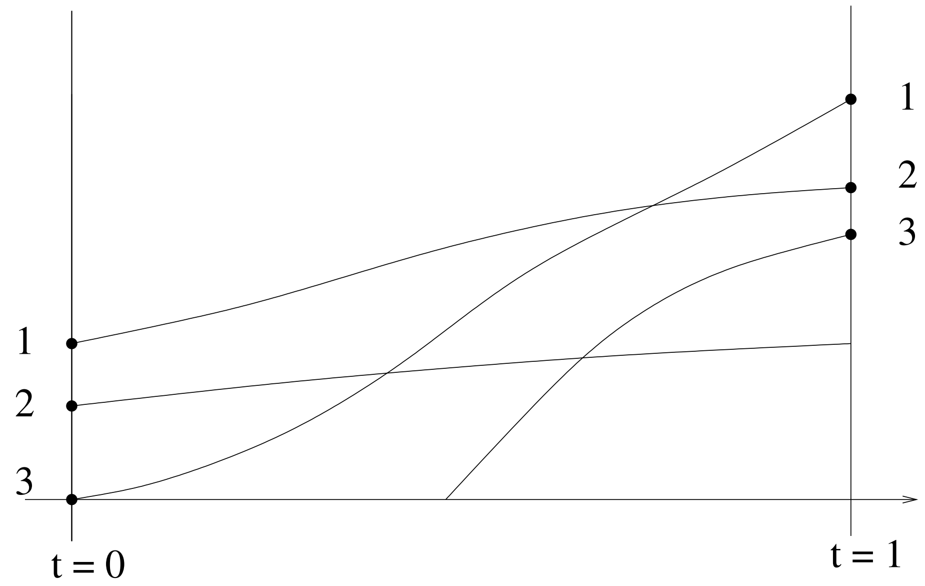
$$\lambda_1^0 \leq \lambda_2^0 \leq \cdots$$

$$\lambda_k^0 \leq \lambda_k^1, \; k = 1, 2, \ldots$$

Analyticity similar to 'type (C)' in the sense of Kato. Derivative

$$\lambda'(t) = \frac{1}{m} Tr\left((H_1^{1/2}P_t)^* C'_\epsilon H_1^{1/2} P_t\right), \quad P_t \text{ eigenprojection.}$$

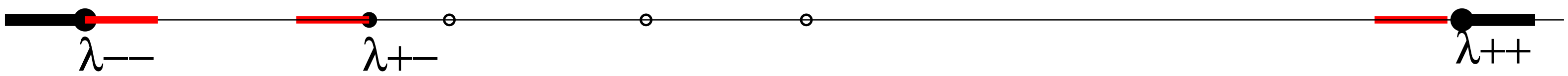
Keeping $\sigma_{ess}(T_t)$ out of (d, d_1) by means of previous spectral inclusions.



Ordering ascending eigenvalues

Reordering eigenvalues for each t they remain continuous and ordered in t.

Now for the eigenvalue bounds:



$T = H + A, \quad \|A\| < \infty, \qquad a_- \le A \le a_+$ (for simplicity).

$I = (\lambda_{--}, \lambda_{++})$ ess. spec. gap, $I' = (\lambda_{--}, \lambda_{+-}) \subseteq I$ spectral gap.

$(\lambda_{--} + a_+, \lambda_{+-} + a_-)$ non void.

$\lambda_1 = \lambda_{+-} \le \lambda_2, \ldots$ eigenv. of H in I.

$$\Longrightarrow \qquad a_- \le \mu_i - \lambda_i \le a_+.$$

Use $H + a_- \le T \le H + a_+$ plus analyticity with

$$T_t = H + ta_+(1-t)A \text{ or } H + ta_-(1-t)A.$$

Evaluating relative bounds? Typically

$$H = H_0 + V, \quad |V| \le a + b|H|, \quad (b < 1),$$

$$T = H + A, \quad |A| \le a_1 + b_1|H|, \quad (b_1 < 1)$$

Bound A by $H = H_0 + V$?.

If H positive semidefinite (Schrödinger) then

$$H_0 \le \frac{a + H}{1 - b} \quad \Longrightarrow \quad |A| \le a_1 + \frac{(a + H)b_1}{1 - b}$$

OK. But if H_0 is indefinite (Dirac)?

Condition $\|V\psi\| \le a\|\psi\| + b\|H\psi\|$ does again but is rather stronger (Coulomb type A with Dirac excluded).

Interesting special case. $H \geq 0, \quad V \leq 0$

Perturb $H = H_0 + V$ into $T = H + V + A$ with

$$b_- V \leq A \leq -b_+ V, \quad 0 \leq b_\pm < 1.$$

– relative 'deformation' of the attractive potential $V \leq 0$.

If A does not change essential spectrum then

$$H_0 + (1 + b_-)(-V) \leq H_0 + V + A \leq H_0 + (1 - b_+)(-V) \Longrightarrow$$

$$\lambda(1 + b_-) \leq \mu \leq \lambda(1 - b_+) \qquad (\lambda(1) = \lambda)$$

$\lambda(t)$ eigenvalues of $H_0 + tV$. Requires knowing $\lambda(t)$ *for a whole interval in* t. For non-relativistic hydrogen $\lambda(t) = \lambda t^2$.

$$2b_-\lambda \approx (2 + b_-)b_-\lambda \leq \mu - \lambda \leq (b_+ - 2)b_+\lambda \approx -2b_+\lambda$$

In Schroedinger case $H_0 = -\Delta$ there are some more such potentials, namely **homogeneous potentials**

$$V \leq 0, \qquad V(\alpha x) = \alpha^s V(x), \qquad -2 < s < 0.$$

Take the multiplicative unitary conformal group in $L_2(\mathbf{R}^n)$

$$U_\alpha \psi(x) = \alpha^{n/2} \psi(\alpha x).$$

Then

$$U_\alpha^{-1}(-\Delta + V(x))U_\alpha = (-\Delta + tV(x))/\alpha^2, \quad t = \alpha^{s+2}.$$

$\Longrightarrow$

$$(1+b_-)^{\frac{2}{s+2}}\lambda \leq \mu \leq (1-b_+)^{\frac{2}{s+2}}\lambda.$$

No need to know the unperturbed eigenvalues themselves for any fixed t!

Positive potentials also possible (harm. oscillator).

Back to the questions:

(1) Does

$$H = H_0 + V, \quad |V| \le a + b|H_0|, \quad (b < 1),$$

(all form estimates) imply

$$|H_0| \le c + d|H_0 + V|$$

???

(2) How to control more tightly the eigenvalue derivative λ'_t for $-\Delta + tV(x)$ (beyond the class of homogeneous V-s and apart of the obvious standard formula $\lambda'_t = (V\psi, \psi)/(\psi, \psi)$)?

Cuenin, J.C. Block-diagonalization of operators with gaps,with applications to Dirac operators, Reviews in Mathematical Physics, 24 (2112).

H. Langer and C. Tretter. Diagonalization of certain block operator matrices and applica-tions to Dirac operators, 122 Oper. Theory Adv. Appl., pp. 331-358. Birkhauser, Basel, 2001

K. Veselić, Spectral perturbation bounds for selfadjoint operators I, Operators and Matrices, 2 (2008) 307-340.

K. Veselić, Perturbation bounds for relativistic spectra, talk on the 7th Workshop on Operator Theory in Krein Spaces and Operator Polynomials, Berlin, December 2007 (unpublished)