Decay of bound states of elliptic PDE's

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Review of elements of publication (in preparation)

Decay of bound states of elliptic PDE's,

joint with I. Herbst.

- Introduction, N–body Schrödinger operators.
- Results.
- Elements of proof.

Consider the operator

$$H = -\Delta + V \text{ on } L^2 = L^2(\mathbb{R}^d)$$

for a suitable class of real decaying potentials $V = V(x)$.

For any solution $\phi \in L^2$ to the eigenvalue equation $H\phi = E\phi$, the **critical decay rate** is:

$$\sigma_c = \sup\{\sigma \geq 0 | e^{\sigma|x|}\phi \in L^2\}.$$

Well-known classification:

- $E > 0 \Rightarrow \sigma_c = \infty$ and $\phi = 0$.
- $E < 0$ and $\phi \neq 0 \Rightarrow \sigma_c = (-E)^{1/2}$.
- $E = 0$ and $\phi \neq 0 \Rightarrow \sigma_c = 0$.

The N-body Schrödinger operators (finite masses):

$$H = \sum_{j=1}^{N} -\frac{1}{2m_j}\Delta_{x_j} + \sum_{1\le i<j\le N} V_{ij}(x_i - x_j).$$

Hilbert space $= L^2(\mathbb{R}^{d(N-1)})$ after separation of center of mass motion.

Atomic N-body Schrödinger operators on Hilbert space $L^2(\mathbb{R}^{dN})$:

$$H = \sum_{j=1}^{N} \Big(-\frac{1}{2m_j}\Delta_{x_j} + V_j^{\mathrm{ncl}}(x_j)\Big) + \sum_{1\le i<j\le N} V_{ij}^{\mathrm{elec}}(x_i - x_j).$$

Atomic N-body Schrödinger operators with obstacle: Hamiltonian as above. Particles confined to the exterior of a bounded obstacle $\overline{\Theta} \subset \mathbb{R}^d$. Hilbert space $= L^2(\Omega)$,

$$\Omega = (\Omega_1)^N = \Omega_1 \times \cdots \times \Omega_1, \qquad \Omega_1 = \mathbb{R}^d \setminus \overline{\Theta}.$$

H defined by Dirichlet boundary condition.

Example (Coulomb interactions for $d \ge 2$)

$V_j^{\mathrm{ncl}}(y) = q_j q^{\mathrm{ncl}} |y|^{-1}$ and $V_{ij}^{\mathrm{elec}}(y) = q_i q_j |y|^{-1}$

For any bound state $H\phi = E\phi$, $0 \neq \phi \in L^2$,
the **critical decay rate** is:

$$\sigma_{\mathrm{c}} = \sup\{\sigma \geq 0 | \mathrm{e}^{\sigma|x|}\phi \in L^2\}.$$

Computation of the decay rate? Possibilities?

N-body Schrödinger operators take form $H = -\Delta + V$.
<u>Sub-Hamiltonians:</u>

$$H^a = -\Delta_{x^a} + V^a(x^a), \quad x = x^a \oplus x_a; \quad a \in \mathcal{A}.$$

<u>Thresholds of H:</u>

$$\mathcal{T} = \bigcup_{a \in \mathcal{A}, H^a \neq H} \sigma_{\mathrm{pp}}(H^a).$$

Set $\mathcal{T} \ni 0$, closed and countable, and (HVZ-theorem)

$$\sigma_{\mathrm{ess}}(H) = [\min \mathcal{T}, \infty).$$

Under decay conditions on pair-potentials:

Theorem (FH,IS)

For any bound state $H\phi = E\phi$, $\phi \neq 0$:

- $\sigma_{\rm c} < \infty$.
- $0 < \sigma_{\rm c}$ *for* $E \notin \mathcal{T}$.
- $E + \sigma_{\rm c}^2 \in \mathcal{T}$.

FH R. Froese, I. Herbst, *Exponential bounds and absence of positive eigenvalues for N-body Schrödinger operators*, Commun. Math. Phys. **87** no. 3 (1982/83), 429–447.

IS K. Ito, E. Skibsted, *Absence of positive eigenvalues for hard-core N-body interactions*, Institut Mittag-Leffler preprint, fall 2012 no. 31.

Absence of positive thresholds and eigenvalues. Example:

Theorem (IS, obstacle + Coulomb interactions)

For N charged $d \geq 2$ dimensional particles confined to the exterior of a bounded obstacle $\overline{\Theta} \subset \mathbb{R}^d$ with $0 \in \Theta$ and $\Omega_1 = \mathbb{R}^d \setminus \overline{\Theta}$ connected, the obstacle Hamiltonian H with Coulomb interactions

$$V_j^{\rm ncl}(y) = q_j q^{\rm ncl} |y|^{-1} \text{ and } V_{ij}^{\rm elec}(y) = q_i q_j |y|^{-1},$$

does not have positive thresholds nor positive eigenvalues.

Bilaplacian Δ^2

Consider

$$H = Q(p) + V, \quad Q(\xi) = (\xi^2)^2, \quad p = -\mathrm{i}\nabla.$$

For any bound state $H\phi = E\phi$, $0 \neq \phi \in L^2$,
the **critical decay rate** is:

$$\sigma_\mathrm{c} = \sup\{\sigma \geq 0 | \mathrm{e}^{\sigma|x|}\phi \in L^2\}.$$

Possible decay rates?

For $E \neq 0$:

- $E > 0 \Rightarrow \sigma_\mathrm{c} = E^{1/4}$.
- $E < 0 \Rightarrow \sigma_\mathrm{c} = (-E/4)^{1/4}$.

Conversely

$$\sigma = \begin{cases} E^{1/4} & \text{for } E > 0, \\ (-E/4)^{1/4} & \text{for } E < 0 \end{cases}$$

is the **critical decay rate** for a bound state with energy E for **some potential** V, possibly for a V with compact support.

General elliptic polynomial

Consider any real elliptic polynomial on $\mathbb{R}^d$ and

$$H = Q(p) + V.$$

for a suitable class of real decaying potentials $V = V(x)$.

For any bound state $H\phi = E\phi$, $0 \neq \phi \in L^2$, the **critical decay rate** is:

$$\sigma_{\mathrm{c}} = \sup\{\sigma \geq 0 | \mathrm{e}^{\sigma|x|}\phi \in L^2\}.$$

Possible decay rates?

Critical values: If $Q(\xi) = C$ and $\nabla Q(\xi) = 0$ for some $\xi \in \mathbb{R}^d$, C is a **critical value** of Q.

Theorem (HS)

For $H\phi = E\phi$, $\phi \neq 0$,

- $\sigma_c < \infty$.
- $\sigma_{\mathrm{c}} > 0$ *if E is a non-critical value of Q.*
- *If $\sigma_{\mathrm{c}} > 0$ there exists $(\omega, \xi) \in S^{d-1} \times \mathbb{R}^d$ such that with $\sigma = \sigma_{\mathrm{c}}$:*

$$\begin{aligned} Q(\xi + \mathrm{i}\sigma\omega) &= E, \\ \nabla_\xi Q(\xi + \mathrm{i}\sigma\omega) &= \mu\omega; \ \mu = \omega \cdot \nabla_\xi Q(\xi + \mathrm{i}\sigma\omega). \end{aligned} \quad (1)$$

If the system (1) has a solution for a given $\sigma > 0$ we call σ **exceptional** at E.

Exceptional points, rotationally invariant case $Q(\xi) = G(\xi^2)$

Suppose $Q(\xi) = G(\xi^2)$. Note

$$\text{degree}(G) = q/2 \text{ for } q = \text{degree}(Q).$$

General facts:

- There are $\leq q/2$ critical values of Q.
- There are $\leq q/2$ exceptional points away from $\leq q/2 - 1$ energies, more precisely at any real non-critical value E of $G : \mathbb{C} \to \mathbb{C}$.

Example (Exactly $q/2$ exceptional points at non-critical value of Q)

Consider

$$Q(\xi) = G(\xi^2); \quad G(z) = \prod_{j=1}^{n}(z + \sigma_j^2), \quad 0 < \sigma_1 < \cdots < \sigma_n.$$

Properties:

- $C = \prod_{j=1}^{n} \sigma_j^2$ is the only critical value of Q, and $\sigma_{\text{ess}}(Q(p) + V) = [C, \infty)$.
- The numbers $\sigma_1 < \cdots < \sigma_n$ are the exceptional points at $E = 0$, and 0 is not a critical value of $z \to G(z)$.
- For each $j \in \{1, \ldots, n\}$ there exists a compactly supported potential V:

$$\sigma_j \text{ is the critical decay rate for some bound state, } (Q(p) + V)\phi = 0.$$

Theorem (HS) is proved by commutator methods.

Two different approaches needed:

- $\sigma_{\mathrm{c}} < \infty$, proved by calculus of differential operators and combinatorics. “Sub-leading symbols” are used.
- Other statements in Theorem (HS), proved by microlocal analysis. Poisson bracket (i.e. “leading order”) calculations suffice. Results can be generalized to variable coefficient PDE’s.

Why system (1)?

Suppose $H\phi = E\phi$ and $\sigma_{\mathrm{c}} > 0$. Introduce

$$r(x) = r_1(x) = (1 + x^2)^{1/2}, \quad \omega(x) = \mathrm{grad}\, r(x).$$

For $\sigma < \sigma_{\mathrm{c}}$ put

$$\phi_\sigma = \mathrm{e}^{\sigma r}\phi,$$

and compute

$$(Q(p + \mathrm{i}\sigma\omega(x)) - E + V)\phi_\sigma = 0$$

For a decaying potential the **principal symbol** is

$$Q(\xi + \mathrm{i}\sigma\omega(x)) - E \approx Q(\xi + \mathrm{i}\sigma\hat{x}) - E, \quad \hat{x} = \tfrac{x}{|x|}.$$

Whence by energy bounds
1st system of equations:

$$Q(\xi + \mathrm{i}\sigma\omega) = E \text{ for some } (\omega, \xi) \in S^{d-1} \times \mathbb{R}^d.$$

2nd system of equations

To obtain the 2nd system of equations of the system (1) write

$$Q(\xi + \mathrm{i}\sigma\omega(x)) - E = (X + \mathrm{i}Y)(\xi + \mathrm{i}\sigma\omega(x)).$$

Conjugate symbol:

$$a = rY(\xi + \mathrm{i}\sigma\omega(x)).$$

Poisson bracket calculation:

$$\sigma^{-1}\{X, Y\} = \partial_\xi X\omega'(x)\partial_\xi^T X + \partial_\xi Y\omega'(x)\partial_\xi^T Y \geq 0. \tag{2a}$$

Quantizing:

$$\mathrm{Op}^{\mathrm{w}}(X) + \mathrm{i}\mathrm{Op}^{\mathrm{w}}(Y) \approx \tilde{X} + \mathrm{i}\tilde{Y} := Q(p + \mathrm{i}\sigma\omega(x)) - E,$$

$$\mathrm{Op}^{\mathrm{w}}(a) \approx A := \mathrm{Re}\,(r\tilde{Y}).$$

Commutator identity, virial type argument:

$$\mathrm{i}[H - E, \mathrm{e}^{\sigma r}A\mathrm{e}^{\sigma r}] = \mathrm{e}^{\sigma r}\big(\mathrm{i}[\tilde{X}, A] + 2\mathrm{Re}\,(\tilde{Y}A)\big)e^{\sigma r} + \mathrm{e}^{\sigma r}\mathrm{i}[V, A]\mathrm{e}^{\sigma r}.$$

Near energy surface $S_\sigma := \{X = Y = 0\}$:

$$\begin{aligned}\{X, a\} + 2rY^2 &= r\{X, Y\} + 2rY^2 + \{X, r\}Y \\ &\geq rY^2 - Cr^{-1}.\end{aligned} \tag{2b}$$

Improvement: If the system (1) does not have solutions, (2a) is strictly positive (for $\sigma < \sigma_{\mathrm{c}}$, but close, and on S_σ), and (2b) is improved as

$$\{X, a\} + 2rY^2 \geq rY^2 + c \geq c > 0.$$

Absence of super-exponentially decaying states

Suppose $H\phi = E\phi$ and

$$\phi_\sigma = \mathrm{e}^{\sigma r}\phi \in L^2 \text{ for all } \sigma > 0.$$

Want to show that $\phi = 0$.

Examine possible positivity of $[\tilde{X}, \tilde{Y}]$? Introducing

$$B = (b_1, \dots, b_d) = \mathrm{e}^{-\sigma r} p \mathrm{e}^{\sigma r} = p - \mathrm{i}\sigma\omega,$$

we have

$$\tilde{X} - \mathrm{i}\tilde{Y} = Q(B) - \lambda \text{ and } \tilde{X} + \mathrm{i}\tilde{Y} = Q(B^*) - \lambda,$$

and

$$2\mathrm{i}[\tilde{X}, \tilde{Y}] = [Q(B), Q(B^*)].$$

Is $[Q(B), Q(B^*)]$ positive?

Note that $p_{kl} := [b_k, b_l^*] = 2\sigma\partial_l\omega_k$, and whence that $P := (p_{kl}) \geq 0$. Maybe

$$[Q(B), Q(B^*)] \approx Q'(B)PQ'(B^*)^T?$$

Better to replace $r = r_1$ by

$$r(x) = r_\epsilon(x) = \langle x \rangle - \langle x \rangle^{1-\epsilon} + 1; \quad \epsilon \in (0, 1).$$

Then

$$P = (p_{kl}) = 2\sigma\omega' \geq c_\epsilon \sigma r^{-1-\epsilon}; \quad \omega(x) = \mathrm{grad}\, r_\epsilon(x).$$

Commutator P is strictly positive.

Abstractly, look at commuting operators $b_1, \dots, b_d$ on a Hilbert space $\mathcal{H}$,

$$B = (b_1, \dots, b_d), \quad B^* = (b_1^*, \dots, b_d^*), \quad p_{kl} = [b_k, b_l^*];\ k, l \leq d,$$

assuming

$$P := (p_{kl}) \geq 0 \text{ and } [b_j^\#, p_{kl}] = 0;\ j, k, l \leq d.$$

Representation of commutator:

$$[Q(B), Q(B^*)] = \sum_{m \geq 1} (-1)^{m+1} \sum_{|\alpha|, |\beta| = m} Q^{(\alpha)}(B)\, F_{\alpha\beta}\, Q^{(\beta)}(B^*); \tag{3a}$$

here

$$F_{\alpha\beta} = \sum_{(m_{kl}) \in \mathcal{M}_{\alpha\beta}} \prod_{k,l \leq d} \frac{p_{kl}^{m_{kl}}}{m_{kl}!},$$

$$\mathcal{M}_{\alpha\beta} = \{(m_{kl}) \in \mathbb{N}_0^{d^2} \mid \sum_k m_{kl} = \beta_l,\ \sum_l m_{kl} = \alpha_k\}.$$

Alternating series. Is the commutator positive?

Another representation:

$$[Q(B), Q(B^*)] = \sum_{m \geq 1} \sum_{|\alpha|, |\beta| = m} Q^{(\alpha)}(B^*)\, F_{\alpha\beta}\, Q^{(\beta)}(B). \tag{3b}$$

Positive series. Answer, yes.

Improved positivity for toy model

Better representation:

$$[Q(B), Q(B^*)] = \sum_{m\geq 1} \sum_{|\alpha|,|\beta|=m} \Big(d_m Q^{(\alpha)}(B)\ F_{\alpha\beta}\ Q^{(\beta)}(B^*) + e_m Q^{(\alpha)}(B^*)\ F_{\alpha\beta}\ Q^{(\beta)}(B) \Big),$$

for combinatorial positive constants d_m and e_m, d_m small; $m = 1, \ldots, \text{degree}(Q)$.

Example ($Q(\xi) = \xi^2$)

Toy model formula reads:

$$[Q(B), Q(B^*)] \approx 4d_1 BP(B^*)^T + 4(1-d_1)B^* PB^T + (2-4d_1)|P|^2_{\mathrm{HiSc}}$$

Exact expression (including multiple commutators):

$$[Q(B), Q(B^*)] = 4d_1 BP(B^*)^T + 4(1-d_1)B^* PB^T + (2-4d_1)|P|^2_{\mathrm{HiSc}} + L;$$

here L is linear in the $b_i^{\#}$'s with coefficients of the form $\sigma O(r^{-2})$. Note

$$P \geq c\sigma r^{-1-\epsilon} \quad \text{and} \quad |P|^2_{\mathrm{HiSc}} \geq c\sigma^2 r^{-2(1+\epsilon)}.$$

By Cauchy-Schwarz: For $\epsilon \leq 1/3$ and for all big σ

$$[Q(B), Q(B^*)] \geq c\sigma \sum_i \Big(b_i r^{-1-\epsilon} b_i^* + b_i^* r^{-1-\epsilon} b_i + \sigma r^{-2(1+\epsilon)} \Big)$$
$$\geq 2c\sigma^3 \omega(x)^2 r^{-1-\epsilon}.$$