

Perturbation of embedded eigenvalues for Schrödinger type operators

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Himeji PDE Conference, 6 March 2015

Background

I will give a survey of results obtained in collaboration with Horia Cornean (Aalborg) and Gheorghe Nenciu (Bucarest) during the last ten years.

Two of the papers are

- ▶ A. Jensen, G. Nenciu: Uniqueness results for transient dynamics of quantum systems. *Contemp. Math.* **447** (2007), 165-174.
- ▶ H. Cornean, A. Jensen, G. Nenciu, Metastable states when the Fermi Golden Rule constant vanishes, *Comm. Math. Phys.* **334** (2015), 1189-1218.

The Problem

We consider a self-adjoint operator H on a Hilbert space \mathcal{H} such that H has an eigenvalue embedded in its continuous spectrum.

We assume the eigenvalue is $\lambda = 0$, is non-degenerate, and has normalized eigenfunction Ψ_0 .

Assumption

There exists $a_0 > 0$ such that for all $0 < a < a_0$ with $J_a = (-a, a)$ we have

$$J_a \cap \sigma_{\text{pp}}(H) = \{0\}, \quad J_a \cap \sigma_{\text{sc}}(H) = \emptyset, \quad \text{and} \quad J_a \cap \sigma_{\text{ac}}(H) \neq \emptyset.$$

The Problem

For the perturbation W we assume

Assumption

W is self-adjoint and bounded.

The family of operators is then

$$H(\varepsilon) = H + \varepsilon W, \quad \varepsilon > 0.$$

The problem to be solved is to describe what happens to the embedded eigenvalue for sufficiently small ε .

I concentrate on the case where the eigenvalue is properly embedded, Case 1 below.

Case 1 

Case 2 

Case 3 

Methods to solve the problem

There are several different ways of getting results on this problem. Two of the major methods are:

- ▶ Spectral deformation methods.
- ▶ Time-dependent methods.

The spectral deformation methods have a long history. I will not review it, but mention two methods.

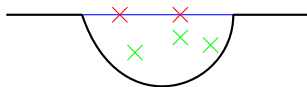
Very important is the dilation-analytic method of Aguilar-Balslev-Combes (1971) with significant extensions by Simon (1972).

The general spectral deformation technique was given a foundation by Hunziker (1996) and then many other authors extended the results.

Main results include a unified perturbation theory for embedded eigenvalues and resonances.

Spectral deformation methods

General picture of spectral deformation. The \times are embedded eigenvalues revealed as isolated eigenvalues by spectral deformation. The \times are resonances revealed by spectral deformation.



Spectral deformation methods

The method used is to continue matrix elements of the resolvent $R(z) = (H - z)^{-1}$, viz. $\langle \psi, R(z)\psi \rangle$, from the upper half plane $\text{Im } z > 0$ into a region in the lower half plane, crossing the absolutely continuous spectrum. This continuation should exist for a dense set of vectors ψ .

Embedded eigenvalues give rise to poles on the real axis in the continued matrix elements. Poles of the continued matrix element in the lower half plane are **defined** to be resonances.

To get a meaningful definition of a resonance one needs further conditions. I will not enter into details on this point now.

Spectral deformation methods

Discussion of spectral deformation methods.

Advantages:

- ▶ Covers many important quantum systems, including atoms and molecules.
- ▶ Gives a consistent definition of a resonance and in many cases makes available the full power of analytic perturbation theory for both resonances and embedded eigenvalues.

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Disadvantage:

- ▶ Dilation analyticity (or other forms of analyticity) of perturbations is a strong assumption.

Time-dependent methods

My interest is in time-dependent methods and I will concentrate on this aspect from this point.

The time-dependent methods are well adapted to a family

$$H(\varepsilon) = H + \varepsilon W, \quad \varepsilon > 0.$$

The results I present are for **small** ε . So it is an asymptotic theory.

First some general results. The set-up is: H is self-adjoint on \mathcal{H} with an eigenvalue λ_0 and eigenprojection P_0 assumed to be of finite rank. We assume that we have constructed an **effective Hamiltonian** $h(\varepsilon)$ on $P_0\mathcal{H}$.

We assume that we have

$$P_0 e^{-itH(\varepsilon)} P_0 = e^{-it h(\varepsilon)} P_0 + \delta(\varepsilon, t) \quad (1)$$

with

$$\sup_{t \geq 0} \|\delta(\varepsilon, t)\| \leq C\varepsilon^p, \quad p > 0. \quad (2)$$

Time-dependent methods

This framework is general enough to cover both the case when the eigenvalue remains (e.g. if λ_0 is isolated) and the case where it becomes a resonance.

Thus $h(\varepsilon)$ describes the short time behaviour of the evolution in the subspace $P_0\mathcal{H}$. If $h(\varepsilon)$ has an asymptotic expansion as $\varepsilon \rightarrow 0$ we have a **uniqueness** result.

Theorem

(i) Assume that $h^1(\varepsilon)$ and $h^2(\varepsilon)$ both satisfy (1) and (2) with the same $p > 0$. Assume that for some $\varepsilon_0 > 0$ $h^1(\varepsilon)$ satisfies

$$h^1(\varepsilon) = \lambda_0 P_0 + \varepsilon h_1^1 + \varepsilon f^1(\varepsilon), \quad 0 \leq \varepsilon < \varepsilon_0,$$

such that $h_1^1 = (h_1^1)^*$, $\text{Im } f^1(\varepsilon) \leq 0$, and $f^1(\varepsilon) = o(1)$. Then for ε_0 sufficiently small we have

$$\|h^1(\varepsilon) - h^2(\varepsilon)\| \leq C\varepsilon^{p+1}, \quad 0 \leq \varepsilon < \varepsilon_0.$$

Time-dependent methods

Continuation:

Theorem

(ii) Assume that $h^1(\varepsilon)$ and $h^2(\varepsilon)$ both satisfy (1) and (2) with $p = 2$. Assume that for some $\varepsilon_0 > 0$ $h^1(\varepsilon)$ satisfies

$$h^1(\varepsilon) = \lambda_0 P_0 + \varepsilon h_1 + \varepsilon^2 h_2 + o(\varepsilon^2), \quad 0 \leq \varepsilon < \varepsilon_0,$$

such that $h_1 = h_1^*$ and $\text{Im } h^1(\varepsilon) \leq 0$. Then there exists a family of invertible operators $U(\varepsilon)$ on $P_0 \mathcal{H}$ with $U(\varepsilon) = P_0 + O(\varepsilon^2)$ such that for sufficiently small ε_0 we have

$$\|h^1(\varepsilon) - U(\varepsilon)h^2(\varepsilon)U(\varepsilon)^{-1}\| \leq C\varepsilon^4, \quad 0 \leq \varepsilon < \varepsilon_0.$$

Reference:

Rank $P_0 = 1$: Cattaneo-Graf-Hunziker 2006

General case: J.-Nenciu 2007.

If $\text{Im } h_2 \neq 0$ we speak of resonance behaviour.

Time-dependent methods

The quantity of interest for a simple eigenvalue is the transition probability amplitude

$$A^0(\varepsilon, t) = \langle \Psi_0, e^{-itH(\varepsilon)} \Psi_0 \rangle.$$

Let us consider the case when $\lambda_0 = 0$ is an isolated eigenvalue. and take $h(\varepsilon) = \lambda(\varepsilon)P_0$, with $\lambda(\varepsilon)$ from eigenvalue perturbation theory. Then

$$|A^0(\varepsilon, t) - e^{-it\lambda(\varepsilon)}| \leq C\varepsilon^2.$$

Time-dependent methods

In general, if we restrict to $P_0\mathcal{H}$ for the effective Hamiltonian, then we can do no better. This holds even in the case of an embedded eigenvalue, if an eigenvalue moves but persists under perturbation.

Proposition

Assume that for sufficiently small ε there exists exactly one eigenvalue $\lambda(\varepsilon)$ ($\lambda(\varepsilon) \rightarrow 0$ for $\varepsilon \rightarrow 0$), with eigenfunction $\Psi(\varepsilon)$. Assume that there exists a $\Psi_1 \neq 0$ such that $\|\Psi(\varepsilon) - \Psi_0 - \varepsilon\Psi_1\| = o(\varepsilon)$ and $\langle \Psi_0, \Psi_1 \rangle = 0$. Then there exists $C > 0$ such that

$$\sup_{t \geq 0} \|A^0(\varepsilon, t) - e^{-it\lambda(\varepsilon)}\| \geq C\varepsilon^2.$$

Time-dependent methods

Results on embedded eigenvalues

We now state the first result on perturbation of embedded eigenvalues. This requires some preparation.

Assumption

Assume there exists a Hilbert space \mathcal{K} and bounded operators $A \in \mathcal{B}(\mathcal{H}, \mathcal{K})$ and $D \in \mathcal{B}(\mathcal{K})$ such that $W = A^*DA$. Here $D = D^*$ and $D^2 = I$ is assumed.

Let $Q_0 = I - P_0$. Define

$$G(z) = AQ_0(H - z)^{-1}Q_0A^*,$$

and

$$F^0(z, \varepsilon) = \varepsilon \langle \Psi_0, W\Psi_0 \rangle - z \\ - \varepsilon^2 \langle \Psi_0, A^*D\{G(z) - \varepsilon G(z)[D + \varepsilon G(z)]^{-1}G(z)\}DA\Psi_0 \rangle.$$

Time-dependent methods

Results on embedded eigenvalues

Using the Stone formula and the Schur-Livsic-Feshbach-Grushin (SLFG) formula we obtain our starting point:

$$A^0(\varepsilon, t) = \lim_{\eta \searrow 0} \frac{1}{2\pi i} \int_{\mathbb{R}} dx e^{-ixt} \left(\frac{1}{F^0(x + i\eta, \varepsilon)} - \frac{1}{F^0(x - i\eta, \varepsilon)} \right).$$

We need conditions on $G(z)$. Let

$$D_a = \{z = x + i\eta \in \mathbb{C} \mid x \in J_a = (-a, a), 0 < \eta < 1\}.$$

For $0 < \theta < 1$ we use the Hölder space $C^{1,\theta}(D_a, \mathcal{B}(\mathcal{K}))$.

Assumption

For some $0 < \theta < 1$ we have $G(\cdot) \in C^{1,\theta}(D_a, \mathcal{B}(\mathcal{K}))$.

This assumption can be verified using Mourre theory, Agmon-Herbst-Skibsted 1989.

Time-dependent methods

Results on embedded eigenvalues

Theorem (J.-Nenciu 2006)

Under the above Assumptions and $0 < \varepsilon < \varepsilon_0$ taken sufficiently small we have $F^0(\cdot, \varepsilon) \in C^{1,\theta}(D_a; \mathbb{C})$.

In particular, this function has an extension to the real axis with the same smoothness properties

$F^0(x, \varepsilon) := \lim_{\eta \searrow 0} F^0(x + i\eta, \varepsilon) \in C^{1,\theta}(J_a; \mathbb{C})$.

Let $R^0(x, \varepsilon)$ and $I^0(x, \varepsilon)$ be the real and imaginary part of $F^0(x, \varepsilon)$, respectively, viz. $F^0(x, \varepsilon) =: R^0(x, \varepsilon) + iI^0(x, \varepsilon)$.

For a fixed ε sufficiently small the equation $R^0(x, \varepsilon) = 0$ has a unique solution $x^0(\varepsilon)$ in $J_{a/2}$, which obeys the estimate $|x^0(\varepsilon)| \lesssim \varepsilon$. Define $\lambda^0(\varepsilon) := x^0(\varepsilon) + iI^0(x^0(\varepsilon), \varepsilon)$. Then for sufficiently small ε we have:

$$|A^0(\varepsilon, t) - e^{-it\lambda^0(\varepsilon)}| \lesssim \varepsilon^2. \quad (3)$$

Time-dependent methods

Results on embedded eigenvalues

We call $\lambda^0(\varepsilon)$ the **resonance position**. The uniqueness results show that it is asymptotically well defined.

Comments

- ▶ The estimate (3) has exactly the same form as for the case of eigenvalues, with the perturbed eigenvalue replaced by the ‘resonance position’, $\lambda^0(\varepsilon)$. In particular, the Proposition above shows that in general, the error in (3) cannot be made smaller.

Time-dependent methods

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Comments

- ▷ The estimate (3) has exactly the same form as for the case of eigenvalues, with the perturbed eigenvalue replaced by the ‘resonance position’, $\lambda^0(\varepsilon)$. In particular, the Proposition above shows that in general, the error in (3) cannot be made smaller.
- ▷ The computation of $I^0(x^0(\varepsilon), \varepsilon)$, using $|x^0(\varepsilon)| \lesssim \varepsilon$, leads to $I^0(x^0(\varepsilon), \varepsilon) = -\varepsilon^2 \Gamma_{\text{FGR}} + O(\varepsilon^3)$, with

$$\Gamma_{\text{FGR}} := \pi \langle \Psi_0, W \delta(Q_0 H Q_0) W \Psi_0 \rangle,$$

which coincides with the result given by the Dirac computation. Here

$$W \delta(Q_0 H Q_0) W = \lim_{\eta \searrow 0} \text{Im } W (Q_0 H Q_0 - i\eta)^{-1} W.$$

Time-dependent methods

Results on embedded eigenvalues

- ▶ Note that **no condition $\Gamma_{\text{FGR}} > 0$ or $I^0(x^0(\varepsilon), \varepsilon) < 0$** is required for this result, in contrast to other authors. Orth 1990 has proved that $I^0(x^0(\varepsilon), \varepsilon) = 0$ if and only if $x^0(\varepsilon)$ is an eigenvalue.

Time-dependent methods

Results on embedded eigenvalues

- ▶ Note that **no condition $\Gamma_{\text{FGR}} > 0$ or $I^0(x^0(\varepsilon), \varepsilon) < 0$** is required for this result, in contrast to other authors. Orth 1990 has proved that $I^0(x^0(\varepsilon), \varepsilon) = 0$ if and only if $x^0(\varepsilon)$ is an eigenvalue.
- ▶ In the analytic case, the resonance position is spectrally defined as a pole of the analytically continued resolvent and coincides with the zero $z_r = x_r + iy_r$ of the analytic continuation of $F^0(z, \varepsilon)$. In our case its definition also involves Ψ_0 since it is given via the limit values of $F^0(z, \varepsilon)$. Comparing the decay law given by the Theorem with the one given by Hunziker 1990 in the analytic case, one can show that $|\lambda^0(\varepsilon) - z_r| \lesssim \varepsilon^2 |y_r|$, i.e. up to some order in ε , $\lambda^0(\varepsilon)$ is indeed a spectral object of the family $H(\varepsilon)$, due to the uniqueness result.

Time-dependent methods

Results on embedded eigenvalues

Can one improve the above results with respect to the error term by replacing Ψ_0 by another choice?

In the dilation analytic framework Hunziker 1990 proved that if the eigenvalue $\lambda_0 (= 0)$ initially is isolated and the formal Rayleigh-Schrödinger (R-S) expansion for the perturbed eigenfunction is well defined up to order ε^N then taking as the resonance function the truncated R-S series one can prove that both $\text{Im} \lambda(\varepsilon)$ and the error term are of order ε^{2N+2} . The result applies to the Stark Hamiltonian to any order N .

We want to obtain similar results in the framework of finite regularity instead of analyticity.

Under the assumption that $\Gamma_{\text{FGR}} = 0$ it turns out that one can deal with the case $N = 1$ in the R-S expansion.

Time-dependent methods

Results on embedded eigenvalues

The detailed construction of a better resonance function is rather technical. I will not give the details. The result is a family $\Psi^1(\varepsilon)$. We define

$$A^1(\varepsilon, t) = \langle \Psi^1(\varepsilon), e^{-itH(\varepsilon)} \Psi^1(\varepsilon) \rangle$$

and we define $F^1(z, \varepsilon)$ in a manner analogous to $F^0(z, \varepsilon)$. The required assumptions are

Assumption

- (i) For some $0 < \theta < 1$ we have $G(\cdot) \in C^{1,\theta}(D_a, \mathcal{B}(\mathcal{K}))$.
- (ii) We have $\Gamma_{\text{FGR}} = 0$.

Under these assumptions we have for the boundary values

$$F^1(x, \varepsilon) := \lim_{\eta \searrow 0} F^1(x + i\eta, \varepsilon) \in C^{1,\theta}(J_{a/2}; \mathbb{C})$$

Time-dependent methods

Results on embedded eigenvalues

Theorem (Cornean-J.-Nenciu 2015)

Under the above assumptions we have the following results. Let $F^1(x, \varepsilon) =: R^1(x, \varepsilon) + iI^1(x, \varepsilon)$. For a fixed ε the equation $R^1(x, \varepsilon) = 0$ has a unique solution $x^1(\varepsilon)$ in $J_{a/2}$, with $|x^1(\varepsilon)| \lesssim \varepsilon$. Define

$$\lambda^1(\varepsilon) := x^1(\varepsilon) + iI^1(x^1(\varepsilon), \varepsilon).$$

Then for sufficiently small ε we have

$$|A^1(\varepsilon, t) - e^{-it\lambda^1(\varepsilon)}| \lesssim \varepsilon^4. \quad (4)$$

Time-dependent methods

High order R-S

One obvious question is whether we can continue the construction of better $\Psi^N(\varepsilon)$ in the finite regularity case for perturbation of a simple embedded eigenvalue. Looking at the formula in Kato's book it looks hopeless with the present approach.

Time-dependent methods

Eigenvalue at threshold

We recall the illustration

Case 1 

Case 2 

Case 3 

A question we have also dealt with is what happens in Case 2 above.

Case 2 our results I

I will briefly review some of the results obtained with G. Nenciu on this problem some time ago.

Resolvent smoothness is replaced by asymptotic expansion of the resolvent around threshold. Results in **odd dimensions**.

Definition of **zero resonance** for Schrödinger operator.

$H = -\Delta + V$ on $L^2(\mathbb{R}^d)$, $V(x)$ real-valued, $|V(x)| \leq C|x|^{-\beta}$, $\beta \gg 2$. Assume $(-\Delta + V)\Psi = 0$. Ψ is a **zero resonance function**, if

▷ **$d = 1$** : $\Psi(x) = c_0 + f$, $c_0 \neq 0$, $f \in L^2(\mathbb{R}^1)$.

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- ▷ $d = 1$: $\Psi(x) = c_0 + f$, $c_0 \neq 0$, $f \in L^2(\mathbb{R}^1)$.
- ▷ $d = 3$: $\Psi(x) = \frac{c_0}{|x|} + f$, $c_0 \neq 0$, $f \in L^2(\mathbb{R}^3)$.

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- ▷ **$d = 1$** : $\Psi(x) = c_0 + f$, $c_0 \neq 0$, $f \in L^2(\mathbb{R}^1)$.
- ▷ **$d = 3$** : $\Psi(x) = \frac{c_0}{|x|} + f$, $c_0 \neq 0$, $f \in L^2(\mathbb{R}^3)$.
- ▷ **$d \geq 5$** : No zero resonance function exists.

Case 2 our results I

H Schrödinger operator on \mathcal{H} . Assumptions are

- ▶ There exists $a > 0$, such that $(-a, 0) \subset \rho(H)$ and $[0, a] \subset \sigma_{\text{ess}}(H)$

Case 2 our results I

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- ▶ There exists $a > 0$, such that $(-a, 0) \subset \rho(H)$ and $[0, a] \subset \sigma_{\text{ess}}(H)$
- ▶ Assume that zero is a **non-degenerate eigenvalue** of H : $H\Psi_0 = 0$, with $\|\Psi_0\| = 1$, and there are no other eigenvalues in $[0, a]$. Let $P_0 = |\Psi_0\rangle\langle\Psi_0|$ be the orthogonal projection onto the one-dimensional eigenspace.

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- ▷ Assume $\langle\Psi_0, W\Psi_0\rangle = b > 0$.

Case 2 our results I

- ▷ For $\operatorname{Re} \kappa \geq 0$ and $z \in \mathbf{C} \setminus [0, \infty)$ we let $\kappa = -i\sqrt{z}$, $z = -\kappa^2$.
 There exist $N_0 \in \mathbf{N}$ and $\delta_0 > 0$, such that for
 $\kappa \in \{\kappa \in \mathbf{C} \mid 0 < |\kappa| < \delta_0, \operatorname{Re} \kappa \geq 0\}$ we have (recall
 $G(z) = AQ_0(H - z)^{-1}Q_0A^*$)

$$G(z) = \sum_{j=-1}^{N_0} \tilde{G}_j \kappa^j + \kappa^{N_0+1} \tilde{G}_{N_0}(\kappa),$$

where

- \tilde{G}_j are bounded and self-adjoint,
- \tilde{G}_{-1} is of finite rank and self-adjoint,
- $\tilde{G}_{N_0}(\kappa)$ is uniformly bounded in κ .

Case 2 our results I

- ▷ From the expansion we get

$$\langle \Psi_0, A^* D G(z) D A \Psi_0 \rangle = \sum_{j=-1}^{N_0} g_j \kappa^j + \kappa^{N_0+1} g_{N_0}(\kappa),$$

where

$$g_j = \langle \Psi_0, A^* D \tilde{G}_j D A \Psi_0 \rangle,$$

$$g_{N_0}(\kappa) = \langle \Psi_0, A^* D \tilde{G}_{N_0}(\kappa) D A \Psi_0 \rangle.$$

Notice that we have $g_j = \bar{g}_j$.

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Notice that we have $g_j = \bar{g}_j$.

- ▷ There exists an odd integer, $-1 \leq \nu \leq N_0$, such that $g_\nu \neq 0$, $\tilde{G}_j = 0$ for $j = -1, 1, \dots, \nu - 2$.

Case 2 our results I

Theorem

Let the above assumptions hold. Then for sufficiently small $\varepsilon > 0$ we have

$$|\langle \Psi_0, e^{-itH(\varepsilon)} \Psi_0 \rangle - e^{-it(x_0(\varepsilon) - i\Gamma(\varepsilon))}| \leq C\varepsilon^{p(\nu)}.$$

Here $p(\nu) = \min\{2, (2 + \nu)/2\}$, and

$$\begin{aligned}\Gamma(\varepsilon) &= -i^{\nu-1} g_\nu b^{\nu/2} \varepsilon^{2+(\nu/2)} (1 + O(\varepsilon)), \\ x_0(\varepsilon) &= b\varepsilon (1 + O(\varepsilon)).\end{aligned}$$

Recall that $\nu = -1, 1, 3, 5, \dots$