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Fermi Golden Rule, Feshbach Method and embedded point spectrum.

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Abstract

A method to study the embedded point spectrum of self-adjoint operators is described. The method combines the Mourre theory and the Limiting Absorption Principle with the Feshbach Projection Method. A more complete description of this method is contained in a joint paper with V. Jakšić, where it is applied to a study of embedded point spectrum of Pauli-Fierz Hamiltonians.

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1 Introduction

In this lecture I would like to describe some of the main ideas of my joint paper with V. Jakšić “Spectral theory of Pauli-Fierz Hamiltonians I” [DJ] devoted to precise estimates on the location and multiplicity of the embedded point spectrum of Pauli-Fierz Hamiltonians. Pauli-Fierz Hamiltonians are models describing interaction of a quantum system with a bosonic field (eg. with radiation). The method described [DJ] is quite general and is not restricted to the case of Pauli-Fierz Hamiltonians. In this lecture I will present a simplified version of this method in an abstract setting. For the proofs and additional results the reader should consult [DJ].

2 Perturbation theory around an isolated eigenvalue

Perturbation theory for isolated eigenvalues is much easier and better known than perturbation theory for embedded eigenvalues. For comparison let us recall some of its main points [Kato, RS4].

In what follows, the spectrum and point spectrum of a self-adjoint operator B will be denoted by $\sigma(B)$ and $\sigma_{\text{pp}}(B)$ respectively. $\mathbf{1}_{\Theta}(B)$ will denote the spectral projection of B onto Θ .

Suppose that $H_{\lambda} := H_0 + \lambda V$ is a family of self-adjoint operators on a Hilbert space \mathcal{H} . To simplify, let us assume that V is bounded. Let e be an isolated point of the spectrum of H_0 . It is well known that, for a small coupling constant λ , a nonempty subset of $\sigma(H_{\lambda})$ of the total multiplicity equal to $\dim \mathbf{1}_{\{e\}}$ will be situated near e .

In order to describe the approximate location and multiplicity of this part of spectrum, it is convenient to represent \mathcal{H} as a direct sum $\mathcal{H}^v \oplus \mathcal{H}^{\bar{v}}$ where $\mathcal{H}^0 := \text{Ran} \mathbf{1}_{\{e\}}(H_0)$. Operators on \mathcal{H} can be represented as 2×2 matrices, for instance,

$$H_{\lambda} = \begin{bmatrix} H_{\lambda}^{v\bar{v}} & H_{\lambda}^{v\bar{v}} \\ H_{\lambda}^{\bar{v}v} & H_{\lambda}^{\bar{v}v} \end{bmatrix}. \quad (2.1)$$

Note, in particular, that $H_0^{\bar{v}v} = e$, $H_0^{v\bar{v}} = H_0^{\bar{v}v} = 0$. Let us assume that $V^{v\bar{v}} = 0$ – this assumption will eliminate the first order corrections in the perturbation expansion. Define an auxiliary operator

$$w(e) := V^{v\bar{v}}(e - H_0^{\bar{v}v})^{-1}V^{\bar{v}v}.$$

Note that, since e is an isolated point of $\sigma(H_0)$, $w(e)$ is a well defined bounded self-adjoint operator.

The following theorem can be easily shown by the methods of [Kato]:

Theorem 2.1 *There exist $\epsilon > 0$, $C > 0$, $\Lambda > 0$ such that for $|\lambda| < \Lambda$ the following is true:*

- 1) $\sigma(H_{\lambda}) \cap [e - \epsilon, e + \epsilon] \subset e + \lambda^2 \sigma(w(e)) + [-C\lambda^3, C\lambda^3]$.
- 2) *If m is an isolated point of $\sigma(w(e))$, then*

$$\dim \mathbf{1}_{\{e + \lambda^2 m\} + [-C\lambda^3, C\lambda^3]} = \dim \mathbf{1}_{\{m\}}(w(e)).$$

3 Heuristic perturbation theory around an embedded eigenvalue

Now suppose that $e \in \sigma_{\text{pp}}(H_0)$ is not isolated in $\sigma(H_0)$. Then, clearly, Theorem 2.1 needs a modification.

A priori, $w(e)$ is not even well defined. It is however reasonable to assume that there exists the limit

$$w(e + i0) := \lim_{\epsilon \downarrow 0} V^{\overline{v}}(e + i\epsilon - H^{\overline{v}})^{-1} V^{\overline{v}}. \quad (3.2)$$

It is easy to see that if the limit (3.2) exists, then it will be dissipative. (We say that B is dissipative if $B + B^* \leq 0$). Clearly, $\sigma(w(e + i0))$ lies in the closed lower half plane. Heuristically, one expects that for small nonzero λ no eigenvalues of H_λ should be associated with nonreal eigenvalues of $w(e + i0)$. If the Hamiltonian allows an analytic continuation, these eigenvalues will be associated with resonances. The real eigenvalues of $w(e + i0)$ either will give rise to eigenvalues of H_λ , or they will also “dissolve in the continuum” by the effects of a higher order in λ .

These heuristic expectations are expressed in the following conjecture:

Conjecture 3.1 *Set $\mathcal{T}_e := \mathbf{R} \cap \sigma(w(e + i0))$. There exist $\epsilon > 0$, $C > 0$, $\kappa > 0$, $\Lambda > 0$ such that for $0 < |\lambda| < \Lambda$ the following is true:*

$$1) \quad \sigma(H_\lambda) \cap [e - \epsilon, e + \epsilon] \subset e + \lambda^2 \mathcal{T}_e + [-C\lambda^{2+\kappa}, C\lambda^{2+\kappa}].$$

2) *If m is an isolated point of \mathcal{T}_e , then*

$$\dim \mathbf{1}_{\{e + \lambda^2 m\} + [-C\lambda^{2+\kappa}, C\lambda^{2+\kappa}]}^{\text{pp}} \leq \dim \mathbf{1}_{\{m\}}(w(e + i0)).$$

Note that the above conjecture is well rooted in practical computations of physicists. In the physics literature, the real part of $\sigma(w(e + i0))$ is sometimes called the Lamb shift and the imaginary part of $\sigma(w(e + i0))$ is called the Fermi Golden Rule [He].

Clearly, Conjecture 3.1 is true only under certain technical assumptions. A set of relatively weak assumptions implying Conjecture 3.1 will be presented later in this lecture.

4 Do embedded eigenvalues survive a perturbation?

In this section I would like to explain why proving Conjecture 3.1 may have important consequences for some physical systems. I ask the reader to forgive me a rather vague and imprecise style of this section.

The most interesting and difficult part of Conjecture 3.1 is the estimate of Part 2). Its proof simplifies considerably if we make the assumption

$$\mathcal{T}_e = \emptyset. \quad (4.3)$$

(4.3) will be called the Fermi Golden Rule Assumption. Under this assumption, if the Conjecture 3.1 is true, then H_λ should have no eigenvalues near e for $0 < |\lambda| < \Lambda$. It should be noted that results similar to Conjecture 3.1 with the assumption (4.3) can be found in the literature, in particular in [BFS1], [BFSS].

The conventional wisdom, widespread among physicists, says that in the case of embedded spectrum the Fermi Golden Rule Assumption is satisfied for a generic perturbation (unless there are some “superselection sectors”, so that both the perturbation and the free Hamiltonian preserve a certain subspace). Furthermore, the conventional wisdom says that, generically, at a non-zero coupling constant all the embedded eigenvalues disappear (see eg. [JL] for a rigorous justification for this claim in a context of a certain class of Anderson models).

It turns out, however, that the above conventional wisdom is not always true. I know at least two examples of physically important classes of Hamiltonians with embedded eigenvalues that survive switching on a perturbation, in spite of the fact that there is no “superselection sector” responsible for this survival.

1) KMS states. Let \mathfrak{M} be a von Neumann algebra, ω_0 a faithful state given by a vector Ω_0 and H_0 the corresponding modular operator. In other words, ω_0 is a KMS state for the dynamics $\sigma_{0,t}(a) := e^{itH_0} a e^{-itH_0}$. In typical examples (eg. in a free gas of bosons in an infinite volume) $\sigma(H_0) = \mathbf{R}$. A result of Araki [BR] says that if $V \in \mathfrak{M}$, then for any λ the perturbed dynamics $\sigma_{\lambda,t}(a) := e^{itH_\lambda} a e^{-itH_\lambda}$ has a KMS state given by a vector Ω_λ . Here $H_\lambda := H_0 + \lambda V - \lambda J V J$, where J is the modular conjugation. The vector Ω_λ satisfies $H_\lambda \Omega_\lambda = 0$. Thus for any λ we have $0 \in \sigma_{\text{pp}}(H_\lambda)$.

A typical example of such a situation is furnished by Pauli-Fierz Hamiltonians describing systems at a positive temperature (see [JP1, JP2, DJP])

2) Ground states of Pauli-Fierz Hamiltonians. Let H_0 be a free Pauli-Fierz Hamiltonian with massless bosons of positive energy. Obviously, H_0 has a ground state (which is not isolated from the rest of the spectrum – it is on the tip of the continuous spectrum). Let V be a perturbation typical for Pauli-Fierz Hamiltonians that has a sufficiently mild infra-red behavior. Then one can show that H_λ has also a ground state (see [BFS1], [AH], [Ge]).

It is not difficult to see that in both these examples, for generic systems, $w(e + i0)$ has only one eigenvalue. Therefore, if Conjecture 3.1 is true, for $0 < |\lambda| < \Lambda$, generically the Hamiltonian H_λ will have only one, nondegenerate eigenvalue. This eigenvalue will correspond to the KMS/ground state (see [DJP]).

Note that this fact will have important implications for the conceptual foundations of quantum statistical physics. In particular, it can be used to show the so-called return to equilibrium property of the system.

5 The conjugate operator method

Let H be a self-adjoint operator and Θ a fixed open subset of the real line. In this section we would like to describe two well-known rigorous methods used in the study of the spectrum of the operator H inside Θ : the analytic deformation method and the Mourre theory. These two methods have a lot in common and can be viewed as two versions of

one method that we will call the conjugate operator method. Although in this lecture we will concentrate on the Mourre theory, it is helpful to keep in mind the intuition derived from the analytic deformation method.

(1) The analytic deformation approach. One considers a family of operators

$$H(\xi) := e^{i\xi S} H e^{-i\xi S}, \quad (5.4)$$

where S is an appropriately chosen self-adjoint operator (sometimes called a conjugate operator). The basic assumptions that one imposes on H and S are the following:

(a) The family $(z - H(\xi))^{-1}$ is analytic in some strip $|\operatorname{Im}\xi| < a$.

(b) For $\operatorname{Im}\xi < 0$, the essential spectrum of $H(\xi)$ “moves down” below Θ , uncovering a region below the real axis, which belongs to the unphysical sheet of the complex plane.

In the uncovered region, $H(\xi)$ may have some discrete eigenvalues. One can show that these eigenvalues do not depend on ξ and that the eigenvalues of $H(\xi)$ contained in $\Theta \subset \mathbf{R}$ coincide with $\sigma_{\text{pp}}(H) \cap \Theta$. The non-real eigenvalues of $H(\xi)$ are called resonances. All these eigenvalues can be studied by standard methods of perturbation theory developed for isolated eigenvalues.

Note that (a) and (b) imply that

$$z \mapsto e^{-a\langle S \rangle} (z - H)^{-1} e^{-a\langle S \rangle} \quad (5.5)$$

is a meromorphic function in a certain region below Θ . ($\langle S \rangle$ denotes $(1 + S^2)^{\frac{1}{2}}$.)

(2) Mourre’s theory and Limiting Absorption Principle. This is an infinitesimal version of the analytic deformation approach. Probably the most advanced version of the Mourre theory can be found in [BG]. Below we briefly describe the Mourre theory following essentially [BG].

One considers again a family of operators (5.4), where now ξ is restricted to the real line. The basic assumptions of the Mourre theory are:

(a $_{\nu}$) Let $\nu > 0$. Then $\xi \mapsto (z - H(\xi))^{-1}$ is ν -Hölder continuous. (If $n = 0, 1, \dots$, $0 \leq \theta < 1$ and $\nu = n + \theta$, then a function is ν -Hölder continuous if its n th derivative is θ -Hölder continuous in the usual sense).

(b) (The Mourre estimate). For any $x \in \Theta$ there exists an open interval $I \ni x$, a positive number $C_0 > 0$ and a compact operator K such that

$$\mathbf{1}_I(H) i[S, H] \mathbf{1}_I(H) \geq C_0 \mathbf{1}_I(H) + K. \quad (5.6)$$

If (a $_{\nu}$) with $\nu = 1$, (b) and some other technical assumptions hold, then one can show that $\sigma_{\text{pp}}(H) \cap \Theta$ is a discrete set which consists of eigenvalues of finite multiplicity. If in addition $\nu > 1$ and $\mu > \frac{1}{2}$, then for $x \in \Theta \setminus \sigma_{\text{pp}}(H)$ one can establish the existence of

$$\langle S \rangle^{-\mu} (x + i0 - H)^{-1} \langle S \rangle^{-\mu} := \lim_{y \downarrow 0} \langle S \rangle^{-\mu} (x + iy - H)^{-1} \langle S \rangle^{-\mu}. \quad (5.7)$$

Note that (5.7) implies the absence of singular continuous spectrum in Θ and is an analog of (5.5). Moreover, if $\nu \geq \mu + \frac{1}{2}$ then the function (5.7) is $\mu - \frac{1}{2}$ -Hölder continuous outside in $\Theta \setminus \sigma_{\text{pp}}(H)$. Statements similar to the existence of (5.7) usually go under the name of the Limiting Absorption Principle.

The weakness of the Mourre method in the form described above is that it does not give much information about the location and the multiplicity of $\sigma_{\text{pp}}(H)$. However, if for all $x \in \Theta$ there is no compact operator K in the Mourre estimate (5.6), then $\sigma_{\text{pp}}(H) \cap \Theta$ is empty.

The two methods described above are complementary. The analytic deformation method typically yields stronger results and allows to study resonances, which are of considerable physical interest. This method, however, is usually applicable to a restricted class of Hamiltonians that meet the analyticity condition. The Mourre theory approach is of much wider applicability but it yields weaker results. In particular, resonances cannot be studied with this approach.

The analytic deformation technique was started in [AC], [BC]. For more information about the early literature on this subject see [Si], [RS4].

The Mourre theory originated in [Mo] and was further developed in [PSS], [JMP], [AHS], [BG],

6 The Feshbach Method

Suppose now that the Hilbert space \mathcal{H} is decomposed into a direct sum

$$\mathcal{H} = \mathcal{H}^v \oplus \mathcal{H}^{\bar{v}}. \quad (6.8)$$

With respect to this decomposition, an operator H can be written as a 2×2 matrix

$$H = \begin{bmatrix} H^{vv} & H^{v\bar{v}} \\ H^{\bar{v}v} & H^{\bar{v}\bar{v}} \end{bmatrix}. \quad (6.9)$$

We will use a similar notation for other operators, for instance,

$$\mathbf{1} = \begin{bmatrix} \mathbf{1}^{vv} & 0 \\ 0 & \mathbf{1}^{\bar{v}\bar{v}} \end{bmatrix}. \quad (6.10)$$

For $z \notin \sigma(H^{\bar{v}\bar{v}})$ we introduce the following objects:

$$\begin{aligned} W_v(z) &:= H^{v\bar{v}}(z\mathbf{1}^{\bar{v}\bar{v}} - H^{\bar{v}\bar{v}})^{-1}H^{\bar{v}v}, \\ G_v(z) &:= z\mathbf{1}^{vv} - H^{vv} - W_v(z). \end{aligned} \quad (6.11)$$

In the physics literature, the operator $W_v(z)$ is sometimes called *the self-energy*. In [DJ] we proposed to call $G_v(z)$ *the resonance function*.

One can easily show

Theorem 6.1 *Let $z \notin \sigma(H^{\overline{v\overline{v}}})$. Then $z \notin \sigma(H)$ iff $0 \notin \sigma(G_v(z))$. Moreover,*

$$\dim \mathbf{1}_{\{z\}}(H) = \dim \mathbf{1}_{\{0\}}(G_v(z)).$$

Theorem (6.1) usually goes under the name of *the Feshbach projection method* (or also *the Grushin, Krein or Livshic method* – see [BFS1] or [MeMo] for further discussion). Theorem 6.1 is easy and well known (it follows eg. from [GGK], [BFS1], see also [DJ]). The following theorem, which extends Theorem 6.1 to $\sigma(H^{\overline{v\overline{v}}})$, is proven in [DJ]:

Theorem 6.2 *Let $x \in \mathbf{R}$. Assume that $W(x+i0) := \lim_{\epsilon \downarrow 0} W(x+i\epsilon)$ exists and that $z \rightarrow W(z)$ is of class C^1 in $\mathbf{C}_+ \cup \{x\}$. Assume (for simplicity) that \mathcal{H}^v is finite dimensional. Then $x \notin \sigma_{\text{pp}}(H)$ iff $0 \notin \sigma(G_v(x+i0))$. Moreover,*

$$\dim \mathbf{1}_{\{x\}}(H) = \dim \text{Ker}(G_v(x+i0)).$$

7 Combining the Feshbach Method with the Mourre Theory

Let us recall that the main weakness of the Mourre theory is the presence of the compact operator K in (5.6) and the resulting lack of control of the point spectrum. Let us explain how one can eliminate this weakness by combining the Mourre theory with the Feshbach Method.

To this end one should choose a splitting of the Hilbert space (6.8) in a clever way. In this splitting, \mathcal{H}^v should be close to the subspace spanned by the eigenvectors of H with eigenvalues near e . Moreover, the Mourre estimate without a compact operator should hold for $H^{\overline{v\overline{v}}}$ and an appropriate conjugate operator $S^{\overline{v\overline{v}}}$

Let us be more precise. Suppose that an operator S on \mathcal{H} has the form

$$S = \begin{bmatrix} 0 & 0 \\ 0 & S^{\overline{v\overline{v}}} \end{bmatrix}. \quad (7.12)$$

Moreover, assume that

- (a' $_{\nu}$) The family $H(\xi)^{\overline{v\overline{v}}}$ satisfies an assumption analogous to (a $_{\nu}$) of Section 5.
- (b') For some open $I \ni e$ and $C_0 > 0$, the following Mourre estimate holds:

$$i\mathbf{1}_I(H^{\overline{v\overline{v}}})[S^{\overline{v\overline{v}}}, H^{\overline{v\overline{v}}}]_I(H^{\overline{v\overline{v}}}) \geq C_0 \mathbf{1}_I(H^{\overline{v\overline{v}}}). \quad (7.13)$$

- (c' $_{\nu}$) $V^{\overline{v\overline{v}}}\langle S^{\overline{v\overline{v}}} \rangle^{\nu-\frac{1}{2}}$ is bounded.

Using (a'_ν) with ν > 1, (b') and some additional technical assumptions, we can develop the Mourre theory for $H^{\overline{\nu\nu}}$, which implies that $H^{\overline{\nu\nu}}$ satisfies the Limiting Absorption Principle near e . More precisely, for $\mu > \frac{1}{2}$ we can prove that the limit

$$\lim_{y \downarrow 0} \langle S^{\overline{\nu\nu}} \rangle^{-\mu} ((x + iy) \mathbf{1}^{\overline{\nu\nu}} - H^{\overline{\nu\nu}})^{-1} \langle S^{\overline{\nu\nu}} \rangle^{-\mu} \quad (7.14)$$

exists for x near e . Moreover, if $\nu \geq \mu + \frac{1}{2}$, then the function (7.14) is $\mu - \frac{1}{2}$ -Hölder continuous.

If additionally (c'_ν) holds one easily shows, using (7.14), that the limit

$$W_\nu(x + i0) := \lim_{y \downarrow 0} W_\nu(x + iy)$$

exists for x near e . Now we see that the assumptions of Theorem 6.2 are true and we can use it to study the point spectrum of H .

8 Rigorous perturbation theory near an embedded eigenvalue

Let us return to the setting of Conjecture 3.1. We would like to state assumptions that imply this conjecture.

Recall that in Section 2 and 3 we considered a family of self-adjoint operators $H_\lambda := H_0 + \lambda V$ such that

$$H_0 = \begin{bmatrix} e & 0 \\ 0 & H_0^{\overline{\nu\nu}} \end{bmatrix}, \quad V = \begin{bmatrix} 0 & V^{\nu\overline{\nu}} \\ V^{\overline{\nu\nu}} & V^{\overline{\nu\nu}} \end{bmatrix}.$$

For simplicity, we assume that V is bounded and \mathcal{H}^ν is finite dimensional. We suppose that S has the form (7.12) and satisfies

(a''_ν) the functions $t \mapsto (z - e^{itS^{\overline{\nu\nu}}} H_0^{\overline{\nu\nu}} e^{-itS^{\overline{\nu\nu}}})^{-1}$ and $t \mapsto e^{itS^{\overline{\nu\nu}}} V^{\overline{\nu\nu}} e^{-itS^{\overline{\nu\nu}}}$ are ν -Hölder continuous;

(b'') for some open $I \ni e$ and $C_0 > 0$

$$\mathbf{1}_I(H_0^{\overline{\nu\nu}}) i[S^{\overline{\nu\nu}}, H_0^{\overline{\nu\nu}}] \mathbf{1}_I(H_0^{\overline{\nu\nu}}) \geq C_0 \mathbf{1}_I(H_0^{\overline{\nu\nu}})$$

(c''_ν) $V^{\nu\overline{\nu}} \langle S^{\overline{\nu\nu}} \rangle^{\nu - \frac{1}{2}}$ is bounded.

Recall also that we introduced

$$w(z) := V^{\nu\overline{\nu}} (z \mathbf{1}^{\overline{\nu\nu}} - H_0^{\overline{\nu\nu}})^{-1} V^{\overline{\nu\nu}}.$$

and we defined $\mathcal{T}_e := \mathbf{R} \cap \sigma(w(e + i0))$. Then by following the ideas of [DJ] one can show the following results:

Theorem 8.1 We assume (a''_ν) , (b'') , (c''_ν) with $\nu > 1$. Let $\kappa := 1 - \nu^{-1}$. Then there exists C and $\Lambda > 0$ such that for $0 < |\lambda| < \Lambda$ the spectrum of H_λ in $I \setminus (\{e\} + \lambda^2 \mathcal{T}_e + [-C\lambda^{2+\kappa}, C\lambda^{2+\kappa}])$ is absolutely continuous and the Limiting Absorption Principle holds, that is

$$\lim_{\epsilon \downarrow 0} \langle S \rangle^{-\mu} (x - i\epsilon - H_\lambda)^{-1} \langle S \rangle^{-\mu}$$

exists.

Theorem 8.2 We assume (a''_ν) , (b'') , (c''_ν) with $\nu > 2$. Let Λ, C, κ be as in the previous theorem and $0 < |\lambda| < \Lambda$. Let $m \in \mathcal{T}_e$ and let $p_{e,m}$ be the projection of $w(e + i0)$ onto m . Then we have

$$\dim \mathbf{1}_{\{e+\lambda^2 m\}+[-C\lambda^{2+\kappa}, C\lambda^{2+\kappa}]}^{\text{pp}}(H_\lambda) \leq \dim p_{e,m}.$$

Moreover, the Limiting Absorption Principle holds in $I \setminus \sigma_{\text{pp}}(H)$.

In the above results we tried to make the regularity assumptions as weak as possible, that is, we tried to make ν as small as possible. This is not a purely technical question, in fact in some physical systems ν gives a restriction on the infrared behavior of the perturbation. It seems that the condition $\nu > 1$ is optimal in Theorem 8.1. We do not know whether the condition $\nu > 2$ is an optimal assumption in the Theorem 8.2 or whether it is an artifact of our method.

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