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Adiabatic Theorem and Spectral Concentration

I. Arbitrary Order Spectral Concentration for the Stark Effect in Atomic Physics

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Abstract. The spectral concentration of arbitrary order for the Stark effect is proved to exist for a large class of Hamiltonians appearing in nonrelativistic and relativistic quantum mechanics. The results are consequences of an abstract result about the spectral concentration for self-adjoint operators. A general form of the adiabatic theorem of quantum mechanics, generalizing an earlier result of the author as well as some results by Lenard, is also proved.

1. Introduction

This is the first in a series of papers devoted to the study of some asymptotic phenomena appearing in the spectral theory of linear operators and in the theory of evolution equations in Hilbert (or, more generally, Banach) spaces. Common to all the papers in the series will be the method employed which is, we believe, a new and rather general way of performing the asymptotic expansions. In a less abstract form, the basic ideas of our method have already appeared in [1–3].

In this paper we shall prove two results. The first one (Theorem 1) gives the existence of asymptotically invariant subspaces (see Sect. 2 for precise definitions) for a class of families, H_ε, $\varepsilon \geqq 0$, of self-adjoint operators in Hilbert spaces. For finite dimensional asymptotically invariant subspaces our result has a close relation to the abstract theory of spectral concentration as developed in [4, 5] (see also [6, Chap. VIII, Sect. 5] and [7, Chap. XII]). The second result (Theorem 2) is an adiabatic theorem "to an arbitrary order" generalizing a recent result of the author [1] as well as some results of Lenard [8].

As an application of Theorem 1 we shall prove the existence of spectral concentration of arbitrary order for the Stark Hamiltonians of atomic physics: atoms and molecules, impurity states in solids, relativistic hydrogen atom etc., as well as for Hamiltonians describing barrier penetration phenomena.

Concerning the Stark effect in atomic physics, some remarks are in order. In the framework of the abstract theory of spectral concentration, Riddell [4] and (in

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a less explicit form) Conley and Rejto [5] gave criteria for the existence of the spectral concentration of order p, $p=1,2,\ldots$. For $p=1$ the hypotheses of the Riddell-Conley-Rejto criterion are easily verified for the Stark Hamiltonian of general atoms and molecules (see [7, notes to Chap. XII.5]). For $p>1$ the situation seems to be less clear. The hypotheses of Riddell-Conley-Rejto criteria implying the spectral concentration of arbitrary order, have been verified by Riddell [4] and Conley-Rejto [5] for the hydrogen atom and by Rejto [9] for the helium atom. Their verification is not very simple even for the hydrogen atom, and it is really complicated for the helium atom. Moreover, we are not aware of a published verification for more general situations. However, it is a simple matter to verify the hypotheses of Riddell-Conley-Rejto criteria, implying the spectral concentration of *arbitrary order* for *general* Stark Hamiltonians appearing in atomic physics. More exactly, the assumptions of Theorem 1, which are readily verified (see Sect. 3) are easily seen to imply the Riddell-Conley-Rejto hypotheses (see Sect. 2). Of course, we cannot exclude that the existence of the arbitrary order spectral concentration for general Stark Hamiltonians was known as folklore, prior to our proof and to the other recent results we are now going to quote. Namely, recently the complex and powerful machineries of dilatation analyticity, translation analyticity and complex scaling have been used to obtain a remarkably detailed description of the Stark effect in hydrogen [10–13]. Moreover, similar results for arbitrary atoms are announced [13][1]. The price one has to pay is that the proofs are far from being simple and depend on some peculiar (and remarkable) properties of the concrete hamiltonians involved $\left(\text{e.g. the fact that } -\frac{d^2}{dx^2}+\varepsilon x \text{ has empty spectrum for } \operatorname{Im}\varepsilon \neq 0\ [11]\right)$.

Section 2 contains the main results. Section 3 contains applications to the Stark effect and to the barrier penetration phenomena. For the sake of simplicity, we shall not state and prove the results in the most general form. Some simple extensions are pointed out in Remarks.

2. The General Theory

We shall start with the following definition.

Definition 1. Let H_ε, P_ε, $\varepsilon \geqq 0$ be families of self-adjoint operators and orthogonal projections, respectively, in a Hilbert space, $\mathscr{H}$, satisfying the conditions:

i) $$\lim_{\varepsilon\to 0} \|P_\varepsilon - P_0\| = 0. \tag{2.1}$$

ii) Let p be a positive integer. There exist $c_p<\infty$, $\varepsilon_p>0$ and bounded self-adjoint operators B_ε defined for $\varepsilon\in[0,\varepsilon_p]$ such that

$$\|B_\varepsilon\| \leqq c_p \varepsilon^{p+1} \tag{2.2}$$

and $P_\varepsilon\mathscr{H}$ are invariant subspaces of $H_\varepsilon + B_\varepsilon$. Then the family $P_\varepsilon\mathscr{H}$ of subspaces is said to be an asymptotically invariant family of subspaces of order p for H_ε.

1 After the first version of this paper was finished, Graffi and Grecchi published [14] results similar to those announced in [13]

Remarks. 1. The definition requires that $P_0\mathscr{H}$ is an invariant subspace of H_0.

2. For ε sufficiently small, $\dim P_\varepsilon = \dim P_0$. The case $\dim P_0 = \infty$ appears naturally in some problems of solid state physics [3]. For $\dim P_0 < \infty$ there is a close connection between the above definition and the spectral concentration.

Definition 2 [4, 5]. Let λ_0 be an isolated eigenvalue of H_0 with finite multiplicity m; $J = [\alpha, \beta]$ an interval containing λ_0 but no other points of the spectrum of H_0; $E_\varepsilon(\lambda)$ the spectral measure of H_ε; P_0 the spectral projector of H_0 corresponding to λ_0; and p a positive number. Then

i) The spectrum of H_ε contained in J is said to be concentrated to order p provided there are sets $C_\varepsilon \subset J$ such that $s\text{-}\lim_{\varepsilon\to 0}(E_\varepsilon(C_\varepsilon) - P_0) = 0$ and $\lim_{\varepsilon\to 0} \varepsilon^{-p}\mu(C_\varepsilon) = 0$ (μ denotes the Lebesque measure).

ii) The set of unit vectors $\{\varphi_i(\varepsilon)\}_{i=1}^{\dim P_0}$, $\varphi_i(\varepsilon) \in \mathscr{D}(H_\varepsilon)$ is said to be an asymptotic basis of order p for $E_\varepsilon(J)$ if:

a) $\lim_{\varepsilon\to 0} \|(1-P_0)\varphi_i(\varepsilon)\| = 0$, $\lim_{\varepsilon\to 0} (\varphi_i(\varepsilon), \varphi_j(\varepsilon)) = \delta_{ij}$,

b) there are real numbers $\lambda_i(\varepsilon)$ such that

$$\lim_{\varepsilon\to 0} \varepsilon^{-p}\|(H_\varepsilon - \lambda_i(\varepsilon))\varphi_i(\varepsilon)\| = 0, \; i = 1, 2, \dots, \dim P_0.$$

The vectors $\varphi_i(\varepsilon)$ and the numbers $\lambda_i(\varepsilon)$ are called pseudo-eigenvectors and pseudo-eigenvalues, respectively.

The main result of Riddell [4] (see also [5] for the proof of the "if" part of the theorem) reads

Theorem R1 [4]. *Under the conditions described in Definition 2, the spectrum of H_ε contained in J is concentrated to order p if and only if there is an asymptotic basis of order p for $E_\varepsilon(J)$.*

As one expects, the existence of asymptotically invariant subspaces implies the spectral concentration.

Proposition 1. *Suppose that:*

i) *H_ε has an asymptotically invariant family of subspaces of order p, with P_0 corresponding to an isolated finitely degenerated eigenvalue λ_0.*

ii) *$H_\varepsilon \to H_0$ in the strong resolvent sense* [6] *as $\varepsilon \to 0$. Then in every interval J containing λ_0 but no other points of the spectrum of H_0, the spectrum is concentrated to order p.*

Proof. For ε small enough $\dim P_\varepsilon = \dim P_0 < \infty$ and then

$$\exp(-i(H_\varepsilon + B_\varepsilon)t)P_\varepsilon\mathscr{H} = P_\varepsilon\mathscr{H}$$

implies that there exist $\lambda_j(\varepsilon)$, $\varphi_j(\varepsilon)$, $j = 1, 2, \dots, \dim P_0$, $(\varphi_i(\varepsilon), \varphi_j(\varepsilon)) = \delta_{ij}$, $\varphi_j(\varepsilon) \in \mathscr{D}(H_\varepsilon)$, $\{\varphi_j(\varepsilon)\}_{j=1}^{\dim P_0}$ is a basis in $P_\varepsilon\mathscr{H}$, and

$$(H_\varepsilon + B_\varepsilon)\varphi_j(\varepsilon) = \lambda_j(\varepsilon)\varphi_j(\varepsilon). \tag{2.3}$$

Then (2.1), (2.2) imply that $\{\varphi_j(\varepsilon)\}_{j=1}^{\dim P_0}$ is an asymptotic basis of order p and the spectral concentration is implied by the "if" part of Riddell's theorem.

Remarks. 3. The condition $\dim P_0 < \infty$ in Proposition 1 is crucial. For an example of what can happen when $\dim P_0 = \infty$ see [3].

As expected, $P_\varepsilon \mathscr{H}$ are almost invariant under the evolution given by H_ε.

Proposition 2. *Suppose H_ε has an asymptotically invariant family of subspaces, $P_\varepsilon \mathscr{H}$, of order p. Then*

$$\|(1-P_\varepsilon)\exp(-iH_\varepsilon t)P_\varepsilon\| \leqq c_p \varepsilon^{p+1}|t|. \tag{2.4}$$

Proof. The inequality (2.4) follows from Definition 1 and

$$\exp(-iH_\varepsilon t) = \exp(-i(H_\varepsilon + B_\varepsilon)t) + i\int_0^t \exp(-i(H_\varepsilon + B_\varepsilon)(t-t'))B_\varepsilon \exp(-iH_\varepsilon t')dt'.$$

In particular if $P_\varepsilon = (\varphi_\varepsilon, \cdot)\varphi_\varepsilon$ is one-dimensional, then due to (2.4), φ_ε has, for small ε a rather long lifetime. This, together with the fact that $\lim_{\varepsilon \to 0} \|P_\varepsilon - P_0\| = 0$ says, in the language of physicists, that φ_ε describes a metastable state.

Suppose now that H_ε is of the form $H_0 + \varepsilon X_0$ where H_0, X_0 are self-adjoint operators in $\mathscr{H}$. The problem is to find conditions on pair H_0, X_0 under which one can prove the existence of asymptotically invariant subspaces for H_ε. The following heuristic discussion gives a hint. Let $\tau_t(X_0; \cdot)$ be the automorphism of $\mathscr{B}(\mathscr{H})$ (the Banach algebra of bounded operators in $\mathscr{H}$) given by

$$\tau_t(X_0; A) = \exp(iX_0 t)A\exp(-iX_0 t) \tag{2.5}$$

and $\mathrm{ad}X_0$ its generator. Suppose that $H_0 \in \ker(\mathrm{ad}X_0)$ in the sense that $(H_0 - z)^{-1} \in \ker(\mathrm{ad}X_0)$ for all $z \in \varrho(H_0)$. Then all the invariant subspaces of H_0 are invariant subspaces of H_ε. On the other hand, if X_0 is bounded, i.e., the domain of $\mathrm{ad}X_0$ is the whole $\mathscr{B}(\mathscr{H})$, then for an arbitrary H_0 the usual perturbation theory provides convergent sequences of asymptotically invariant subspaces of H_ε. By some rearrangements of the perturbation series one can see that objects like $(\mathrm{ad}X_0)^p(H_0 - z)^{-1}$ appear. The above extreme situations suggest that, when X_0 is unbounded, one may still hope that some sort of perturbation theory can be performed if $(H_0 - z)^{-1} \in \mathscr{D}((\mathrm{ad}X_0)^p)$, $p = 1, 2, \ldots$. That this is indeed the case says Theorem 1 below. Before stating the theorem, let us remark that $(H_0 - z)^{-1} \in \mathscr{D}((\mathrm{ad}X_0)^p)$ is equivalent with the fact that $\tau_t(X_0; (H_0 - z)^{-1})$ is p times norm differentiable with respect to t.

Theorem 1. *Suppose that:*

i) *$H_\varepsilon = H_0 + \varepsilon X_0$ is essentially self-adjoint on $\mathscr{D}(H_0) \cap \mathscr{D}(X_0)$.*

ii) *$\tau_t(X_0; (H_0 \pm i)^{-1})$ is $p+1$ times norm differentiable.*

iii) *There exist, $-\infty < \lambda_1 < \lambda_2 < \infty$, such that the spectrum σ_0 of H_0 has the properties: $\sigma_0 = \sigma_0^1 \cup \sigma_0^2$, $\sigma_0^1 \subset [\lambda_1, \lambda_2]$, $\mathrm{dist}(\sigma_0^1, \sigma_0^2) = d > 0$.*

Let P_0 be the spectral projection of H_0 corresponding to σ_0^1. Then H_ε has asymptotically invariant families of subspaces, of order q, $P_\varepsilon^q \mathscr{H}$, $q = 0, 1, \ldots, p$ with $P_0^q = P_0$.

Proof. For simplicity, and having in mind the examples in Sect. 3, we shall consider the case $p = \infty$. The proof is by construction and is divided in a series of steps.

1. We shall start with the following, almost trivial lemma.

Lemma 1. *Let* $H_0(t)$ *be defined by*

$$\exp(i\varepsilon X_0 t)H_0 \exp(-i\varepsilon X_0 t) = H_0(t), \qquad R_0(t;z) = \tau_{\varepsilon t}(X_0; (H_0 - z)^{-1})$$

be its resolvent and $P_0(t) = \tau_{\varepsilon t}(X_0; P_0)$ *its spectral projection corresponding to* σ_0^1. *Then* $R_0(t;z)$, $z \in \varrho(H_0)$, $P_0(t)$ *are infinitely norm differentiable and there exist finite constants* $b_{0,m}(z)$, $c_{0,m}$; $m = 1, 2, \ldots$ *such that*

$$\left\| \frac{d^m}{dt^m} R_0(t;z) \right\| = \left\| \left[\frac{d^m}{dt^m} R_0(t;z) \right]_{t=0} \right\| \leqq b_{0,m}(z)\varepsilon^m, \tag{2.6}$$

$$\left\| \frac{d^m}{dt^m} P_0(t) \right\| = \left\| \left[\frac{d^m}{dt^m} P_0(t) \right]_{t=0} \right\| \leqq c_{0,m}\varepsilon^m. \tag{2.7}$$

Proof. For $z = \pm i$, (2.6) holds by hypothesis. For arbitrary $z \in \varrho(H_0)$, one has to use the identity

$$R_0(t;z) = R_0(t;z_0)[1 + (z - z_0)R_0(t;z_0)]^{-1}. \tag{2.8}$$

Finally, (2.7) follows from (2.6) and the usual formula relating the resolvent and spectral projections.

2. We shall use the following construction, which has been given by Kato [6, 15].

Lemma 2. *Let* $P(t)$ *be a norm differentiable family of orthogonal projections, with norm continuous derivative.*

i) *If* $K(t)$ *is defined by*

$$K(t) = i(1 - 2P(t))\frac{d}{dt}P(t), \tag{2.9}$$

then $K(t)$ *is self-adjoint.*

ii) *The equation*

$$i\frac{d}{dt}A(t) = K(t)A(t); \qquad A(0) = 1 \tag{2.10}$$

has a unique solution satisfying $A^{-1}(t) = A^*(t)$ *and*

$$P(t) = A(t)P(0)A^*(t). \tag{2.11}$$

3. Let $K_0(t)$, $A_0(t)$ be given by Lemma 2 applied to $P_0(t)$ and

$$B_0 = \varepsilon^{-1}K_0(0). \tag{2.12}$$

Note that $\|B_0\| \leqq c_{0,1}$. Consider now the self-adjoint operator

$$X_1 = X_0 + B_0; \qquad \mathscr{D}(X_1) = \mathscr{D}(X_0). \tag{2.13}$$

By the Stone theorem, for all $f \in \mathscr{D}(X_0)$

$$i\frac{d}{dt}(\exp(i\varepsilon X_0 t)\exp(-i\varepsilon X_1 t))f = K_0(t)\exp(i\varepsilon X_0 t)\exp(-i\varepsilon X_1 t)f,$$

which together with Lemma 2 implies

$$A_0(t) = \exp(i\varepsilon X_0 t)\exp(-i\varepsilon X_1 t). \tag{2.14}$$

From (2.11), (2.14) one has

$$P_0 = \exp(i\varepsilon X_1 t) P_0 \exp(-i\varepsilon X_1 t), \tag{2.15}$$

which implies that for $f \in \mathscr{D}(X_0) \cap \mathscr{D}(H_0)$

$$P_0(H_0 + \varepsilon X_1) f - (H_0 + \varepsilon X_1) P_0 f = 0. \tag{2.16}$$

Since $H_0 + \varepsilon X_1 = H_\varepsilon + \varepsilon B_0$ is essentially self-adjoint on $\mathscr{D}(X_0) \cap \mathscr{D}(H_0)$ it follows that

$$[P_0, \exp(-i(H_\varepsilon + \varepsilon B_0)t)] = 0, \tag{2.17}$$

which says that $P_\varepsilon^0 \equiv P_0$ is asymptotically invariant of order zero for H_ε.

4. Consider now $H_1(t)$ given by

$$H_1(t) = A_0^*(t)[H_0(t) - K_0(t)] A(t). \tag{2.18}$$

From the identity

$$\begin{aligned} R_1(t;z) &\equiv (H_1(t) - z)^{-1} \\ &= A_0^*(t) R_0(t;z)[1 - K_0(t) R_0(t;z)]^{-1} A_0(t) \end{aligned} \tag{2.19}$$

and Lemma 1 it follows that $R_1(t;z)$ is infinitely norm differentiable. Note that if $H_1(\varepsilon)$ is defined by

$$H_1(\varepsilon) = H_0 - \varepsilon B_0,$$

then

$$\begin{aligned} H_1(t) &= \exp(i\varepsilon X_1 t) H_1(\varepsilon) \exp(-i\varepsilon X_1 t) \\ H_\varepsilon &= H_1(\varepsilon) + \varepsilon X_1. \end{aligned}$$

5. For $\varepsilon < \varepsilon_0 \equiv d/2\|B_0\|$ the spectrum of $H_1(\varepsilon)$ is still separated and we can repeat the whole construction. Obviously one can continue this process indefinitely. Namely, for $n = 0, 1, \ldots$ starting from H_ε written in the form

$$H_\varepsilon = H_n(\varepsilon) + \varepsilon X_n, \tag{2.20}$$

where $\sigma(H_n(\varepsilon)) \equiv \sigma_n = \sigma_n^1 \cup \sigma_n^2$; $\operatorname{dist}(\sigma_n^1, \sigma_n^2) > 0$ (σ_n^1 coincide with σ_0^1 in the limit $\varepsilon \to 0$), we define

$$\begin{aligned} &P_\varepsilon^n = \text{the spectral projection of } H_n(\varepsilon) \text{ corresponding to } \sigma_n^1, \\ &H_n(t) = \exp(i\varepsilon X_n t) H_n(\varepsilon) \exp(-i\varepsilon X_n t), \\ &P_n(t) = \exp(i\varepsilon X_n t) P_\varepsilon^n \exp(-i\varepsilon X_n t), \\ &K_n(t) = i(1 - 2P_n(t)) \frac{d}{dt} P_n(t), \\ &i \frac{d}{dt} A_n(t) = K_n(t) A_n(t); \qquad A_n(0) = 1, \\ &B_n = \varepsilon^{-1} K_n(0), \\ &H_{n+1}(\varepsilon) = H_n(\varepsilon) - \varepsilon B_n, \\ &X_{n+1} = X_n + B_n. \end{aligned} \tag{2.21}$$

Obviously

$$H_\varepsilon = H_{n+1}(\varepsilon) + \varepsilon X_{n+1},$$
$$H_{n+1}(t) = A_n^*(t)[H_n(t) - K_n(t)]A_n(t),$$

and the whole procedure can be carried further as far as

$$\varepsilon < \varepsilon_n \equiv d/2\left(\sum_{j=0}^{n} \|B_j\|\right)$$

[which assures that the spectrum of $H_{n+1}(\varepsilon)$ is still separated]. Since by construction

$$[P_\varepsilon^n, \exp(-i(H_\varepsilon + \varepsilon B_n)t)] = 0, \tag{2.22}$$

the only thing we have to do in order to finish the proof of the theorem is to obtain bounds on $\|B_n\|$, $n = 0, 1, \ldots$.

6. The needed bounds are consequences of the following Lemma which is the main (and only) technical point of our paper.

Lemma 3. *Let Γ be a contour (of finite length) surrounding σ_0^1, satisfying* $\operatorname{dist}(\Gamma, \sigma_0) = d/2$. *Then there exist constants $b_{p,m}$, $c_{p,m}$; $p = 0, 1, \ldots$; $m = 1, 2, \ldots$ such that for $\varepsilon < \varepsilon_{p-1}$ (by definition $\varepsilon_{-1} = \infty$) and $z \in \Gamma$*

$$\left\|\frac{d^m}{dt^m} R_p(t; z)\right\| \leqq b_{p,m}\varepsilon^m; \qquad R_p(t; z) \equiv (H_p(t) - z)^{-1}, \tag{2.23}$$

$$\left\|\frac{d^m}{dt^m} P_p(t)\right\| \leqq c_{p,m}\varepsilon^{p+m}. \tag{2.24}$$

Proof. The proof is by induction over p. The case $p = 0$ is contained in Lemma 1. Suppose (2.23), (2.24) be true for $p-1$. Then (2.23) for p follows from a formula similar to (2.19) relating $R_p(t; z)$ and $R_{p-1}(t; z)$ and the induction hypothesis. For (2.24) the following observation [1] is crucial. From

$$P_{p-1}(t) = A_{p-1}(t)P_{p-1}(0)A_{p-1}^*(t)$$

it follows that $P_{p-1}(0)$ is the spectral projection of $A_{p-1}^*(t)H_{p-1}(t)A_{p-1}(t)$ corresponding to σ_{p-1}^1, for all $t \in \mathbb{R}$. Then one can write

$$P_p(t) - P_{p-1}(0) = (2\pi i)^{-1} A_{p-1}^*(t) \cdot \left[\int_\Gamma (H_{p-1}(t) - K_{p-1}(t) - z)^{-1} K_{p-1}(t) R_{p-1}(t; z) dz\right] A_{p-1}(t). \tag{2.25}$$

Now, (2.25) and the induction hypothesis implies (2.24) for p to be true and the proof of the Lemma is finished.

7. From the definition of $K_p(t)$ and (2.24) for $m = 1$ it follows

$$\|B_p\| \leqq c_{p,1}\varepsilon^p, \qquad \varepsilon < \varepsilon_{p-1}, \tag{2.26}$$

which finishes the proof of the Theorem 1.

Remarks. 4. One can relax the condition that σ_0^1 be bounded, but then one needs $\left\|\frac{d^m}{dt^m} R_0(t;z)\right\|$ to have sufficiently rapid decrease in $\mathrm{dist}(z,\sigma_0)$, to assure the convergence of integrals appearing in $\frac{d^m}{dt^m} P_0(t)$.

5. The whole proof works for H_ε of the type

$$H_\varepsilon = H_0 + X_0(\varepsilon)$$

as long as $R_0(t;z) = \tau_t(X_0(\varepsilon);(H_0-z)^{-1})$ is infinitely norm differentiable and satisfies (2.6).

6. The assumption ii) of Theorem 1 already implies that $\mathscr{D}(H_0)\cap\mathscr{D}(X_0)$ is dense in $\mathscr{H}$. In fact, we suspect that it implies assumption i). The assumption i) has been used to obtain (2.17) from (2.16). If $H_0+\varepsilon X_0$ has several self-adjoint extensions and $\dim P_0<\infty$, then (2.16) implies (2.17) for any self-adjoint extension of $H_0+\varepsilon X_0$.

Formally, the recurrent construction in the proof of Theorem 1 is the following

$$\begin{aligned} &B_q = (1-2P_\varepsilon^q)[P_\varepsilon^q, X_q]\,; \qquad P_\varepsilon^0 \equiv P_0\,, \\ &X_{q+1} = X_q + B_q\,; \qquad H_{q+1}(\varepsilon) = H_q(\varepsilon) - \varepsilon B_q\,. \end{aligned} \tag{2.27}$$

The observation in (2.25) is nothing but

$$[P_\varepsilon^q, X_q] = [P_\varepsilon^q - P_\varepsilon^{q-1}, X_q]\,. \tag{2.28}$$

If X_0 is H_0-bounded, one expects that the recurrent construction (2.27) converges.

Proposition 3. *Suppose that*

i) X_0 *is* H_0*-bounded.*

ii) H_0 *satisfies the spectrum condition iii) of Theorem 1. Let* Γ *be the contour in Lemma 3,*

$$b = (d/2)\sup_{z\in\Gamma}\|X_0(H_0-z)^{-1}\|\,, \qquad k = (1/2\pi)\int_\Gamma |dz|\,, \qquad a_0 = 4bk/d\,.$$

Then for

$$\varepsilon \leqq d^2/(2^8 k a_0) \equiv \varepsilon_c\,, \tag{2.29}$$

$$\|B_n\| \leqq (\varepsilon/2\varepsilon_c)^n a_0\,. \tag{2.30}$$

Proof. The proof is by induction. Note that $\|B_0\|\leqq a_0$.

Denoting $a_n = \|B_n\|$ using $R_n = R_0\left[1-\varepsilon\left(\sum_{i=0}^{n-1} B_i\right)R_0\right]^{-1}$ and the fact that $b<a_0$, we have from (2.28)

$$a_n \leqq 8\varepsilon k d^{-2} a_{n-1}\left(1-2\varepsilon d^{-1}\sum_{i=0}^{n-1} a_i\right)^{-2}\sum_{i=0}^{n-1} a_i\,; \qquad n=1,2,\ldots \tag{2.31}$$

as long as

$$2\varepsilon d^{-1}\sum_{i=0}^{n-1} a_i < 1\,.$$

Then (2.30) follows from (2.29) and (2.31) by induction.

Proposition 3 shows that for regular perturbations the construction in Theorem 1 is nothing but a different way to perform the perturbation theory. Moreover, using (2.27) and (2.28) one can give a "time independent" proof of Theorem 1. Translated in the "time independent" language, Lemma 3 says, in particular, that $(H_n(\varepsilon)-z)^{-1}$, P^n_ε, B_n, $n=0,1,\ldots$ are all in $\mathscr{D}((\mathrm{ad}X_0)^\infty)$. Using this, the recurrent construction given by (2.27), (2.28) and the identity

$$(A+B-z)^{-1}=(A-z)^{-1}\sum_{j=0}^{N}(-1)^j(B(A-z)^{-1})^j + (-1)^{N+1}((A-z)^{-1}B)^{N+1}(A+B-z)^{-1},$$

one can easily see that for arbitrary integers n, N (and sufficiently small ε)

$$P^n_\varepsilon=\sum_{j=0}^{N}P^n_j\varepsilon^j+\varepsilon^{N+1}\tilde{P}^n_N(\varepsilon), \tag{2.32}$$

where P^n_j does not depend on ε, and all P^n_j, $\tilde{P}^n_N(\varepsilon)$ are in $\mathscr{D}(\mathrm{ad}X_0)$.

Due to (2.26)

$$P^n_j=P^{n+1}_j, \quad j=0,1,\ldots,n,$$

which together with (2.32) shows that

$$P^n_\varepsilon=\sum_{j=0}^{n}P_j\varepsilon^j+\varepsilon^{n+1}\tilde{P}_n(\varepsilon), \tag{2.33}$$

where P_j does not depend on n and ε. Moreover, by construction $\limsup_{\varepsilon\to 0}\|\tilde{P}_n(\varepsilon)\|<\infty$ and

$$P_j\mathscr{H}\subset\mathscr{D}(H_0)\,; \qquad \tilde{P}_n(\varepsilon)\mathscr{H}\subset\mathscr{D}(H_0)\,.$$

Suppose now X_0 to be H_0-bounded and let P_ε be the spectral projection of H_ε corresponding to the part of the spectrum which coincides with σ^1_0 in the limit $\varepsilon\to 0$. By the usual theory of perturbation [6, Chap. II, Sect. 2]

$$P_\varepsilon=\sum_{j=0}^{\infty}\varepsilon^j\frac{(-1)^j}{2\pi i}\int_\Gamma((H_0-z)^{-1}X_0)^j(H_0-z)^{-1}dz\,.$$

By Proposition 3, $\|P_\varepsilon-P^n_\varepsilon\|\sim\varepsilon^{n+1}$, which together with (2.33) implies that P_j are nothing but

$$(-1)^j(1/2\pi i)\int_\Gamma((H_0-z)^{-1}X_0)^j(H_0-z)^{-1}dz,$$

rewritten in a form which still has a definite meaning even if X_0 is not bounded (but of course the hypotheses of Theorem 1 are fulfilled). Let us check this explicitly for P_1. Writing

$$X_0=P_0X_0P_0+(1-P_0)X_0(1-P_0)-B_0,$$

and taking into account that

$$(H_0-z)^{-1}P_0X_0P_0(H_0-z)^{-1}, \quad (H_0-z)^{-1}(1-P_0)X_0(1-P_0)(H_0-z)^{-1}$$

are analytic outside, respectively inside Γ, it follows that

$$\int_\Gamma (H_0-z)^{-1}X_0(H_0-z)^{-1}dz = -\int_\Gamma (H_0-z)^{-1}B_0(H_0-z)^{-1}dz,$$

which is the desired equality.

Suppose now σ_0^1 to be an isolated eigenvalue with finite multiplicity. In this case more detailed results can be obtained. More exactly, we shall briefly outline the proof of the fact that for an arbitrary integer n, one can construct an asymptotic basis of order n having the form

$$\varphi_i(\varepsilon) = \sum_{j=0}^{n} \varphi_{i,j}\varepsilon^j + O(\varepsilon^{n+1})$$

$$\lambda_i(\varepsilon) = \sum_{j=0}^{n} \lambda_{i,j}\varepsilon^j + O(\varepsilon^{n+1})$$

$$i = 1, 2, \ldots, \dim P_0 .$$

The proof consists in reducing the problem to a finite dimensional one, in close analogy with the theory of regular perturbations [7, Chap. XII, Sect. 2].

Consider, for sufficiently small ε, the operator [16, 6, Chap. II, Sect. 4 and Chap. VIII, 2]

$$A_\varepsilon^n = [1-(P_\varepsilon^n - P_0)^2]^{-1/2}(P_\varepsilon^n P_0 + (1-P_\varepsilon^n)(1-P_0)).$$

Using (2.33) one can write for A_ε^n the expansion

$$A_\varepsilon^n = 1 + \sum_{j=1}^{n} A_j\varepsilon^j + \varepsilon^{n+1}\tilde{A}_n(\varepsilon). \tag{2.34}$$

From the corresponding properties of P_j, $\tilde{P}_n(\varepsilon)$ it follows that

$$\begin{aligned} &A_j, \tilde{A}_n(\varepsilon) \in \mathscr{D}(\operatorname{ad} X_0); \quad j=1,\ldots,n, \\ &A_j\mathscr{H} \subset \mathscr{D}(H_0), \quad \tilde{A}_n(\varepsilon)\mathscr{H} \subset \mathscr{D}(H_0). \end{aligned} \tag{2.35}$$

It is easily verified that A_ε^n is unitary and

$$A_\varepsilon^n P_0 A_\varepsilon^{n*} = P_\varepsilon^n ,$$

which together with (2.22) implies that $P_0\mathscr{H}$ is an invariant subspace of $A_\varepsilon^{n*}(H_\varepsilon + \varepsilon B_n)A_\varepsilon^n$. Defining the "reduced" hamiltonian, $H_{\text{red}}^n(\varepsilon)$ by

$$H_{\text{red}}^n(\varepsilon) = P_0 A_\varepsilon^{n*}(H_\varepsilon + \varepsilon B_n)A_\varepsilon^n P_0 ,$$

one can write, using (2.34)

$$H_{\text{red}}^n(\varepsilon) = \sum_{j=0}^{n} H_j\varepsilon^j + \varepsilon^{n+1}\tilde{H}_{\text{red}}^n(\varepsilon). \tag{2.36}$$

Some care is to be taken at this point to make sure that all the operators appearing in the right hand side of (2.36) are well defined. All of them have the form $P_0Q^*YQP_0$ where Y is either a bounded operator, H_0 or X_0 and Q is 1, A_j or $\tilde{A}_n(\varepsilon)$. Due to (2.35) the terms containing H_0 give no difficulties. Concerning terms containing X_0 one has to observe that $X_0QP_0=[X_0,Q]P_0+QX_0P_0$ and due to (2.35) the only thing one has to prove is that X_0P_0 is bounded. For further use we shall prove more, namely that $X_0^mP_0$ is bounded for $m=1,2,\ldots$. Indeed, from

$$\exp(itX_0)P_0=\exp(itX_0)P_0\exp(-itX_0)\exp(itX_0),$$

it follows that for $\phi\in\mathscr{D}(X_0^m)$, $\exp(itX_0)P_0\phi$ is m times differentiable so that $X_0^mP_0$ is bounded on $\mathscr{D}(X_0^m)$ which implies $X_0^mP_0$ to be bounded due to the fact that P_0 is finite dimensional (if $\dim P_0=\infty$, in general not even X_0P_0 is bounded).

Let $\psi_i(\varepsilon)$, $\mu_i(\varepsilon)$, $i=1,\ldots,\dim P_0$ be the eigenvectors and eigenvalues of $\sum_{j=0}^{n}H_j\varepsilon^j$ (considered as an operator in $P_0\mathscr{H}$). Due to the Rellich theorem [6, Chap. II, Sect. 6; 7, Chap. XII.1] $\psi_i(\varepsilon)$ and $\mu_i(\varepsilon)$ are analytic in a neighborhood of $\varepsilon=0$ so that

$$\psi_i(\varepsilon)=\sum_{j=0}^{\infty}\psi_{i,j}\varepsilon^j;\qquad \mu_i(\varepsilon)=\sum_{j=0}^{\infty}\mu_{i,j}\varepsilon^j.$$

Clearly $\lambda_i(\varepsilon)=\mu_i(\varepsilon)$, $\varphi_i(\varepsilon)=A_\varepsilon^{n*}\psi_i(\varepsilon)$ have all the desired properties.

At this point we can make the connection with the following result obtained by Riddell [4] and by Conley and Rejto [5], concerning the existence of asymptotic bases.

Theorem R2. *Suppose H_0 is essentially self-adjoint on $\mathscr{D}=\mathscr{D}(H_0)\cap\mathscr{D}(X_0)$ and let H_ε be a self-adjoint extension of $H_0+\varepsilon X_0$ defined on $\mathscr{D}$. If, under the conditions described in Definition 2, all the operators $X_1X_2\ldots X_nP_0$, where X_i is either the reduced resolvent of H_0 at λ_0, S, either SX_0 are bounded, then the perturbation method yields an asymptotic basis of order n.*

Since the hypotheses in Theorem R2 are nothing but the conditions needed for solving the formal Reyleigh-Schrödinger perturbation equations, one can expect that these hypotheses are implied by the hypotheses of Theorem 1. Indeed, as already said in the introduction, it is easy to see that this is true. Using the following formula [6, Chap. II, Sect. 2] for S

$$S=\frac{1}{2\pi i}\int_\Gamma(H_0-z)^{-1}(z-\lambda_0)^{-1}dz,$$

it follows that $S\in\mathscr{D}((\mathrm{ad}X_0)^\infty)$. Consider now an operator of the form $X_1X_2\ldots X_nP_0$. After commuting X_0 past all the reduced resolvents, one is left with $X_0^qP_0$, $q\leqq n$ which is bounded.

Remarks. 7. As already said, using (2.27) and (2.28) one can give a "time independent" proof of Theorem 1. We preferred the above proof, since with few modifications it gives also a rather general form of the adiabatic theorem in quantum mechanics, which in some sense is the generalization of Theorem 1 to time-dependent Hamiltonians (see Theorem 2 below). Here we shall state and prove the adiabatic theorem only for bounded Hamiltonians, in order not to obscure the simplicity of the proof. In the second paper of this series we shall consider the general case of unbounded time-dependent Hamiltonians, where some technical points related to the possible nondifferentiability of the unitary propagators arise [7, Chap. X.12].

8. Under the conditions of Theorem 1, one cannot expect to obtain bounds on $c_{p,1}$ in (2.26) as a function of p. In the third paper of this series we shall explore the consequences of replacing condition ii) of Theorem 1, by the following stronger one: $R_0(t;z)$ is, as a funtion of t, analytic in the strip $|\mathrm{Im}\,t|<a$ for some $a>0$, or in other words $(H_0-z)^{-1}$ is an analytic vector for adX_0.

Theorem 2. *Let $H(s)$, $s\in I=[0,S]$ be a norm continuous family of bounded self-adjoint operators satisfying the conditions*

i) $\sigma(H(s))=\sigma_1(s)\cup\sigma_2(s)$,

$$\inf_{s\in I}\mathrm{dist}\,(\sigma_1(s),\sigma_2(s))=d>0\,.$$

ii) $R(s;\pm i)\equiv(H(s)\mp i)^{-1}$ *are infinitely norm differentiable.*

Let $U_\varepsilon(s)$ be the unique solution of the Schrödinger equation

$$i\varepsilon\frac{dU_\varepsilon(s)}{ds}=H(s)U_\varepsilon(s)\,;\qquad U_\varepsilon(0)=1\,,$$

and $P_0(s)$ be the spectral projection of $H(s)$ corresponding to $\sigma_1(s)$.

Then, for every positive integer q, there exist $\varepsilon_q>0$, $a_q<\infty$ and orthogonal projections $P_q^\varepsilon(s)$ defined for $0<\varepsilon\leqq\varepsilon_q$ such that

$$\lim_{\varepsilon\to 0}\|P_q^\varepsilon(s)-P_0(s)\|=0\,,$$
$$\|U_\varepsilon(s)P_q^\varepsilon(0)-P_q^\varepsilon(s)U_\varepsilon(s)\|\leqq a_q s\varepsilon^q\,;\qquad s\in I\,. \tag{2.37}$$

Proof. Let $H_0(t)$ be defined by $H_0(t)=H(\varepsilon t)$. The construction in the proof of Theorem 1 gives $H_q(t)$, $P_q(t)$, $K_q(t)$, $A_q(t)$ and the existence of a_q, ε_q such that

$$\|K_q(t)\|\leqq a_q\varepsilon^{q+1}\,;\qquad t\in[0,\varepsilon^{-1}S]\,;\qquad 0<\varepsilon\leqq\varepsilon_q\,;\qquad q=0,1,\ldots\,. \tag{2.38}$$

Denote $Z_q(t)=\prod_{i=0}^{q-1}A_i(t)$, $q=1,2,\ldots$,

$$B_0(t)=K_0(t)\,;\qquad B_q(t)=Z_q(t)K_q(t)Z_q^*(t) \tag{2.39}$$

and

$$H^q(t)=H_0(t)+\sum_{i=0}^{q-1}B_i(t)\,;\qquad q=1,2,\ldots\,. \tag{2.40}$$

By construction

$$H^q(t)=Z_q(t)H_q(t)Z_q^*(t)\,.$$

Let $P_\varepsilon^q(t)$ be the spectral projection of $H^q(t)$ corresponding to the part of the spectrum which coincides with $\sigma_1(t)$ in the limit $\varepsilon\to 0$. Obviously

$$P_\varepsilon^q(t)=Z_q(t)P_q(t)Z_q^*(t)\,. \tag{2.41}$$

Let $U(t)$, $V_q(t)$, $W_q(t)$ be defined by

$$U(t)=U_\varepsilon(\varepsilon t)\,; \qquad t\in[0,\varepsilon^{-1}S]\,, \tag{2.42}$$

$$i\frac{d}{dt}V_q(t)=A_q^*(t)H_q(t)A_q(t)V_q(t)\,; \qquad V_q(0)=1\,, \tag{2.43}$$

$$U(t)=Z_q(t)A_q(t)V_q(t)W_q(t)\,. \tag{2.44}$$

By construction, since $P_\varepsilon^q(0)=P_q(0)$,

$$[A_q^*(t)H_q(t)A_q(t), P_\varepsilon^q(0)]=0\,,$$

and hence

$$[V_q(t), P_\varepsilon^q(0)]=0\,. \tag{2.45}$$

By construction

$$i\frac{d}{dt}W_q(t)=-V_q^*(t)A_q^*(t)K_q(t)A_q(t)V_q(t)W_q(t)\,,$$

which together with (2.38) gives

$$\|W_q(t)-1\|\leqq a_q|t|\varepsilon^{q+1}\,. \tag{2.46}$$

On the other hand from (2.41) and (2.45)

$$Z_q(t)A_q(t)V_q(t)P_\varepsilon^q(0)=P_\varepsilon^q(t)Z_q(t)A_q(t)V_q(t)\,,$$

which together with (2.44) and (2.46) implies

$$\|P_\varepsilon^q(t)U(t)-U(t)P_\varepsilon^q(0)\|\leqq a_q t\varepsilon^{q+1}\,, \tag{2.47}$$

which is nothing but (2.37) with the identifications (2.42) and $P_q^\varepsilon(s)=P_\varepsilon^q(\varepsilon^{-1}s)$.

Remarks. 9. Suppose that $H(s)$ is constant in some neighborhoods of 0 and S. Then $P_0(0)=P_q^\varepsilon(0)$, $P_0(S)=P_q^\varepsilon(S)$ for all q and in this case (2.37) for $s=S$ reduces to an infinite-dimensional generalization of Lenard's results [8].

3. Applications

1. Let M be a positive integer and $\alpha=\{\alpha_{ij}\}_{i,j=1}^M$ be a real, strictly positive $M\times M$ matrix. Consider in the Hilbert space $L^2(\mathbb{R}^M)$ the operators T, V, X_0 defined by

$$T=\sum_{i,j=1}^M \alpha_j P_i P_j\,; \qquad P_k=-i\partial/\partial x_k\,; \qquad x=(x_1,\dots,x_M)\,; \qquad k=1,2,\dots,M, \tag{3.1}$$

$$(Vf)(x)=V(x)f(x)\,, \tag{3.2}$$

$$(X_0 f)(x)=\left(\sum_{j=1}^M c_j x_j\right)f(x)\,, \qquad c_j\in\mathbb{R} \tag{3.3}$$

on their natural domains. Suppose that V is T-bounded with relative bound less than one, so that $T+V$ is self-adjoint on $\mathscr{D}(T)$ [7, Chap. X.2].

Proposition 4. *The operators $H_0 = T + V$ and X_0 defined by* (3.1)–(3.3) *satisfy the conditions i), ii) of Theorem 1.*

Proof. For condition i), see [7, Theorem X.38]. For condition ii): remark that

$$\begin{aligned} H_0(t) &= \exp(i\varepsilon X_0 t) H_0 \exp(-i\varepsilon X_0 t) \\ &= \sum_{i,j=1}^{M} \alpha_{ij}(P_i + \varepsilon c_i t)(P_j + \varepsilon c_j t) + V, \end{aligned} \tag{3.4}$$

from which the verification is straightforward. Obviously, this example covers the Stark effect in arbitrary atoms and molecules (see for example the form of the Hamiltonian in Zhislin's theorem [7, Theorem XIII.7]). For $M = 3, \alpha_{ij} = \frac{1}{2m}\delta_{ij}$, $V(x) = V_1(x) + V_2(x)$, where V_1 is periodic and locally L^2 (see [7, Theorem XIII.96]) and $V_2 \in L^2(\mathbb{R}^3) + L^p(\mathbb{R}^3)$, $2 \leqq p < \infty$, the above example describes the Stark effect for impurity states in solid state physics.

2. (The Dirac Equation.) The Hilbert space is $(L^2(\mathbb{R}^3))^4$,

$$T = \sum_{i=1}^{3} \alpha_i P_i + \beta m\,; \qquad P_k = -i\partial/\partial x_k\,, \tag{3.5}$$

where α_i, β are the Dirac 4×4 constant matrices

$$(V\psi)_i(x) = \sum_{j=1}^{4} V_{ij}(x)\psi_j(x)\,; \qquad V_{ij}(x) = \overline{V_{ji}(x)}\,, \tag{3.6}$$

and

$$(X_0\psi)_i(x) = \left(\sum_{j=1}^{3} c_j x_j\right)\psi_i(x)\,, \qquad x = (x_1, x_2, x_3)\,. \tag{3.7}$$

Again we shall suppose that V is T-bounded with relative bound less then one so that $H_0 = T + V$ is self-adjoint on $\mathscr{D}(T)$.

Proposition 5. *The operators H_0, X_0 defined by* (3.5)–(3.7) *satisfy the conditions i), ii) of Theorem 1.*

Proof. For i) see [17]. For ii) see the proof of Proposition 4.

3. (Barrier Penetration (for details see [18]).)

Consider in $L^2(\mathbb{R}^3)$ the operators

$$H_\varepsilon = -\Delta + V(x) + X_0(\varepsilon) = H_0 + X_0(\varepsilon) \tag{3.8}$$

with $V \in L^2(\mathbb{R}^3)$ and

$$(X_0(\varepsilon)f)(x) = K(\exp(-\varepsilon|x|) - 1)f(x)\,; \qquad K > 0\,, \qquad \varepsilon > 0\,. \tag{3.9}$$

Suppose that H_0 has eigenvalues in $(-K, 0)$. For all $\varepsilon > 0$, $(-K, 0)$ is contained in the continuum spectrum of H_ε. As $\varepsilon \to 0$ the spectrum of H_ε contained in $(-K, 0)$ shows arbitrary order spectral concentration. In this case the self-adjointness problem is trivial. Concerning the condition ii) in Theorem 1 see Remark 5.

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