On asymptotic perturbation theory for Quantum Mechanics: Almost invariant subspaces and gauge invariant magnetic perturbation theory

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Abstract

Singular perturbation theory for Quantum Mechanics is considered in a framework generalising the spectral concentration theory. Under very general conditions, asymptotic estimations on the Rayleigh-Schrödinger expansions of the perturbed spectral projections are obtained. As a consequence almost invariant subspaces of exponential order are constructed. The results covers practically all singular perturbations considered in nonrelativistic quantum mechanics. In the magnetic field case, under the condition that the magnetic field does not increase at infinity, a gauge invariant perturbation theory leading to convergent series with field dependent coefficients is developed.

1 Introduction

While the regular perturbation theory achived its final form in the papers of Sz-Nagy, Rellich and Kato (see [14] , [22] and references therein), in the case singular perturbations (Stark and Zeeman effects in quanum mechanics are in this class) the progress has been much slower, at least for the degenerate eigenvalues case. In the general framework laid down in Kato's book a systematic theory of asymptotic Rayleigh-Schrödinger perturbation theory for degenerate eigenvalues has been developed, fairly recently by Hunziker and coworkers [27], [13] , [12] (see the beautiful review paper by Hunziker [12] and also the recent book by Hislop and Sigal [10] for detailed exposition and extensive bibliography). The key condition which selects the allowed class of perturbations is the so called "stability condition"; in the cases where the considered eigenvalues are not stable one considers, in the spirit of Aguilar-Balslev-Combes theory [1], [3] , a related (e.g. dilated) hamiltonian for which the stability condition holds true. The main point of the theory is that the stability condition, together with the exponential decay of unperturbed eigenvectors given by Combes-Thomas theory [4], [12] , allows to obtain powerfull asymptotic estimates. The price to be paid are strong conditions (e.g. dilation analyticity) on the perturbation. Also, at the technical level the theory is far from being elementary since one has to deal with non-self-adjoint operators, analytic continuation etc. In addition, as far as we understand, it does not seem easy to obtain informations on the perturbed eigenvectors.

In this paper which , with the exception of the last section, is a continuation of [16] we follow a different route, closer in its spirit with the theory of spectral concentration, in which the main objects are the perturbed subspaces. The aim is twofold: first, using the results in [17] we push the estimations in [16], [20] up to exponential order; second, and more important, we extend the analysis to cases where the techniques in [16], [17] , based on adiabatic expansions do not apply.

The content of the paper is as follows. In Section 2 we set up the framework. Almost invariant subspaces of families of self-adjoint operators are defined and it is shown that their existence gives (up to some errors) similar spectral and evolution informations as the existence of invariant subspaces. In this context we give a very general form of the Hylleraas-Wigner "2n+1" theorem: "the knowledge of eigenfunction up to errors of order δ, gives the knovledge of the corresponding eigenvalue up to errors of order δ^2". Section 3, again of general nature, is devoted to the construction of almost invariant subspaces out of asymptotic Rayleigh- Schrödinger series of the perturbed projection. Section 4 contains one of the main results of the paper: for the Schrödinger operator in $\mathbb{R}^3$ (actually all the arguments work in an appropriate abstract setting), under very general conditions on the perturbing potential, we are able to construct formal Rayleigh-Schrödinger expansions for the perturbed projection (see also [11]) and to obtain good asymptotic estimates on the coefficients of this expansions. The results (or their easy extensions to $\mathbb{R}^n$) cover the perturbations by polynomially bounded potentials of bound states in atomic, molecular and solid state physics . Also for perturbing potentials growing up at infinity at most linearly (as in the case of the Stark effect) one can treat the perturbations of the energy bands in solids (the Stark-Wannier problem). In all this cases one obtains that the perturbed subspaces are almost invariant up to exponentially long times, which in the present setting is the anlog of the fact that the imaginary part of the corresponding resonances (in the cases when they can be defined) are exponentially small.

Section 5, the last one, concernes with perturbations given by magnetic fields which do not grow at infinity (the most important particular case being the Zeeman effect i.e. the case of constant magnetic field) and can be read independently of the rest of the paper. The main result is that this case is closer to regular perturbation theory. More exactly one finds that *after factorising* the so called "nonintegrable gauge phase factor" on can write down a gauge invariant *convergent* perturbation series for the integral kernel of the perturbed resolvent, with coefficients depending themselvs upon the perturbing magnetic field. This dependence comes from *phase factors* containing fluxes through some polygonal contours and the asymptotic nature of the usual expansions comes *solely* from expanding these phase factors. In particular this leads (for the first time to our best knowledge) to a convergent expansion for the usual Zeeman effect. The fact that the factorisation of the non-integrable gauge phase factor makes the perturbation given by magnetic fields less singular has been used many times in the physical literature (see e.g. [15], [18] and references therein in connection with the Peierls-Onsager problem) and has been fully used recently [6] in connection with decay of eigenfunctions (see also [5] for the use of the same ideea to control the thermodynamic limit for quantum gases in constant magnetic field).

2 Almost invariant subspaces. General theory.

We start with the definition of almost invariant subspaces (a.s.i.).

Definition 2.1. *Let $H_\varepsilon, P_\varepsilon, \quad \varepsilon \in [0, \varepsilon_0], \varepsilon_0 > 0$ be families of self-adjoint operators and orthogonal projections respectively, in a separable Hilbert space , $\mathcal{H}$, satisfying the conditions*

i.

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

ii. $P_\varepsilon \mathcal{D}(H_\varepsilon) \subset \mathcal{D}(H_\varepsilon)$ where $\mathcal{D}(H_\varepsilon)$ is the domain of H_ε and on $\mathcal{D}(H_\varepsilon)$:

$$\| [H_\varepsilon P_\varepsilon] \| \leq \delta(\varepsilon), \quad 0 \leq \delta(\varepsilon) < \infty, \quad \lim_{\varepsilon \to 0} \delta(\varepsilon) = 0. \tag{2.2}$$

Then we say that $P_\varepsilon \mathcal{H}$ are almost invariant subspaces of order $\delta(\varepsilon)$ for H_ε.

The definition implies that $P_0\mathcal{H}$ is an invariant subspace of H_0. In what follows we shall restrict ourselves to the case when P_0 is the spectral projection of H_0 corresponding to a bounded isolated part, σ_0, of $\sigma(H_0)$ i.e.

iii.

$$P_0 = \frac{i}{2\pi} \oint_\Gamma (H_0 - z)^{-1} dz \tag{2.3}$$

where Γ is a contour enclosing σ_0. In particular, we shall not consider the perturbation of embedded eigenvalues.

Remarks

2.1 The condition (2.1) implies that for sufficiently small ε (for which $\| P_\varepsilon - P_0 \| \leq 1$) P_ε and P_0 are unitarily equivalent; in particular $\dim P_\varepsilon \mathcal{H} = dim P_0 \mathcal{H}$. Notice that (2.1) cannot be replaced by $s - \lim_{\varepsilon\to 0} P_\varepsilon = P_0$ even if $\dim P_0\mathcal{H} < \infty$ and $H_\varepsilon \to H_0$ in the strong resolvent sense (see e.g. [12])

2.2 The condition ii. is equivalent with the following one: $P_\varepsilon \mathcal{D}_\varepsilon \subset \mathcal{D}(H_\varepsilon)$ where $\mathcal{D}_\varepsilon$ is a core of H_ε and 2.2 holds true on $\mathcal{D}_\varepsilon$.

If we write H_ε in a matrix form according to the decomposition $\mathcal{H} = P_\varepsilon\mathcal{H} \oplus (1 - P_\varepsilon)\mathcal{H}$ then the off-diagonal part, B_ε:

$$B_\varepsilon = P_\varepsilon H(1 - P_\varepsilon) + (1 - P_\varepsilon) H P_\varepsilon = (1 - 2P_\varepsilon)[H_\varepsilon, P_\varepsilon]. \tag{2.4}$$

is bounded on $\mathcal{D}(H_\varepsilon)$

$$\| B_\varepsilon \| \leq \delta(\varepsilon). \tag{2.5}$$

It follows that both $P_\varepsilon H_\varepsilon P_\varepsilon$ and $(1 - P_\varepsilon)H_\varepsilon(1 - P_\varepsilon)$ are self-adjoint on $P_\varepsilon \mathcal{D}(H_\varepsilon)$ and $(1 - P_\varepsilon)\mathcal{D}(H_\varepsilon)$ respectively. Notice that $P_\varepsilon H_\varepsilon P_\varepsilon$ need not be bounded.

In what follows we shall use the notations:

$$H_{\varepsilon,D} \equiv H_\varepsilon - B_\varepsilon = P_\varepsilon H_\varepsilon P_\varepsilon + (1 - P_\varepsilon)H_\varepsilon(1 - P_\varepsilon), \tag{2.6}$$

$$h_\varepsilon \equiv P_\varepsilon H_\varepsilon P_\varepsilon : P_\varepsilon \mathcal{D}(H_\varepsilon) \to P_\varepsilon \mathcal{H}. \tag{2.7}$$

Taking into account (2.4-2.7) the above definition of a.s.i. coincide with the definition of asymptotic invariant subspaces in [16].

One expects that the existence of a.s.i. to give (up to some errors controlled by $\delta(\varepsilon)$) similar spectral informations on H_ε as the existence of invariant subspaces.

Proposition 2.2. *If $P_\varepsilon\mathcal{H}$ are a.i.s. of order $\delta(\varepsilon)$ for H_ε then:*

$$\| (1-P_\varepsilon)exp(-itH_\varepsilon)P_\varepsilon \| \leq |\, t \,|\, \delta(\varepsilon). \tag{2.8}$$

If h_ε has an eigenvalue E_ε and

$$h_\varepsilon\psi_\varepsilon = E_\varepsilon\psi_\varepsilon \tag{2.9}$$

then

$$exp(-itH_\varepsilon)\psi_\varepsilon = exp(-itE_\varepsilon)\psi_\varepsilon + \chi_\varepsilon(t) \tag{2.10}$$

with

$$\| \chi_\varepsilon(t) \| \leq |\, t \,|\, \delta(\varepsilon). \tag{2.11}$$

In particular

$$|< \psi_\varepsilon, exp(-itH_\varepsilon)\psi_\varepsilon >| \geq 1 - |\, t \,|\, \delta(\varepsilon) \tag{2.12}$$

i.e. in the physicists language ψ_ε describes a metastable state.

Proof. Direct consequence of the definition and of the formula:

$$exp(-itH_\varepsilon) = exp(-itH_{\varepsilon,D}) - i\int_0^t exp(-itH_{\varepsilon,D}(t-s))B_\varepsilon exp(-isH_\varepsilon)ds. \tag{2.13}$$

Remarks

2.3. Iterating once (2.13) and taking into account that B_ε is off-diagonal one can improve (2.12) to

$$|< \psi_\varepsilon, exp(-itH_\varepsilon)\psi\varepsilon >| \geq 1 - |\, t \,|^2\, \delta(\varepsilon)^2/2 \tag{2.14}$$

Consider now the case when $H_\varepsilon \to H_0$ in the strong resolvent sense and $\sigma_0 = \{\lambda_0\}$ with λ_0 an isolated, m-degenerate eigenvalue so that

$$dim P_0\mathcal{H} = m < \infty. \tag{2.15}$$

From (1.1) it follows that for sufficiently small ε

$$dim P_\varepsilon\mathcal{H} = m < \infty. \tag{2.16}$$

In this case the existence of a.i.s. of order $\delta(\varepsilon)$ is equivalent [16] with the spectral concentration as defined in [23], [14]. Indeed suppose $P_\varepsilon\mathcal{H}$ are a.i.s. of order $\delta(\varepsilon)$ for H_ε. Since $P_\varepsilon\mathcal{H}$ are finite dimensional there exist

$$\phi_{\varepsilon,j} \in P_\varepsilon\mathcal{H}, \quad <\phi_{\varepsilon,j}, \phi_{\varepsilon,k}>= \delta_{j,k}, \quad \tilde{\lambda}_{\varepsilon,j} \in \mathbf{R}; \quad j,k = 1,2,...m$$

such that

$$h_\varepsilon \phi_{\varepsilon,j} = \tilde{\lambda}_{\varepsilon,j}\phi_{\varepsilon,j} \tag{2.17}$$

From (2.1), (2.2) and (2.6) it follows that

$$\lim_{\varepsilon\to 0} \| (1-P_0)\phi_{\varepsilon,j} \| = 0 \tag{2.18}$$

$$\| (H_\varepsilon - \tilde{\lambda}_{\varepsilon,j})\phi_{\varepsilon,j} \| \leq \delta_\varepsilon \tag{2.19}$$

i.e. $\phi_{\varepsilon,j}, \tilde{\lambda}_{\varepsilon,j})$ are pseudo eigenvectors and pseudo eigenvalues of all orders $p \in \mathbf{N}$ for which $\lim_{\varepsilon\to 0}\varepsilon^{-p}\delta(\varepsilon) = 0$ and this is equivalent with the spectral concentration according to the Riddel's theorem [23]. Conversely if $\tilde{\lambda}_{\varepsilon,j}$ and $\phi_{\varepsilon,j}$ satisfying (2.18) and (2.19) exist then $P_\varepsilon\mathcal{H}$ with

$$P_\varepsilon = \sum_{j=1}^{m} <\phi_{\varepsilon,j}, \cdot> \phi_{\varepsilon,j} \tag{2.20}$$

are a.i.s. of order $\delta(\varepsilon)$ for H_ε.

Finnaly let us consider the case when, in addition, λ_0 is stable [12] (see also [14], [10]). From the definition of stability there exist $d > 0, \varepsilon_1 > 0$ such that for $\varepsilon \in [0, \varepsilon_1]$, $\Gamma = \{z \mid | z - \lambda_0 | = d\} \subset \rho(H_\varepsilon)$ and

$$\inf_{z\in\Gamma} dist(z, \sigma(H_\varepsilon)) \geq d/2. \tag{2.21}$$

In addition, if

$$Q_\varepsilon = \oint_\Gamma (H_\varepsilon - z)^{-1} dz \tag{2.22}$$

then

$$\lim_{\varepsilon\to 0} \| Q_\varepsilon - P_0 \| = 0. \tag{2.23}$$

From (2.1), (2.2) and (2.23) there exist $\varepsilon_2 > 0$ such that for all $\varepsilon \in [0, \varepsilon_2]$ one has:

$$\| Q_\varepsilon - P_0 \| < 1/6, \ \ \| P_\varepsilon - P_0 \| < 1/6, \ \ \delta(\varepsilon) \leq d/8. \tag{2.24}$$

As expected Q_ε and the spectrum of $Q_\varepsilon H_\varepsilon Q_\varepsilon$ (as an operator in the m-dimensional space $Q_\varepsilon\mathcal{H}$) are close to P_ε and $\sigma(h_\varepsilon)$ respectively.

Proposition 2.3. *For* $\varepsilon \in [0, min\{\varepsilon_1, \varepsilon_2\}]$

$$\| P_\varepsilon - Q_\varepsilon \| \leq c_1(d)\delta(\varepsilon) \tag{2.25}$$

$$dist(\sigma(Q_\varepsilon H_\varepsilon Q_\varepsilon), \sigma(h_\varepsilon) \leq c_2(d)\delta(\varepsilon)^2 \tag{2.26}$$

Remarks

2.4. The proof gives the following (nonoptimal) values for $c_i(d)$: $c_1(d) = 16/3d$, $c_2(d) = \frac{512}{9d}$.

2.5. The interesting part of Proposition 2.3 is (2.26) which is a general form of the so called Hylleraas-Wigner "$2n+1$" theorem in perturbation theory (see [8] and references therein): the knowledge of the perturbed wave function to order $\delta(\varepsilon)$ gives the perturbed eigenvalue with errors of order $\delta(\varepsilon)^2$. To see the connection, consider the elementary case of regular perturbations of nondegenerate isolated eigenvalues. Let $H_\varepsilon \psi_\varepsilon = \lambda_\varepsilon \psi_\varepsilon$ and suppose that one knows an approximate *normalised* wave function $\tilde{\psi}_\varepsilon$, $\| \tilde{\psi}_\varepsilon \| = 1$ with $\| \tilde{\psi}_\varepsilon - \psi_\varepsilon \| \leq \delta(\varepsilon)$, $\| H_\varepsilon(\tilde{\psi}_\varepsilon - \psi_\varepsilon) \| \leq M\delta(\varepsilon)$; M uniformly bounded as $\varepsilon \to 0$. Then if

$$P_\varepsilon = < \tilde{\psi}_\varepsilon, \cdot > \tilde{\psi}_\varepsilon$$

one has

$$\| [P_\varepsilon, H_\varepsilon] \| \leq 2(M + | \lambda_\varepsilon |)\delta(\varepsilon)$$

which according to Proposition 2.3 gives

$$| \lambda_\varepsilon - < \tilde{\psi}_\varepsilon, H_\varepsilon \tilde{\psi}_\varepsilon > | \leq \text{const.}\delta(\varepsilon)^2. \tag{2.27}$$

Actually in this simple case one can obtain (2.27) at once from:

$$| \lambda_\varepsilon - < \tilde{\psi}_\varepsilon, H_\varepsilon \tilde{\psi}_\varepsilon > | = | < \tilde{\psi}_\varepsilon, (H_\varepsilon - \lambda_\varepsilon)\tilde{\psi}_\varepsilon > | =$$

$$| < \tilde{\psi}_\varepsilon, (H_\varepsilon - \lambda_\varepsilon)(\tilde{\psi}_\varepsilon - \psi_\varepsilon) > | = | < (H_\varepsilon - \lambda_\varepsilon)(\tilde{\psi}_\varepsilon - \psi_\varepsilon), \tilde{\psi}_\varepsilon - \psi_\varepsilon > |$$

Notice however that the above argument cannot be generalised directly to the degenerate case and actually we do not know a reference for the Hylleraas-Wigner theorem in the degenerate case in spite of the fact that it is probably known to experts. The reason for the quadratic estimation in (2.26) is the fact that B_ε is an off-diagonal perturbation of $H_{\varepsilon,D}$. Let us stress that the condition $P_\varepsilon = P_\varepsilon^2$ is essential for (2.26) to hold true; actually it replaces the condition that $\tilde{\psi}_\varepsilon$, in the above proof of Hylleraas-Wigner theorem, is normalised.

2.6. Proposition 2.3 can be easily extended to the case when σ_0 is a stable, bounded isolated part of the spectrum oh H_0 but the constants in

(2.25), (2.26) becomes more complicated and depend also upon the diameter of σ_0.

Proof of Proposition 2.3. We apply regular perturbation theory to the pair $H_{\varepsilon,D}, H_\varepsilon = H_{\varepsilon,D} + B_\varepsilon$. From (2.5),(2.6) and (2.24) ,

$$dist(\Gamma, \sigma(H_{\varepsilon,D})) \geq 3d/8. \tag{2.28}$$

If

$$T_\varepsilon = \frac{i}{2\pi} \oint_\Gamma (H_{\varepsilon,D} - z)^{-1} dz \tag{2.29}$$

then

$$Q_\varepsilon - T_\varepsilon = -\frac{i}{2\pi} \oint_\Gamma (H_{\varepsilon,D} - z)^{-1} B_\varepsilon (H_\varepsilon - z)^{-1} dz \tag{2.30}$$

which gives

$$\| Q_\varepsilon - T_\varepsilon \| \leq 16\delta(\varepsilon)/3d < 2/3 \tag{2.31}$$

From (2.24) and (2.31) one has

$$\| P_\varepsilon - T_\varepsilon \| < 1. \tag{2.32}$$

Now (2.32) implies that

$$P_\varepsilon = T_\varepsilon \tag{2.33}$$

which together with (2.31) gives (2.25). Indeed since $P_\varepsilon,\ T_\varepsilon$ are orthogonal projections commuting with $H_{\varepsilon,D}$, in a $L^2(M, d\mu)$ representation of $H_{\varepsilon,D}$ they are multiplications with some characteristic functions so $P_\varepsilon - T_\varepsilon$ is the multiplication with a function taking only the values 0 and ± 1. As the values ± 1 are ruled out by (2.32) the equality (2.33) follows.

For the proof of (2.26) consider consider the Sz-Nagy transformation matrix [14] corresponding to the pair $P_\varepsilon,\ Q_\varepsilon$

$$U_\varepsilon = (1 - (Q_\varepsilon - P_\varepsilon)^2)^{-1/2} [Q_\varepsilon P_\varepsilon + (1 - Q_\varepsilon)(1 - P_\varepsilon)]. \tag{2.34}$$

As well known U_ε is unitary and intertwines Q_ε and P_ε

$$Q_\varepsilon = U_\varepsilon P_\varepsilon U_\varepsilon^*. \tag{2.35}$$

As a consequence

$$U_\varepsilon^* Q_\varepsilon H_\varepsilon Q_\varepsilon U_\varepsilon = P_\varepsilon U_\varepsilon^* H_\varepsilon U_\varepsilon P_\varepsilon \tag{2.36}$$

i.e. $Q_\varepsilon H_\varepsilon Q_\varepsilon$ is unitarily equivalent with the "effective" hamiltonian $P_\varepsilon U_\varepsilon^* H_\varepsilon U_\varepsilon P_\varepsilon$. On the other hand the analytic perturbation theory applied to the pair $H_{\varepsilon,D},\ H_\varepsilon = H_{\varepsilon,D} + B_\varepsilon$ gives for $P_\varepsilon U_\varepsilon^* H_\varepsilon U_\varepsilon P_\varepsilon$ [14]:

$$P_\varepsilon U_\varepsilon^* H_\varepsilon U_\varepsilon P_\varepsilon = h_\varepsilon + P_\varepsilon B_\varepsilon P_\varepsilon + \mathcal{O}(B_\varepsilon^2) \tag{2.37}$$

so that (since the second term in the r.h.s. vanishes)

$$\| P_\varepsilon U_\varepsilon^* H_\varepsilon U_\varepsilon P_\varepsilon - h_\varepsilon \| \leq \mathcal{O}(B_\varepsilon^2) \tag{2.38}$$

which in particular implies (2.26). The computation below gives a precise form of the error in terms of $\delta(\varepsilon)$ and d. Without restricting the generality on can take $\lambda_0 = 0$. Using

$$Q_\varepsilon H_\varepsilon Q_\varepsilon = \frac{i}{2\pi} \oint_\Gamma z(H_\varepsilon - z)^{-1} dz \tag{2.39}$$

and

$$\begin{aligned}(H_\varepsilon - z)^{-1} =& (H_{\varepsilon,D} - z)^{-1} - (H_{\varepsilon,D} - z)^{-1} B_\varepsilon (H_{\varepsilon,D} - z)^{-1} \\ &+ (H_\varepsilon - z)^{-1} B_\varepsilon (H_{\varepsilon,D} - z)^{-1} B_\varepsilon (H_{\varepsilon,D} - z)^{-1}\end{aligned} \tag{2.40}$$

one has

$$\begin{aligned}P_\varepsilon Q_\varepsilon H_\varepsilon Q_\varepsilon P_\varepsilon =& P_\varepsilon \frac{i}{2\pi} \oint_\Gamma z(H_{\varepsilon,D} - z)^{-1} dz P_\varepsilon \\ &- P_\varepsilon \frac{i}{2\pi} \oint_\Gamma z(H_{\varepsilon,D} - z)^{-1} B_\varepsilon (H_{\varepsilon,D} - z)^{-1} dz P_\varepsilon \\ &+ P_\varepsilon \frac{i}{2\pi} \oint_\Gamma z(H_\varepsilon - z)^{-1} B_\varepsilon (H_{\varepsilon,D} - z)^{-1} B_\varepsilon \\ &(H_{\varepsilon,D} - z)^{-1} dz P_\varepsilon\end{aligned} \tag{2.41}$$

Now from (2.39) written for $H_{\varepsilon,D}$, the first term in the r.h.s. of (2.41) gives h_ε while the second vanishes due to the fact that B_ε is off-diagonal and P_ε commutes with $H_{\varepsilon,D}$. Then estimating brutally the third term in the r.h.s. of (2.41) one obtains

$$\| P_\varepsilon Q_\varepsilon H_\varepsilon Q_\varepsilon P_\varepsilon - h_\varepsilon \| \leq 128\delta(\varepsilon)^2/9d \tag{2.42}$$

On the other hand

$$\begin{aligned}P_\varepsilon U_\varepsilon^* H_\varepsilon U_\varepsilon P_\varepsilon - P_\varepsilon Q_\varepsilon H_\varepsilon Q_\varepsilon P_\varepsilon =& (P_\varepsilon U_\varepsilon^* - P_\varepsilon Q_\varepsilon) Q_\varepsilon H_\varepsilon Q_\varepsilon U_\varepsilon P_\varepsilon \\ &+ P_\varepsilon Q_\varepsilon H_\varepsilon Q_\varepsilon (U_\varepsilon P_\varepsilon - Q_\varepsilon P_\varepsilon)\end{aligned} \tag{2.43}$$

and then

$$\| U_\varepsilon^* Q_\varepsilon H_\varepsilon Q_\varepsilon U_\varepsilon - P_\varepsilon Q_\varepsilon H_\varepsilon Q_\varepsilon P_\varepsilon \| \leq 2 \| U_\varepsilon Q_\varepsilon - Q_\varepsilon P_\varepsilon \| \cdot \| Q_\varepsilon H_\varepsilon Q_\varepsilon \| \quad (2.44)$$

Now from

$$U_\varepsilon P_\varepsilon - Q_\varepsilon P_\varepsilon = [(1 - (Q_\varepsilon - P_\varepsilon)^2)^{-1/2}) - 1] Q_\varepsilon P_\varepsilon \quad (2.45)$$

one obtains (see (2.31) and (2.33))

$$\| U_\varepsilon P_\varepsilon - Q_\varepsilon P_\varepsilon \| = \| P_\varepsilon U_\varepsilon^* - P_\varepsilon Q_\varepsilon \| \leq 128 \delta(\varepsilon)^2 / 3d^2 \quad (2.46)$$

Since (remember that we took $\lambda_0 = 0$)

$$\| Q_\varepsilon H_\varepsilon Q_\varepsilon \| \leq d/2, \quad (2.47)$$

puting all together one obtains

$$\| P_\varepsilon U_\varepsilon^* H_\varepsilon U_\varepsilon P_\varepsilon - h_\varepsilon \| \leq \frac{512}{9d} \delta(\varepsilon)^2 \quad (2.48)$$

which gives in particular (2.26)with the value of c_2 given in Remark 2.5.

3 Perturbative construction of almost invariant subspaces

We turn now to the problem of constructing a.i.s. for families, H_ε, of self-adjoint operators. The setting we shall consider, which is sufficiently general to cover practically all physical situations in nonrelativistic quantum mechanics, is as follows: $\varepsilon > 0$ is a small parameter $\varepsilon \in [0, \varepsilon_0]$; H_0 and $V(\varepsilon)$ are self-adjoint operators such that there exists a dense subspace, $\mathcal{D}$, $\mathcal{D} \subset \mathcal{D}(H_0) \cap \mathcal{D}(V(\varepsilon))$ on which $H_0 + \varepsilon V(\varepsilon)$ has self-adjoint extensions (in most examples $H_0 + \varepsilon V(\varepsilon)$ is essentially self-adjoint on $\mathcal{D}$); we shall denote by H_ε any of its self-adjoint extensions with the property $\mathcal{D}(H_\varepsilon) \supset \mathcal{D}(H_0) \cap \mathcal{D}(V_\varepsilon)$

We shall consider explicitely only the particular case when $V(\varepsilon) = V$ is independent on ε, and in this case $\mathcal{D} = \mathcal{D}(H_0) \cap \mathcal{D}(V)$, but all the results generalise as far as $V(\varepsilon)$ obeys the needed technical conditions uniformly in ε. Indeed in this case one obtains results (uniformly in $\eta \in [0, \varepsilon_0]$) for

$$H_{\varepsilon,\eta} = H_0 + \varepsilon V(\eta)$$

and at the end one sets $\eta = \varepsilon$.

At the heuristic level the problem of finding a.i.s for H_ε can be wieved as the search for solutions of the equations

$$[H_\varepsilon, P_\varepsilon] = [H_0, P_\varepsilon] + \varepsilon[V, P_\varepsilon] \simeq 0, \tag{3.1}$$

$$P_\varepsilon^2 - P_\varepsilon \simeq 0. \tag{3.2}$$

Making the "perturbational" ansatz

$$P_\varepsilon \simeq \sum_j E_j \varepsilon^j \tag{3.3}$$

one is led to the problem of solving the following equations for E_j, $j = 1, 2, ...$

$$P_0 = E_0, \tag{3.4}$$

$$[H_0, E_j] = -[V, E_{j-1}], \tag{3.5}$$

$$\sum_{l=0}^{j} E_l E_{j-l} = E_j. \tag{3.6}$$

The equation (3.4) is nothing but (2.1) for $\varepsilon = 0$ while (3.5) and (3.6) follow from pluging (3.3) into (3.1) and (3.2) respectively.

In the rest of this section we shall outline how the existence of solutions, E_0, $E_1, ..., E_N$; $N \leq \infty$ of (3.4-3.6) together with estimates on the norm of E_j and $[V, E_j]$ gives the existence of a.i.s. in the sense of (2.1-2.2) with control on the constant $\delta(\varepsilon)$. Of course the technical core of the theory is the proof of existence of solutions of (3.4-3.6) with bounds on their norms and this question will be addressed in the next section.

Suppose $E_j L^2(\mathbb{R}^3) \subset \mathcal{D}(H_0) \cap \mathcal{D}(V)$, $j = 0, 1, ...N$ and there satisfy (3.4-3.6). In addition:

$$\| E_j \| \leq e_j, \tag{3.7}$$

$$\| [V, E_j] \| \leq f_j \quad j = 1, 2, ..., N \tag{3.8}$$

Consider

$$T_N(\varepsilon) = \sum_{j=0}^{N} E_j \varepsilon^j. \tag{3.9}$$

where N can depend upon ε. Unfortunately $T_N(\varepsilon)$ is not a projection (in particular $T_N(\varepsilon)^2 \neq T_N(\varepsilon)$ and even if $T_N(\varepsilon)$ is self-adjoint $i[\frac{d}{d\varepsilon}T_N(\varepsilon), T_N(\varepsilon)]$ is not self-adjoint; this point has been overlooked in [11] but without consequences on the result there). So the first step is to construct out of $T_N(\varepsilon)$ a projection operator,$P_N(\varepsilon)$ whose expansion in ε should coincide with $T_N(\varepsilon)$ up to order N. Of course such a "completion" is far from being unique; we shall use the method employed in [17] since it gives an easy control on $\| [H_\varepsilon, P_N(\varepsilon)] \|$

We need a few elementary facts about projections. Here we consider the self-adjoint case; for the non self-adjoint case see Appendix where a more elaborate version of (elementary) Proposition 3 in [17] is given. Let T be a bounded self-adjoint operator satisfying

$$\| T^2 - T \| \leq \delta < 1/4. \tag{3.10}$$

Then by the spectral theorem

$$\rho(T) \subset (\frac{1-\sqrt{1+4\delta}}{2}, \frac{1-\sqrt{1-4\delta}}{2}) \cup (\frac{1+\sqrt{1-4\delta}}{2}, \frac{1+\sqrt{1+4\delta}}{2})$$

In particular $1/2 \in \rho(T)$, $\| T \| \leq \frac{1+\sqrt{1+4\delta}}{2}$ and

$$\sup_{|z-1|=1/2} \| (T-z)^{-1} \| \leq \frac{2}{\sqrt{1-4\delta}} \tag{3.11}$$

Now, if P is the spectral projection of T corresponding to the part of the spectrum around 1 :

$$P = \frac{i}{2\pi} \oint_{|z-1|=1/2} (T-z)^{-1} dz \tag{3.12}$$

then again by the spectral theorem

$$\| T - P \| \leq \frac{1-\sqrt{1-4\delta}}{2} = \frac{2\delta}{1+\sqrt{1-4\delta}}. \tag{3.13}$$

Consider now $T_N(\varepsilon)$.Due to (3.6) and (3.7) $\| T_N(\varepsilon)^2 - T_N(\varepsilon) \| \sim \mathcal{O}(\varepsilon^{N+1})$ i.e. for sufficiently small ε ,

$$\| T_N(\varepsilon)^2 - T_N(\varepsilon) \| < 1/4$$

and one can define $P_N(\varepsilon)$ by

$$P_N(\varepsilon) = \frac{i}{2\pi} \oint_{|z-1|=1/2} (T_N(\varepsilon) - z)^{-1} dz. \tag{3.14}$$

$P_N(\varepsilon)$ is a projection and according to (3.13)

$$\| P_N(\varepsilon) - T_N(\varepsilon) \| \sim \mathcal{O}(\varepsilon^{N+1}) \tag{3.15}$$

We compute now $[H_\varepsilon, P_N(\varepsilon)]$. Notice first that due to the identity

$$(T-z)^{-1} = z^{-1}(T(T-z)^{-1} - 1)$$

$[H_\varepsilon, P_N(\varepsilon)]$ is well defined on a dense subspace and the following computation can be done. From (3.5)

$$[H_\varepsilon, T_N(\varepsilon)] = \varepsilon^{N+1}[V, E_N]$$

and then

$$\begin{aligned}[H_\varepsilon, P_N(\varepsilon)] &= -\frac{i}{2\pi}\oint_{|z-1|=1/2} (T_N(\varepsilon)-z)^{-1}[H_\varepsilon, T_N(\varepsilon)](T_N(\varepsilon)-z)^{-1}dz \\ &= -\varepsilon^{N+1}\frac{i}{2\pi}\oint_{|z-1|=1/2} (T_N(\varepsilon)-z)^{-1}[V, E_N](T_N(\varepsilon)-z)^{-1}dz\end{aligned} \tag{3.16}$$

We summarise the above discussion in the following lemma:

Lemma 3.1. *Suppose E_j satisfy (3.4-3.8), $T_N(\varepsilon)$ be given by (3.9) and let ε_N be the positive solution of the equation:*

$$\sum_{l=N+1}^{2N} \varepsilon^l a_l = 1/8 \tag{3.17}$$

where

$$a_l = \sum_{j+m=l, 0\le j,m\le N} e_j e_m$$

Then for $0 \le \varepsilon \le \varepsilon_N$:

$$\| T_N(\varepsilon)^2 - T_N(\varepsilon) \| \le \sum_{l=N+1}^{2N} \varepsilon^l a_l \equiv \delta_N(\varepsilon) \le 1/8 \tag{3.18}$$

and if $P_N(\varepsilon)$ is given by (3.14)

$$\| P_N(\varepsilon) - T_N(\varepsilon) \| \le 2\delta_N(\varepsilon), \tag{3.19}$$

$$\| [H_\varepsilon, P_N(\varepsilon)] \| \le \varepsilon^{N+1} \| [V, E_N] \| \equiv \varepsilon^{N+1} f_N. \tag{3.20}$$

Proof.

For (3.18) notice that from (3.6)

$$T_N(\varepsilon)^2 - T_N(\varepsilon) = \sum_{l=N+1}^{2N} \varepsilon^l \Big(\sum_{j+m=l, 0\le j,m\le N} E_j E_m \Big).$$

Then (3.19) follows from (3.18) and (3.14) while (3.20) follows from (3.16) and (3.19).

Remarks

3.1 The main point of the lemma is the estimate (3.20).

3.2 Notice that in each particular case one has still to prove that $P_\varepsilon \mathcal{D}_\varepsilon \subset \mathcal{D}(H_\varepsilon)$ (see Remark 2.2 and remind that $\mathcal{D}_\varepsilon$ is a core of H_ε).

At a more elaborate level of perturbation theory the task is to obtain, under specific conditions on H_0, V and P_0 the dependence on j of e_j, f_j; the rate of increase of these constants "measures" the singularity of the perturbation. The simplest case is when $e_j \le e^j$ for some finite constant e ; this corresponds to the well known regular perturbations and there is no need for further discussion. The most interesting case is when $N = \infty$ and there exist constants $g < \infty, \;\; \alpha > 0$ such that

$$e_j \le g^j (j!)^\alpha, \;\; f_j \le g^{j+1}((j+1)!)^\alpha, \;\; j = 1, 2, ... \tag{3.21}$$

In this case the series in (3.3) is not convergent and the idea here is to use a best remainder estimate a la Necharosev i.e. to take N depending on ε in (3.9) in order to have the r.h.s. of (3.16) as small as possible. This requirement leads to N_ε given by

$$N_\varepsilon + 1 = [(\frac{1}{g\varepsilon})^{1/\alpha}] \tag{3.22}$$

where $[\ldots]$ means the integer part. Pluging (3.22) into (3.9) one obtains:

Lemma 3.2. *Let N_ε be given by (3.22). Then there exists $\varepsilon_0 > 0$ such that for $\varepsilon \in [0, \varepsilon_0]$, (3.18) holds true and $P_\varepsilon \equiv P_{N_\varepsilon}$ satisfies (2.2) with*

$$\delta(\varepsilon) = (2\pi)^\alpha \frac{1}{(g\,\varepsilon)^{1/2}} exp(-\frac{\alpha}{(g\,\varepsilon)^{1/\alpha}}). \tag{3.23}$$

Proof. From (3.21)

$$a_l \le \sum_{j=0}^{l} e_j e_{l-j} \le g^l (l+1)(l!)^\alpha. \tag{3.24}$$

From the Stirling formula (K is an absolute constant)

$$j! \leq K j^{j+1/2} e^{-j} \tag{3.25}$$

and the fact that for all $N_\varepsilon + 1 \leq k \leq 2N_\varepsilon$:

$$\alpha \ln k \leq \alpha \ln 2N_\varepsilon \leq \alpha \ln 2 - \ln(g\,\varepsilon) \tag{3.26}$$

one obtains

$$\varepsilon^j\, a_j \leq K^\alpha (j+1)^{1+\alpha/2} e^{-j\alpha(1-\ln 2)} \tag{3.27}$$

so

$$\delta_N(\varepsilon) \leq K^\alpha \sum_{j=N_\varepsilon+1}^{\infty} (j+1)^{\alpha+1/2} e^{-\alpha(1-ln2)j}. \tag{3.28}$$

Since $N_\varepsilon \to \infty$ as $\varepsilon \to 0$ the first part of the lemma is proved. Then (3.23) follows from (3.20),(3.22) and the Stirling formula.

Remark 3.3 If $g\,\varepsilon < 1$, in the limit $\alpha \to 0$ one has $\delta(\varepsilon) \to 0$ which fits with the fact that for $\alpha = 0$ the series in (3.3) is convergent for $\varepsilon < g^{-1}$.

4 Asymptotic estimations.

In this section we consider the problem of finding solutions E_j of (3.4-3.6) satisfying estimations like (3.7-3.8). In spite of the fact that all the arguments below work in an appropriate abstract setting, for definiteness we shall discuss a simple Schrodinger case in $\mathbb{R}^3$

$$H_\varepsilon = -\Delta + V_0(\mathbf{x}) + \varepsilon V(\mathbf{x}) \equiv H_0 + \varepsilon V(\mathbf{x}) \tag{4.1}$$

with

$$V_0 \in L^2_{uloc} \;\; i.e. \sup_{\mathbf{x}\in\mathbb{R}^3} \int_{|\mathbf{x}-\mathbf{y}|\leq 1} \mid V_0(\mathbf{y}) \mid^2 d\mathbf{y} < \infty \tag{4.2}$$

and

$$\mid V(\mathbf{x}) \mid \leq \; < \mathbf{x} >^\beta, \; < \mathbf{x} >= (1+\mathbf{x}^2)^{1/2}, \; \beta \in \mathbf{R}. \tag{4.3}$$

In particular H_0 is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3)$ [21]. I what follows H_ε is *any* self-adjoint extension of $H_0 + \varepsilon V_(\mathbf{x})$ defined on $\mathcal{D}(H_0) \cap \mathcal{D}(V) \supset \mathcal{C}_0^\infty(\mathbb{R}^3)$. We remind the following elementary result from Combes-Thomas theory ([4]), ([12]), ([18]):

Proposition 4.1. *Let $K \subset \rho(H_0)$ be compact, λ_0 an isolated finite degenerate eigenvalue of H_0. Then there exist $\gamma_0 > 0, \;\; M < \infty$ such that for all $\gamma \in [0, \gamma_0]$:*

$$\| e^{\gamma<\cdot>} P_0 e^{\gamma<\cdot>} \| \leq M \tag{4.4}$$

$$\sup_{z \in K} \| R_{0,\gamma}(z) \| \leq M \tag{4.5}$$

where

$$R_{0,\gamma}(z) = e^{\gamma<\cdot>}(H_0 - z)^{-1} e^{-\gamma<\cdot>} \tag{4.6}$$

and P_0 is the spectral projection of H_0 corresponding to λ_0.

If $\beta \in (-\infty, 0]$ then $VR_0(z)$ ($R_0(z) = (H_0 - z)^{-1}$) is bounded and E_j given by the well known perturbation formula

$$E_j = (-1)^j \frac{i}{2\pi} \oint R_0(z)(VR_0(z))^j dz \tag{4.7}$$

satisfy (3.4-3.6) and (3.7-3.8) with $\alpha = 0$. Now, if $\beta > 0, \;\; VR_0(z)$ is not bounded and one cannot decide at once from (4.7) whether E_j are bounded or not and the main idea in what follows is to find alternative formulae for E_j which make sense for $\beta > 0$.

Lemma 4.2. *For all $\beta \in \mathbb{R}$, E_j given by (4.7) are well defined on $\mathcal{C}_0^\infty(\mathbb{R}^3)$ and satisfy (3.4-3.6).*

Proof. The key observation ([12]) is that due to (4.3) and (4.5-4.5) expressions like $R_0(z)(VR_0(z))^l, \;\; VR_0(z)(VR_0(z))^l V$ are well defined on $\mathcal{C}_0^\infty(\mathbb{R}^3)$. In particular from (4.7), for $u \in \mathcal{C}_0^\infty(\mathbb{R}^3)$, $E_j u$ is well defined:

$$E_j u = (-1)^j \frac{i}{2\pi} \oint R_0(z)(Ve^{-\frac{\gamma}{j}})R_{0,\frac{\gamma}{j}}(z)...R_{0,\gamma}(z)e^{\gamma<\cdot>}u dz. \tag{4.8}$$

For all $z \neq z' \in \rho(H_0), \;\; j = 1, ...$ and $u \in \mathcal{C}_0^\infty(\mathbf{R}^3)$

$$\frac{1}{z - z'}[R_0(z)(VR_0(z))^j - R_0(z')(VR_0(z'))^j]u =$$

$$= \sum_{l=0}^{j} [R_0(z)(VR_0(z))^l][R_0(z')(VR_0(z'))^{j-l}]u. \tag{4.9}$$

Indeed from the resolvent formula

$$
\begin{aligned}
&(z-z')\sum_{l=0}^{j}[R_0(z)(VR_0(z))^l][R_0(z')(VR_0(z'))^{j-l}]u = \\
&= (R_0(z)-R_0(z'))VR_0(z')...VR_0(z')u + R_0(z)(R_0(z) \\
&- R_0(z'))VR_0(z')...VR_0(z')u + ... + R_0(z)VR_0(z)...(R_0(z)-R_0(z'))u \\
&= R_0(z)(VR_0(z))^j - R_0(z')(VR_0(z'))^j u.
\end{aligned}
$$

Integrating (4.9) on two contours $\Gamma, \quad \Gamma' \subset \rho(H_0), \quad \Gamma' \subset Int\Gamma$ enclosing σ_0 one obtains

$$E_j u = \sum_{l=0}^{j} E_l E_{j-l} u. \tag{4.10}$$

From $H_0R_0(z) = 1 + zR_0(z)$, again on $u \in \mathcal{C}_0^\infty(\mathbb{R}^3)$

$$
\begin{aligned}
&H_0R_0(z)(VR_0(z))^jVR_0(z)u - R_0(z)(VR_0(z))^jVR_0(z)H_0u \\
&= (VR_0(z))^jVR_0(z)u - R_0(z)(VR_0(z))^jVu
\end{aligned}
$$

which after the integration on Γ gives

$$[H_0, E_{j+1}]u = -[V, E_j]u$$

and the proof is finished.

Consider now the case when $\sigma_0 = \{\lambda_0\}$ with λ_0 a finite degenerate, isolated eigenvalue of H_0:

$$dist(\lambda_0, \sigma(H_0) \setminus \lambda_0) = d_0 > 0, \;\; dim\ P_0 = m < \infty, \; \Gamma = \{z \mid\mid \lambda_0 - z \mid= d_0/2\}. \tag{4.11}$$

Then by the residue theorem [14]

$$E_j u = (-1)^{j-1} \sum_{\nu_1,\nu_2...\nu_{j+1};\nu_l\geq 0;\sum_{l=1}^{j+1}\nu_l = j} S^{\nu_1}VS^{\nu_2}V...VS^{\nu_{j+1}} \tag{4.12}$$

where S is the reduced resolvent at λ_0:

$$S = \frac{i}{2\pi}\oint_\Gamma R_0(z)(\lambda_0 - z)^{-1}dz \tag{4.13}$$

and by convention

$$S^0 = -P_0. \tag{4.14}$$

Notice that from (4.5) and (4.13)

$$\| e^{\gamma<\cdot>} S e^{-\gamma<\cdot>} \| \leq M, \quad \text{all} \quad \gamma \in [0, \gamma_0]. \tag{4.15}$$

The main point about (4.12) is that all terms in its r.h.s. contain at *least* one P_0; this together with the decay propery (4.4) of P_0 and (4.15) which allows to propagate this decay in order to control the unboundedness od V implies that E_j defined initially on $\mathcal{C}_0^\infty(\mathbb{R}^3)$ are bounded and their extensions by continuity are given by (4.12) and satisfy (3.5)-(3.6). More precisely we have

Theorem 4.3. *Let β, γ_0, d_0 as given by (4.3 -4.5) and (4.11). Then the operators E_j, $j = 0, 1, 2, ...$ defined by (4.12) have the following properties:*

$$E_0 = P_0, \tag{4.16}$$

$$E_j L^2(\mathbb{R}^3) \subset \mathcal{D}(H_0) \cap \mathcal{D}(V), \tag{4.17}$$

$$E_j = \sum_{l=0}^{j} E_l E_{j-l}, \tag{4.18}$$

$$[H_0, E_j]u = -[V, E_j]u, \;\; \textit{all} \;\; u \in \mathcal{D}(H_0) \cap \mathcal{D}(V), \tag{4.19}$$

$$\| E_j \| \leq g^j j^{\beta j}, \tag{4.20}$$

$$\| [V, E_j] \| \leq d_0 g^{j+1} j^{\beta(j+1)}, \;\; j = 1, 2, ... \tag{4.21}$$

with

$$g = 3fM(\beta / e\gamma_0)^\beta \tag{4.22}$$

where f is the (absolute) constant appearing in the inequality:

$$\sum_{l=1}^{j-1} \frac{1}{l^2 (j-l)^2} \leq \frac{f}{j^2}. \tag{4.23}$$

Proof. (3.4,3.5,3.6) can be read directly from (4.12), Proposition 3.1, and Lemma3.1. Consider now the estimations (4.20), (4.21) . One can see directly that each term in (4.12) is bounded by

$$M^{j+1} \parallel V^j e^{-\gamma_0 <\cdot>} \parallel$$

so that

$$\parallel E_j \parallel \leq N(j) M^{j+1} \parallel V^j e^{-\gamma_0 <\cdot>} \parallel \tag{4.24}$$

where $N(j)$ is the number of terms in the r.h.s. of (4.12). Unfortunately, due to the fact that $N(j)$ is at least of order $j!$ (4.24) is much weaker than the expected estimation; for example if $\beta = 1$ one expects $\parallel E_j \parallel \leq const.e^j j!$ while (4.24) gives at best $const.e^j (j!)^2$. We shall prove (4.20,4.21) by recurrence using the identity (4.18) in the form:

$$E_j = P_0 E_j + E_j P_0 + \sum_{l=1}^{j-1} E_l E_{j-l} \tag{4.25}$$

and taking the advantage of the extra P_0 in $P_0 E_j$ and $E_j P_0$ which allows to use (4.7) instead of (4.12).

From

$$\parallel V^j e^{-\gamma <\cdot>} \parallel \leq \sup_{a>0} a^{\beta j} e^{-\gamma_0 a} = (\beta j / e\gamma_0)^{\beta j} \tag{4.26}$$

4.4, 4.5 and 4.7 one obtains

$$\parallel P_0 E_j \parallel = \parallel E_j P_0 \parallel \leq \mu^j j^{\beta j} \tag{4.27}$$

where

$$\mu = M(\beta / e\gamma_0)^\beta. \tag{4.28}$$

In particular since $E_1 = P_0 E_1 + E_1 P_0$ one has

$$\parallel E_1 \parallel \leq 2\mu. \tag{4.29}$$

Let now f be the constant appearing in the inequality

$$\sum_{l=1}^{j-1} \frac{1}{l^2 (j-l)^2} \leq \frac{f}{j^2}; \quad j = 2, 3, ... \tag{4.30}$$

Notice that $f \geq 4$. We now prove by induction that for $j = 1, 2, ...$

$$\| E_j \| \leq \frac{2}{j^2} A^{j-1} \mu^j j^{\beta j} \tag{4.31}$$

and

$$\| [V, E_j] \| \leq \frac{2d_0}{j^2} A^{j-1} \mu^{j+1} j^{\beta(j+1)} \tag{4.32}$$

with

$$A = 3f. \tag{4.33}$$

Consider first (4.31). From (4.25- 4.27) and taking into account that for $\beta \geq 0$, $(\frac{l^l (j-l)^{j-l}}{j^j})^\beta \leq 1$ one gets

$$\begin{aligned} \| E_j \| &\leq 2\mu^j j^{\beta j} + \frac{4f}{j^2} A^{j-2} \mu^j j^{\beta j} \\ &= \frac{2}{j^2} A^{j-1} \mu^j j^{\beta j} [\frac{j^2}{A^{j-1}} + \frac{2f}{A}]. \end{aligned} \tag{4.34}$$

For $A = 3f$ the square braket in the r.h.s. of (4.34) is smaller than one for all $j = 2, 3, ...$ and the proof of 4.31 is finished. Consider now (4.32):

$$[V, E_j] = [V, E_j P_0] + [V, P_0 E_j] + \sum_{l=1}^{j-1} ([V, E_l] E_{j-l} + E_l [V, E_{j-l}]). \tag{4.35}$$

As before

$$\| [V, E_j P_0] \| \leq d_0 \mu^{j+1} (j+1)^{\beta(j+1)} \tag{4.36}$$

$$\| [V, E_1] \| \leq 2 d_0 \mu^2 2^{2\beta} \tag{4.37}$$

Indeed, for example

$$\begin{aligned} \| V E_j P_0 \| &\leq \frac{1}{2\pi} \int_\Gamma \| V e^{-\frac{\gamma_0}{j+1} <\cdot>} R_{0, \frac{\gamma_0}{j+1}}(z) ... R_{0,\gamma_0}(z) e^{\gamma_0 <\cdot>} P_0 \| | dz | \\ &\leq \frac{d_0}{2} M^{j+1} \| V^{j+1} e^{-\gamma_0 <\cdot>} \| . \end{aligned}$$

Inserting in (4.35) the inequalities (4.36), (4.37) and (4.32) for $j = 2, ..., j-1$ one obtains

$$\| [V, E_j] \| \leq 2d_0 \mu^{j+1}(j+1)^{\beta(j+1)} + \frac{8d_0 f}{j^2} A^{j-2} \mu^{j+1} j^{\beta(j+1)}$$
$$\leq \frac{2d_0}{j^2} A^{j-1} \mu^{j+1} j^{\beta(j+1)} [\frac{j^2}{A^{j-1}} + \frac{2f}{A}]$$

and the proof is finished since for all $j = 2, 3, ...$ $[\frac{j^2}{A^{j-1}} + \frac{2f}{A}] \leq 1$.

Remarks

4.1. By Stirling's formula $j^{\beta j} \leq e^{\beta j}(j!)^\beta$ so (4.20), (4.21) can be rewritten as:

$$\| E_j \| \leq \tilde{g}^j (j!)^\beta, \tag{4.38}$$

$$\| [V, E_j] \| \leq d_0 \tilde{g}^{j+1}((j+1)!)^\beta \tag{4.39}$$

with

$$\tilde{g} = 3fM(\beta/\gamma_0)^\beta.$$

4.2. As already said the result in Theorem 4.3. can be extended in a variety of situations as for example for Zeeman effect

$$H_\varepsilon = (\mathbf{P} - \varepsilon \mathbf{a})^2 + V_0; \;\; \mathbf{P} = -i\nabla$$

with (4.3) replaced by

$$| \mathbf{a} | + | \nabla \cdot \mathbf{a} | \leq < \mathbf{x} >^\beta$$

Also if $V_0(\mathbf{x}) \to \infty$ as $| \mathbf{x} | \to \infty$ one can replace the decay factor $e^{-\gamma_0 <\cdot>}$ by a better one; e.g. in the "harmonic oscillator" case $V_0(\mathbf{x}) \sim | \mathbf{x} |^2$ as $| \mathbf{x} | \to \infty$ one can take (see [12]) $e^{-\gamma_0 <\cdot>^2}$ instead of $e^{-\gamma_0 <\cdot>}$ and in this case the asymptotic estimations are in terms of $\| V^j e^{-\gamma_0 <\cdot>^2} \|$. Notice also that even in the case (4.3) one can allow $| V(\mathbf{x}) | \leq e^{\eta <\cdot>}$ with η sufficiently small, but in this case only a finite number of E_j can be controlled.

4.3.There is another way of proving that E_j given by (4.12) satisfy (4.18) and (4.19) namely starting with a cut-off perturbation , $V_\lambda(\mathbf{x}) = V(\mathbf{x})$ if $| V(\mathbf{x}) | \leq \lambda$ and zero orhervise, for which (4.18) and (4.19) are true (since the series $P_{\varepsilon,\lambda} = \sum_{j=0}^\infty \varepsilon^j E_{j,\lambda}$ is convergent and satisfies $-\varepsilon[P_{\varepsilon,\lambda}, V_\lambda] = -[P_{\varepsilon,\lambda}, H_0]$, $P_{\varepsilon,\lambda} = P_{\varepsilon,\lambda}^2$) and then taking the limit $\lambda \to \infty$. Yet another proof can be found in [11].

The proof of Theorem 4.1 rests heavily on exponential decay of eigenfunctions (see (4.4)) that is on the fact that $dim\ P_0 < \infty$. We consider now the case $dim\ P_0 = \infty$ when (4.4) does not hold true. Still, as far as $\beta \leq 1$ (see (4.3)) on can find solutions of (3.4)-(3.6). More exactly:

Theorem 4.4. *Suppose* $d_0 = dist(\sigma_0, \sigma(H_0) \setminus \sigma_0) > 0,\ D_0 = \sup_{\lambda,\mu \in \sigma_0} < \infty$ *and*

$$\sup_{\mathbf{x} \in \mathbb{R}^3} \mid \nabla V(\mathbf{x}) \mid \leq 1. \tag{4.40}$$

i. E_j *given recurently by*

$$E_0 = P_0,$$

$$\begin{aligned} E_{j+1} =& \frac{i}{2\pi} \oint_\Gamma R_0(z) \{ P_0 [V, E_j] Q_0 - Q_0 [V, E_j] P_0 \} R_0(z) dz \\ &+ S_j - 2 P_0 S_j P_0 \end{aligned} \tag{4.41}$$

where

$$Q_0 = 1 - P_0, \tag{4.42}$$

$$S_j = \sum_{k=1}^{k=j} E_k E_{j+1-k} \tag{4.43}$$

have the properties:

$$E_j \mathcal{D}(V) \subset \mathcal{D}(H_0) \cap \mathcal{D}(V), \tag{4.44}$$

$$\| E_j \| \leq g^j j!, \tag{4.45}$$

$$\| [V, E_{j-1}] \| \leq g^j j! \tag{4.46}$$

for some $g < \infty$ *and satisfy (3.4)-(3.6).*

ii. Let P_ε *as given by (3.14), (3.9)and (3.22) with* $\alpha = 1$*. Let* H_ε *be the (unique by Faris-Lavine theorem [21]) self-adjoint extension of* $H_0 + \varepsilon V$ *defined on* $\mathcal{D}(H_0) \cap \mathcal{D}(V)$*. Then*

$$P_\varepsilon \mathcal{D}(H_0) \cap \mathcal{D}(V) \subset \mathcal{D}(H_0) \cap \mathcal{D}(V) \tag{4.47}$$

and on $\mathcal{D}(H_0) \cap \mathcal{D}(V)$

$$\| [H_\varepsilon, P_\varepsilon] \| \leq \frac{2\pi}{g\,\varepsilon} \exp(-\frac{1}{g\,\varepsilon}) \tag{4.48}$$

Remark

4.4. In order to see why bounded E_j should however exist consider $E_j u$ with $u \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ as given by (4.7). Then

$$\begin{aligned} E_j u &= -\frac{i}{2\pi}(\oint_\Gamma R_0(z) V R_0(z) dz) u \\ &= -\frac{i}{2\pi}(\oint_\Gamma R_0^2(z) V dz) u - \frac{i}{2\pi}(\oint_\Gamma R_0(z)[V, R_0(z)] dz) u. \end{aligned} \tag{4.49}$$

Now for $u \in \mathcal{C}_0^\infty(\mathbb{R}^3)$

$$[V, R_0(z)] u = i R_0(z)(\mathbf{P} \cdot \nabla V + \nabla V \cdot \mathbf{P}) R_0(z) u \tag{4.50}$$

so the operator in the last term in the r.h.s. of (4.49) is bounded. On the other hand , by residue theorem, the first term in the r.h. s. of (4.49) vanishes. It follows that E_1 as given by (4.49) is bounded on $\mathcal{C}_0^\infty(\mathbb{R}^3$ and then it has an bounded extension by continuity. In addition it follovs that $E_1 L^2(\mathbb{R}^3 \subset \mathcal{D}(H_0)$ and one can argue that (see the proof of Lemma 4.2) that $E_1 \mathcal{D}(V) \subset \mathcal{D}(V)$. Actually one can prove the existence of E_j "rewriting" (4.7) in a form in which V enters only in multiple commutators $[V, [V ... [V, R_0(z)] ...]$. Instead of doing that we shall use the results in [17] about adiabatic expansions.

Proof of Theorem 4.4

As already said Theorem 4.4 follows from the treatement of the Stark effect in [16], [20] combined with the adiabatic exponential estimations in [17], so we shall only outline the main points.

Consider the family of self-adjoint operators

$$H(s) = e^{isV} H_0 e^{-isV} = (\mathbf{P} - is\nabla V)^2 + V_0 \tag{4.51}$$

Let $\Gamma \subset \rho(H_0)$ be a contour of finite length enclosing σ_0. By regular perturbation theory, $(H(s) - z)^{-1}$ is, for all $z \in \Gamma$, analytic in s, in a strip around real axis and uniformly bounded there so we can apply the methods in [17]. In the Lemma below we collect some results from [17] in an appropriate form.

Lemma 4.5. *[17]*

i. Let

$$P_0(s) = e^{isV} P_0 e^{-isV}, \quad R(s; z) \equiv (H(s) - z)^{-1} = e^{isV}(H_0 - z)^{-1} e^{-isV}. \tag{4.52}$$

Then $E_j(s)$ given by the reccurence formula

$$\begin{aligned} E_{j+1}(s) =& \frac{i}{2\pi}\oint_\Gamma R(s;z)\{P_0(s)\frac{d}{ds}E_j(s)Q_0(s) - Q_0(s)\frac{d}{ds}E_j(s)P_0(s)\}R(s;z)dz \\ &+ S_j(s) - 2P_0(s)S_j(s)P_0(s) \end{aligned} \tag{4.53}$$

where

$$Q_0(s) = 1 - P_0(s), \tag{4.54}$$

$$S_j(s) = \sum_{k=1}^{k=j-1} E_k(s) E_{j-k}(s). \tag{4.55}$$

are the unique solution of

$$E_0(s) = e^{isV} P_0 e^{-isV} \equiv P_0(s), \tag{4.56}$$

$$i\frac{d}{ds} E_j(s) = [H(s), E_{j+1}(s)], \tag{4.57}$$

$$E_j(s) = \sum_{k=0}^{k=j} E_k(s) E_{j-k}(s), \tag{4.58}$$

are norm differentiable, and satisfy

$$E_j(s) L^2(\mathbb{R}^3) \subset \mathcal{D}(H(s)) \tag{4.59}$$

$$\| E_j(s) \| \leq g^j j!, \quad \| \frac{d}{ds} E_j(s) \| \leq g^{j+1}(j+1)!, \tag{4.60}$$

for some $g < \infty$

ii. Let $P_\varepsilon(s)$ *as given by (3.14), (3.9)and (3.22) with* $\alpha = 1$. *Then* $P_\varepsilon(s)$ *is norm differentiable*

$$P_\varepsilon(s) L^2(\mathbb{R}^3) \subset \mathcal{D}(H(s)) \tag{4.61}$$

and there exists $\varepsilon_0 > 0$ *such that for* $\varepsilon \in [0, \varepsilon_0]$*:*

$$\| \varepsilon \frac{d}{ds} P_\varepsilon(s) - [H(s), P_\varepsilon(s)] \| \leq \frac{1}{g\,\varepsilon} \exp(-\frac{1}{g\,\varepsilon}). \tag{4.62}$$

Let A be a bounded operator, such that $A(s) = e^{isV} A e^{-isV}$ is norm differentiable. Then from Stone's theorem for $f \in \mathcal{D}(V)$ one has $Af \in \mathcal{D}(V)$ and

$$i\frac{d}{ds} A(s) f = e^{isV}[A, V] e^{-isV} f. \tag{4.63}$$

Notice that $[A,V]$ is bounded on $\mathcal{D}(V)$. Since $E_0(s) = e^{isV}P_0e^{-isV}$, from (4.53) and (4.63) it follows that $E_j(s)$ are of the form

$$E_j(s) = e^{isV}E_je^{-isV} \tag{4.64}$$

where E_j have all the properties stated in Theorem 4.4.i.

By the same argument (see (3.14))

$$P_\varepsilon(s) = e^{isV}P_\varepsilon e^{-isV}, \quad P_\varepsilon\mathcal{D}(V) \subset \mathcal{D}(V), \tag{4.65}$$

and

$$i\,\varepsilon\,\frac{d}{ds}P_\varepsilon(s) = \varepsilon\, e^{isV}[P_\varepsilon, V]e^{-isV} \tag{4.66}$$

which together with $P_\varepsilon L^2(\mathbb{R}^3) \subset \mathcal{D}(H_0)$ and (4.23) finishes the proof ot Theorem 4.4.

5 Magnetic Schrodinger operators: gauge invariant perturbation theory.

The aim of this section (which can be read independently of the rest of the paper) is to point out how the gauge covariance can be used to control the singularitiy of perturbations given by magnetic fields which do not wanish (or decay very slowly) as $|\,\mathbf{x}\,| \to \infty$. In order not to obscure the main ideas we shall consider here a particular case: a particle in $\mathbb{R}^3$, subjected to a magnetic field $\mathbf{b}(\mathbf{x})$, and an electric potential $V_0(\mathbf{x})$. Also the proofs of some technical Lemmae below will be given at the end of the section.

Concerning the magnetic field, $\mathbf{b}(\mathbf{x})$, we suppose that:

$$|\,\mathbf{b}(\mathbf{x})\,| + \sum_{j=1}^{d} |\,\partial_j\mathbf{b}(\mathbf{x})\,| \leq < \cdot >^{\beta}, \;\; \beta \leq 0. \tag{5.1}$$

and for $V_0(\mathbf{x})$ as before, we suppose to be uniformly L^2_{loc} i.e.

$$\sup_{\mathbf{x}\in\mathbb{R}^3} \int |\,V_0(\mathbf{y})\,|^2\, d\mathbf{y} < \infty \tag{5.2}$$

As well known [7], for a large class of vector potentials, $\mathbf{a}(\mathbf{x})$, corresponding to $\mathbf{b}(\mathbf{x})$ and $\varepsilon \in [0,\infty)$ the hamiltonian

$$H_{\varepsilon,\mathbf{a}} = (\mathbf{P} - \varepsilon\mathbf{a})^2 + V \tag{5.3}$$

is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3)$ [7] and we shall denote by the same symbol its self-adjoint closure. As before, the unperturbed hamiltonian (i.e. $\varepsilon = 0$) is denoted by H_0

$$H_0 = \mathbf{P}^2 + V. \tag{5.4}$$

The results below can be extended in many directions: arbitrary dimensions; more (locally) singular $\mathbf{b}(\mathbf{x})$ and $V(\mathbf{x})$; many particle systems; the presence of a fixed magnetic field which amounts to replace in (4.4) $\mathbf{P}$ by $(\mathbf{P} - \mathbf{A}_0)$ where where $\mathbf{A}_0(\mathbf{x})$ corresponds to a *fixed* magnetic field, $\mathbf{B}_0(\mathbf{x})$; Dirac operators etc.

Suppose that H_0 has an isolated and bounded part, σ_0, of the spectrum i.e.

$$\sigma(H_0) = \sigma_0 \cup \sigma_1; \quad dist(\sigma_0, \sigma_1) = d > 0 \tag{5.5}$$

and let P_0 be the spectral projection of H_0 corresponding to σ_0. The problem is to study the "deformation" of σ_0 and P_0 when $\varepsilon \neq 0, \ \ \varepsilon \to 0$. If β in (5.1) is less than 0 then there exist magnetic potentials which are uniformly bounded (e.g. the transversal gauge, see below) there is nothing new to say since in that case

$$H_{\varepsilon,\mathbf{a}} = H_0 - \varepsilon(\mathbf{P}\cdot\mathbf{a} - \mathbf{a}\cdot\mathbf{P} + \varepsilon^2 \mid \mathbf{a} \mid^2) \equiv H_0 - \varepsilon W_{\varepsilon,\mathbf{a}} \tag{5.6}$$

where $W_{\varepsilon,\mathbf{a}}$ is a regular perturbation of H_0 and the analytic perturbation theory works.

On the contrary, if in (5.1), $\beta \geq 0$ it is not possible in general to find $\mathbf{a}$ which is uniformly bounded and this implies that $W_{\varepsilon,\mathbf{a}}(H_0 - z)^{-1}$ is not bounded so one cannot obtain an expansion in ε of $(H_{\varepsilon,\mathbf{a}} - z)^{-1}$ from

$$(H_{\varepsilon,\mathbf{a}} - z)(H_0 - z)^{-1} = 1 - \varepsilon W_{\varepsilon,\mathbf{a}}(H_0 - z)^{-1} \tag{5.7}$$

If $\sigma_0 \subset \sigma_{discr}(H_0)$ the asymptotic perturbation theory developed in previous sections works for all $\beta \in \mathbb{R}$ and gives asymptotic expansions for perturbed eigenvalues and corresponding eigenvectors. The situation is more involved when σ_0 is not contained in the discrete spectrum of H_0. On one hand for $\beta \leq 0$ i.e. for magnetic fields which are uniformly bounded, it has been proved by Avron and Simon [2] in a particular case and by Nenciu [19] and Helffer and Sjostrand [9] in the general case that the spactrum (sa a set) is stable and then for sufficiently small ε one can still define the spectral projection $P_{\varepsilon,\mathbf{a}}$ of $H_{\varepsilon,\mathbf{a}}$ corresponding to the part of $\sigma(H_{\varepsilon,\mathbf{a}})$ coinciding with σ_0 in the limit $\varepsilon \to 0$. Now the singularity of the perturbation manifests itself in the "non smooth" behaviour of $P_{\varepsilon,\mathbf{a}}$ as $\varepsilon \to 0$; There are examples in solid state theory (i.e. V periodic and $\mathbf{b}$ constant where [18]):

$$\lim_{\varepsilon \to 0} \| P_{\varepsilon,\mathbf{a}} - P_0 \| = 1 \tag{5.8}$$

(of course one still has $s - \lim_{\varepsilon \to 0} P_{\varepsilon,\mathbf{a}} = P_0$) so there is no room for a (norm) asymptotic expansion of $P_{\varepsilon,\mathbf{a}}$. Since, in contrast with $\sigma(H_{\varepsilon,\mathbf{a}})$, $P_{\varepsilon,\mathbf{a}}$ is not a gauge invariant quantity, the above discussion suggests that, in general, the gauge invariant quantities behave much more smoothly in the limit $\varepsilon \to 0$ than the non gauge invariant ones. In other words if one wants to develop a perturbation theory, one has to consider gauge invariant quantities. The problem is that, in almost all perturbation schemes, the basic object is the resolvent which is not a gauge invariant quantity.

Fortunately, one can "factor" out the non gauge invariant party. Let $G_{\varepsilon,\mathbf{a}}(\mathbf{x}, \mathbf{y}; z)$, $z \in \rho(H_{\varepsilon,\mathbf{a}})$ be the integral kernel (we shall prove below that it exists) of $(H_{\varepsilon,\mathbf{a}} - z)^{-1}$ and $\phi_{\mathbf{a}}(\mathbf{x}, \mathbf{y})$ be the famous nonintegrable phase factor corresponding to $\mathbf{a}$ i.e.

$$\phi_{\mathbf{a}}(\mathbf{x}, \mathbf{y}) = \int_{\mathbf{y}}^{\mathbf{x}} \mathbf{a}(\mathbf{u}) \cdot d\mathbf{u} \tag{5.9}$$

where the integral ia along the straightline joining $\mathbf{x}$ and $\mathbf{y}$. Alternatively one can write (5.9) as

$$\phi_{\mathbf{a}}(\mathbf{x}, \mathbf{y}) = (\int_0^1 \mathbf{a}(\mathbf{y} + t(\mathbf{x} - \mathbf{y}))dt) \cdot (\mathbf{x} - \mathbf{y}). \tag{5.10}$$

Then as one can easily check

$$K_{\varepsilon}(\mathbf{x}, \mathbf{y}; z) = e^{-i\varepsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})} G_{\varepsilon,\mathbf{a}}(\mathbf{x}, \mathbf{y}; z) \tag{5.11}$$

is a gauge invariant quantity. In other words we have to make the ansatz

$$G_{\varepsilon,\mathbf{a}}(\mathbf{x}, \mathbf{y}; z) = e^{i\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})} K_{\varepsilon}(\mathbf{x}, \mathbf{y}; z) \tag{5.12}$$

and seek a perturbation expansion for $K_{\varepsilon}(\mathbf{x}, \mathbf{y}; z)$. The formula (5.12) is crucial for all what follows; it says that the whole gauge noninvariance of the integral kernel of the resolvent (and then for other related objects like as spectral projections, evolution etc) is contained in an exponential factor

$e^{i\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}$. Coming back to perturbation theory, (5.12) suggests to take as the "zero'th" approximation for $(H_{\varepsilon,\mathbf{a}}-z)^{-1}$ the operator $S_{\varepsilon,\mathbf{a}}(z)$, given by the following integral kernel ("twisted" unperturbed resolvent)

$$(S_{\varepsilon,\mathbf{a}}(z)f)(\mathbf{x}) = \int_{\mathbf{R}^3} e^{i\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})} G_0(\mathbf{x},\mathbf{y};z) f(\mathbf{y}) d\mathbf{y} \tag{5.13}$$

where $G_0(\mathbf{x},\mathbf{y};z)$ is the integral kernel of $(H_0-z)^{-1}$. Let's consider now (5.7) with $(H_0-z)^{-1}$ replaced by $S_{\varepsilon,\mathbf{a}}(z)$ and define $T_{\varepsilon,\mathbf{a}}(z)$ by

$$(H_{\varepsilon,\mathbf{a}}-z)S_{\varepsilon,\mathbf{a}}(z) = 1-\varepsilon\, T_{\varepsilon,\mathbf{a}}(z) \tag{5.14}$$

Before computing $T_{\varepsilon,\mathbf{a}}(z)$ let us give the following gauge covariance formula

Lemma 5.1. *Let $\mathbf{a}(\mathbf{x})$ be an arbitrary continuous vector potential corresponding to $\mathbf{b}(\mathbf{x})$, $\mathbf{c}\in\mathbf{R}^3$ and $\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})$ the corresponding nonintegrable phase factor. Then*

$$e^{-i\varepsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})}(\mathbf{P}_{\mathbf{x}}-\varepsilon\mathbf{a}(\mathbf{x}))e^{i\varepsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})} = (\mathbf{P}_{\mathbf{x}}-\varepsilon\mathbf{a}_{\mathbf{c}}(\mathbf{x})) \tag{5.15}$$

where $\mathbf{P}_{\mathbf{x}}=-i\nabla_{\mathbf{x}}$ and $\mathbf{a}_{\mathbf{c}}(\mathbf{x})$ is the vector potential given by the transversal (Poincare) gauge relative to the point $\mathbf{c}$:

$$\mathbf{a}_{\mathbf{c}}(\mathbf{x}) = (\int_0^1 t\mathbf{b}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))dt)\wedge(\mathbf{x}-\mathbf{c}) \tag{5.16}$$

Notice that $\mathbf{a}_{\mathbf{0}}(\mathbf{x})$ is the usual transversal gauge [26]:

$$\mathbf{a}_{\mathbf{0}}(\mathbf{x}) = (\int_0^1 t\mathbf{b}(t\mathbf{x})dt)\wedge\mathbf{x} \tag{5.17}$$

The most interesting properties of $\mathbf{a}_{\mathbf{c}}(\mathbf{x})$ and $\phi_{\mathbf{a}_{\mathbf{c}}}(\mathbf{x},\mathbf{y})$ are given in the following:

Lemma 5.2. *i.*

$$\phi_{\mathbf{a}_{\mathbf{c}}}(\mathbf{x},\mathbf{y}) = -(\int_0^1 dt\int_0^1 ds s\mathbf{b}(st(\mathbf{x}-\mathbf{y})+s(\mathbf{y}-\mathbf{c}))\cdot(\mathbf{x}-\mathbf{c}\wedge\mathbf{y}-\mathbf{c}) \tag{5.18}$$

i.e. $\phi_{\mathbf{a}_{\mathbf{c}}}(\mathbf{x},\mathbf{y})$ is the flux through the triangle $\mathbf{x}\,\mathbf{c}\,\mathbf{y}$.

ii.

$$|\ \mathbf{a}_{\mathbf{c}}(\mathbf{x})\ |\le|\ \mathbf{x}-\mathbf{c}\ |/2 \tag{5.19}$$

$$| \nabla \mathbf{a}_{\mathbf{c}}(\mathbf{x}) | \leq 2 | \mathbf{x} - \mathbf{c} | \tag{5.20}$$

iii.

If $\mathbf{b}(\mathbf{x}) = \mathbf{b}_0 = const$ *then*

$$\mathbf{a}_{\mathbf{c}}(\mathbf{x}) = \mathbf{b}_0 \wedge (\mathbf{x} - \mathbf{c})/2, \tag{5.21}$$

$$\phi_{\mathbf{a}_{\mathbf{c}}}(\mathbf{x}, \mathbf{y}) = \mathbf{b}_0 \cdot ((\mathbf{x} - \mathbf{c}) \wedge (\mathbf{y} - \mathbf{c}))/2 \tag{5.22}$$

Computing the r.h.s. of (5.14) applied to $f \in \mathcal{C}_0^\infty(\mathbf{R}^3)$ by using Lemma 4.1. one finds:

$$(T_{\varepsilon,\mathbf{a}}(z)f)(\mathbf{x}) = \int_{\mathbf{R}^3} e^{i\varepsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})} M_\varepsilon(\mathbf{x}, \mathbf{y}; z) f(\mathbf{y}) d\mathbf{y} \tag{5.23}$$

where

$$M_\varepsilon(\mathbf{x}, \mathbf{y}; z) = (-2i\mathbf{a}_{\mathbf{y}}(\mathbf{x}) \cdot \nabla_{\mathbf{x}} - i(\nabla_{\mathbf{x}} \mathbf{a}_{\mathbf{y}}(\mathbf{x})) - \varepsilon | \mathbf{a}_{\mathbf{y}}(\mathbf{x}) |^2) G_0(\mathbf{x}, \mathbf{y}; z) \tag{5.24}$$

Notice that M_ε depends only upon $\mathbf{b}$ i.e. is gauge invariant. Up to now the discussion was at the heuristic formal level. The main technical point of this section is contained in

Theorem 5.3. *Suppose (5.1) and (5.2) hold true,* $z \in \rho(H_0)$, $\varepsilon \in [0, \varepsilon_0]$, $\varepsilon_0 < \infty$, $K \subset \rho(H_0)$ *compact.Then (5.23), (5.24) define a bounded operator in* $L^2(\mathbb{R}^3)$ *and there exist* $t(z) < \infty$ *(dependind upon* V, $\mathbf{b}$, *and* ε_0 *but not upon* $\mathbf{a}$*) such that uniformly for* $\varepsilon \in [0, \varepsilon_0]$ *and* $z \in K$:

$$\| T_{\varepsilon,\mathbf{a}}(z) \| \leq t(z). \tag{5.25}$$

As a direct consequence we obtain the following perturbation formula for $(H_{\varepsilon,\mathbf{a}} - z)^{-1}$:

Lemma 5.4. *If* $\varepsilon \in [0, t(z)^{-1}]$ *then* $z \in \rho(H_{\varepsilon,\mathbf{a}})$ *and*

$$(H_{\varepsilon,\mathbf{a}} - z)_{-1} = S_{\varepsilon,\mathbf{a}}(z) \sum_{j=0}^{\infty} \varepsilon^j T_{\varepsilon,\mathbf{a}}(z)^j \tag{5.26}$$

as a norm convergent series.

Combining (5.13), (5.23) and (5.26) one can write down the expansion for $K_\varepsilon(\mathbf{x},\mathbf{y};z)$:

$$K_\varepsilon(\mathbf{x},\mathbf{y};z) = G_0(\mathbf{x},\mathbf{y};z) + \sum_{j=1}^{\infty} \varepsilon^j \, K_{\varepsilon,j}(\mathbf{x},\mathbf{y};z) \tag{5.27}$$

where

$$\begin{aligned} K_{\varepsilon,j}(\mathbf{x},\mathbf{y};z) = \int \cdots \int d\mathbf{u}_1 d\mathbf{u}_2 ... d\mathbf{u}_j e^{i\varepsilon\Phi(\mathbf{x},\mathbf{u}_1,\mathbf{u}_2...\mathbf{u}_j,\mathbf{y})} \\ G_0(\mathbf{x},\mathbf{u}_1;z) M_\varepsilon(\mathbf{u}_1,\mathbf{u}_2;z) ... M_\varepsilon(\mathbf{u}_j,\mathbf{y};z) \end{aligned} \tag{5.28}$$

and

$$\Phi(\mathbf{x},\mathbf{u}_1,\mathbf{u}_2...\mathbf{u}_j,\mathbf{y}) = \phi_{\mathbf{a}}(\mathbf{y},\mathbf{u}_j) + \phi_{\mathbf{a}}(\mathbf{u}_j,\mathbf{u}_{j-1}) + ... + \phi_{\mathbf{a}}(\mathbf{u}_1,\mathbf{x}) + \phi_{\mathbf{a}}(\mathbf{x},\mathbf{y}). \tag{5.29}$$

Notice that Φ is gauge invariant and is the flux through the polygonal contour $\mathbf{y}\mathbf{u}_j\mathbf{u}_{j-1}...\mathbf{x}\mathbf{y}$. In terms of integral kernels, (5.26) rewrites as:

$$G_{\varepsilon,\mathbf{a}}(\mathbf{x},\mathbf{y};z) = e^{i\varepsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}\{G_0(\mathbf{x},\mathbf{y};z) + \sum_{j=1}^{\infty} \varepsilon^j K_{\varepsilon,j}(\mathbf{x},\mathbf{y};z)\}. \tag{5.30}$$

The formulae (5.28), (5.30) are the main result of this section.

Starting from (5.30), as in the analytic perturbations case , on can compute all physical quantities as convergent series in ε but with coefficients which depend themselvs upon ε. For example, if $\sigma_0 = \{\lambda_0\}$ where λ_0 is non-degenerate, then for sufficiently small ε the perturbed eigenvalue, $\lambda(\varepsilon)$, has an expansion:

$$\lambda(\varepsilon) = \sum_{j=0}^{\infty} \varepsilon^j \lambda_{\varepsilon,j}, \quad | \lambda_{\varepsilon,j} | \leq k^j \ \text{ for some } \ k < \infty. \tag{5.31}$$

The expressions for $\lambda_{\varepsilon,j}$ can be obtained from:

$$\lambda(\varepsilon) = Tr(H_{\varepsilon,\mathbf{a}} P_{\varepsilon,\mathbf{a}}) = Tr \frac{i}{2\pi} \oint_\Gamma z (H_{\varepsilon,\mathbf{a}} - z)^{-1} dz$$

where Γ is a contour enclosing λ_0. Notice that ($\psi_0(\mathbf{x})$ is the eigenfunction of H_0 corresponding to λ_0)

$$\lambda_{\varepsilon,0} = \frac{i}{2\pi} \int_{\mathbf{R}^3} d\mathbf{x} \oint_\Gamma z \frac{| \psi_0(\mathbf{x}) |^2}{\lambda_0 - z} dz = \lambda_0. \tag{5.32}$$

For $j \geq 1$, due to the fact that $K_{j,\varepsilon}(\mathbf{x},\mathbf{x})$ is finite one can write:

$$\lambda_{\varepsilon,j} = \frac{i}{2\pi}\int_{\mathbf{R}^3} d\mathbf{x} \oint_\Gamma K_{\varepsilon,j}(\mathbf{x},\mathbf{x};z)dz. \tag{5.33}$$

Further details and applications of Theorem 5.3 will be given elsewhere.

The rest of this section is devoted to the proofs of Lemmae 5.1.-5.2 and Theorem 5.3.

Proof of Lemma 5.1. By the usual computation

$$e^{-i\varepsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})}(\mathbf{P}_{\mathbf{x}} - \varepsilon\mathbf{a}(\mathbf{x}))e^{i\varepsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})} = (\mathbf{P}_{\mathbf{x}} - \varepsilon(\mathbf{a}(\mathbf{x}) - \nabla\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})) \tag{5.34}$$

To compute $\nabla_{\mathbf{x}}\phi_{\mathbf{a}}$ one uses (5.10) and the vector analysis formula [25]

$$\begin{aligned}\nabla(\mathbf{A}(\mathbf{x})\cdot\mathbf{B}(\mathbf{x})) =& \mathbf{B}(\mathbf{x}) \wedge (\nabla \wedge \mathbf{A}(\mathbf{x})) + \mathbf{A}(\mathbf{x}) \wedge (\nabla \wedge \mathbf{B}(\mathbf{x})) \\ &+ (\mathbf{B}(\mathbf{x})\cdot\nabla)\mathbf{A}(\mathbf{x}) + (\mathbf{B}(\mathbf{x})\cdot\nabla)\mathbf{A}(\mathbf{x})\end{aligned} \tag{5.35}$$

with

$$\mathbf{A}(\mathbf{x}) = \int_0^1 \mathbf{a}(\mathbf{c} + t(\mathbf{x}-\mathbf{c}))dt$$

$$\mathbf{B}(\mathbf{x}) = (\mathbf{x}-\mathbf{c})$$

One obtains four terms; the first one gives $-\mathbf{a}_{\mathbf{c}}(\mathbf{x})$, the second vanishes and the fourth gives $\int_0^1 \mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))dt$. Observing that

$$t\frac{d}{dt}\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c})) = ((\mathbf{x}-\mathbf{c})\cdot\nabla_{\mathbf{x}})\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))$$

the third term gives $\int_0^1 t\frac{d}{dt}\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))dt$ and then, after integration by parts $\mathbf{a}(\mathbf{x}) - \int_0^1 \mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))dt$. Summing up all the terms one obtains (5.34).

Proof of Lemma 5.2. The only thing to be proved is (5.18) since (5.19)-(5.22) can be read directly from (5.10) and (5.1). Now (5.18) follows, either directly by direct computation from (5.10) and (5.16) or from Stokes's theorem by observing that

$$\int_{\mathbf{c}}^{\mathbf{x}} \mathbf{a}_{\mathbf{c}}(\mathbf{u})\cdot d\mathbf{u} = \int_{\mathbf{c}}^{\mathbf{y}} \mathbf{a}_{\mathbf{c}}(\mathbf{u})\cdot d\mathbf{u} = 0$$

Proof of Theorem 5.3. We have to estimate $M_\varepsilon(\mathbf{x},\mathbf{y};z)$. The key fact is that (see (5.19) and (5.20)) $\mathbf{a}_{\mathbf{y}}(\mathbf{x})$ and $\nabla_{\mathbf{x}}\cdot\mathbf{a}_{\mathbf{y}}(\mathbf{x})$ diverge only when $|\mathbf{x}-\mathbf{y}| \to \infty$ and this divergence is canceled by the decay of $G_0(\mathbf{x},\mathbf{y};z)$ and $\nabla_{\mathbf{x}}\cdot G_0(\mathbf{x},\mathbf{y};z)$ as given by the proposition below which is the pointwise analog of Proposition 4.1.

Proposition 5.5. *i. For all $z \in \rho)H_0)$, $(H_0 - z)^{-1}$ is a Carleman operator; in particular it has an integral kernel $G_0(\mathbf{x}, \mathbf{y}; z)$.*

ii. Let $K \subset \rho(H_0)$ be compact. Then there exist $C < \infty$, $\gamma > 0$ such that uniformly in $z \in K$:

$$\mid G_0(\mathbf{x}, \mathbf{y}; z) \mid \leq \frac{C}{\mid \mathbf{x} - \mathbf{y} \mid} e^{-\gamma|\mathbf{x}-\mathbf{y}|} \tag{5.36}$$

$$\mid \nabla_{\mathbf{x}} G_0(\mathbf{x}, \mathbf{y}; z) \mid \leq \frac{C}{\mid \mathbf{x} - \mathbf{y} \mid^2} e^{-\gamma|\mathbf{x}-\mathbf{y}|}. \tag{5.37}$$

From

$$\sup_{r>0} r^m e^{-\nu r} = M(m, \nu) < \infty, \quad m \geq 0, \nu > 0 \tag{5.38}$$

(5.19), (5.20),(5.36), (5.37) and (5.24) one obtains that uniformly for $\varepsilon \in [0, \varepsilon_0]$, $z \in K$

$$\mid M_\varepsilon(\mathbf{x}, \mathbf{y}; z) \mid \leq \text{const} \frac{1}{\mid \mathbf{x} - \mathbf{y} \mid} e^{-\gamma|\mathbf{x}-\mathbf{y}|/2} \tag{5.39}$$

and then by Young inequality

$$\parallel T_\varepsilon f \parallel \leq \text{const}\left(\int_{\mathbb{R}^3} \frac{e^{-\gamma|\mathbf{x}|/2}}{\mid \mathbf{x} \mid} d\mathbf{x}\right) \parallel f \parallel \tag{5.40}$$

and the proof is finished.

Proof of Proposition 5.5. The proposition follows from the results in [24], so we shall only outline the proof. The fact that $(H_0 - z)^{-1}$ is a Carleman operator follows from the fact that V_0 is $-\Delta$ bounded and then $(H_0 - z)^{-1} \in \mathcal{B}(L^2(\mathbb{R}^3), L^\infty(\mathbb{R}^3))$ (see Corollary A.1.2 in [Si]). The inequality (5.36) follows from Theorem B 7.2. in [24] (actually Theorem B 7.2. in [24] is stated for a fixed z but the proof covers the given case).

For $z = -a$, $a > 0$ and sufficiently large

$$\begin{aligned} G_0(\mathbf{x}, \mathbf{y}; -a) =& \frac{1}{4\pi \mid \mathbf{x} - \mathbf{y} \mid} e^{-a^{1/2}|\mathbf{x}-\mathbf{y}|} \\ &- \int_{\mathbb{R}^3} \frac{1}{4\pi \mid \mathbf{x} - \mathbf{u} \mid} e^{-a^{1/2}|\mathbf{x}-\mathbf{u}|} V(u) G_0(\mathbf{u}, \mathbf{y}; -a) d\mathbf{u} \end{aligned} \tag{5.41}$$

and then

$$\begin{aligned} \nabla_{\mathbf{x}} G_0(\mathbf{x}, \mathbf{y}; -a) =& \nabla_{\mathbf{x}}\left(\frac{1}{4\pi \mid \mathbf{x} - \mathbf{y} \mid} e^{-a^{1/2}|\mathbf{x}-\mathbf{y}|}\right) \\ &- \int_{\mathbb{R}^3} \nabla_{\mathbf{x}}\left(\frac{1}{4\pi \mid \mathbf{x} - \mathbf{u} \mid} e^{-a^{1/2}|\mathbf{x}-\mathbf{u}|}\right) V(u) G_0(\mathbf{u}, \mathbf{y}; -a) d\mathbf{u} \end{aligned} \tag{5.42}$$

which gives (5.37) for $z=-a$. Finally (5.37) is "carried" from $-a$ to $z \in K$ via the resolvent equation

$$\nabla_{\mathbf{x}} G_0(\mathbf{x},\mathbf{y};z) = \nabla_{\mathbf{x}} G_0(\mathbf{x},\mathbf{y};-a) \tag{5.43}$$

$$+ (z+a) \int_{\mathbb{R}^3} \nabla_{\mathbf{x}} G_0(\mathbf{x},\mathbf{u};-a) G_0(\mathbf{u},\mathbf{y};z) d\mathbf{u}. \tag{5.44}$$

6 Appendix

Although the Proposition 3 in [17] provides the nedeed construction we shall give below a more aestetical form of it.

Let P be a bounded idempotent. Then (see e.g [14] Ch. III. 4) $\mathcal{H} = \mathcal{M} + \mathcal{N}$ such that if $f = m + n, \quad m \in \mathcal{M}, \quad n \in \mathcal{N}$ then $Pf = m$ i.e. P is a projection. By direct computation

$$(P-z)(P+z-1) = z(z-1)$$

which in particular implies that $\sigma(P) = \{0,1\}$. Moreover it gives the following formula for the resolvent of P

$$(P-z)^{-1} = \frac{(P+z-1)}{z(z-1)}$$

Let now T be bounded and "almost" idempotent(but not necessarily self-adjoint). The problem is whether T is close to an idempotent.

Proposition 6.1. *Let T be a bounded operator, $\Delta = T^2 - T$. Then for $\| \Delta \| \equiv \delta \leq 1/4$, $\{| z-1 | = 1/2\} \subset \rho(T)$ and*

$$\| T - \frac{1}{2\pi i} \oint_{|z-1|=1/2} (T-z)^{-1} dz \| \leq \frac{4\delta(2 \| T \| + 1)}{1-4\delta} \tag{6.1}$$

Proof

By direct computation,

$$(T-z)(T+z-1) = z(z-1)[1 + \Delta/z(z-1)]$$

whereof for $\| \Delta \| / | z(z-1) | < 1$

$$(T-z)^{-1} = \frac{T+z-1}{z(1-z)}[1 + \frac{\Delta}{z(1-z)}]^{-1} =$$

$$(\frac{T}{z(1-z)}-\frac{1}{z})[1-\frac{\Delta}{z(1-z)}(1+\frac{\Delta}{z(1-z)})^{-1}] \tag{6.2}$$

whereof for $\delta < 1/4$

$$P-T=-\Delta\frac{1}{2\pi i}\oint_{|z-1|=1/2}\frac{1}{z(1-z)}(\frac{T}{z(1-z)}+1)(1+\frac{\Delta}{z(1-z)})^{-1}dz \tag{6.3}$$

which gives (6.1)

Remarks

6.1. If T is self-adjoint then P is also self-adjoint.

6.2. By performing the integral in (6.2) using the residue theorem one can show that

$$\begin{aligned} P-T &= (T-1/2)[(1+4\Delta)^{-1/2}-1] \\ &= 4\Delta(T-1/2)(1+4\Delta)^{-1/2})[(1+4\Delta)^{-1/2}+1]^{-1/2} \end{aligned} \tag{6.4}$$

which gives the estimation

$$\| P-T \| \leq \frac{2\delta(2 \| T \| +1)}{1-4\delta} \tag{6.5}$$

which is better than (6.1) by a factor of 2.

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