

Gell-Mann and Low formula for degenerate unperturbed states

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Abstract

The Gell-Mann and Low switching allows to transform eigenstates of an unperturbed Hamiltonian H_0 into eigenstates of the modified Hamiltonian $H_0 + V$. This switching can be performed when the initial eigenstate is not degenerate, under some gap conditions with the remainder of the spectrum. We show here how to extend this approach to the case when the ground state of the unperturbed Hamiltonian is degenerate. More precisely, we prove that the switching procedure can still be performed when the initial states are eigenstates of the finite rank self-adjoint operator $\mathcal{P}_0 V \mathcal{P}_0$, where \mathcal{P}_0 is the projection onto a degenerate eigenspace of H_0 .

1 Introduction

Adiabatic switching is a crucial ingredient of many-body theory. It provides a way to express the eigenstates of a Hamiltonian $H_0 + V$ in terms of the eigenstates of H_0 . Its basic idea is to switch very slowly the interaction V , *i. e.* to transform $H_0 + V$ into a time-dependent Hamiltonian of the typical form $H_0 + e^{-\varepsilon|t|}V$, where the small parameter $\varepsilon > 0$ eventually vanishes. It may be expected that an eigenstate of $H_0 + V$ is obtained by taking the limit of an eigenstate of H_0 , evolved according to the time-dependent Hamiltonian $H_0 + e^{-\varepsilon|t|}V$ when ε tends to zero. It turns out that this naive expectation is not justified since the time-dependent eigenstate has no limit when $\varepsilon \rightarrow 0$ because of some non-convergent phase factor. When the initial state belongs to a non degenerate eigenspace, Gell-Mann and Low solved the problem by dividing out the oscillations by a suitable factor [7]. The ratio becomes, in the limit $\varepsilon \rightarrow 0$, the Gell-Mann and Low wavefunction. Mathematically, the convergence of this procedure has been proved in 1989 by Nenciu and Rasche [16], elaborating on the adiabatic theorem [3, 12, 6].

On the other side, the physics community realized about fifty years ago [2] that a generalization of the Gell-Mann and Low formula is needed in the case of a degenerate eigenvalue of H_0 . This happens in many practical situations, for instance when the system contains unfilled shells. This problem has been discussed in several fields, including nuclear physics, solid state physics, quantum chemistry and atomic physics, see the references in [4, 5]. In most cases, it

is assumed that there is *some* eigenstate in the degenerate eigenspace \mathcal{E}_0 of H_0 for which the Gell-Mann and Low formula holds. In general however, the Gell-Mann and Low formula is not applicable when this state is chosen at random in the degenerate subspace, as illustrated in the simple model analytically studied in [4].

We show in this paper that the switching can be performed provided the initial eigenstates are also eigenstates of $\mathcal{P}_0 V \mathcal{P}_0|_{\mathcal{E}_0}$, the perturbation restricted to act on the degenerate eigenspace. If the latter operator has itself degenerate eigenvalues, a further analysis is required, as discussed in Section 3.4. The result is based on the recent progress in the mathematical analysis of adiabatic problems, see [15, 1, 8, 21, 9, 14, 17, 22, 10] and references therein.

The physical consequences of our result are discussed in the companion physics paper [5], where we also comment on the formal relation with different types of Green's functions.

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2 Statement of the results

2.1 Spectral structure of the problem

Consider a Hilbert space \mathcal{H} , a self-adjoint operator H_0 , with dense domain $D(H_0) \subset \mathcal{H}$, and a symmetric perturbation V , H_0 -bounded with relative bound $a < 1$. Then, according to the Kato-Rellich theorem (Theorem X.12 in [18]), $H_0 + \lambda V$ is self-adjoint on $D(H_0)$ for any $0 \leq \lambda \leq 1$. We denote¹

$$\tilde{H}(\lambda) = H_0 + \lambda V,$$

with $\lambda \in [0, 1]$. In all this study, we will assume that the spectrum has the following structure.

Assumption 1 (Structure of the spectrum). *The spectrum of $\tilde{H}(\lambda) = H_0 + \lambda V$, $\lambda \in [0, 1]$, consists of two disconnected pieces*

$$\sigma(\tilde{H}(\lambda)) = \sigma_N(\lambda) \cup \left(\sigma(\tilde{H}(\lambda)) \setminus \sigma_N(\lambda) \right)$$

where $\sigma_N(\lambda)$ is a finite subset of the discrete spectrum:

$$\sigma_N(\lambda) = \left\{ \tilde{E}_j(\lambda), j = 1, \dots, N \right\} \subset \sigma_{\text{disc}}(\tilde{H}(\lambda)),$$

and the initial state is degenerate: $\tilde{E}_j(0) = \tilde{E}_k(0)$ for all $1 \leq j, k \leq N$.

In order to apply results and techniques from adiabatic theory [3, 12, 15, 1], we make the following standard assumption on the existence of a gap in the spectrum.

Assumption 2 (Gap condition). *There is a gap between the two parts of the spectrum, in the sense that:*

$$\Delta(\lambda) = \min_{j=1, \dots, N} \left(\min \left\{ \left| \tilde{E}_j(\lambda) - E \right|, E \in \sigma(H(\lambda)) \setminus \{ \tilde{E}_1(\lambda), \dots, \tilde{E}_N(\lambda) \} \right\} \right),$$

¹ For reasons that will become clear once a time variable is introduced, we will always denote with a $\tilde{}$ functions of the variable $\lambda \in [0, 1]$. Untilded functions will have time as an argument.

is bounded from below by a positive constant:

$$\inf_{\lambda \in [0,1]} \Delta(\lambda) = \Delta^* > 0.$$

The projectors associated with the N eigenvalues $\tilde{E}_j(\lambda)$ (counted with their multiplicities) are denoted by $\tilde{P}_j(\lambda)$, for $1 \leq j \leq M$ with $M \leq N$. The projector onto the subspace orthogonal to the eigenspace spanned by the N eigenvectors is $\tilde{P}_{N+1}(\lambda) = \mathbb{I} - \sum_{j=1}^M \tilde{P}_j(\lambda)$. We denote in the sequel

$$\mathcal{P}_0 = \sum_{j=1}^M \tilde{P}_j(0)$$

the projector onto the eigenspace $\mathcal{E}_0 = \text{Ran}(\mathcal{P}_0)$ spanned by the N degenerate eigenstates of H_0 . For simplicity, we assume that the perturbation V is sufficient to split the degeneracy (so that $M = N$), in the sense that the following assumption holds true.

Assumption 3 (Degeneracy splitting). *The finite rank self-adjoint operator $\mathcal{P}_0 V \mathcal{P}_0 : \mathcal{E}_0 \rightarrow \mathcal{E}_0$ has non-degenerate eigenvalues, and there is a gap between the N first levels in the interval $(0, 1]$: for any $\lambda^* > 0$, there exists α (depending on λ^*) such that*

$$\inf_{\lambda^* \leq \lambda \leq 1} \min_{k \neq l} \left| \tilde{E}_k(\lambda) - \tilde{E}_l(\lambda) \right| \geq \alpha > 0. \quad (2.1)$$

This implies that the projectors $\tilde{P}_j(\lambda)$ are rank-1 projectors for any $\lambda > 0$ (since it can be proved that the perturbation V is enough to split the eigensubspaces, and the gap condition on $(0, 1]$ ensures that no crossing can happen; see Section 3.1 for more details).

Remark 4. *Assumption 3 may be relaxed in several ways. First, the operator $\mathcal{P}_0 V \mathcal{P}_0$ can have degenerate eigenvalues, but then higher order terms should be considered in the perturbative expansion of the eigenvalues. The gap assumption can be relaxed as well, and some crossings could be allowed. Besides, the general case of $M < N$ projectors of ranks greater or equal to 1 can be treated similarly upon modifying the condition $\left\| \tilde{P}_j(1) - \tilde{P}_j(0) \right\| < 1$ required in Theorem 7 below. All these extensions are discussed in Section 3.4.*

2.2 Switching procedure

Consider, for $\tau \in (-\infty, 0]$,

$$H(\tau) = \tilde{H}(f(\tau)) = H_0 + f(\tau)V.$$

where the switching function f has values in $[0, 1]$ (in order for the operator $H(\tau)$ to be well-defined as a self-adjoint operator on $D(H_0)$). We denote by $P_j(\tau)$ the eigenprojectors and eigenvalues corresponding to the first N eigenvalues $E_j(\tau)$ of $H(\tau)$; also, $P_{N+1}(\tau) = \mathbb{I} - \sum_{k=1}^N P_k(\tau)$. Of course,

$$P_j(\tau) = \tilde{P}_j(f(\tau)), \quad E_j(\tau) = \tilde{E}_j(f(\tau)).$$

For the subsequent analysis, we assume that

Assumption 5. *The switching function $f : (-\infty, 0] \rightarrow [0, 1]$ is a C^2 function such that*

(i) *f is non-decreasing;*

(ii) *$f(0) = 1$ and $\lim_{\tau \rightarrow -\infty} f(\tau) = 0$;*

(iii) *$f, f'' \in L^1((-\infty, 0])$.*

The most common choice in practice is $f(\tau) = e^\tau$. Notice however that any C^2 non-decreasing compactly supported function satisfies the above assumptions. In the latter case, the monotonicity of f implies that the support of f is a compact interval $[R_f, 0]$, and $f(t) > 0$ for $t \in (R_f, 0]$. The assumption $f \in C^2$ ensures that the adiabatic evolution (see (3.13) below) is well-defined.

As a consequence of these assumptions, $f' \geq 0$ and $f' \in L^1((-\infty, 0]) \cap L^\infty((-\infty, 0])$, hence $f' \in L^2((-\infty, 0])$. Indeed, the boundedness of f' is a consequence of the fundamental theorem of calculus and the fact that $f'' \in L^1((-\infty, 0])$. Besides, $\int_t^0 f' = f(0) - f(t) \leq 1$, and $f' \geq 0$, hence $f' \in L^1((-\infty, 0])$.

Remark 6. *It can be shown that eigenprojectors and eigenvectors are analytic with respect to $\lambda = f(s)$ (see Section 3.1). When the switching function f is analytic, the eigenvalues $E_j(\tau)$ (and the associated eigenvectors and eigenprojectors) are also analytic with respect to τ .*

We denote by $U_\varepsilon(s, s_0)$ the unitary evolution generated by $H(\varepsilon s)$, i. e. the unique solution (which is well-defined by Theorem X.70 in [18]) of the problem:

$$i \frac{dU_\varepsilon(s, s_0)}{ds} = H(\varepsilon s) U_\varepsilon(s, s_0), \quad U_\varepsilon(s_0, s_0) = \mathbb{I}.$$

In order to remove divergent phase factors (see the proof in Section 3.3.1), it is convenient to consider evolution operators in the interaction picture:

$$U_{\varepsilon, \text{int}}(s, s_0) = e^{isH_0} U_\varepsilon(s, s_0) e^{-is_0 H_0}.$$

It is actually more convenient to rescale the time and to consider a macroscopic time $t = \varepsilon s$. The unitary evolution $U^\varepsilon(t, t_0)$ in terms of the macroscopic time is the solution of

$$i\varepsilon \frac{dU^\varepsilon(t, t_0)}{dt} = H(t) U^\varepsilon(t, t_0), \quad U^\varepsilon(t_0, t_0) = \mathbb{I},$$

and, in the interaction picture,

$$U_{\text{int}}^\varepsilon(t, t_0) = e^{itH_0/\varepsilon} U^\varepsilon(t, t_0) e^{-it_0 H_0/\varepsilon}.$$

Standard results show that $U_{\text{int}}^\varepsilon(t, -\infty)\psi = \lim_{t_0 \rightarrow -\infty} U_{\text{int}}^\varepsilon(t, t_0)\psi$ exists for $\psi \in D(H_0)$ (for instance, by using a standard Cook's type argument and rewriting this operator as the integral of its derivative with respect to t_0).

2.3 Main results

We are now in position to state our main results.

Theorem 7. *Suppose that the gap conditions on H_0 and V (Assumptions 1 and 2) are satisfied, and that the perturbation term V lifts the degeneracy (Assumption 3). Consider a switching function verifying Assumption 5. Let (ψ_1, \dots, ψ_N) be an orthonormal basis of \mathcal{E}_0 which diagonalizes the bounded operator $\mathcal{P}_0 V \mathcal{P}_0|_{\mathcal{E}_0}$. Then, if*

$$\|P_j(-\infty) - P_j(0)\| < 1, \quad (2.2)$$

the limit

$$\Psi_j = \lim_{\varepsilon \rightarrow 0} \frac{U_{\text{int}}^\varepsilon(0, -\infty)\psi_j}{\langle \psi_j | U_{\text{int}}^\varepsilon(0, -\infty)\psi_j \rangle} \quad (2.3)$$

exists and is an eigenstate of $H_0 + V$ corresponding to $E_j(0) = \tilde{E}_j(1)$.

Notice that, for a generic state $\psi \in \text{Ran } \mathcal{P}_0$ which is not an eigenvector of $\mathcal{P}_0 V \mathcal{P}_0|_{\mathcal{E}_0}$ the above limit generically does not exist, as showed in [4] by using a simple toy model. It is therefore crucial to select the appropriate initial states, so that the Gell-Mann & Low limit (2.3) does exist.

As an intermediate step, the eigenprojector $P_j(0)$ and a corresponding eigenfunction Ψ_j can be recovered by Kato's geometric evolution [12].

Definition 8. *The Kato evolution operator $A(s, s_0)$, for $s, s_0 \in \mathbb{R}$ is the unique solution of the problem*

$$\frac{dA(s, s_0)}{ds} = K(s) A(s, s_0), \quad A(s_0, s_0) = \mathbb{I}, \quad (2.4)$$

with

$$K(s) = - \sum_{j=1}^{N+1} P_j(s) \frac{dP_j}{ds}(s).$$

By our assumptions, the operator $K(s)$ is uniformly bounded (see the comment after Definition 11). The Kato evolution operator is a unitary operator which intertwines the spectral subspaces of $H(s)$ and $H(s_0)$, in the sense that

$$A(s, s_0)P_j(s_0) = P_j(s)A(s, s_0).$$

Equipped with this notation, we have the following result, where no condition analogous to (2.2) is assumed.

Proposition 9. *Let Assumptions 1, 2, 3 and 5 be satisfied. Let (ψ_1, \dots, ψ_N) be an orthonormal basis of \mathcal{E}_0 which diagonalizes the operator $\mathcal{P}_0 V \mathcal{P}_0|_{\mathcal{E}_0}$. Then*

$$\Psi_j := A(0, -\infty)\psi_j$$

is an eigenvector of $H_0 + V$ corresponding to the eigenvalue $E_j(0)$.

It is actually much simpler to consider the geometric evolution operator A rather than the evolution operator $U_{\text{int}}^\varepsilon$ since less conditions are required. Indeed, there is no denominator which needs to be considered in order to remove a divergent phase. However, the many-body theory used in physics is defined in terms of $U_{\text{int}}^\varepsilon$ and not in terms of A .

We sketch shortly the structure of the proof, which is done in four steps:

- (i) first, we use the Kato geometric evolution backward in time, in order to identify, though in a non explicit manner, the initial subspaces of \mathcal{P}_0 whose vectors can be considered as convenient initial states;
- (ii) In a second step (Section 3.2), we give an explicit description of these initial subspaces, in terms of the eigenvectors of $\mathcal{P}_0 V \mathcal{P}_0|_{\mathcal{E}_0}$. At this stage, we are already in position to prove Proposition 9;
- (iii) Then, we show how the limit of the full evolution $U_{\text{int}}^\varepsilon$ can be related to the geometric evolution as $\varepsilon \rightarrow 0$ (Section 3.3). A first step is to introduce an intermediate concept, the adiabatic evolution, which takes some dynamics into account (arising from the Hamiltonian operator). The adiabatic evolution is also an intertwiner. Since intertwiners differ only by a phase (in sense to be made precise), and, provided this phase can be removed, the adiabatic evolution can be reduced to the geometric one (see Section 3.3.2);
- (iv) the last point is to show that the limit as $\varepsilon \rightarrow 0$ of the full evolution is the adiabatic evolution (see Section 3.3.1).

Steps (iii) and (iv) are straightforward extensions of previous results in adiabatic theory, and we heavily relied on the paper by Nenciu and Rasche [16] for Section 3.3.1 and the book by Teufel [22] for Section 3.3.2.

3 Proof of the results

3.1 Geometric evolution and definition of the initial states

In view of the local gap assumption, the projectors and eigenvalues of $\tilde{H}(\lambda)$ are real analytic functions of $\lambda \in (0, 1]$. Besides, Theorem II.6.1 in [13] shows that the eigenvalues \tilde{E}_j and projectors \tilde{P}_j can be analytically continued in the limit $\lambda \rightarrow 0$. The Kato construction of unitary operators A intertwining projectors can then be performed, see for instance Theorem XII.12 in [19] or Sections II.4 and II.6.2 in [13]. Consider the operator

$$\tilde{K}(\lambda) = - \sum_{j=1}^{N+1} \tilde{P}_j(\lambda) \frac{d\tilde{P}_j}{d\lambda}(\lambda),$$

first proposed in [12], and the unique solution of

$$\frac{d\tilde{A}(\lambda, \lambda_0)}{d\lambda} = \tilde{K}(\lambda) \tilde{A}(\lambda, \lambda_0), \quad \tilde{A}(\lambda_0, \lambda_0) = \mathbb{I}. \quad (3.1)$$

Since $\tilde{K}(\lambda)$ is uniformly bounded, the operator $\tilde{A}(\lambda, \lambda_0)$ is well-defined and strongly continuous (see Theorem X.69 in [18]). Besides, $\tilde{A}(\lambda, \lambda_0)$ is unitary, and intertwines the spectral subspaces:

$$\tilde{P}_j(\lambda) = \tilde{A}(\lambda, \lambda_0) \tilde{P}_j(\lambda_0) \tilde{A}(\lambda, \lambda_0)^*.$$

It is also easily shown that $\tilde{A}(\lambda_2, \lambda_1)\tilde{A}(\lambda_1, \lambda_0) = \tilde{A}(\lambda_2, \lambda_0)$, for instance by computing the derivative of both expressions with respect to λ_2 and using the uniqueness of the solution of (3.1).

We define the *initial subspaces* by evolving backwards eigenstates of the Hamiltonian $\tilde{H}(\lambda)$ for which the perturbation has split the degeneracy: the corresponding eigenprojector is defined as

$$P_j^{\text{init}} := \tilde{A}(0, \lambda)\tilde{P}_j(\lambda), \quad (3.2)$$

the definition being independent of $\lambda > 0$.

Eigenstates of $\tilde{H}(1) = H_0 + V$ are then obtained by evolving initial states belonging to the range of P_j^{init} according to the Kato evolution operator. Indeed, $\tilde{A}(1, 0)P_j^{\text{init}} = \tilde{A}(1, 0)\tilde{A}(0, \lambda)\tilde{P}_j(\lambda) = \tilde{A}(1, \lambda)\tilde{P}_j(\lambda)$. Thanks to the intertwining property of A , it holds

$$\tilde{P}_j(1) = \tilde{A}(1, 0)P_j^{\text{init}}. \quad (3.3)$$

3.2 Characterization of the initial states

The above paragraph shows that the evolution can be performed for states belonging to $\text{Ran}(P_j^{\text{init}})$. We now *characterize* these states by an explicit condition.

General expressions of the eigenvalues and eigenvectors. Since the eigenvalues and eigenprojectors of $\tilde{H}(\lambda)$ are analytic in $\lambda \in [0, 1]$, the following expansions are valid for $1 \leq j \leq N$:

$$\tilde{E}_j(\lambda) = \sum_{n=0}^{+\infty} \lambda^n E_{j,n}, \quad (3.4)$$

and

$$\tilde{P}_j(\lambda) = \sum_{n=0}^{+\infty} \lambda^n P_{j,n}.$$

Of course, $E_{j,0} = E_0 = \tilde{E}_j(0)$, the common value of the energy in the degenerate ground-state. Notice also that the operators $P_{j,n}$ are not necessarily orthogonal projectors.

To define $\tilde{P}_j(\lambda)$, it is more convenient to consider an eigenvector $\phi_j(\lambda)$ associated with $\tilde{E}_j(\lambda)$, i. e. a non-zero element of \mathcal{H} satisfying

$$\tilde{H}(\lambda)\phi_j(\lambda) = \tilde{E}_j(\lambda)\phi_j(\lambda). \quad (3.5)$$

Such an eigenvector can be chosen to be analytic, by the same results which allow to conclude to the analyticity of the eigenprojectors. We therefore write

$$\phi_j(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \varphi_{j,n}. \quad (3.6)$$

Once such an eigenvector is known, the analytic eigenprojector can be constructed as

$$\tilde{P}_j(\lambda) = \left| \frac{\phi_j(\lambda)}{\|\phi_j(\lambda)\|} \right\rangle \left\langle \frac{\phi_j(\lambda)}{\|\phi_j(\lambda)\|} \right|.$$

The aim of this section is to provide an explicit expression of the leading terms of the above expansions, in order to have a more explicit definition of P_j^{init} . To this end, we first construct a basis of \mathcal{E}_0 , which will turn out to be particularly useful to characterize the terms in the expansions (3.4) and (3.6).

Diagonalization of $\mathcal{P}_0 V \mathcal{P}_0$. Since $\mathcal{P}_0 V \mathcal{P}_0$ and \mathcal{P}_0 commute, it is possible to construct an orthonormal basis $(\varphi_{1,0}, \dots, \varphi_{N,0})$ of \mathcal{E}_0 such that

$$\mathcal{P}_0 V \mathcal{P}_0 \varphi_{j,0} = \alpha_j \varphi_{j,0} \quad (3.7)$$

for some real numbers $\alpha_1, \dots, \alpha_N$, and

$$\forall j \neq k, \quad \langle \varphi_{k,0} | \mathcal{P}_0 V \mathcal{P}_0 | \varphi_{j,0} \rangle = 0. \quad (3.8)$$

Expressions for the terms in the expansions (3.4)-(3.6) at order 1. We identify the terms associated with the same powers of λ in (3.5). An additional normalization condition should be added in order to uniquely define the solution, so we impose

$$\forall \lambda \in [0, 1], \quad \langle \varphi_{j,0} | \phi_j(\lambda) \rangle = 1, \quad (3.9)$$

as is done in [20]. As will be seen below, this condition is simpler to work with than the standard condition $\|\phi_j(\lambda)\| = 1$. The identification of the terms in (3.5) gives, for $1 \leq j \leq N$, the following hierarchy of equations:

$$\begin{aligned} (H_0 - E_0)\varphi_{j,0} &= 0, \\ (H_0 - E_0)\varphi_{j,1} &= (E_{j,1} - V)\varphi_{j,0}, \\ (H_0 - E_0)\varphi_{j,2} &= (E_{j,1} - V)\varphi_{j,1} + E_{j,2}\varphi_{j,0}, \end{aligned}$$

and, for general $n \geq 2$,

$$(H_0 - E_0)\varphi_{j,n+1} = (E_{j,1} - V)\varphi_{j,n} + \sum_{m=0}^{n-1} E_{j,n+1-m}\varphi_{j,m}. \quad (3.10)$$

The equation on the terms of order zero does not give any information on the choice of the initial states $\varphi_{j,0}$. This information can be obtained from the first order condition:

$$(H_0 - E_0)\varphi_{j,1} = (E_{j,1} - V)\varphi_{j,0}. \quad (3.11)$$

A necessary condition for this equation to have a solution is that the right-hand side belongs to \mathcal{E}_0^\perp (since the left-hand side does):

$$\forall 1 \leq j, k \leq N, \quad \langle \varphi_{k,0}, (E_{j,1} - V)\varphi_{j,0} \rangle = 0. \quad (3.12)$$

This requires

$$E_{j,1} = \langle \varphi_{j,0}, V \varphi_{j,0} \rangle,$$

and

$$\forall k \neq j, \quad \langle \varphi_{k,0}, V \varphi_{j,0} \rangle = 0.$$

Therefore, the conditions (3.12) for $k \neq j$ cannot be fulfilled for a general basis. A necessary condition is that the basis $\{\varphi_{k,0}\}_{k=1,\dots,N}$ of \mathcal{E}_0 diagonalizes $\mathcal{P}_0 V \mathcal{P}_0$. Besides, the first-order term in the energy shifts are exactly the eigenvalues of $\mathcal{P}_0 V \mathcal{P}_0$. This condition determines uniquely the basis when $\mathcal{P}_0 V \mathcal{P}_0$ has non-degenerate eigenvalues. If this is not the case, information of the higher order equations in the hierarchy is needed (see Section 3.4).

Remark 10. *Assuming that the bands do not recross after the initial splitting, and if the degenerate state is the ground state of H_0 , then the ground state of $H_0 + V$ is obtained by following the eigenstate associated with the lowest $E_{j,1}$.*

Once the initial basis and the first energy shifts have been defined, the first order term in the variation of the eigenstates can be obtained from (3.11) as the sum of the reduced resolvent applied to the right-hand side, and some solution of the homogeneous equation $(H_0 - E_0)\psi = 0$:

$$\begin{aligned}\varphi_{j,1} &= \sum_{k=1}^N c_{j,k}^1 \varphi_{k,0} + (H_0 - E_0)^{-1} \Big|_{\mathcal{E}_0^\perp} (E_{j,1} - V) \varphi_{j,0} \\ &= \sum_{k \neq j} c_{j,k}^1 \varphi_{k,0} - R_0 V \varphi_{j,0},\end{aligned}$$

where

$$R_0 = (H_0 - E_0)^{-1} \Big|_{\mathcal{E}_0^\perp} = (\mathbb{I} - \mathcal{P}_0) (H_0 - E_0)^{-1} (\mathbb{I} - \mathcal{P}_0)$$

is a bounded operator from \mathcal{E}_0^\perp to $\mathcal{E}_0^\perp \cap D(H_0)$, and $c_{j,j}^1 = 0$ in view of the normalization condition (3.9). The coefficients $c_{k,j}^1$ (for $k \neq j$) are undetermined at this stage. They have to be chosen so that the right hand side of the next equation in the hierarchy is in \mathcal{E}_0^\perp .

Conclusion: characterization of the initial subspaces. The above computations show that $\tilde{P}_j(\lambda) = P_{j,0} + \mathcal{O}(\lambda)$, with $P_{j,0} = |\varphi_{j,0}\rangle\langle\varphi_{j,0}|$. Besides, $\|\tilde{A}(0, \lambda) - \mathbb{I}\| = \mathcal{O}(\lambda)$ in view of the differential equation (3.1) satisfied by \tilde{A} . The initial subspace (3.2) is therefore

$$P_j^{\text{init}} = \tilde{A}(0, \lambda) P_j(\lambda) = \lim_{\lambda \rightarrow 0} \tilde{A}(0, \lambda) [P_{j,0} + \mathcal{O}(\lambda)] = P_{j,0}.$$

Proof of Proposition 9. Let $\psi \in \mathcal{E}_0$ be an eigenvector of $\mathcal{P}_0 V \mathcal{P}_0$. Then, for some j , $\psi \in \text{Ran}(P_{j,0}) = \text{Ran}(P_j^{\text{init}})$. Using (3.3), it follows

$$A(0, -\infty)\psi_j = \tilde{A}(1, 0)\psi_j \in \text{Ran}\left(\tilde{P}_j(1)\right),$$

which proves the claim.

3.3 Adiabatic evolution and limit of the full evolution

Definition 11. *The adiabatic evolution operator $U_A(s, s_0)$ is defined for $(s, s_0) \in \mathbb{R}^2$ as the unique solution of the problem*

$$i \frac{dU_A(s, s_0)}{ds} = H_A(s) U_A(s, s_0), \quad U_A(s_0, s_0) = \mathbb{I}, \quad (3.13)$$

where the adiabatic Hamiltonian is

$$H_A(s) = H(s) + iK(s),$$

with

$$K(s) = - \sum_{j=1}^{N+1} P_j(s) \frac{dP_j}{ds}(s).$$

Notice that $K(s) = f'(s) \tilde{K}(f(s))$ so that

$$\|K(s)\| \leq C f'(s) \quad (3.14)$$

for some constant $C > 0$. Therefore, $K(s)$ is uniformly bounded since f' is bounded by our assumptions on the switching function.

Compared to the geometric evolution (3.1), a Hamiltonian term has been added, which will be at the origin of some dynamical phase factor in the dynamics. The adiabatic dynamics is well-defined in view of the assumptions made on H_0 , V and f (see Theorem X.70 in [18]). A simple computation shows that it intertwines the spectral subspaces:

$$P_j(s) = U_A(s, s_0) P_j(s_0) U_A(s, s_0)^*.$$

Switching to the interaction picture, we define

$$U_{A,\text{int}}(s, s_0) = e^{isH_0} U_A(s, s_0) e^{-is_0H_0}.$$

The factor ε is introduced by slowing down the switching as

$$i \frac{dU_{\varepsilon,A}(s, s_0)}{ds} = H_A(\varepsilon s) U_{\varepsilon,A}(s, s_0), \quad U_{\varepsilon,A}(s_0, s_0) = \mathbb{I}, \quad (3.15)$$

and the corresponding operator in the interaction picture is $e^{isH_0} U_{\varepsilon,A}(s, s_0) e^{-is_0H_0}$. It is convenient to rewrite the evolution (3.15) in the rescaled time variable $t = \varepsilon s$:

$$i\varepsilon \frac{dU_A^\varepsilon(t, t_0)}{dt} = H_A^\varepsilon(t) U_A^\varepsilon(t, t_0), \quad U_A^\varepsilon(t_0, t_0) = \mathbb{I}, \quad (3.16)$$

with $H_A^\varepsilon(t) = H(t) + i\varepsilon K(t)$. The associated operator in the interaction picture is

$$U_{A,\text{int}}^\varepsilon(t, t_0) = e^{itH_0/\varepsilon} U_A^\varepsilon(t, t_0) e^{-it_0H_0/\varepsilon}.$$

Theorem 7 is then a consequence of the following results.

Lemma 12. *Let $\psi_j \in P_j^{\text{init}}$ (defined by (3.2)). Then, under the assumptions of Theorem 7, the vector*

$$\frac{U_{A,\text{int}}^\varepsilon(0, -\infty)\psi_j}{\langle \psi_j | U_{A,\text{int}}^\varepsilon(0, -\infty)\psi_j \rangle} = \frac{U_{A,\text{int}}(0, -\infty)\psi_j}{\langle \psi_j | U_{A,\text{int}}(0, -\infty)\psi_j \rangle} \quad (3.17)$$

is an eigenstate of H_0 .

Lemma 13. *Let $\psi_j \in P_j^{\text{init}}$. Then, under the assumptions of Theorem 7,*

$$\lim_{\varepsilon \rightarrow 0} \left(\frac{U_{\text{int}}^\varepsilon(0, -\infty)\psi_j}{\langle \psi_j | U_{\text{int}}^\varepsilon(0, -\infty)\psi_j \rangle} - \frac{U_{A,\text{int}}^\varepsilon(0, -\infty)\psi_j}{\langle \psi_j | U_{A,\text{int}}^\varepsilon(0, -\infty)\psi_j \rangle} \right) = 0.$$

3.3.1 Proof of Lemma 12

We show first in this section that ψ_j can be transformed into an eigenstate of $H(0) = \tilde{H}(1)$ using the adiabatic evolution defined from (3.13), and then the equality of the ratios (3.17). The proof presented here reproduces the argument of Nenciu and Rasche [16], which was given in the case $N = 1$ with our notation, but can be applied *mutatis mutandis* to the case considered here. We however present the proof for completeness.

Evolution in the case $\varepsilon = 1$. Since both U_A and A are intertwiners, they differ only by a phase which commutes with the spectral projectors. Indeed, define

$$\Phi(s, s_0) = A(s, s_0)^* U_A(s, s_0),$$

so that $U_A(s, s_0) = A(s, s_0) \Phi(s, s_0)$. Then,

$$[\Phi(s, s_0), P_j(s_0)] = 0.$$

as can be seen using the intertwining properties:

$$\begin{aligned} [\Phi(s, s_0), P_j(s_0)] &= A(s, s_0)^* U_A(s, s_0) P_j(s_0) - P_j(s_0) A(s, s_0)^* U_A(s, s_0) \\ &= A(s, s_0)^* P_j(s) U_A(s, s_0) - A(s, s_0)^* P_j(s) U_A(s, s_0) = 0. \end{aligned}$$

The time-evolution of the phase matrix can be simplified due to this commutation property. First,

$$\frac{d\Phi(s, s_0)}{ds} = -iA(s, s_0)^* H(s) U_A(s, s_0),$$

since $K(s)^* = -K(s)$. Besides,

$$\Phi(s, s_0) = \left(\sum_{k=1}^{N+1} P_k(s_0) \right) \Phi(s, s_0) \left(\sum_{k=1}^{N+1} P_k(s_0) \right) = \sum_{k=1}^{N+1} \Phi_k(s, s_0),$$

where $\Phi_k(s, s_0) = P_k(s_0) \Phi(s, s_0) P_k(s_0)$. The time evolution of the projected phase-matrix is a scalar phase since

$$\frac{d}{ds} \Phi_k(s, s_0) = -iE_k(s) \Phi_k(s, s_0),$$

hence

$$\Phi(s, s_0) P_j(s_0) = \exp \left(-i \int_{s_0}^s E_j(r) dr \right) P_j(s_0).$$

The geometric evolution and the adiabatic evolution are therefore related through some global dynamical phase:

$$U_A(s, s_0) P_j(s_0) = A(s, s_0) \Phi(s, s_0) P_j(s_0) = \exp \left(-i \int_{s_0}^s E_j(r) dr \right) A(s, s_0) P_j(s_0).$$

To describe the evolution, we follow closely the approach of [16]. In order for $U_A(s, s_0) P_j(s_0)$ to be defined in the limit $s_0 \rightarrow -\infty$, it is important to work in the interaction picture. Then,

$$\begin{aligned} U_{A,\text{int}}(s, s_0) P_j(-\infty) &= e^{isH_0} A(s, s_0) \Phi(s, s_0) e^{-is_0H_0} P_j(-\infty) \\ &= e^{-is_0E_0} e^{isH_0} A(s, s_0) e^{-isH_0} e^{isH_0} \Phi(s, s_0) P_j(-\infty). \end{aligned}$$

Using

$$\Phi(s, s_0)P_j(s_0) = P_j(s_0)\Phi(s, s_0)P_j(s_0) = \exp\left(-i \int_{s_0}^s E_j(r) dr\right) P_j(s_0),$$

it holds

$$\begin{aligned} & e^{-is_0E_0}e^{isH_0}\Phi(s, s_0)P_j(-\infty) \\ &= e^{-is_0E_0}e^{isH_0}\Phi(s, s_0)P_j(s_0) + e^{-is_0E_0}e^{isH_0}\Phi(s, s_0)(P_j(-\infty) - P_j(s_0)) \\ &= \exp\left(-i \int_{s_0}^s E_j(r) dr - is_0E_0\right) e^{isH_0}P_j(s_0) + e^{-is_0E_0}e^{isH_0}\Phi(s, s_0)(P_j(-\infty) - P_j(s_0)) \\ &= \exp\left(-i \int_{s_0}^s E_j(r) dr - is_0E_0\right) [e^{isH_0}P_j(-\infty) + e^{isH_0}(P_j(s_0) - P_j(-\infty))] \\ &\quad + e^{-is_0E_0}e^{isH_0}\Phi(s, s_0)(P_j(-\infty) - P_j(s_0)) \\ &= e^{-isE_0} \exp\left(-i \int_{s_0}^s E_j(r) - E_0 dr\right) P_j(-\infty) + W(s, s_0)(P_j(s_0) - P_j(-\infty)), \end{aligned}$$

where $\|W\| \leq 2$. Since $\lambda \mapsto E_j(\lambda)$ is C^1 on the compact interval $[0, 1]$, there exists a constant $C > 0$ such that

$$|E_j(r) - E_0| = \left| \tilde{E}_j(f(r)) - \tilde{E}_j(0) \right| \leq Cf(r).$$

Since $f \in L^1((-\infty, 0])$, this shows that the function $r \mapsto E_j(r) - E_0$ is integrable on $(-\infty, 0]$. Besides, $P(s_0) \rightarrow P_j(-\infty)$ when $s_0 \rightarrow -\infty$. The limit $s_0 \rightarrow -\infty$ of $U_{A,\text{int}}(s, s_0)P_j(-\infty)$ is therefore well-defined:

$$U_{A,\text{int}}(s, -\infty)P_j(-\infty) = e^{-isE_0} \exp\left(-i \int_{-\infty}^s E_j(r) - E_0 dr\right) e^{isH_0} A(s, -\infty) e^{-isH_0} P_j(-\infty). \quad (3.18)$$

The above equality reads, for $s = 0$,

$$U_{A,\text{int}}(0, -\infty)P_j(-\infty) = \exp\left(-i \int_{-\infty}^0 E_j(r) - E_0 dr\right) A(0, -\infty)P_j(-\infty).$$

Since $P_j(0)A(0, -\infty) = A(0, -\infty)P_j(-\infty)$, it holds, for $\psi_j \in P_j^{\text{init}} = P_j(-\infty) = \text{Ran}(\varphi_{j,0})$,

$$P_j(0)\psi_j = A(0, -\infty)P_j(-\infty)A(0, -\infty)^*\psi_j = \langle \psi_j | A(0, -\infty)^*\psi_j \rangle A(0, -\infty)\psi_j. \quad (3.19)$$

Finally,

$$\frac{P_j(0)\psi_j}{\|P_j(0)\psi_j\|^2} = \frac{P_j(0)\psi_j}{\langle \psi_j | P_j(0)\psi_j \rangle} = \frac{A(0, -\infty)\psi_j}{\langle \psi_j | A(0, -\infty)\psi_j \rangle} = \frac{U_{A,\text{int}}(0, -\infty)\psi_j}{\langle \psi_j | U_{A,\text{int}}(0, -\infty)\psi_j \rangle},$$

which shows that the adiabatic evolution transforms the initial eigenstate into an eigenstate of $H(1)$ provided $\|P_j(0)\psi_j\| \neq 0$, which is the case when $\|P_j(0) - P_j(-\infty)\| < 1$.

Evolution in the case $\varepsilon > 0$. Let us conclude this section by proving the equality (3.17). Computations similar to the ones performed in the case $\varepsilon = 1$ lead to

$$U_{A,\text{int}}^\varepsilon(0, -\infty)P_j(-\infty) = \exp\left(-\frac{i}{\varepsilon} \int_{-\infty}^0 E_j(\tau) - E_0 d\tau\right) A(0, -\infty)P_j(-\infty).$$

This can be seen for instance by noticing that (3.16) can be rewritten in the form (3.13), upon considering the Hamiltonian H/ε . Therefore, $U_{A,\text{int}}^\varepsilon(0, -\infty)P_j(-\infty)$ is equal, up to the ε -dependence in the phase factor, to $U_{A,\text{int}}(0, -\infty)P_j(-\infty)$. The non convergent phase factor can be eliminated precisely by considering the Gell-Mann and Low ratio (3.17).

3.3.2 Proof of Lemma 13

It is sufficient to prove that

$$\lim_{\varepsilon \rightarrow 0} \|U^\varepsilon(0, -\infty) - U_A^\varepsilon(0, -\infty)\| = 0,$$

which indeed gives the result since

$$\|U_{\text{int}}^\varepsilon(t, t_0) - U_{A,\text{int}}^\varepsilon(t, t_0)\| = \|U^\varepsilon(t, t_0) - U_A^\varepsilon(t, t_0)\|.$$

Notice that, although none of the operators $U^\varepsilon(0, -\infty), U_A^\varepsilon(0, -\infty)$ has a limit when $\varepsilon \rightarrow 0$, the difference goes to 0 in this limit.

The proof is based on the proofs of Theorem 2.2 and Corollary 2.5 in the book by Teufel [22], which are extended to the case of non-compactly supported switching functions and $N > 1$ with our notation. In this section, C and C' denote constants, which may change from line to line, but are always independent of t, ε , etc, and depends only on the relative H_0 -bound of V , on N , on Δ^* and on bounds on the functions \tilde{P}_j and their derivatives on $[0, 1]$.

We denote by $\delta_j(t) \geq 0$ the local gap around $E_j(t)$:

$$\delta_j(t) = \min \left\{ |E_j(t) - E|, E \in \sigma(H(t)) \setminus \{E_j(t)\} \right\}.$$

Notice that $\delta_j(t) > 0$ when $f(t) > 0$, but $\delta_j(t) \rightarrow 0$ when $f(t) \rightarrow 0$ since the initial eigenvalue is N -fold degenerate (see Assumption 3). In fact, the analysis of Section 3.2 shows that there exist $\alpha_1, \alpha_2 > 0$ such that

$$\alpha_1 \leq \left| \frac{\delta_j(t)}{f(t)} \right| \leq \alpha_2 \tag{3.20}$$

when $f(t) > 0$.

Rewriting the difference as an integral. The difference between the two unitary evolution is rewritten as the integral of the derivative, as:

$$\begin{aligned} U^\varepsilon(t, t_0) - U_A^\varepsilon(t, t_0) &= -U^\varepsilon(t, t_0) \int_{t_0}^t \frac{d}{dt'} (U^\varepsilon(t_0, t') U_A^\varepsilon(t', t_0)) dt' \\ &= -\frac{i}{\varepsilon} U^\varepsilon(t, t_0) \int_{t_0}^t U^\varepsilon(t_0, t') [H(t') - H_A(t')] U_A^\varepsilon(t', t_0) dt' \\ &= -U^\varepsilon(t, t_0) \int_{t_0}^t U^\varepsilon(t_0, t') K(t') U_A^\varepsilon(t', t_0) dt'. \end{aligned}$$

The idea is to rewrite $K(t)$ as a commutator, so that $t \mapsto U^\varepsilon(t_0, t)K(t)U_A^\varepsilon(t, t_0)$ is the derivative of a function (up to negligible terms), and an integration by parts gives the required estimates. The proof proposed here is an extension of the proof presented in [22, Chapter 2] in the case when several pieces of the discrete spectrum are considered independently. It would also have been possible to use the twiddle operation introduced in [1], which is, in some sense, the inverse operation of the commutator with the Hamiltonian.

Construction of the function used in the commutator. Consider $-\infty < t \leq 0$ such that $f(t) > 0$ (for compactly supported switching functions, this means that t is in the interior of the support). Define

$$F(t) = -\frac{1}{2} \left(\sum_{j=1}^{N+1} F_j(t) + G_j(t) \right),$$

with, for $1 \leq j \leq N$,

$$F_j(t) = \frac{1}{2i\pi} \oint_{\Gamma_j(t)} P_j^\perp(t) R(z, t) \dot{R}(z, t) dz, \quad (3.21)$$

$$G_j(t) = \frac{1}{2i\pi} \oint_{\Gamma_j(t)} \dot{R}(z, t) R(z, t) P_j^\perp(t) dz, \quad (3.22)$$

where

$$R(z, t) = (H(t) - z)^{-1}, \quad \dot{R}(z, t) = \frac{d}{dt} [(H(t) - z)^{-1}] = -R(z, t) \frac{dH(t)}{dt} R(z, t),$$

and $\Gamma_j(t)$ is a contour enclosing $E_j(t)$ and no other element of the spectrum (such a contour exists in view of Assumption 3). For $j = N + 1$, we denote by $\Gamma_{N+1}(t)$ a contour enclosing all the first N eigenvalues $E_k(t)$, $k = 1, \dots, N$, and separated from the remainder of the spectrum (such a contour exists in view of Assumption 2), and define

$$F_{N+1}(t) = -\frac{1}{2i\pi} \oint_{\Gamma_{N+1}(t)} \left(\sum_{k=1}^N P_k(t) \right)^\perp R(z, t) \dot{R}(z, t) dz, \quad (3.23)$$

$$G_{N+1}(t) = -\frac{1}{2i\pi} \oint_{\Gamma_{N+1}(t)} \dot{R}(z, t) R(z, t) \left(\sum_{k=1}^N P_k(t) \right)^\perp dz. \quad (3.24)$$

By definition of the contours,

$$-\frac{1}{2i\pi} \oint_{\Gamma_j(t)} R(z, t) dz = P_j(t), \quad 1 \leq j \leq N,$$

and

$$-\frac{1}{2i\pi} \oint_{\Gamma_{N+1}(t)} R(z, t) dz = \sum_{k=1}^N P_k(t) = P_{N+1}^\perp(t).$$

Besides, in view of the continuity of $t \mapsto E_j(t)$ for all $1 \leq j \leq N$, it is possible to use contours which are locally constant in time, *i.e.* for a given $t > -\infty$ such that $f(t) > 0$, there exists a (small) time interval $(t - \tau, t + \tau)$ and a contour Γ_j^t such that

$$\forall s \in (t - \tau, t + \tau), \quad -\frac{1}{2i\pi} \oint_{\Gamma_j^t} R(z, s) dz = P_j(s)$$

for $1 \leq j \leq N$, a similar result holding for $j = N + 1$. Using such locally constant contours, the time derivative of the contour integral defining the projector can be restated as a contour integral of the time derivative of the resolvent:

$$-\frac{1}{2i\pi} \oint_{\Gamma_j(t)} \dot{R}(z, t) dz = \frac{dP_j(t)}{dt}, \quad 1 \leq j \leq N,$$

and

$$-\frac{1}{2i\pi} \oint_{\Gamma_{N+1}(t)} \dot{R}(z, t) dz = \sum_{k=1}^N \frac{dP_k(t)}{dt} = -\frac{dP_{N+1}(t)}{dt}.$$

Boundedness of F . The operator $F(t)$ is bounded. To see this, we first rewrite F_j ($1 \leq j \leq N$) as

$$F_j(t) = P_j^\perp(t)R(E_j(t), t)P_j^\perp(t) \frac{dP_j(t)}{dt}. \quad (3.25)$$

Indeed, using the expression (3.21) of F_j ,

$$\begin{aligned} & F_j(t) - P_j^\perp(t)R(E_j(t), t)P_j^\perp(t) \frac{dP_j(t)}{dt} \\ &= \frac{1}{2i\pi} \oint_{\Gamma_j(t)} P_j^\perp(t)(R(z, t) - R(E_j(t), t))P_j^\perp(t) \dot{R}(z, t) dz \\ &= -\frac{1}{2i\pi} \oint_{\Gamma_j(t)} P_j^\perp(t)(R(z, t) - R(E_j(t), t))R(z, t)P_j^\perp(t) \dot{H}(t)R(z, t) dz. \end{aligned}$$

When the contour encircles closely enough $E_j(t)$,

$$\|R(z, t)\| \leq \frac{1}{|z - E_j(t)|}.$$

Using the resolvent identity, it follows

$$\begin{aligned} \|P_j^\perp(t)(R(z, t) - R(E_j(t), t))R(z, t)P_j^\perp(t)\| &= |z - E_j(t)| \cdot \|P_j^\perp(t)R(z, t)R(E_j(t), t)R(z, t)P_j^\perp(t)\| \\ &\leq \frac{|z - E_j(t)|}{\delta_j(t)^3}. \end{aligned}$$

Then, the difference

$$\left\| \oint_{\Gamma_j(t)} P_j^\perp(t)(R(z, t) - R(E_j(t), t))R(z, t)P_j^\perp(t) \dot{H}(t)R(z, t) dz \right\| \leq C \frac{f'(t)}{\delta_j(t)^3} |\Gamma_j(t)|$$

can be made arbitrarily small by decreasing the radius of the contour $\Gamma_j(t)$, with a constant C depending on the relative H_0 -bound of V .

From the expression (3.25), and the bound $\|P_j^\perp(t)R(E_j(t), t)P_j^\perp(t)\| \leq \delta_j(t)^{-1}$, it holds finally

$$\|F_j(t)\| \leq \frac{\|\dot{P}_j(t)\|}{\delta_j(t)} \leq C \frac{f'(t)}{f(t)},$$

where we recall that both f and f' are non-negative. This shows that $F_j(t)$ is a bounded operator when $f(t) > 0$. A similar bound holds for G_j .

The terms $F_{N+1}(t), G_{N+1}(t)$ require a different treatment. In this case, the uniformity of the gap between the N eigenvalues encircled by $\Gamma_{N+1}(t)$, and the remainder of the spectrum may be used to construct a contour $\Gamma_{N+1}(t)$ such that

$$\forall z \in \Gamma_{N+1}(t), \quad \|R(z, t)\| \leq \frac{4}{\Delta(t)}.$$

This can be done by ensuring that the contour remains far away enough from the remainder of the spectrum, while still being at a finite distance of the first N eigenvalues. In particular, it is possible to construct a contour intersecting the real axis at point γ such that $|\gamma - E_N(t)| \geq \Delta(t)/4$ and

$$\inf \left\{ |\gamma - E|, E \in \sigma(H(t)) \setminus \{E_1(t), \dots, E_N(t)\} \right\} \geq \Delta(t)/4.$$

Then,

$$\|F_{N+1}(t)\| = \left\| \frac{f'(t)}{2i\pi} \oint_{\Gamma_{N+1}(t)} \left(\sum_{k=1}^N P_k(t) \right)^\perp R(z, t)^2 V R(z, t) dz \right\| \leq C \frac{f'(t)}{\Delta(t)^3}, \quad (3.26)$$

and so F_{N+1} is bounded since $\Delta(t) \geq \Delta^* > 0$ and f' is bounded. A similar bound holds for G_{N+1} .

In conclusion,

$$\|F(t)\| \leq C_F \frac{f'(t)}{f(t)}, \quad (3.27)$$

for some constant C_F independent of t .

Computation of the commutator. It is easily seen that $F(t)$ maps the Hilbert space \mathcal{H} to $D(H_0)$. The commutator $[H(t), F(t)]$ can then be defined as an unbounded operator with domain $D(H(t)) = D(H_0)$. For a given $1 \leq j \leq N$, it holds, using the commutation property $P_j^\perp(t)H(t) = H(t)P_j^\perp(t)$,

$$\begin{aligned} [H(t), F_j(t)] &= \frac{1}{2i\pi} \oint_{\Gamma_j(t)} [H(t), P_j^\perp(t)R(z, t)\dot{R}(z, t)] dz \\ &= \frac{1}{2i\pi} \oint_{\Gamma_j(t)} [H(t) - z, P_j^\perp(t)R(z, t)\dot{R}(z, t)] dz \\ &= \frac{1}{2i\pi} \oint_{\Gamma_j(t)} P_j^\perp(t)\dot{R}(z, t) - P_j^\perp(t)R(z, t)\dot{R}(z, t)(H(t) - z) dz \\ &= -P_j^\perp(t)\frac{dP_j(t)}{dt} + P_j^\perp(t) \left(\frac{1}{2i\pi} \oint_{\Gamma_j(t)} R(z, t)^2 dz \right) \dot{H}(t) \\ &= -(\mathbb{I} - P_j(t))\frac{dP_j(t)}{dt}, \end{aligned}$$

following the proof of Theorem 2.2 in [22]. Similar computations show

$$[H(t), G_j(t)] = \frac{dP_j(t)}{dt}(\mathbb{I} - P_j(t)).$$

Finally, for $1 \leq j \leq N$,

$$[H(t), F_j(t) + G_j(t)] = \left[P_j(t), \frac{dP_j(t)}{dt} \right].$$

Similarly,

$$[H(t), F_{N+1}(t) + G_{N+1}(t)] = - \left[P_{N+1}(t), \frac{dP_{N+1}^\perp(t)}{dt} \right] = \left[P_{N+1}(t), \frac{dP_{N+1}(t)}{dt} \right].$$

Since

$$K(t) = - \sum_{j=1}^{N+1} P_j(t) \frac{dP_j(t)}{dt} = -\frac{1}{2} \sum_{j=1}^{N+1} \left[P_j(t), \frac{dP_j(t)}{dt} \right],$$

it holds

$$[H(t), F(t)] = K(t). \quad (3.28)$$

Integration by parts. Consider now $-\infty < t_0 < t \leq 0$ such that $f(t_0) > 0$ (hence $f(t) > 0$ since f is non-decreasing). Define

$$\mathcal{K}(t) = -i\varepsilon U^\varepsilon(t_0, t) F(t) U^\varepsilon(t, t_0).$$

Then

$$\mathcal{K}'(t) = U^\varepsilon(t_0, t) [H(t), F(t)] U^\varepsilon(t, t_0) - i\varepsilon U^\varepsilon(t_0, t) F'(t) U^\varepsilon(t, t_0).$$

In view of (3.28), the difference between the evolution operators is rewritten as

$$\begin{aligned} U^\varepsilon(t, t_0) - U_A^\varepsilon(t, t_0) &= -U^\varepsilon(t, t_0) \int_{t_0}^t U^\varepsilon(t_0, t') K(t') U_A^\varepsilon(t', t_0) dt' \\ &= -U^\varepsilon(t, t_0) \int_{t_0}^t \left(\frac{d\mathcal{K}(t')}{dt'} + i\varepsilon U^\varepsilon(t_0, t') \frac{dF(t')}{dt'} U^\varepsilon(t', t_0) \right) U^\varepsilon(t_0, t') U_A^\varepsilon(t', t_0) dt', \end{aligned} \quad (3.29)$$

so that, after an integration by parts,

$$\begin{aligned} \|U^\varepsilon(t, t_0) - U_A^\varepsilon(t, t_0)\| &= \left\| \int_{t_0}^t U^\varepsilon(t_0, t') K(t') U_A^\varepsilon(t', t_0) dt' \right\| \quad (3.30) \\ &\leq \|K(t)\| + \|K(t_0)\| + \varepsilon \int_{t_0}^t \|F'\| + \left\| \int_{t_0}^t \mathcal{K}(t') \frac{d}{dt'} (U^\varepsilon(t_0, t') U_A^\varepsilon(t', t_0)) dt' \right\| \\ &\leq \varepsilon \left(\|F(t)\| + \|F(t_0)\| + \int_{t_0}^t \|F'(t')\| dt' + \int_{t_0}^t \|F(t')\| \|K(t')\| dt' \right). \end{aligned} \quad (3.31)$$

The first two terms in the above equality are bounded with the bound (3.27) on F . For the last one, we use again the bound (3.27) on F , and the fact that K is uniformly bounded (see (3.14)), so that

$$\int_{t_0}^t \|F(t')\| \|K(t')\| dt' \leq C \int_{t_0}^t \frac{(f')^2}{f} \leq \frac{C}{f(t_0)} \int_{t_0}^t (f')^2. \quad (3.32)$$

We now turn to the central term. For $1 \leq j \leq N$, and using (3.25),

$$\begin{aligned}
\int_{t_0}^t \|F'_j(t')\| dt' &\leq \int_{t_0}^t \frac{\|\ddot{P}_j(t')\|}{\delta_j(t')} dt' + \int_{t_0}^t \|\dot{P}_j(t')\| \left\| \frac{d}{dt'} \left(P_j^\perp(t') R(E_j(t'), t') P_j^\perp(t') \right) \right\| dt' \\
&\leq \int_{t_0}^t \frac{\|\ddot{P}_j(t')\|}{\delta_j(t')} dt' + \int_{t_0}^t \frac{2\|\dot{P}_j(t')\|^2}{\delta_j(t')} dt' \\
&\quad + \int_{t_0}^t \|\dot{P}_j(t')\| \|P_j^\perp(t') R(E_j(t'), t') V R(E_j(t'), t') P_j^\perp(t')\| f'(t') dt' \\
&\leq \int_{t_0}^t \frac{\|\ddot{P}_j(t')\|}{\delta_j(t')} + \frac{2\|\dot{P}_j(t')\|^2}{\delta_j(t')} + C f'(t) \frac{\|\dot{P}_j(t')\|}{\delta_j(t')^2} dt' \\
&\leq C' \int_{t_0}^t \left| \frac{f''(t')}{f(t')} \right| + 3 \frac{f'(t')^2}{f(t')} + \left(\frac{f'(t')}{f(t')} \right)^2 dt' \\
&\leq C' \left(\frac{1}{f(t_0)} \int_{t_0}^t (|f''| + 3(f')^2) + \frac{1}{f(t_0)^2} \int_{t_0}^t (f')^2 \right),
\end{aligned}$$

for some constants $C, C' > 0$ (related to the relative H_0 -bound of V). Similar expressions can be obtained for G_j ($1 \leq j \leq N$). Straightforward estimates can be used for F_{N+1}, G_{N+1} , following a treatment similar to what was done to obtain (3.26), upon deriving the terms appearing in the contour integral:

$$\|F'_{N+1}(t)\| \leq C \left(\frac{|f''(t)|}{\Delta(t)^3} + \frac{f'(t)}{\Delta(t)^3} \sum_{k=1}^N \|\dot{P}_k(t)\| + \frac{f'(t)^2}{\Delta(t)^4} \right),$$

with

$$\|\dot{P}_k(t)\| = f'(t) \left\| \partial_\lambda \tilde{P}(f(t)) \right\| \leq C f'(t).$$

In conclusion,

$$\int_{t_0}^t \|F'(t')\| dt' \leq C \left(\frac{1}{f(t_0)} \int_{t_0}^t (|f''| + (f')^2) + \frac{1}{f(t_0)^2} \int_{t_0}^t (f')^2 \right), \quad (3.33)$$

for some constant $C > 0$.

Decomposition of the integral close to the degeneracy. In order to avoid the singularities when $f(t_0) \rightarrow 0$, the difference of the unitary operators is separated into two contributions as

$$\begin{aligned}
U^\varepsilon(0, t_0) - U_A^\varepsilon(0, t_0) &= -U^\varepsilon(0, t_0) \int_{t_0}^T U^\varepsilon(t_0, t) K(t) U_A^\varepsilon(t, t_0) dt \\
&\quad - U^\varepsilon(0, t_0) \int_T^0 U^\varepsilon(t_0, t) K(t) U_A^\varepsilon(t, t_0) dt,
\end{aligned}$$

where T is chosen such that $f(T) > 0$. The first term is bounded using the straightforward estimate

$$\left\| U^\varepsilon(0, t_0) \int_{t_0}^T U^\varepsilon(t_0, t) K(t) U_A^\varepsilon(t, t_0) dt \right\| \leq C \int_{t_0}^T \sum_{k=1}^N \|\dot{P}_k(t)\| dt \leq C' \int_{t_0}^T f'(t) dt \leq C' f(T). \quad (3.34)$$

For $t \in [T, 0]$, $f(t) \geq f(T) > 0$ and there is a gap proportional to $f(T)$ between the eigenvalues:

$$\forall 1 \leq j \leq N, \quad \forall t \in [0, T], \quad \delta_j(t) \geq \alpha f(T),$$

for some $\alpha > 0$. The inequality (3.30), combined with (3.27), (3.32) and (3.33), allows to bound the second term as

$$\begin{aligned} \left\| U^\varepsilon(0, t_0) \int_T^0 U^\varepsilon(t_0, t) K(t) U_A^\varepsilon(t, t_0) dt \right\| &= \left\| \int_T^0 U^\varepsilon(T, t) K(t) U_A^\varepsilon(t, T) dt \right\| \\ &\leq C\varepsilon \left(\frac{f'(0)}{f(0)} + \frac{1 + f'(T)}{f(T)} + \frac{1}{f(T)} \int_T^0 (|f''| + (f')^2) + \frac{1}{f(T)^2} \int_T^0 (f')^2 \right). \end{aligned} \quad (3.35)$$

The limit $t_0 \rightarrow -\infty$ can then be taken in the above expressions. Moreover, upon choosing T small enough so that $f(T) = \varepsilon^{1/3} \ll 1$, it follows, adding (3.34) and (3.35), and using the fact that $f' \in L^1((-\infty, 0]) \cap L^\infty((-\infty, 0])$ and $f'' \in L^1((-\infty, 0])$,

$$\|U^\varepsilon(0, -\infty) - U_A^\varepsilon(0, -\infty)\| \leq C \left(f(T) + \varepsilon \left(1 + \frac{1}{f(T)^2} \right) \right) \leq 3C\varepsilon^{1/3}. \quad (3.36)$$

This concludes the proof.

3.4 Extensions

The above proofs can be straightforwardly extended to the following cases (see Section 3 for the notation).

Definition of the initial states when $\mathcal{P}_0 V \mathcal{P}_0$ has degenerate eigenvalues. Two changes should be made in the proofs presented in this paper: (i) the estimate obtained in the adiabatic limit degrades; (ii) more conditions are required to define the initial states.

Denote by $\mathcal{E}_{0,i}$ the $M < N$ eigenspaces associated with the eigenvalues of $\mathcal{P}_0 V \mathcal{P}_0$, set $n_i = \dim(\mathcal{E}_{0,i})$, and define

$$\mathcal{N}_i = \left\{ k \in \{1, \dots, N\} \mid \varphi_{k,0} \in \mathcal{E}_{0,i} \right\},$$

the set of indices corresponding to the i -th eigenspace of $\mathcal{P}_0 V \mathcal{P}_0$. Of course,

$$\sum_{i=1}^M n_i = N, \quad \text{Card}(\mathcal{N}_i) = n_i.$$

In view of Assumption 3, for any $(k, l) \in \mathcal{N}_i^2$, $k \neq l$, there exists an integer $p_{k,l} \geq 2$ and an analytic function $e_{kl}(\lambda)$ such that

$$E_k(\lambda) - E_l(\lambda) = \lambda^{p_{k,l}} e_{kl}(\lambda), \quad e_{k,l}(0) \neq 0.$$

Denote by p_* the maximal integer for all couples $1 \leq k, l \leq N$. Then, the final estimate (3.36) in the proof of the adiabatic limit reads

$$\|U^\varepsilon(0, -\infty) - U_A^\varepsilon(0, -\infty)\| \leq C \left(f(T) + \varepsilon \left(1 + \frac{1}{f(T)^{2p_*}} \right) \right) \leq 3C\varepsilon^{1/(2p_*+1)},$$

which is indeed larger than the $\varepsilon^{1/3}$ bound found in the case $p = 1$ (no degeneracy of the perturbation restricted to \mathcal{E}_0).

We now describe an iterative procedure which determines the initial states in a unique manner, using the higher order equations in the hierarchy (3.10). We start with the conditions of order 2. A necessary condition for (3.10) to have a solution is that its right-hand side belongs to \mathcal{E}_0^\perp . With (3.13), this requires

$$\forall 1 \leq j, k \leq N, \quad \langle \varphi_{k,0}, VR_0V\varphi_{j,0} \rangle + E_{j,2}\delta_{j,k} + (E_{j,1} - E_{k,1})c_{j,k}^1 = 0, \quad (3.37)$$

where $\delta_{a,b}$ is the Kronecker symbol. In particular,

$$\forall i \in \{1, \dots, M\}, \quad \forall (j, k) \in \mathcal{N}_i^2, \quad \langle \varphi_{k,0}, VR_0V\varphi_{j,0} \rangle + E_{j,2}\delta_{j,k} = 0.$$

Therefore, $\{\varphi_{j,0}\}_{j \in \mathcal{N}_i}$ has to be an eigenbasis of $\mathcal{P}_{0,i}VR_0V\mathcal{P}_{0,i}$ where $\mathcal{P}_{0,i}$ denotes the projector onto $\mathcal{E}_{0,i}$. If $\mathcal{P}_{0,i}VR_0V\mathcal{P}_{0,i}$ has non-degenerate eigenvalues, the initial eigenfunctions $\{\varphi_{k,0}\}_{k \in \mathcal{N}_i}$ are uniquely defined.

Otherwise, the procedure must be repeated. Recall that there exists an integer p_* such that after p_* steps the degeneracy has no further split (see the discussion at the beginning of this paragraph). The procedure can therefore be repeated until the degeneracy is totally split, which allows to determine the initial states in a unique manner. See for instance [11]. In many practical cases however, degeneracy is never totally split because V shares some symmetries with H_0 . In this case, permanent degeneracy has to be taken into account (see below).

Decomposition of the switching. In the case when (2.2) is not satisfied, *i. e.* $\|P_j(0) - P(-\infty)\| = 1$ or equivalently $\|P_j(0)\psi_j\| = 0$ (since the eigenspaces are assumed to be one-dimensional), the switching should be done in several steps. The intermediate steps can be chosen by finding a finite number of values $\lambda_k \in [0, 1]$ ($k = 1, \dots, N-1$), with $\lambda_0 = 0$ and $\lambda_N = 1$, such that $\|\tilde{P}_j(\lambda_{k+1}) - \tilde{P}_j(\lambda_k)\| < 1$. This is possible since \tilde{P}_j is continuous on the compact interval $[0, 1]$.

The initial state ψ_0 is evolved into a state ψ_1 by switching from H_0 to $H_0 + \lambda_1 V$ as

$$\psi_1 = \lim_{\varepsilon_1 \rightarrow 0} \frac{U_{\text{int}, \lambda_1}^{\varepsilon_1}(0, -\infty)\psi_0}{\langle \psi_0 | U_{\text{int}, \lambda_1}^{\varepsilon_1}(0, -\infty)\psi_0 \rangle},$$

where the evolution operator

$$U_{\text{int}, \lambda_1}^\varepsilon(t, t_0) = e^{itH_0/\varepsilon} U_{\lambda_1}^\varepsilon(t, t_0) e^{-it_0H_0/\varepsilon}$$

is the following operator in the interaction picture:

$$i\varepsilon \frac{dU_{\lambda_1}^\varepsilon(t, t_0)}{dt} = \left(H_0 + \lambda_1 f(t)V \right) U_{\lambda_1}^\varepsilon(t, t_0), \quad U_{\lambda_1}^\varepsilon(t_0, t_0) = \mathbb{I}.$$

The state ψ_1 is then evolved into a state ψ_2 by switching $H_0 + \lambda_1 V$ to $H_0 + \lambda_2 V$ as

$$\psi_2 = \lim_{\varepsilon_2 \rightarrow 0} \frac{U_{\text{int}, \lambda_2, \lambda_1}^{\varepsilon_2}(0, -\infty)\psi_1}{\langle \psi_0 | U_{\text{int}, \lambda_2, \lambda_1}^{\varepsilon_2}(0, -\infty)\psi_0 \rangle},$$

where the evolution operator

$$U_{\text{int}, \lambda_2, \lambda_1}^\varepsilon(t, t_0) = e^{itH_0/\varepsilon} U_{\lambda_2, \lambda_1}^\varepsilon(t, t_0) e^{-it_0H_0/\varepsilon}$$

is defined as the following operator in the interaction picture:

$$i\varepsilon \frac{dU_{\lambda_2, \lambda_1}^\varepsilon(t, t_0)}{dt} = \left(H_0 + \lambda_1 V + (\lambda_2 - \lambda_1) f(t) V \right) U_{\lambda_2, \lambda_1}^\varepsilon(t, t_0), \quad U_{\lambda_2, \lambda_1}^\varepsilon(t_0, t_0) = \mathbb{I}.$$

This construction is repeated until an eigenstate ψ_N of $H_0 + V = H_0 + \lambda_N V$ is obtained. Notice that it is important to do the procedure sequentially.

Permanently degenerate eigenspaces. When there are permanently degenerate eigenspaces associated with one of the eigenvalues $\tilde{E}_j(\lambda)$ or $E_j(t)$, the determination of the initial basis can still be performed as it is presented in Section 3.2. However, the argument leading to (3.19) in Section 3.3.1 cannot be extended as such to the case when $\text{Ran } \tilde{P}_j(0)$ is of dimension larger or equal to 2. This is not a problem since $A(0, -\infty)\psi_j$ is still an eigenvector of $P_j(0)$, and its phase can be removed upon considering

$$\frac{U_{A, \text{int}}^\varepsilon(0, -\infty)\psi_j}{\langle \phi | U_{A, \text{int}}^\varepsilon(0, -\infty)\psi_j \rangle} = \frac{A(0, -\infty)\psi_j}{\langle \phi | A(0, -\infty)\psi_j \rangle}$$

for some fixed state ϕ , provided the denominator is non zero. In Theorem 7, the choice $\phi = \psi_j$ is done, together with the assumption $\langle \phi | A(0, -\infty)\psi_j \rangle \neq 0$. This assumption could in this specific case be translated into an assumption on $\|P_j(0) - P_j(-\infty)\|$, but in general it should then be assumed that there exists $\phi \in \mathcal{H}$ such that $\langle \phi | A(0, -\infty)\psi_j \rangle \neq 0$.

Existence of finitely many crossings. The projectors being analytic, the Kato operator can still be defined when there are eigenvalue crossings. The main issue in extending the Gell-Mann and Low formula to this case is therefore the proof of the adiabatic limit, which can however still be handled with [22, Corollary 2.5] since the crossings are regular (again, because the eigenvalues are analytic).

Initial subspace composed of several degenerate spaces $\mathcal{E}_0, \mathcal{E}_1, \dots$ In this case, the operator V should be diagonalized in each subspaces, *i. e.* the self-adjoint finite-rank operators $\mathcal{P}_j V \mathcal{P}_j|_{\mathcal{E}_j}$ are diagonalized in order to construct a basis of \mathcal{E}_j . A global basis is then obtained by concatenation (direct sum).

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