

Adiabatic switching for degenerate ground states

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- The Gell-Mann and Low formula is a fundamental tool in Quantum Field Theory, used to obtain expressions of the Green's function amenable to a perturbative treatment
- Allow to **transform an eigenstate** of some unperturbed Hamiltonian H_0 into an eigenstate of $H = H_0 + V$ where the interaction term has been turned on (e.g Coulomb interactions between electrons)
- However, eigenspaces of H_0 (even for the ground-state) may be **degenerate**. It is unclear how to **choose the initial state** so that the Gell-Mann and Low formula remains valid
- Outline
 - Some **background** on the spectral theory of Schrödinger operators
 - Proof in the case when the initial eigenspace is **not degenerate**
 - Extension to the **degenerate** case (is there a way to **choose** the initial eigenstates?)

First, some background material...

Quantum description of molecular systems

- Fixed nuclei of charges z_m located at $R_m \in \mathbb{R}^3$ (Born-Oppenheimer approximation)
- **Wavefunction** $\psi((x_1, \sigma_1), \dots, (x_N, \sigma_N)) \in \bigwedge_{i=1}^N L^2(\mathbb{R}^3 \times \{-1, 1\})$ with

$$\|\psi\|_{L^2} = 1$$

- The spin variable will be omitted in the sequel
- **Hamiltonian** operator (in atomic units)

$$H = \sum_{i=1}^N \left(-\frac{1}{2} \Delta_{x_i} + V_{\text{nuc}}(x_i) \right) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}$$

with domain $D(H) = \bigwedge_{i=1}^N H^2(\mathbb{R}^3) \subset \mathcal{H} = \bigwedge_{i=1}^N L^2(\mathbb{R}^3)$ and where

$$V_{\text{nuc}}(x) = - \sum_{m=1}^M \frac{z_m}{|x - R_m|}$$

Spectrum of a linear operator (1)

- Linear operator $A : D(A) \subset \mathcal{H} \rightarrow \mathcal{H}$ on a Hilbert space, with **dense domain** $D(A)$
- A is injective if $\text{Ker}(A) = \{\phi \in D(A) \mid A\phi = 0\} = \{0\}$
- If A is injective, it is possible to define its **inverse**, which is an operator with domain

$$D(A^{-1}) = \text{Ran}(A) = \left\{ \psi \in \mathcal{H} \mid \exists \phi \in D(A), \psi = A\phi \right\}$$

such that $\phi = A^{-1}\psi \Leftrightarrow \psi = A\phi$

- A is **invertible** if it has a bounded inverse defined on $D(A^{-1}) = \mathcal{H}$
- If A is closed and one-to-one $D(A) \rightarrow \mathcal{H}$, the operator $A^{-1} : \mathcal{H} \rightarrow D(A)$ is automatically bounded by the closed graph theorem
- Resolvent set $\rho(A) =$ (open) set of $\lambda \in \mathbb{C}$ such that $\lambda - A$ is invertible
- The **spectrum** $\sigma(A) = \mathbb{C} \setminus \rho(A)$ is closed

Spectrum of a linear operator (2)

- The spectrum can be decomposed as $\sigma(A) = \sigma_p(A) \cup \sigma_r(A) \cup \sigma_c(A)$, where (“by decreasing defaults of invertibility”)
 - $\lambda \in \sigma_p(A)$ iff $\text{Ker}(\lambda - A) \neq \{0\}$ [**eigenvalues**]
 - $\lambda \in \sigma_r(A)$ iff $\lambda - A$ is injective but $\overline{\text{Ran}(\lambda - A)} \neq \mathcal{H}$ [the inverse is not uniquely defined]
 - $\lambda \in \sigma_c(A)$ iff $\lambda - A$ is injective, $\overline{\text{Ran}(\lambda - A)} = \mathcal{H}$ but $\text{Ran}(\lambda - A) \neq \mathcal{H}$ [the inverse is unbounded with dense domain; **generalized eigenvalues**]
- Other decomposition: $\sigma(A) = \sigma_d(A) \cup \sigma_{\text{ess}}(A)$, where the **discrete spectrum** $\sigma_d(A) \subset \sigma_p(A)$ = isolated eigenvalues of finite multiplicity
- Examples (necessarily infinite dimensional)
 - **Residual** spectrum: shift operator τ_d on $l^2(\mathbb{N}, \mathbb{C})$ with $\tau_d(z_0, z_1, z_2, \dots) = (0, z_0, z_1, \dots)$
 - **Continuous** spectrum: $A\psi(x) = x\psi(x)$ on $L^2(\mathbb{R})$

- Adjoint of an unbounded operator = closed operator with domain

$$\begin{aligned} D(A^*) &= \left\{ \phi \in \mathcal{H} \mid \forall \psi \in D(A), |\langle A\psi, \phi \rangle| \leq C_\phi \|\psi\| \right\} \\ &= \left\{ \phi \in \mathcal{H} \mid \exists \varphi \in \mathcal{H}, \forall \psi \in D(A), \langle A\psi, \phi \rangle = \langle \psi, \varphi \rangle \right\} \end{aligned}$$

defined by $A^* \phi = \varphi$

- **Symmetric** operator: $\forall (\phi, \psi) \in D(A)^2, \langle A\phi, \psi \rangle = \langle \phi, A\psi \rangle$ (i.e. $A \subset A^*$)
- A symmetric operator is self-adjoint if $A = A^*$ (i.e. $D(A) = D(A^*)$)
- For self-adjoint operators, $\sigma(A) \subset \mathbb{R}$ and $\sigma_r(A) = \emptyset$
- An operator V is H_0 -bounded if $D(H_0) \subset D(V)$ and
$$\forall \phi \in D(H_0), \quad \|V\phi\| \leq a\|H_0\phi\| + b\|\phi\|$$
- **Kato-Rellich criterion**: If H_0 is self-adjoint and V is symmetric and H_0 -bounded with **relative bound** $a < 1$, then $H = H_0 + V$ defined on $D(H) = D(H_0)$ is self-adjoint

Important example: the molecular Hamiltonian

- Consider $D(H_0^N) = \bigwedge_{i=1}^N H^2(\mathbb{R}^3)$

$$H_0^N = \sum_{i=1}^N \left(-\frac{1}{2} \Delta_{x_i} + V_{\text{nuc}}(x_i) \right), \quad V^N = \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}$$

- (Kato) Using the **Hardy inequality**

$$\forall \phi \in H^1(\mathbb{R}^3), \quad \int_{\mathbb{R}^3} \frac{|\phi(x)|^2}{|x|^2} dx \leq 4 \int_{\mathbb{R}^3} |\nabla \phi(x)|^2 dx,$$

it can be shown that $H^N = H_0^N + V^N$ is self-adjoint on $\mathcal{H}_N = \bigwedge_{i=1}^N L^2(\mathbb{R}^3)$

- HVZ theorem:** $\sigma_{\text{ess}}(H^N) = [E^{N-1}, +\infty[$, where

$$E^{N-1} = \inf \sigma(H^{N-1})$$

- If $N < Z + 1$, then there are **infinitely many eigenvalues** of finite multiplicity below the essential spectrum

The Gell-Mann and Low formula for nondegenerate states

Switching procedure (1)

- Consider, on a given Hilbert space \mathcal{H} ,
 - a self-adjoint operator H_0 , bounded from below and with dense domain $D(H_0) \subset \mathcal{H}$
 - a symmetric perturbation V , H_0 -bounded with relative bound $a < 1$.
 - Set $\tilde{H}(\lambda) = H_0 + \lambda V$ with $\lambda \in [0, 1]$
- Switching function $f \in C^1\left((-\infty, 0], [0, 1]\right)$
 - integrable
 - $f(0) = 1$ and $\lim_{\tau \rightarrow -\infty} f(\tau) = 0$
 - for $\tau \in (-\infty, 0]$, define $H(\tau) = H_0 + f(\tau) V$
- Denote by $U_\varepsilon(s, s_0)$ the unitary evolution generated by $H(\varepsilon s)$, i.e. the unique solution of the problem:

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

Switching procedure (2)

- **Divergent phase** as $\varepsilon \rightarrow 0$! Consider $V = 0$ and ϕ an eigenstate of H_0 :

$$U_\varepsilon(s, s_0) \phi = \exp\left(-\frac{iE_0(s - s_0)}{\varepsilon}\right) \phi$$

- Remove divergence by working in the **interaction picture**:

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

- **Macroscopic time** $t = \varepsilon s$, then unitary evolution

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

so that, in the interaction picture, $U_{\text{int}}^\varepsilon(t, t_0) = e^{itH_0/\varepsilon} U^\varepsilon(t, t_0) e^{-it_0H_0/\varepsilon}$

- Standard results show that, for $\psi \in D(H_0)$, the following limit exists:

$$U_{\text{int}}^\varepsilon(t, -\infty) \psi = \lim_{t_0 \rightarrow -\infty} U_{\text{int}}^\varepsilon(t, t_0) \psi$$

- In order for eigenstates to be **stable** during the switching procedure, some **gap** conditions are required
- The spectrum of $\tilde{H}(\lambda) = H_0 + \lambda V$, $\lambda \in [0, 1]$, consists of **two disconnected pieces**

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

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

- There is **a uniform gap** between the two parts of the spectrum, and between the elements of $\sigma_N(\lambda)$, in the sense that:

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

$$\delta(\lambda) = \min \left\{ \left| \tilde{E}_j(\lambda) - \tilde{E}_i(\lambda) \right|, 1 \leq i < j \leq N \right\}$$

are bounded from below by a positive constant for all $\lambda \in [0, 1]$

The Gell-Mann and Low formula

- For simplicity, eigenvalues $E_j(\tau) = \tilde{E}_j(f(\tau))$ of multiplicity 1
- Then, for an **eigenstate** ψ_j of H_0 associated with $E_j(-\infty)$, if

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

the limit

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

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

- Extension to the case of eigenspaces of multiplicity higher than 1 provided some direction ϕ exists such that the denominator does not vanish...
- Proposed by GELL-MANN and LOW (*Phys. Rev.* 1951), first proof due to NENCIU and RASCHE (*Helvetica Physica Acta*, 1989)

First step of the proof: Geometric evolution

- **Kato intertwining** operator: $\frac{d\tilde{A}(\lambda, \lambda_0)}{d\lambda} = \tilde{K}(\lambda) \tilde{A}(\lambda, \lambda_0)$ with $\tilde{A}(\lambda_0, \lambda_0) = \mathbb{I}$
- Generator $\tilde{K}(\lambda) = - \sum_{j=1}^{N+1} \tilde{P}_j(\lambda) \frac{d\tilde{P}_j}{d\lambda}(\lambda)$, with $\tilde{P}_{N+1}(\lambda) = \mathbb{I} - \sum_{j=1}^N \tilde{P}_j(\lambda)$
- Since $\tilde{K}(\lambda)$ is uniformly bounded (gap, hence projectors smooth), the operator $\tilde{A}(\lambda, \lambda_0)$ is well-defined and strongly continuous
- $\tilde{A}(\lambda, \lambda_0)$ is **unitary** (since $K^* = -K$), and intertwines the spectral subspaces:

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

- Denoting by $A(s, s_0) = \tilde{A}(f(s), f(s_0))$,

$$P_j(0) A(0, -\infty) \psi_j = A(0, -\infty) P_j(-\infty) \psi_j = A(0, -\infty) \psi_j,$$

so that $A(0, -\infty) \psi_j$ is an **eigenstate** of $H(0) = H_0 + V$

Second step: Adiabatic evolution (adding the dynamical phase)

- **Adiabatic evolution** operator $U_A(s, s_0)$ is defined as the unique solution of

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

where the **adiabatic Hamiltonian** is $H_A(s) = H(s) + iK(s)$

- Since both U_A and A are intertwiners, they **differ only by a phase** which commutes with the spectral projectors: 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, $[\Phi(s, s_0), P_j(s_0)] = 0$

- The **time-evolution of the phase** matrix is then easily obtained and

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

Second step: Adiabatic evolution (2)

- Important again to work in the **interaction picture** to remove the divergent (dynamical) phase: $U_{A,\text{int}}(s, s_0) = e^{isH_0} U_A(s, s_0) e^{-is_0H_0}$

- It can be shown that

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

- Phase well-defined since $|E_j(r) - E_0| = |\tilde{E}_j(f(r)) - \tilde{E}_j(0)| \leq C f(r)$

- In the **time-rescaled** variable $t = \varepsilon s$,

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

- **Eliminate the phase** using

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

Third step: Adiabatic limit of the full evolution

- **Compare** the adiabatic and full evolutions in the rescaled time-variable:

$$i\varepsilon \frac{dU_A^\varepsilon(t, t_0)}{dt} = \left(H(t) + i\varepsilon K(t) \right) U_A^\varepsilon(t, t_0), \quad i\varepsilon \frac{dU^\varepsilon(t, t_0)}{dt} = H(t) U^\varepsilon(t, t_0)$$

- Prove the **uniform convergence** $\lim_{\varepsilon \rightarrow 0} \|U^\varepsilon(0, -\infty) - U_A^\varepsilon(0, -\infty)\| = 0$
(although $U^\varepsilon(0, -\infty), U_A^\varepsilon(0, -\infty)$ do not have a limit as $\varepsilon \rightarrow 0$)
- Strategy from (TEUFEL, *Adiabatic perturbation theory in quantum dynamics*, 2003):

$$U^\varepsilon(t, t_0) - U_A^\varepsilon(t, t_0) = -U^\varepsilon(t, t_0) \int_{t_0}^t U^\varepsilon(t_0, t') K(t') U_A^\varepsilon(t', t_0) dt'$$

- Define $\mathcal{K}(t) = -i\varepsilon U^\varepsilon(t_0, t) F(t) U^\varepsilon(t, t_0)$ with $[H(t), F(t)] = K(t)$. Then

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

- **Similar to** $\int_0^t e^{-i\tau/\varepsilon} d\tau = i\varepsilon \left(e^{-it/\varepsilon} - 1 \right) =$ highly oscillatory integral

The degenerate case

Structure of the spectrum

- Initial state is **degenerate**: $\tilde{E}_j(0) = \tilde{E}_k(0)$ for all $1 \leq j, k \leq N$
- **Degeneracy splitting** (for simplicity): $\mathcal{P}_0 V \mathcal{P}_0$ has non-degenerate eigenvalues and for any $\lambda^* > 0$, there exists α such that

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

- Switching function f **analytic**, such that $f \in W^{2,1}((-\infty, 0])$, and f'/f and f' belong to $L^\infty((-\infty, 0])$ (In addition to the previous constraints)
- For example, $f(s) = e^s$
- Let (ψ_1, \dots, ψ_N) be an basis of \mathcal{E}_0 which **diagonalizes the bounded operator** $\mathcal{P}_0 V \mathcal{P}_0|_{\mathcal{E}_0}$. Then, if $\|P_j(-\infty) - P_j(0)\| < 1$, the limit

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

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

Characterization of the initial states

- Theorem II.6.1 in (KATO, *Perturbation Theory for Linear Operators*) shows that the eigenvalues \tilde{E}_j and projectors \tilde{P}_j are **analytic** functions
- Eigenvectors satisfy $\tilde{H}(\lambda) \phi_j(\lambda) = \tilde{E}_j(\lambda) \phi_j(\lambda)$ with

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

- Hierarchy of equations. First order condition

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

- A **necessary** condition for this equation to have a solution is that the right-hand side belongs to \mathcal{E}_0^\perp
- This requires $E_{j,1} = \langle \varphi_{j,0}, V \varphi_{j,0} \rangle$ and $\forall k \neq j, \langle \varphi_{k,0}, V \varphi_{j,0} \rangle = 0$ so that the basis **diagonalizes** $\mathcal{P}_0 V \mathcal{P}_0|_{\mathcal{E}_0}$
- When degeneracies of $\mathcal{P}_0 V \mathcal{P}_0$: higher order conditions

Idea of the proof and further references

- Geometric and adiabatic evolutions: **unchanged**, since the regularity of the projectors is obtained with the theorem of Kato
- Adiabatic limit: **decomposition** of the evolution into
 - an evolution on $[T, 0]$, for Hamiltonians operators with (small) **gaps**
 - an evolution on the time-frame $(-\infty, T]$, with **T small enough** so that the unitary evolutions are not very different
- References:
 - C. BROUDER, G. STOLTZ AND G. PANATI, Adiabatic approximation, Gell-Mann and Low theorem and degeneracies: A pedagogical example, *Phys. Rev. A* **72** (2008) 042102
 - C. BROUDER, G. PANATI AND G. STOLTZ, Gell-Mann and Low formula for degenerate unperturbed states **[the math paper!]**
 - C. BROUDER, G. PANATI AND G. STOLTZ, The Green function of degenerate systems, submitted to *Phys. Rev. Lett.*

Application to Green functions (formal...)

- Operator A expressed in the **Heisenberg** picture $A_{\text{hsnbrg}}(t) = e^{itH} A e^{-itH}$ and, in the **interaction** picture, $A_{\text{int}}(t) = e^{itH_0} A e^{-itH_0}$
- Correlation function $C_{A,B}(t, t') = \langle \psi | T [A_{\text{hsnbrg}}(t) B_{\text{hsnbrg}}(t')] | \psi \rangle$
- Technical lemma (proof to be done...):

$$s\text{-}\lim_{\varepsilon \rightarrow 0} U_{\varepsilon, \text{int}}(t, 0)^* A_{\text{int}}(t) U_{\varepsilon, \text{int}}(t, t') B_{\text{int}}(t') U_{\varepsilon, \text{int}}(t', 0) = A_{\text{hsnbrg}}(t) B_{\text{hsnbrg}}(t')$$

- Using the Gell-Mann and Low formula, it can then be shown that

$$C_{A,B}(t, t') = \lim_{\varepsilon \rightarrow 0} \frac{\langle \psi_0 | T [A_{\text{int}}(t) B_{\text{int}}(t') U_{\varepsilon, \text{int}}(+\infty, -\infty)] | \psi_0 \rangle}{\langle \psi_0 | U_{\varepsilon, \text{int}}(+\infty, -\infty) | \psi_0 \rangle}.$$

- Formal extension to the case when A, B are **field operators**
- Basis for a **perturbative treatment** of the Green's function, where the operators $U_{\varepsilon, \text{int}}(+\infty, -\infty)$ in the numerator and denominator are expanded using Feynman diagrams.