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On the smooth Feshbach–Schur map

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Abstract

A new variant of the Feshbach map, called smooth Feshbach map, has been introduced recently by Bach et al., in connection with the renormalization analysis of non-relativistic quantum electrodynamics. We analyze and clarify its algebraic and analytic properties, and we generalize it to non-selfadjoint partition operators χ and $\overline{\chi}$.

Keywords: Schur complement; Feshbach map; Quantum electrodynamics; Renormalization transform

1. Introduction

For the spectral analysis of non-relativistic QED a *renormalization transform* was introduced in [1,2] that reduces an eigenvalue problem for the Hamiltonian H to an equal one for an effective Hamiltonian on a smaller Hilbert space, or, more precisely, a Hamiltonian with fewer degrees of freedom. The heart of this renormalization transform is Schur's block-diagonalization of the Hamiltonian H with respect to the decomposition $\mathcal{H} = P\mathcal{H} \oplus \bar{P}\mathcal{H}$ of the Hilbert space $\mathcal{H}$ induced by suitably chosen projections P and $\bar{P} = 1 - P$: assuming that $\bar{P}H\bar{P}$ is invertible on $\bar{P}\mathcal{H}$, the Hamiltonian H is invertible if and only if its Schur complement, or Feshbach map,

$$F_P(H) = PHP - PH\bar{P}(\bar{P}H\bar{P})^{-1}\bar{P}HP, \tag{1}$$

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is invertible on $P\mathcal{H}$ [1,2,7]. Moreover, the kernels of H and $F_P(H)$ have equal dimensions. In the renormalization analysis of Bach et al. the projection operator P is the spectral projection $\chi_{[0,\rho]}(H_f)$ of a self-adjoint operator, H_f, the field energy. The spectral problem is solved by iterating the renormalization transform composed of the operator map $H \mapsto F_P(H)$ and a suitable scaling transformation.

In the recent beautiful paper [3] a novel, *smooth Feshbach map* $H = T + W \mapsto F_\chi(H, T)$ with surprisingly nice algebraic properties is introduced. In the definition of $F_\chi(H, T)$, commuting self-adjoint operators χ and $\overline{\chi}$ with $\chi^2 + \overline{\chi}^2 = 1$ and $[\chi, T] = 0 = [\overline{\chi}, T]$ play the roles of P and $\bar{P}$. This allows one, in the application to QED, to choose χ and $\overline{\chi}$ as smooth functions of H_f, which avoids technical problems that were caused by the non-differentiability of the function $\chi_{[0,\rho]}$ defining P in the renormalization map based on (1). Since χ and $\overline{\chi}$ need not be projections, there is no obvious interpretation of the smooth Feshbach map in terms of a block-diagonalization of H. Nevertheless, H is invertible if and only if $F_\chi(H, T)$ is invertible, the kernels of H and $F_\chi(H, T)$ have equal dimensions, and all other properties of $F_P(H)$ that were used in [1,2] have analogs in the smooth Feshbach map. This is the content of the Feshbach theorem, Theorem II.1, in [3].

In the present paper we prove that the Feshbach theorem is still true when the self-adjointness assumption on χ and $\overline{\chi}$ is dropped. This generalization is needed, for example, in the analysis of resonances, and in the perturbation theory of the ground state of models of matter and quantized radiation [4,6]. In the course of modifying the proof of Theorem II.1 [3], we closely examined all of its parts. The result is an improved version of the Feshbach theorem, Theorem 1 below, with weaker assumptions and a stronger statement. Using new algebraic identities, we show, for example, that χ is an isomorphism from the kernel of H onto the kernel of $F_\chi(H, T)$, and we identify its inverse. The renormalization transform based on our generalized Feshbach theorem may again be iterated to solve a given spectral problem.

The Schur complement (for matrices) goes back to Schur [11], see also [9,12], and it is widely used in applied mathematics [12]. In the physics literature H. Feshbach derived an effective Hamiltonian of the form of a Schur complement in a study of nuclear reactions [5]. Subsequently this effective Hamiltonian was written in the form (1) using projection operators P and $Q = 1 - P$ [8], called Feshbach's projection operators [10].

2. The smooth Feshbach map

Let χ and $\overline{\chi}$ be commuting, nonzero bounded operators, acting on a separable Hilbert space $\mathcal{H}$ and satisfying $\chi^2 + \overline{\chi}^2 = 1$. By a *Feshbach pair* (H, T) for χ we mean a pair of closed operators with same domain,

$$H, T : D(H) = D(T) \subset \mathcal{H} \to \mathcal{H}$$

such that $H, T, W := H - T$, and the operators

$$\begin{aligned} W_\chi &:= \chi W \chi, & W_{\overline{\chi}} &:= \overline{\chi} W \overline{\chi}, \\ H_\chi &:= T + W_\chi, & H_{\overline{\chi}} &:= T + W_{\overline{\chi}}, \end{aligned}$$

defined on $D(T)$ satisfy the following assumptions:

(a) $\chi T \subset T \chi$ and $\overline{\chi} T \subset T \overline{\chi}$,

(b) $T, H_{\overline{\chi}} : D(T) \cap \operatorname{Ran} \overline{\chi} \to \operatorname{Ran} \overline{\chi}$ are bijections with bounded inverse,
(c) $\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi : D(T) \subset \mathcal{H} \to \mathcal{H}$ is a bounded operator.

Henceforth we will call an operator $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ *bounded invertible in a subspace* $V \subset \mathcal{H}$ (V not necessarily closed), if $A : D(A) \cap V \to V$ is a bijection with bounded inverse.

Remarks. 1. To verify (a), it suffices to show that $T\chi = \chi T$ and $T\overline{\chi} = \overline{\chi} T$ on a *core* of T.

2. If T is bounded invertible in $\operatorname{Ran} \overline{\chi}$, $\|T^{-1}\overline{\chi} W \overline{\chi}\| < 1$, $\|\overline{\chi} W T^{-1} \overline{\chi}\| < 1$, and $T^{-1}\overline{\chi} W \chi$ is a bounded operator, then the bounded invertibility of $H_{\overline{\chi}}$ and condition (c) follow. See Lemma 3 below.

3. Note that $\operatorname{Ran} \chi$ and $\operatorname{Ran} \overline{\chi}$ need not be closed and are not closed in the application to QED. One can however, replace $\operatorname{Ran} \overline{\chi}$ by $\overline{\operatorname{Ran} \overline{\chi}}$ both in condition (b) and in the statement of Theorem 1 below. Then this theorem continues to hold and the proof remains unchanged.

Since our conditions defining Feshbach pairs are different from those stated in [3], some explanations are necessary. First, our conditions (a) and (b) on Feshbach pairs can also be found in [3, Section 2.1]. The bounded invertibility of T is not mentioned there as an assumption, but it is used in the proof of [3, Theorem 2.1]. Second, there is no condition needed on $\chi W(\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi})$, or a similar operator, since this operator is bounded as a consequence of the domain assumptions. In fact, since H and T are closed on $D(T)$, and since $\operatorname{Ran} \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} \subset D(T)$, the operators $H(\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi})$, $T(\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi})$ are defined on $\mathcal{H}$, closed and hence bounded. Since $W = H - T$, it follows that $W(\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi})$ is bounded. Third, our condition (c) is weaker than the corresponding condition (2.3) of [3], at least in practice, and this is crucial in some applications to QED. Condition (c) is satisfied, for example, if $H = H_\alpha$ is the Hamiltonian of an atom or molecule in the standard model of non-relativistic QED with finestructure constant α and with $T = H_{\alpha=0}$. Condition (2.3) of [3] will not be satisfied in this case.

Given a Feshbach pair (H, T) for χ, the operator

$$F_\chi(H, T) := H_\chi - \chi W \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi \tag{2}$$

on $D(T)$ is called *Feshbach map of* H. The mapping $(H, T) \mapsto F_\chi(H, T)$ is called *Feshbach map*. The auxiliary operators

$$Q_\chi := \chi - \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi,$$
$$Q_\chi^\# := \chi - \chi W \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi},$$

play an important role in the analysis of $F_\chi(H, T)$. By conditions (a), (c), and the explanation above, they are bounded, and Q_χ leaves $D(T)$ invariant. The Feshbach map is isospectral in the sense of the following theorem, which generalizes [3, Theorem 2.1] to non-selfadjoint χ and $\overline{\chi}$.

Theorem 1. *Let* (H, T) *be a Feshbach pair for* χ *on a separable Hilbert space* $\mathcal{H}$. *Then the following holds*:

(i) *Let* V *be a subspace with* $\operatorname{Ran} \chi \subset V \subset \mathcal{H}$,

$$T : D(T) \cap V \to V, \quad \textit{and} \quad \overline{\chi} T^{-1} \overline{\chi} V \subset V. \tag{3}$$

Then $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ is bounded invertible if and only if $F_\chi(H,T) : D(T) \cap V \to V$ is bounded invertible in V. Moreover,

$$H^{-1} = Q_\chi F_\chi(H,T)^{-1} Q_\chi^\# + \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi},$$
$$F_\chi(H,T)^{-1} = \chi H^{-1} \chi + \overline{\chi} T^{-1} \overline{\chi}.$$

(ii) $\chi \operatorname{Ker} H \subset \operatorname{Ker} F_\chi(H,T)$ *and* $Q_\chi \operatorname{Ker} F_\chi(H,T) \subset \operatorname{Ker} H$. *The mappings*

$$\chi : \operatorname{Ker} H \to \operatorname{Ker} F_\chi(H,T), \tag{4}$$
$$Q_\chi : \operatorname{Ker} F_\chi(H,T) \to \operatorname{Ker} H, \tag{5}$$

are linear isomorphisms and inverse to each other.

Remarks. 1. The subspaces $V = \operatorname{Ran} \chi$ and $V = \mathcal{H}$ satisfy the conditions stated in (3).

2. From [3] it is known that χ and Q_χ are one-to-one on $\operatorname{Ker} H$ and $\operatorname{Ker} F_\chi(H,T)$, respectively. The stronger result (ii) will be derived from the new algebraic identities (a) and (b) of the following lemma.

Theorem 1 will easily follow from the next lemma, which is of interest and importance in its own right.

Lemma 2. *Let (H,T) be a Feshbach pair for χ and let $F := F_\chi(H,T)$, $Q := Q_\chi$, and $Q^\# := Q_\chi^\#$ for simplicity. Then the following identities hold*:

(a) $\quad \big(\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi}\big) H = 1 - Q\chi$, *on* $D(T)$, $\qquad H\big(\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi}\big) = 1 - \chi Q^\#$, *on* $\mathcal{H}$,

(b) $\quad \big(\overline{\chi} T^{-1} \overline{\chi}\big) F = 1 - \chi Q$, *on* $D(T)$, $\qquad F\big(\overline{\chi} T^{-1} \overline{\chi}\big) = 1 - Q^\# \chi$, *on* $\mathcal{H}$,

(c) $\quad HQ = \chi F$, *on* $D(T)$, $\qquad Q^\# H = F\chi$, *on* $D(T)$.

Proof. We proof the first equations in (a), (b), and (c) only. The other ones are proved analogously.

(a) Since $\overline{\chi} T \subset \overline{\chi} T$ and $\chi^2 + \overline{\chi}^2 = 1$, on $D(T)$,

$$\begin{aligned}
\big(\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi}\big) H &= \overline{\chi} H_{\overline{\chi}}^{-1} T \overline{\chi} + \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \big(\chi^2 + \overline{\chi}^2\big) \\
&= \overline{\chi} H_{\overline{\chi}}^{-1} (T + W_{\overline{\chi}}) \overline{\chi} + \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi^2 \\
&= \overline{\chi}^2 + \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi^2 \\
&= 1 - Q\chi.
\end{aligned}$$

(b) Using again condition (a) of Feshbach pairs and $\chi^2 + \overline{\chi}^2 = 1$, we find on $D(T)$,

$$\begin{aligned}
\big(\overline{\chi} T^{-1} \overline{\chi}\big) F &= \overline{\chi} T^{-1} \overline{\chi} \big(T + W_\chi - \chi W \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi\big) \\
&= \overline{\chi}^2 + \overline{\chi} T^{-1} \overline{\chi} \chi W \chi - \chi \overline{\chi} T^{-1} W_{\overline{\chi}} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi \\
&= \overline{\chi}^2 + \chi \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi \\
&= 1 - \chi Q,
\end{aligned}$$

where in the third equation we used the resolvent identity $\overline{\chi}(T^{-1} - H_{\overline{\chi}}^{-1})\overline{\chi} = \overline{\chi}T^{-1}W_{\overline{\chi}}H_{\overline{\chi}}^{-1}\overline{\chi}$.

(c) By the second equation of (a), on $D(T)$,

$$\begin{aligned} HQ &= H\big(\chi - \overline{\chi}H_{\overline{\chi}}^{-1}\overline{\chi}W\chi\big) \\ &= \chi T + W\chi - \big(1 - \chi Q^{\#}\big)W\chi \\ &= \chi\big(T + Q^{\#}W\chi\big) = \chi F. \qquad \Box \end{aligned}$$

Remark. Alternatively, one can prove the identities of Lemma 2(b) as follows. By definition of F and the first equation of (c), on $D(T)$,

$$\begin{aligned} \overline{\chi}^2 F = F - \chi^2 F &= (T + \chi W Q) - \chi H Q \\ &= T - \chi T Q = T(1 - \chi Q). \end{aligned}$$

Since the range of $1 - \chi Q = \overline{\chi}^2 + \chi\overline{\chi}H_{\overline{\chi}}^{-1}\overline{\chi}W\chi$ is a subspace of $\operatorname{Ran}\overline{\chi}$, the first identity of Lemma 2(b) follows from condition (b) of Feshbach pairs. The other identity of Lemma 2(b) can be shown similarly.

Proof of Theorem 1. We use the simplified notation of Lemma 2.

(i) Suppose F is bounded invertible in V. Then the operator

$$R := QF^{-1}Q^{\#} + \overline{\chi}H_{\overline{\chi}}^{-1}\overline{\chi}$$

is bounded, and by Lemma 2(a) and (c)

$$\begin{aligned} RH &= QF^{-1}Q^{\#}H + \big(\overline{\chi}H_{\overline{\chi}}^{-1}\overline{\chi}\big)H \\ &= Q\chi + (1 - Q\chi) = 1, \end{aligned}$$

on $D(H)$. Similarly one shows that $HR = 1$ on $\mathcal{H}$. On the other hand, if H is bounded invertible in $\mathcal{H}$, then

$$\widetilde{R} := \chi H^{-1}\chi + \overline{\chi}T^{-1}\overline{\chi}$$

is bounded, and by Lemma 2(c) and (b)

$$\begin{aligned} \widetilde{R}F &= \chi H^{-1}\chi F + \big(\overline{\chi}T^{-1}\overline{\chi}\big)F \\ &= \chi Q + (1 - \chi Q) = 1, \end{aligned}$$

on $D(T)$. Similarly one shows that $F\widetilde{R} = 1$ on $\mathcal{H}$. This shows that F is bounded invertible in $\mathcal{H}$. Finally, from the definitions of F, $\widetilde{R}$ and the properties of V, it follows that $F : D(T) \cap V \to V$ and $\widetilde{R} : V \to D(T) \cap V$. Hence F is also bounded invertible in V.

(ii) On the one hand, by Lemma 2(c), $\chi \operatorname{Ker} H \subset \operatorname{Ker} F$ and $Q \operatorname{Ker} F \subset \operatorname{Ker} H$. On the other hand, by the first equations of part (a) and (b) of that lemma

$$Q\chi = 1 \quad \text{on } \operatorname{Ker} H \quad \text{and} \quad \chi Q = 1 \quad \text{on } \operatorname{Ker} F.$$

This proves statement (ii). $\Box$

Lemma 3. *Conditions* (a), (b), *and* (c) *on Feshbach pairs are satisfied if*:

(a′) $\chi T \subset T\chi$ *and* $\overline{\chi} T \subset T\overline{\chi}$,
(b′) T *is bounded invertible in* $\operatorname{Ran}\overline{\chi}$,
(c′) $\|T^{-1}\overline{\chi}W\overline{\chi}\| < 1$, $\|\overline{\chi}WT^{-1}\overline{\chi}\| < 1$ *and* $T^{-1}\overline{\chi}W\chi$ *is a bounded operator.*

Proof. By assumptions (a′) and (b′), on $D(T) \cap \operatorname{Ran}\overline{\chi}$,

$$H_{\overline{\chi}} = \bigl(1 + \overline{\chi}WT^{-1}\overline{\chi}\bigr)T,$$

and $T : D(T) \cap \operatorname{Ran}\overline{\chi} \to \operatorname{Ran}\overline{\chi}$ is a bijection with bounded inverse. From (c′) it follows that

$$1 + \overline{\chi}WT^{-1}\overline{\chi} : \operatorname{Ran}\overline{\chi} \to \operatorname{Ran}\overline{\chi}$$

is a bijection with bounded inverse. In fact, $(1 + \overline{\chi}WT^{-1}\overline{\chi})\operatorname{Ran}\overline{\chi} \subset \operatorname{Ran}\overline{\chi}$, the Neumann series

$$\sum_{n\geqslant 0}\bigl(-\overline{\chi}WT^{-1}\overline{\chi}\bigr)^n = 1 - \overline{\chi}WT^{-1}\overline{\chi}\sum_{n\geqslant 0}\bigl(-\overline{\chi}WT^{-1}\overline{\chi}\bigr)^n$$

converges and maps $\operatorname{Ran}\overline{\chi}$ to $\operatorname{Ran}\overline{\chi}$. Hence $H_{\overline{\chi}} \restriction \operatorname{Ran}\overline{\chi}$ is bounded invertible.

Finally, from $H_{\overline{\chi}} = T(1 + T^{-1}W_{\overline{\chi}})$ and (c′) it follows that

$$H_{\overline{\chi}}^{-1}\overline{\chi}W\chi = \bigl(1 + T^{-1}W_{\overline{\chi}}\bigr)^{-1}T^{-1}\overline{\chi}W\chi,$$

which, by (c′), is bounded. □

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