Technische
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Mathematics of Interacting Quantum Systems
Summer Semester 25/26
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6. Exercise Sheet 6

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Exercise 6.1 (6)

Let $A, W \in \mathfrak{M}_{3\times 3}(\mathbb{C})$ and define $A_g := A + gW$ with $g \in \mathbb{R}$ as in Eqs. (V.47)–(V.49) of the lecture notes, and let $z \in D(0,1)$ be given by (V.60), where

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 9 \end{pmatrix} \quad \text{and} \quad W = \begin{pmatrix} 0 & i & 2 \\ -i & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix}. \tag{1}$$

Determine $\rho := \|W\|_{op}^{-1} < \infty$ and compute $a_0, a_1, a_2, a_3 \in \mathbb{C}$ and $C_4 < \infty$ such that

$$\left| z - (a_0 + a_1 g + a_2 g^2 + a_3 g^3) \right| \leq C_4 g^4$$

for all $g \in (-\rho, \rho)$.

Solution.

The eigenvalues of A are $1, 5, 9$. Let P be the orthogonal projection onto the eigenspace associated with 1, and let $P^{\perp}$ be the projection onto the orthogonal complement. Explicitly,

$$P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad P^{\perp} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1. \end{pmatrix} \tag{2}$$

One has that $P^{\perp}(A-1)P^{\perp}$ restricted to $Ran(P^{\perp})$ is invertible. Then for $|g|$ and $|z|$ sufficiently small one has that the matrix

$$P^{\perp}(A_g - 1 - z)P^{\perp} = P^{\perp}(A - 1 - z)P^{\perp} + gP^{\perp}WP^{\perp} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 4-z & 0 \\ 0 & 0 & 8-z \end{pmatrix} + gP^{\perp}WP^{\perp},$$

restricted to $Ran(P^{\perp})$ is invertible.

Moreover, one has

$$P^{\perp}(A_g - 1 - z)P^{\perp} = (1 + gP^{\perp}WP^{\perp}R_0^{\perp}(1+z)) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 4-z & 0 \\ 0 & 0 & 8-z \end{pmatrix} \tag{3}$$

where

$$R_0^{\perp}(1+z) = (P^{\perp}(A - 1 - z)P^{\perp})^{-1}P^{\perp} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & (4-z)^{-1} & 0 \\ 0 & 0 & (8-z)^{-1} \end{pmatrix}.$$

If $z \in D(0,1)$ then $\|R_0^{\perp}(1+z)\|_{op} \leq \frac{1}{3}$. Then for $|g| < \|W\|_{op}^{-1}$ one obtains

$$(P^{\perp}(A_g - 1 - z)P^{\perp})^{-1}P^{\perp} = R_0^{\perp}(1+z) \sum_{n=0}^{\infty} (-g)^n (P^{\perp}WP^{\perp}R_0^{\perp}(1+z))^n. \tag{4}$$

Let us consider the Feshbach–Schur map

$$\begin{aligned} F_P(A_g-1-z, A-1-z) &= P(A_g-1-z)P - g^2 PWP^{\perp}(P^{\perp}(A_g-1-z)P^{\perp})^{-1}P^{\perp}WP \\ &= -zP + gPWP - g^2 PWR_0^{\perp}(1+z)\sum_{n=0}^{\infty}(-g)^n(P^{\perp}WP^{\perp}R_0^{\perp}(1+z))^n P^{\perp}WP. \end{aligned} \tag{5}$$

By Theorem V.2 of the notes, $A_g - 1 - z$ is invertible if and only if $F_P(A_g-1-z, A-1-z)$ is invertible. Since F_P is a rank-one matrix, $1+z$ is an eigenvalue of A_g if and only if

$$\begin{aligned} 0 &= \langle e_1 | F_P(A_g-1-z, A-1-z)e_1\rangle \\ &= -z + gW_{1,1} - g^2\sum_{n=0}^{\infty}(-g)^n\langle We_1|R_0^{\perp}(1+z)(P^{\perp}WP^{\perp}R_0^{\perp}(1+z))^n P^{\perp}We_1\rangle. \end{aligned} \tag{6}$$

An explicit computation shows that

$$\langle We_1|R_0^{\perp}(1+z)P^{\perp}We_1\rangle = \frac{1}{4-z} + \frac{4}{8-z}, \qquad \langle We_1|R_0^{\perp}(1+z)P^{\perp}WP^{\perp}R_0^{\perp}(1+z)P^{\perp}We_1\rangle = 0.$$

Then we obtain that $z \in D(0,1)$ satisfies

$$z = -g^2\left(\frac{1}{4-z} + \frac{4}{8-z}\right) - g^4 f(g,z). \tag{7}$$

with $\|f(g,z)\| \leq \|W\|_{op}^2/6$ for all $|g| < \|W\|_{op}^{-1}$. Using Eq. (7) one gets $|z| \leq C_1 g^2$ where $C_1 := 1/3 + 4/7 + 1/6$, then

$$\begin{aligned} |z + 3/4g^2| &= \left| -g^2\left(\frac{1}{4-z} - \frac{1}{4} + \frac{4}{8-z} - \frac{1}{2}\right) - g^4 f(g,z)\right| \\ &\leq g^2\frac{|z|}{4|4-z|} + g^2\frac{|z|}{2|8-z|} + g^4\|W\|_{op}^2/6 \\ &\leq g^4\left(C_1(1/12 + 1/14) + \|W\|_{op}^2/6\right). \end{aligned} \tag{8}$$

Exercise 6.2 (6)

Let $n \in \mathbb{N}$, $T = T^*, W = W^* \in \mathcal{B}(\mathbb{C}^n) \setminus \{0\}$ and $T_g := T + gW$ with $g \in \mathbb{R}$. Let $T_{k,k} = \langle e_k \mid Te_k\rangle = 0$ and $T_{k,\ell} = \langle e_k \mid Te_\ell\rangle < 0$ for all $k \neq l \in \{1, \dots, n\}$, where $\{e_k\}_{k=1}^n \subseteq \mathbb{C}^n$ denotes the canonical orthonormal basis.

(i) Let $\inf\sigma(T) =: \lambda_0$. Show that λ_0 is a strictly negative eigenvalue.

(ii) Let $\psi \in \operatorname{Ker}[T-\lambda_0] \setminus \{0\}$ be an eigenvector corresponding to λ_0. Show that there exists $\alpha \in [0, 2\pi)$ such that $e^{-i\alpha}\langle e_k \mid \psi\rangle > 0$ for all $k \in \{1, \dots, n\}$. Conclude that λ_0 is a simple eigenvalue of T.

(iii) Assume that $\langle\psi \mid W\psi\rangle = 0$, $P^{\perp}W\psi \neq 0$ and $\inf\sigma(T_g) =: \lambda_g$. Show that the map $\mathbb{R} \ni g \mapsto \lambda_g \in \mathbb{R}$ attains a strict local maximum at $g = 0$.

Solution.

(i) Let $\lambda_0 < \lambda_1 \cdots < \lambda_{n-1}$ be the eigenvalues of T. One has

$$\sum_{j=0}^{n-1}\lambda_j = \operatorname{Tr}(T) = \sum_{k=1}^{n}\langle e_k|Te_k\rangle = 0. \tag{9}$$

Since $T = T^*$, $\lambda_j \in \mathbb{R}$. Moreover, since $T \neq 0$, not all eigenvalues are equal to 0. Using the above and Eq. (9), one concludes that $\lambda_0 < 0$.

(ii) Let us set $\varphi = \|\psi\|^{-1}\psi$. We denote $\varphi_k = \langle e_k|\varphi\rangle$, and define $\phi = \sum_{k=1}^{n} |\varphi_k| e_k$. One has that

$$\lambda_0 = \langle \varphi | T\varphi\rangle = \sum_{1\le k<l\le n} (\overline{\varphi_k}\varphi_l + \varphi_k\overline{\varphi_l})T_{k,l} \ge \sum_{1\le k<l\le n} 2|\varphi_k||\varphi_l|T_{k,l} = \langle \phi, T\phi\rangle \ge \lambda_0. \tag{10}$$

Therefore, $\overline{\varphi_k}\varphi_l + \varphi_k\overline{\varphi_l} = |\overline{\varphi_k}\varphi_l|$, which implies that there exists α such that $\varphi_k = e^{i\alpha}|\varphi_k|$. Hence $e^{-i\alpha}\langle e_k|\psi\rangle = |\varphi_k|\|\psi\| \ge 0$. Since $\psi \ne 0$, there exists l such that $e^{-i\alpha}\langle e_l|\psi\rangle > 0$, and thus

$$e^{-i\alpha}\langle e_k|\psi\rangle = \sum_{j=1}^{n} \frac{1}{\lambda_0} T_{k,j} e^{-i\alpha}\langle e_j|\psi\rangle \ge \frac{1}{\lambda_0} T_{k,l} e^{-i\alpha}\langle e_l|\psi\rangle > 0. \tag{11}$$

If $\dim(\mathrm{Ker}(T-\lambda_0)) > 1$, then since $T = T^*$ one can choose orthogonal eigenvectors $\psi, \tilde{\psi}$ associated with λ_0. Taking $\alpha, \tilde{\alpha}$ such that $e^{-i\alpha}\langle e_k|\psi\rangle, e^{-i\tilde{\alpha}}\langle e_k|\tilde{\psi}\rangle > 0$, one would have

$$0 = \langle e^{-i\alpha}\psi | e^{-i\tilde{\alpha}}\tilde{\psi}\rangle = \sum_{k=1}^{n} e^{-i\alpha}\langle e_k|\psi\rangle \cdot e^{-i\tilde{\alpha}}\langle e_k|\tilde{\psi}\rangle > 0, \tag{12}$$

which is impossible.

(iii) Let P be the orthogonal projection onto $\mathrm{Ker}(T-\lambda_0)$ and $P^\perp = 1 - P$. Then $P^\perp(T-\lambda_0)P^\perp$ is invertible in $Ran(P^\perp)$. By definition, one has

$$\langle \phi | T_g \phi\rangle = \langle \phi | T\phi\rangle + g\langle \phi | W\phi\rangle, \tag{13}$$

which implies

$$\lambda_0 + g\|W\| \ge \lambda_g \ge \lambda_0 - g\|W\|. \tag{14}$$

Then one has $\|\lambda_g - \lambda_0\| \le |g|\|W\|$. Hence, for $|g| > 0$ sufficiently small, $P^\perp(T_g - \lambda_g)P^\perp$ is also invertible in $Ran(P^\perp)$, and one can consider the Feshbach–Schur map $F_P(T_g - \lambda_g)$. Moreover, since $T_g - \lambda_g$ is not invertible, $F_P(T_g - \lambda_g)$ is not invertible. Since $\dim \mathrm{Ran}(P) = 1$, one has that for a normalized vector $\psi \in \mathrm{Ran}(P)$,

$$\begin{aligned} 0 &= \langle \psi | F_P(T_g - \lambda_g)\psi\rangle \\ &= \lambda_0 - \lambda_g + g\langle \psi|W\psi\rangle - g^2\langle \psi | WP^\perp(P^\perp TP^\perp + gP^\perp WP^\perp - \lambda_g)^{-1}P^\perp W\psi\rangle \\ &= \lambda_0 - \lambda_g - g^2\langle P^\perp W\psi | (P^\perp TP^\perp + gP^\perp WP^\perp - \lambda_g)^{-1}P^\perp W\psi\rangle \end{aligned} \tag{15}$$

Since $P^\perp TP^\perp - \lambda_0$ restricted to $Ran(P^\perp)$ is strictly positive, one has that for sufficiently small $|g| > 0$,

$$P^\perp TP^\perp + gP^\perp WP^\perp - \lambda_g = P^\perp TP^\perp - \lambda_0 + gP^\perp WP^\perp - (\lambda_g - \lambda_0) > 0,$$

and since $P^\perp W\psi \ne 0$, one obtains

$$\langle P^\perp W\psi | (P^\perp TP^\perp + gP^\perp WP^\perp - \lambda_g)^{-1}P^\perp W\psi\rangle > 0. \tag{16}$$

Eqs. (16) and (15) imply the result.

Exercise 6.3 (12)

Let $n \in \mathbb{N}$, $T = T^*, W = W^* \in \mathcal{B}(\mathbb{C}^n) \setminus \{0\}$, and $T_g := T + gW$, with $g \geq 0$ and $W \geq 0$. Let $\lambda_0 := \inf \sigma(T)$ be a simple eigenvalue with normalized eigenvector $\psi_0 \in \mathbb{C}^n$ and associated orthogonal projection $P_0 := |\psi_0\rangle\langle\psi_0|$. Furthermore, define $R_0^\perp(z) := (T_0 - z)^{-1} P_0^\perp$ and $\lambda_g := \inf \sigma(T_g)$.

(i) Show that there exists $g_0 > 0$ such that λ_g is a simple eigenvalue for $g \in (-g_0, g_0)$.

(ii) Show that there exists $g_0 > 0$ such that λ_g satisfies the estimate

$$\lambda_g \;\geq\; \lambda_0 + g\langle\psi_0|W\psi_0\rangle - g^2\Big\langle\psi_0\Big|W\,R_0^\perp\left[\lambda_0 + g\langle\psi_0|W\psi_0\rangle\right]\,W\psi_0\Big\rangle \tag{17}$$

for $g \in [0, g_0)$.

(iii) Show that there exists $g_0 > 0$ such that λ_g satisfies the estimate

$$\begin{aligned} \lambda_g \;&\leq \lambda_0 + g\langle\psi_0|W\psi_0\rangle \\ &- g^2\Big\langle\psi_0\Big|WR_0^\perp(\lambda_0)W\psi_0\Big\rangle + g^3\Big\langle\psi_0\Big|WR_0^\perp(\lambda_0)WR_0^\perp(\lambda_0)W\psi_0\Big\rangle \end{aligned} \tag{18}$$

for $g \in [0, g_0)$. Hint: Apply the variational principle with the trial vector $\psi_0 - gR_0^\perp(\lambda_0)W\psi_0$. (Why is this a good choice?)

Solutions.

(i) Theorem IV.10 of the notes implies that there exists $r, \rho > 0$ such that for all $g \in (-\rho, \rho)$,

$$\sigma(T_g) \cap D(\lambda_0, r) = \{\mu_g\},$$

where μ_g is a simple eigenvalue of T_g. One also has

$$|\lambda_g - \lambda_0| \leq |g|\|W\|. \tag{19}$$

Taking $g_0 := \min(r/\|W\|, \rho)$ one obtains that for all $g \in (-g_0, g_0)$, $\mu_g = \lambda_g$.

(ii) Using the Feshbach–Schur map one obtains that for g sufficiently small

$$\lambda_g = \lambda_0 + g\langle\psi_0|W\psi_0\rangle - g^2\langle\psi_0|WP_0^\perp(P_0^\perp TP_0^\perp + gP_0^\perp WP_0^\perp - \lambda_g)^{-1}P_0^\perp W\psi_0\rangle. \tag{20}$$

Since $P_0^\perp TP_0^\perp - \lambda_0 > 0$, for $|g|$ sufficiently small one has

$$P_0^\perp TP_0^\perp + gP_0^\perp WP_0^\perp - \lambda_g > 0.$$

Then Eq. (20) implies that

$$\lambda_g \leq \lambda_0 + g\langle\psi_0|W\psi_0\rangle.$$

Let $0 < g_0 < \frac{\lambda_1 - \lambda_0}{\langle\psi_0|W\psi_0\rangle}$, then for all $0 < g < g_0$ one obtains

$$P_0^\perp TP_0^\perp + gP_0^\perp WP_0^\perp - \lambda_g \geq P_0^\perp TP_0^\perp - \lambda_0 - g\langle\psi_0|W\psi_0\rangle > P_0^\perp TP_0^\perp - \lambda_1 \geq 0.$$

Then one has

$$R_0^\perp[\lambda_0 + g\langle\psi_0|W\psi_0\rangle] = (P_0^\perp TP_0^\perp - \lambda_0 - g\langle\psi_0|W\psi_0\rangle)^{-1} \geq (P_0^\perp TP_0^\perp + gP_0^\perp WP_0^\perp - \lambda_g)^{-1}. \tag{21}$$

Using Eq. (20) and (21) one obtains (17).

(iii) Let us denote $\varphi = \psi_0 - gR_0^{\perp}(\lambda_0)W\psi_0$. An explicit computation using that $R_0^{\perp}(\lambda_0)W\psi_0 \in \{\psi_0\}^{\perp}$ shows

$$\begin{aligned}\langle\varphi|T_g\varphi\rangle &= \lambda_0 + g\langle\psi_0|W\psi_0\rangle + \lambda_0 g^2\|R_0^{\perp}(\lambda_0)W\psi_0\|^2 - g^2\langle\psi_0|WR_0^{\perp}(\lambda_0)W\psi_0\rangle \\ &\quad + g^3\langle\psi_0|WR_0^{\perp}(\lambda_0)WR_0^{\perp}(\lambda_0)W\psi_0\rangle \\ &= \lambda_0\|\varphi\|^2 + g\langle\psi_0|(W - gWR_0^{\perp}(\lambda_0)W + g^2WR_0^{\perp}(\lambda_0)WR_0^{\perp}(\lambda_0)W)\psi_0\rangle.\end{aligned} \tag{22}$$

Besides, since $W \geq 0$ for $g > 0$ one has

$$\begin{aligned}&W - gWR_0^{\perp}(\lambda_0)W + g^2WR_0^{\perp}(\lambda_0)WR_0^{\perp}(\lambda_0)W \\ &\qquad \geq W - 2gWR_0^{\perp}(\lambda_0)W + g^2WR_0^{\perp}(\lambda_0)WR_0^{\perp}(\lambda_0)W \\ &\qquad = \sqrt{W}(1 - g\sqrt{W}R_0^{\perp}(\lambda_0)\sqrt{W})^2\sqrt{W} \geq 0.\end{aligned} \tag{23}$$

where in the first inequality one uses that $WR_0^{\perp}(\lambda_0)W \geq 0$. Then using Eq. (22) and that $\|\varphi\|^2 = 1 + g^2\|R_0^{\perp}(\lambda_0)W\psi_0\|^2 \geq 1$ one obtains,

$$\langle\varphi|T_g\varphi\rangle \leq \|\varphi\|^2\Big(\lambda_0 + g\langle\psi_0|(W - gWR_0^{\perp}(\lambda_0)W + g^2WR_0^{\perp}(\lambda_0)WR_0^{\perp}(\lambda_0)W)\psi_0\rangle\Big). \tag{24}$$

Since $\lambda_g \leq \frac{\langle\varphi|T_g\varphi\rangle}{\|\varphi\|^2}$, one obtains the result.