



The discrete Fourier transform &
Applications to 2×2 matrix problems

Homework Problems

34. The Fourier transform of various functions (8 points)

Compute the Fourier coefficients of the following functions on $[-\pi, +\pi]$ and characterize their asymptotic behavior for large $|k|$:

(i) $f(x) = 1 + x$

(ii) $g(x) = \sin 2x$

(iii) $h(x) = \begin{cases} +1 & x \in [0, +\pi] \\ 0 & x \in [-\pi, 0) \end{cases}$

(iv) $j(x) = \begin{cases} +1 & x \in [0, +\pi] \\ -1 & x \in [-\pi, 0) \end{cases}$

Solution:

(i) From $(\mathcal{F}1)(k) = \delta_{k,0}$ and

$$(\mathcal{F}x)(k) = \begin{cases} 0 & k = 0 \\ (-1)^k \frac{i}{k} & k \in \mathbb{Z} \setminus \{0\} \end{cases},$$

we can immediately give the Fourier series of f as

$$(\mathcal{F}f)(k) \stackrel{[2]}{=} \begin{cases} 1 & k = 0 \\ (-1)^k \frac{i}{k} & k \in \mathbb{Z} \setminus \{0\} \end{cases}.$$

The Fourier series decays as $1/|k|$.

(ii) Writing $\sin 2x = \frac{1}{i2}(e^{+i2x} - e^{-i2x})$ in terms of exponential functions immediately yields

$$(\mathcal{F}g)(k) \stackrel{[2]}{=} \begin{cases} -\frac{i}{2} & k = 2 \\ +\frac{i}{2} & k = -2 \\ 0 & \text{else} \end{cases}.$$

The Fourier series has only finitely many non-zero terms, i. e. it decays superpolynomially and superexponentially.

(iii) For $k = 0$, we obtain

$$(\mathcal{F}h)(0) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} dx h(x) = \frac{1}{2\pi} \int_0^{+\pi} dx \stackrel{[1]}{=} \frac{1}{2},$$

while for $k \neq 0$, we get

$$\begin{aligned} (\mathcal{F}h)(k) &= \frac{1}{2\pi} \int_0^{+\pi} dx e^{-ikx} = \left[\frac{1}{2\pi} \frac{1}{-ik} e^{-ikx} \right]_0^{+\pi} \\ &\stackrel{[1]}{=} \frac{i((-1)^k - 1)}{2\pi k}. \end{aligned}$$

The Fourier series decays as $1/|k|$.

(iv) Noticing that $j(x) = 2h(x) - 1$, we deduce

$$(\mathcal{F}j)(k) \stackrel{[2]}{=} \begin{cases} 0 & k = 0 \\ \frac{i((-1)^k - 1)}{\pi k} & k \in \mathbb{Z} \setminus \{0\} \end{cases}.$$

The Fourier series decays as $1/|k|$.

35. The Pauli matrices

Consider the three Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- (i) Prove $\sigma_j \sigma_k = \delta_{jk} \text{id}_{\mathbb{C}^2} + i \sum_{l=1}^3 \epsilon_{jkl} \sigma_l$ where ϵ_{jkl} is the epsilon tensor.
- (ii) Prove that any 2×2 matrix can be written as the linear combination of the identity and the three Pauli matrices with coefficients h_0 and $h = (h_1, h_2, h_3)$,

$$\text{Mat}_{\mathbb{C}}(2) \ni A = (a_{jk})_{1 \leq j, k \leq 2} = h_0 \text{id}_{\mathbb{C}^2} + \sum_{j=1}^3 h_j \sigma_j =: \text{id}_{\mathbb{C}^2} + h \cdot \sigma. \quad (1)$$

Hint: Use that $\text{Mat}_{\mathbb{C}}(2)$ is finite-dimensional.

- (iii) Now assume that the coefficients h_0, \dots, h_3 in equation (1) are real. Show that then the resulting matrix $H = h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma$ is hermitian. Compute the eigenvalues $E_{\pm}(h_0, h)$ of H in terms of the coefficients h_0 and h .
- (iv) Use (i) to prove that for real h_0, \dots, h_3

$$P_{\pm}(h_0, h) = \frac{1}{2} \left(\text{id}_{\mathbb{C}^2} \pm \frac{h \cdot \sigma}{|h|} \right), \quad h \neq 0 \in \mathbb{R}^3, \quad |h| := \sqrt{h_1^2 + h_2^2 + h_3^2},$$

are the projections onto the eigenspaces for the two eigenvalues $E_{\pm}(h_0, h)$ of H .

- (v) Compute the trace of H .

Note: In physics especially, one frequently writes $h \cdot \sigma$ for $\sum_{j=1}^3 h_j \sigma_j$ where $h = (h_1, h_2, h_3)$.

Solution:

- (i) This follows from direct computation: for $j = k$ we obtain

$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = \text{id}_{\mathbb{C}^2}$$

while for $j < k$

$$\begin{aligned} \sigma_1 \sigma_2 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} = \begin{pmatrix} +i & 0 \\ 0 & -i \end{pmatrix} = i \sigma_3 \\ \sigma_1 \sigma_3 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i \sigma_2 \\ \sigma_2 \sigma_3 &= \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & +i \\ +i & 0 \end{pmatrix} = i \sigma_1 \end{aligned}$$

In other words, we have shown (i) for $j < k$.

To show (i) in the remaining cases, we use that the $\sigma_j = \sigma_j^*$ are hermitian matrices, and hence for $j < k$ we obtain

$$\begin{aligned} \sigma_k \sigma_j &= (\sigma_j \sigma_k)^* = \left(\delta_{jk} \text{id}_{\mathbb{C}^2} + i \sum_{l=1}^3 \epsilon_{jkl} \sigma_l \right)^* \\ &= \delta_{jk} \text{id}_{\mathbb{C}^2} - i \sum_{l=1}^3 \epsilon_{jkl} \sigma_l = \delta_{jk} \text{id}_{\mathbb{C}^2} + i \sum_{l=1}^3 \epsilon_{kjl} \sigma_l. \end{aligned}$$

This proves (i).

- (ii) The vector space of 2×2 matrices is four-dimensional, $\dim \text{Mat}_{\mathbb{C}}(2) = 4$, and seeing as the 4 vectors $\{\text{id}_{\mathbb{C}^2}, \sigma_1, \sigma_2, \sigma_3\}$ are linearly independent, they form a basis of $\text{Mat}_{\mathbb{C}}(2)$.
- (iii) In case h_0, \dots, h_3 are real,

$$\begin{aligned} H^* &= (h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma)^* = \overline{h_0} \text{id}_{\mathbb{C}^2} + \overline{h} \cdot \sigma \\ &= h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma = H \end{aligned}$$

is hermitian and we can compute both eigenvalues: the characteristic polynomial of H is

$$\begin{aligned} \chi(\lambda) &= \det(\lambda \text{id}_{\mathbb{C}^2} - H) = \det \begin{pmatrix} \lambda - h_0 - h_3 & h_1 - \text{i} h_2 \\ h_1 + \text{i} h_2 & \lambda - h_0 + h_3 \end{pmatrix} \\ &= ((\lambda - h_0) - h_3) ((\lambda - h_0) + h_3) - (h_1 - \text{i} h_2)(h_1 + \text{i} h_2) \\ &= (\lambda - h_0)^2 - (h_1^2 + h_2^2 + h_3^2) = (\lambda - h_0)^2 - |h|^2, \end{aligned}$$

and hence, the eigenvalues are $E_{\pm}(h_0, h) = h_0 \pm |h|$.

- (iv) The product

$$H P_{\pm} = (h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma) P_{\pm} = h_0 P_{\pm} + \frac{1}{2} \left(h \cdot \sigma \pm \frac{(h \cdot \sigma)^2}{|h|} \right)$$

involves the square of $h \cdot \sigma$ which can be computed with the help of (i):

$$\begin{aligned} (h \cdot \sigma)^2 &= \sum_{j,k=1}^3 h_j h_k \sigma_j \sigma_k \\ &= \sum_{j=1}^3 h_j^2 \text{id}_{\mathbb{C}^2} + \sum_{\substack{j,k,l=1,2,3 \\ j \neq k}} h_j h_k \text{i} \epsilon_{jkl} \sigma_l \\ &= |h|^2 \text{id}_{\mathbb{C}^2} + \text{i} \sum_{l=1}^3 \left(\sum_{\substack{j,k=1,2,3 \\ j \neq k}} h_j h_k \text{i} \epsilon_{jkl} \right) \sigma_l = |h|^2 \text{id}_{\mathbb{C}^2} \end{aligned}$$

Hence, we can factor out E_{\pm} and obtain (iv):

$$\begin{aligned} H P_{\pm} &= h_0 P_{\pm} + \frac{1}{2} \left(h \cdot \sigma \pm \frac{|h|^2 \text{id}_{\mathbb{C}^2}}{|h|} \right) \\ &= h_0 P_{\pm} \pm |h| \frac{1}{2} \left(\text{id}_{\mathbb{C}^2} \pm \frac{h \cdot \sigma}{|h|} \right) \\ &= (h_0 \pm |h|) P_{\pm} = E_{\pm} P_{\pm} \end{aligned}$$

- (v) The trace is just the sum over the diagonal elements of the matrices, and clearly, the Pauli matrices are all traceless. Hence, we compute

$$\begin{aligned} \text{tr} H &= \text{tr}(h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma) \\ &= h_0 \text{tr} \text{id}_{\mathbb{C}^2} + \sum_{j=1}^3 h_j \text{tr} \sigma_j = 2h_0. \end{aligned}$$

36. Functional calculus for 2×2 matrices

Let f be a piecewise continuous function and $H = H^*$ a hermitian 2×2 matrix. Then define

$$f(H) := \sum_{j=\pm} f(E_{\pm}) P_{\pm} \quad (2)$$

where E_{\pm} are the eigenvalues of H and P_{\pm} the two projections from problem 35.

(i) Compute $f(H)$ defined as in equation (2) for $H = h \cdot \sigma$, $h \neq 0$, and

$$f(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}.$$

(ii) Show that $f(H)$ for $f(x) = e^{-itx}$ (defined via (2)) coincides with the matrix exponential, i. e.

$$f(H) = e^{-ith_0} \left(\cos(|h|t) - \frac{i}{|h|} \sin(|h|t) h \cdot \sigma \right) = e^{-itH} = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} H^n. \quad (3)$$

Hint: Use $e^{-it(h_0+h\cdot\sigma)} = e^{-ith_0} e^{-ith\cdot\sigma}$.

(iii) Assuming h_0, h_1, h_2, h_3 are real, compute $\psi(t)$ for the initial condition $\psi(0) = \psi_0 \in \mathbb{C}^2$:

(a) $\frac{d}{dt}\psi(t) = (h_2 \sigma_2 + h_3 \sigma_3)\psi(t)$

(b) $i \frac{d}{dt}\psi(t) = h_2 \sigma_2 \psi(t)$

(c) $-i \frac{d}{dt}\psi(t) = (h_0 \text{id}_{\mathbb{C}^2} + h_3 \sigma_3)\psi(t)$

Solution:

(i) $f(H) = f(|h|) P_+ + f(-|h|) P_- = P_+$

(ii) For $h = 0$, H is a scalar multiple of the identity matrix and equation (3) holds. So let us assume $h \neq 0$. Then we first compute the left-hand side:

$$\begin{aligned} e^{-itx}(H) &= e^{-it(h_0+|h|)} P_+ + e^{-it(h_0-|h|)} P_- \\ &= \frac{1}{2} \left(e^{-it(h_0+|h|)} + e^{-it(h_0-|h|)} \right) \text{id}_{\mathbb{C}^2} + \frac{1}{2} \left(e^{-it(h_0+|h|)} - e^{-it(h_0-|h|)} \right) \frac{h \cdot \sigma}{|h|} \\ &= e^{-ith_0} \left(\cos(|h|t) - \frac{i}{|h|} \sin(|h|t) h \cdot \sigma \right) \end{aligned}$$

To obtain the right-hand side, we note

$$\begin{aligned} (h \cdot \sigma)^2 &= \sum_{j,k=1,2,3} h_j h_k \sigma_j \sigma_k = \sum_{j=1,2,3} h_j^2 \sigma_j^2 + \sum_{\substack{j,k=1,2,3 \\ j \neq k}} h_j h_k \sigma_j \sigma_k \\ &= \sum_{j=1,2,3} h_j^2 \text{id}_{\mathbb{C}^2} + \sum_{l=1,2,3} \sum_{\substack{j,k=1,2,3 \\ j \neq k}} h_j h_k \epsilon_{jkl} \sigma_l = h^2, \end{aligned}$$

and thus we identify a pattern in $(h \cdot \sigma)^n$:

$$\begin{aligned} (h \cdot \sigma)^{2n} &= |h|^{2n} \text{id}_{\mathbb{C}^2} \\ (h \cdot \sigma)^{2n+1} &= (h \cdot \sigma)^{2n} h \cdot \sigma = |h|^{2n} h \cdot \sigma \end{aligned}$$

This means that we can compute the matrix exponential after splitting the sum into even and odd terms:

$$\begin{aligned}
e^{-itH} &= e^{-ith_0} e^{-ith \cdot \sigma} = e^{-ith_0} \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} (h \cdot \sigma)^n \\
&= e^{-ith_0} \sum_{n=0}^{\infty} \frac{(-it)^{2n}}{(2n)!} (h \cdot \sigma)^{2n} + e^{-ith_0} \sum_{n=0}^{\infty} \frac{(-it)^{2n+1}}{(2n+1)!} (h \cdot \sigma)^{2n+1} \\
&= e^{-ith_0} \sum_{n=0}^{\infty} (-1)^n \frac{(|h|t)^{2n}}{(2n)!} \text{id}_{\mathbb{C}^2} - \frac{i}{|h|} e^{-ith_0} \sum_{n=0}^{\infty} (-1)^n \frac{(|h|t)^{2n+1}}{(2n+1)!} h \cdot \sigma \\
&= e^{-ith_0} \left(\cos(|h|t) \text{id}_{\mathbb{C}^2} - \frac{i}{|h|} \sin(|h|t) h \cdot \sigma \right)
\end{aligned}$$

Thus, left- and right-hand side agree.

(iii) (a)

$$\begin{aligned}
\psi(t) &= e^{tH} \psi_0 = e^{t|h|} P_+(0, 0, h_2, h_3) + e^{-t|h|} P_-(0, 0, h_2, h_3) \\
&= \frac{1}{2} (e^{+t|h|} + e^{-t|h|}) \psi_0 + \frac{1}{2} \frac{e^{+t|h|} - e^{-t|h|}}{|h|} (h_2 \sigma_2 + h_3 \sigma_3) \psi_0 \\
&= \cosh(t|h|) \psi_0 + \sinh(t|h|) (h_2 \sigma_2 + h_3 \sigma_3) \psi_0
\end{aligned}$$

$$(b) \quad \psi(t) = e^{-itH} \psi_0 = \cos(t|h_2|) \psi_0 - i \frac{h_2}{|h_2|} \sin(t|h_2|) \sigma_2 \psi_0$$

$$(c) \quad \psi(t) = e^{+itH} \psi_0 = e^{+ith_0} \cos(t|h_2|) \psi_0 + i e^{+ith_0} \frac{h_3}{|h_3|} \sin(t|h_3|) \sigma_3 \psi_0$$

37. A simple model for graphene (12 points)

Consider the nearest-neighbor model for graphene

$$H = \begin{pmatrix} q_3 \text{id}_{\ell^2(\mathbb{Z}^2)} & 1_{\ell^2(\mathbb{Z}^2)} + q_1 \mathfrak{s}_1 + q_2 \mathfrak{s}_2 \\ 1_{\ell^2(\mathbb{Z}^2)} + q_1 \mathfrak{s}_1^* + q_2 \mathfrak{s}_2^* & -q_3 \text{id}_{\ell^2(\mathbb{Z}^2)} \end{pmatrix}.$$

Here, $q_1, q_2 \in \mathbb{R}$ are hopping amplitudes while $q_3 \in \mathbb{R}$ is the so-called stagger parameter. Repeat the analysis in Chapter 6.1.5.2:

- (i) Compute the momentum representation $H^{\mathcal{F}} := \mathcal{F}^{-1} H \mathcal{F}$. What Hilbert space does this operator act on?
- (ii) Find a matrix-valued function $T(k)$ so that $H^{\mathcal{F}} = T(\hat{k})$ is the multiplication operator associated to T .
- (iii) Find the eigenvalues $E_{\pm}(k)$ and eigenprojections $P_{\pm}(k)$ of $T(k)$.
- (iv) Compute the unitary evolution group $U^{\mathcal{F}}(t)$ for $H^{\mathcal{F}}$.
- (v) Compute the unitary evolution group $U(t)$ in position representation.
- (vi) **Voluntary:** Identify the parameter region where the eigenvalues are not separated by a gap, i. e. $\inf_{k \in \mathbb{T}^n} |E_+(k) - E_-(k)| = 0$.

Remark: This nearest-neighbor model with stagger was used to investigate the piezoelectric effect in graphene: *Topological Polarization in Graphene-like Systems*, G. De Nittis and M. Lein, J. Phys. A **46** no. 38, p. 385001, 2013

Solution:

- (i) Using that $\mathcal{F}^{-1} \mathfrak{s}_j \mathcal{F} = e^{+ik_j} [1]$, we obtain

$$\begin{aligned} H^{\mathcal{F}} &= \mathcal{F}^{-1} H \mathcal{F} \\ &\stackrel{[2]}{=} \begin{pmatrix} q_3 \text{id}_{L^2(\mathbb{T}^2)} & \text{id}_{L^2(\mathbb{T}^2)} + q_1 e^{+i\hat{k}_1} + q_2 e^{+i\hat{k}_2} \\ \text{id}_{L^2(\mathbb{T}^2)} + q_1 e^{-i\hat{k}_1} + q_2 e^{-i\hat{k}_2} & -q_3 \text{id}_{L^2(\mathbb{T}^2)} \end{pmatrix} \\ &= \begin{pmatrix} q_3 \text{id}_{L^2(\mathbb{T}^2)} & \omega(\hat{k}) \\ \omega(\hat{k}) & -q_3 \text{id}_{L^2(\mathbb{T}^2)} \end{pmatrix} \end{aligned}$$

where $\omega(k) = 1 + q_1 e^{+ik_1} + q_2 e^{+ik_2}$ is defined just as in the lecture. $H^{\mathcal{F}}$ is a bounded operator acting on $L^2(\mathbb{T}^2, \mathbb{C}^2) [1]$.

- (ii) The matrix-valued function can be read off as

$$T(k) \stackrel{[1]}{=} \begin{pmatrix} q_3 & \omega(k) \\ \omega(k) & -q_3 \end{pmatrix} \stackrel{[1]}{=} \text{Re}(\omega(k)) \sigma_1 - \text{Im}(\omega(k)) \sigma_2 + q_3 \sigma_3.$$

- (iii) The eigenvalues and eigenprojections have already been calculated in problem 35:

$$\begin{aligned} E_{\pm}(k) &\stackrel{[1]}{=} \pm \sqrt{q_3^2 + |\omega(k)|^2} \\ P_{\pm}(k) &\stackrel{[1]}{=} \frac{1}{2} \left(\text{id}_{L^2(\mathbb{T}^2)} \pm \frac{\text{Re}(\omega(k)) \sigma_1 - \text{Im}(\omega(k)) \sigma_2 + q_3 \sigma_3}{E_{\pm}(k)} \right) \end{aligned}$$

(iv) Problem 36 (ii) has introduced an efficient way to compute the unitary time evolution in the momentum representation [1]:

$$U^{\mathcal{F}}(t) = e^{-itH^{\mathcal{F}}} \stackrel{[1]}{=} \cos(E_+(\hat{k})t) \text{id}_{L^2(\mathbb{T}^2, \mathbb{C}^2)} - \frac{i \sin(E_+(\hat{k})t)}{E_+(\hat{k})} T(\hat{k})$$

(v) According to Proposition 6.1.5 (ii), $\mathcal{F}(fg) = \mathcal{F}f * \mathcal{F}g$ holds [1], and hence

$$\begin{aligned} U(t)\psi &\stackrel{[1]}{=} \mathcal{F}U^{\mathcal{F}}(t)\mathcal{F}^{-1}\psi \\ &\stackrel{[1]}{=} \mathcal{F}\left(\cos(E_+t) \text{id}_{L^2(\mathbb{T}^2, \mathbb{C}^2)} - \frac{i \sin(E_+t)}{E_+} T\right) * \psi \end{aligned}$$

(vi) The system has no gap if and only if $E_+(k)^2 = q_3^2 + |\omega(k)|^2 = 0$ for some $k \in \mathbb{T}^2$. This is zero if and only if $q_3 = 0$ and

$$\omega(k) = 1 + q_1 e^{-ik_1} + q_2 e^{-ik_2} \stackrel{!}{=} 0$$

The result is best explained in a graph (Figure 2 (b) in the aforementioned publication):

