

Differential Equations of Mathematical Physics (APM 351 Y)

2013–2014 Problem Sheet 10 (2013.11.21)

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

Homework Problems

34. The Fourier transform of various functions

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

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

35. The Pauli matrices

Consider the three Pauli matrices

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

(i) Prove $\sigma_j \sigma_k = \delta_{jk} \operatorname{id}_{\mathbb{C}^2} + \operatorname{i} \sum_{l=1}^3 \epsilon_{jkl} \sigma_l$ 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 $h = (h_1, h_2, h_3)$,

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

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

- (iii) Now assume that the coefficients h_0, \ldots, h_3 in equation (1) are real. Show that then the resulting matrix $H = h_0 \operatorname{id}_{\mathbb{C}^2} + h \cdot \sigma$ 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, \ldots, h_3

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

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 $h = (h_1, h_2, h_3)$.

36. Functional calculus for 2×2 matrices

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

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

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

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

$$f(H) = e^{-ith_0} \left(\cos(|h|t) - \frac{i}{|h|} \sin(|h|t) h \cdot \sigma \right) = e^{-itH} = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} H^n.$$
(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) $-\mathbf{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = (h_0\,\mathbf{i}\mathrm{d}_{\mathbb{C}^2} + h_3\,\sigma_3)\psi(t)$

37. A simple model for graphene

Consider the nearest-neighbor model for graphene

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

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

Hand in home work on: Thursday, 28 November 2013, before class