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1 Intro to LFT – Exercise sheet 1 2025-04-15

1.1 Exercise 1

Since the new basis $\{b^n\}$ needs to be orthonormal - the allowed transformations are

1. permutation of the basis vectors $\{e^n\}$
2. and then a rigid rotation of the whole basis

This transformations the basis mean ($O \in O(N)$)

$$\begin{aligned}
e^n &= \sum_m O^n_m b^m && (1)\\
\rightarrow v &= \alpha_n e^n && (2)\\
&= \sum_m (\sum_n O^n_m \alpha_n) b^m && (3)\\
&= \sum_m \beta_m b^m && (4)\\
\rightarrow \beta_m &= \sum_n O^n_m \alpha_n && (5)
\end{aligned}$$

Now with $d\beta_m = \sum_n O^n_m d\alpha_n$

$$\begin{aligned}
I'(f) &= \int \left(\prod_i d\beta_i\right) f(\underbrace{\beta_k b^k}_{=\alpha_k a^k}) && (6)\\
&= \int \left(\prod_i \sum_n O^n_i d\alpha_n\right) f(\underbrace{\beta_k b^k}_{=\alpha_k a^k}) && (7)\\
&= \int |\underbrace{\det O}_{\pm 1}| \left(\prod_i d\alpha_n\right) f(\underbrace{\beta_k b^k}_{=\alpha_k a^k}) && (8)\\
&= \int \left(\prod_i d\alpha_n\right) f(\alpha_k a^k) && (9)\\
&= I(f) && (10)
\end{aligned}$$

1.2 Exercise 2

As ususal we try to obtain a complete square

$$-\frac{1}{2}\phi^T A\phi + J^T\phi = -\frac{1}{2}\left(\phi^T A\phi - 2J^T\phi\right) \tag{11}$$
$$= -\frac{1}{2}\left((\phi + x)^T A(\phi + x)\right) + y \tag{12}$$
$$= -\frac{1}{2}\left(\phi^T A\phi + \phi^T Ax + x^T A\phi + x^T Ax\right) + y \tag{13}$$

with $x = -A^{-1}J$

$$-\frac{1}{2}\phi^T A\phi + J^T\phi = -\frac{1}{2}\left(\phi^T A\phi - \phi^T A(A^{-1}J) - (A^{-1}J)^T A\phi + (A^{-1}J)^T A(A^{-1}J)\right) + y \tag{14}$$
$$= -\frac{1}{2}\left(\phi^T A\phi - J^T\phi + \phi^T J + J^T A^{-1}J\right) + \frac{1}{2}J^T A^{-1}J \tag{15}$$
$$= -\frac{1}{2}\left(\phi^T A\phi - J^T\phi + (J^T\phi)^T + J^T A^{-1}J\right) + \frac{1}{2}J^T A^{-1}J \tag{16}$$

and therefore

$$-\frac{1}{2}\phi^T A\phi + J^T\phi = -\frac{1}{2}(\phi - A^{-1}J)^T A(\phi - A^{-1}J) + \frac{1}{2}J^T A^{-1}J \tag{17}$$

So

$$I(J) = \int d\phi\ \exp\left[-\frac{1}{2}(\phi - A^{-1}J)^T A(\phi - A^{-1}J)\right] \cdot \exp\left[\frac{1}{2}J^T A^{-1}J\right] \tag{18}$$
$$= \exp\left[\frac{1}{2}J^T A^{-1}J\right] \cdot \int d\phi\ \exp\left[-\frac{1}{2}(\phi - A^{-1}J)^T A(\phi - A^{-1}J)\right] \tag{19}$$

To calculate the remaining integral will now try to break it into a product of 1d gaussian integrals (which we know how to calculate).

- As A is real and symmetric we can write it as $A = S^T DS$ where D is diagonal (with positive eigenvalues of A on the diagonal) and S is orthogonal $S^{-1} = S^T$

$$I(0) = \int d\phi\ \exp\left[-\frac{1}{2}(\phi - A^{-1}J)^T S^T DS(\phi - A^{-1}J)\right] \tag{20}$$
$$= \int d\phi\ \exp\left[-\frac{1}{2}[S(\phi - A^{-1}J)]^T D[S(\phi - A^{-1}J)]\right] \tag{21}$$
$$= \int d\phi\ \prod_k \exp\left[-\frac{1}{2}[S(\phi - A^{-1}J)]_k^T D_{kk}[S(\phi - A^{-1}J)]_k\right] \tag{22}$$

- Now we can use the result of problem 1 - getting a new orthogonal coordinate system

$$I(0) = \int d\phi\ \prod_k \exp\left[-\frac{1}{2}[S(\phi - A^{-1}J)]_k^T D_{kk}[S(\phi - A^{-1}J)]_k\right] \tag{23}$$
$$= \prod_k \int d\psi_k\ \exp\left[-\frac{1}{2}\psi_k^T D_{kk}\psi_k\right] \tag{24}$$
$$= \prod_k \sqrt{\frac{2\pi}{D_{kk}}} \tag{25}$$
$$= \sqrt{\frac{(2\pi)^N}{detA}} \tag{26}$$

And therefore

$$I(J) = \frac{(2\pi)^{N/2}}{\sqrt{\det A}} \exp\left[\frac{1}{2} J^T A^{-1} J\right] \tag{27}$$

which is finite for every J.

1.3 Exercise 3

With

$$(A\phi)_n = \frac{2\phi_n - \phi_{n\oplus(+1)} - \phi_{n\oplus(-1)}}{a^2} \qquad (n = 1, ..., N) \tag{28}$$

we see that A is the 1d negative discretized Laplacian with periodic boundary conditions (know from finite difference numerics of the heat and Schroedinger equation)

$$A = \frac{1}{a^2}\begin{pmatrix} 2 & -1 & 0 & ... & 0 & 0 & -1 \\ -1 & 2 & -1 & ... & 0 & 0 & 0 \\ 0 & -1 & 2 & ... & 0 & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & ... & 2 & -1 & 0 \\ 0 & 0 & 0 & ... & -1 & 2 & -1 \\ -1 & 0 & 0 & ... & 0 & -1 & 2 \end{pmatrix} \tag{29}$$

This looks like the set of equations of motion for a 1D chain of atoms

$$m\ddot{x}_i = k(u_{i-1} - u_i) + k(u_{i+1} - u_i) \tag{30}$$

in matrix form.

1. We see that A is symmetric - A is positive definite if and only if all eigenvalues are strictly positive - which we might see - once we calculated the eigenvalues.

2. The periodic boundary conditions imply

$$v_0^{(p)} = v_N^{(p)} \quad \to \quad e^{iapN} = 1 \tag{31}$$

$$\to \quad apN = 2\pi k \qquad (k \in \{1, 2, 3, ..., N\}) \tag{32}$$

$$\to \quad p = \frac{2\pi k}{aN} \qquad \text{(Nyquist-Shannon-sampling theorem)} \tag{33}$$

and with $e^{iapN} = 1$ we can calculate

$$(Av^{(p)})_n = (Ae^{iapn})_n \tag{34}$$

$$= \begin{cases} \frac{1}{a^2}(2e^{iap\cdot 1} - e^{iap\cdot 2} - e^{iapN}) = \frac{1}{a^2}(2 - e^{iap} - e^{-iap})e^{iap} & (n = 1) \\ \frac{1}{a^2}(2e^{iapn} - e^{iap(n+1)} - e^{iap(n-1)}) = \frac{1}{a^2}(2 - e^{iap} - e^{-iap})e^{iapn} & \text{else} \\ \frac{1}{a^2}(2e^{iapN} - e^{iap\cdot(1)} - e^{iap\cdot(N-1)}) = \frac{1}{a^2}(2 - e^{iap} - e^{-iap})e^{iapN} & (n = N) \end{cases} \tag{35}$$

$$= \frac{1}{a^2}(2 - e^{iap} - e^{-iap})v_n^{(p)} \tag{36}$$

$$= \frac{2}{a^2}(1 - \cos ap)v_n^{(p)} \tag{37}$$

Now we can read-off the N eigenvectors and eigenvalues are $(1 \leq k \leq N)$

$$v_n^{(k)} = e^{ian\frac{2\pi k}{aN}} = e^{2\pi i\frac{n}{N}k} \tag{38}$$

$$\lambda^{(k)} = \frac{2}{a^2}\left(1 - \cos a\frac{2\pi k}{aN}\right) \tag{39}$$

$$= \frac{2}{a^2}\left(1 - \cos\frac{2\pi k}{N}\right) \tag{40}$$

$$= \frac{2}{a^2}\left(1 - \cos^2\frac{\pi k}{N} + \sin^2\frac{\pi k}{N}\right) \tag{41}$$

$$= \frac{4}{a^2}\sin^2\frac{\pi k}{N} = \left(\frac{2}{a}\sin\frac{\pi k}{N}\right)^2 \tag{42}$$

As expected - this looks like the dispersion relation $\omega(k)$ for a 1D chain of atoms. Now we see that $\lambda^{(N)} = 0$ so A is NOT positive definite but positive semi-definite.

3. Lets rewright

$$v^{(k)} = e^{2\pi i \frac{n}{N} k} = \cos\left(2\pi \frac{n}{N} k\right) + i \sin\left(2\pi \frac{n}{N} k\right) \tag{43}$$

so - using results from elementary Fourier analysis - we rewrite the completeness relation as a (finite) Fourier series

k	$\lambda^{(k)}$	(complex) $v_n^{(k)}$	(real) $u_n^{(k)}$	(real) $u_n^{(k)}$
1	$\frac{4}{a^2}\sin^2\left(\pi\frac{1}{N}\right)$	$\exp\left(2\pi\frac{in}{N}\right)$	$\sqrt{\frac{2}{N}}\cos\left(2\pi\frac{n}{N}\right)$	$\sqrt{\frac{2}{N}}\sin\left(2\pi\frac{n}{N}\right)$
2	$\frac{4}{a^2}\sin^2\left(\pi\frac{2}{N}\right)$	$\exp\left(2\pi\frac{2in}{N}\right)$	$\sqrt{\frac{2}{N}}\cos\left(2\pi\frac{2n}{N}\right)$	$\sqrt{\frac{2}{N}}\sin\left(2\pi\frac{2n}{N}\right)$
...				
$(N/2)$	$\frac{4}{a^2}$	$\exp\left(i\pi n\right)$	$\sqrt{\frac{2}{L}}(-1)^n$	0
...				
$N-2$	$\frac{4}{a^2}\sin^2\left(\pi\frac{2}{N}\right)$	$\exp\left(-2\pi\frac{2in}{N}\right)$	$\sqrt{\frac{2}{N}}\cos\left(2\pi\frac{2n}{N}\right)$	$-\sqrt{\frac{2}{N}}\sin\left(2\pi\frac{2n}{N}\right)$
$N-1$	$\frac{4}{a^2}\sin^2\left(\pi\frac{1}{N}\right)$	$\exp\left(-2\pi\frac{in}{N}\right)$	$\sqrt{\frac{2}{N}}\cos\left(2\pi\frac{n}{N}\right)$	$-\sqrt{\frac{2}{N}}\sin\left(2\pi\frac{n}{N}\right)$
N	0	1	$\sqrt{\frac{1}{N}}$	0

Table 1: Overview of eigensystems

and we see that we can drop half of the sine and cosine eigenfunctions occurring twice (up to a potential sign) - so we can drop them. So depending on N even or odd

$$u^{(N)} = \sqrt{\frac{1}{N}} \tag{44}$$

$$u^{(k)} = \sqrt{\frac{2}{N}} \cos\left(2\pi \frac{n}{N} k\right) \qquad (k = 1..[N-1/2]) \tag{45}$$

$$u^{(N/2+k)} = \sqrt{\frac{2}{N}} \sin\left(2\pi \frac{n}{N} k\right) \qquad (k = 1..[N-1/2]) \tag{46}$$

$$u^{(N/2)} = \sqrt{\frac{2}{N}} (-1)^n \qquad (\text{iff } N \text{ is even}) \tag{47}$$

It looks a bit messy in the write-up but I think its clear.

4. The eigenvalues $\tilde{\lambda}^{(k)}$ of $A + m^2 = A + 1_{N\times N} m^2$ are

$$\tilde{\lambda}^{(k)} = \lambda^{(k)} + m^2 \tag{48}$$

$$= \frac{4}{a^2} \sin^2 \frac{\pi k}{N} + m^2 \tag{49}$$

while the eigenvectors are the same as for A. Using the spectral decomposition to calculate the inverse of $(A+m^2)^{-1}$ (which has the inverse eigenvalues and the same eigenvectors)

$$(A+m^2)^{-1} = \sum_k \frac{1}{\tilde{\lambda}^{(k)}} {u^{(k)}}^T u^{(k)} \tag{50}$$

$$(A+m^2)^{-1}_{ij} = \sum_k \frac{1}{\frac{4}{a^2}\sin^2\frac{\pi k}{N} + m^2} {u_i^{(k)}}^T u_j^{(k)} \tag{51}$$

I tried to find a simple expression using Mathematica - but could not find anything. Alternatively I also tried

$$\frac{1}{A+m^2} = \frac{1}{m^2}\left(1 - \frac{1}{m^2}A + \frac{1}{m^4}A^2 - \frac{1}{m^6}A^3 + ...\right) \tag{52}$$

$$\frac{1}{A+m^2}_{ij} = u^{(i)T}\frac{1}{A+m^2}u^{(j)} \tag{53}$$

$$= \frac{1}{m^2}\left(1 - \frac{1}{m^2}u^{(i)T}Au^{(j)} + \frac{1}{m^4}u^{(i)T}A^2u^{(j)} - \frac{1}{m^6}u^{(i)T}A^3u^{(j)} + ...\right) \tag{54}$$

$$= \frac{1}{m^2}\left(1 - \frac{1}{m^2}u^{(i)T}\lambda^{(j)}u^{(j)} + \frac{1}{m^4}u^{(i)T}(\lambda^{(j)})^2u^{(j)} - \frac{1}{m^6}u^{(i)T}(\lambda^{(j)})^3u^{(j)} + ...\right) \tag{55}$$

$$= \frac{1}{m^2}\left(1 - \frac{\lambda^{(j)}}{m^2}u^{(i)T}u^{(j)} + \frac{(\lambda^{(j)})^2}{m^4}u^{(i)T}u^{(j)} - \frac{(\lambda^{(j)})^3}{m^6}u^{(i)T}u^{(j)} + ...\right) \tag{56}$$

but got nowhere.