Laplacian eigenmodes in twisted periodic topologies for new physics models

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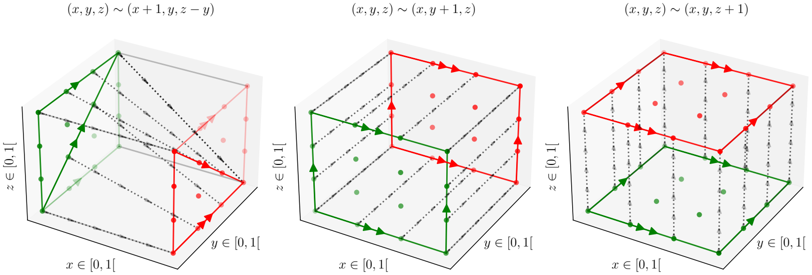
Outline

1. $\mathcal{M}_3$ Laplacian & similar examples:
   - Möbius strip,
   - $R\mathbb{P}^2$,
   - $\mathbb{T}^3$.
2. Physics-informed neural networks
   - Architecture,
   - Optimisation algorithm,
   - Implementation.
3. Numerical results
4. Summary & Outlook

$\mathcal{M}_3$ i.e. 3-nilmanifold

- $\mathcal{M}_3$ negatively curved spaces ($\mathcal{R} < 0$) built from solvable Lie groups & algebras.
- **Motivations:** Kaluza-Klein type models with compactified extra-dimensions.
- Discrete/Twist identifications ("boundary conditions"):

$$(x, y, z) \sim (x+1, y, z-y) \sim (x, y+1, z) \sim (x, y, z+1)$$



Exact $\mathcal{M}_3$ eigenmodes

- Special/simplest case of $\mathcal{M}_3$ metric:

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = dx^2 + dy^2 + (dz^2 + xdy)^2.$$

- Laplacian (RHS):

$$\nabla^2 u_{k,l,n} = (\partial_x^2 + (\partial_y - x\partial_z)^2 + \partial_z^2)u_{k,l,n}, \quad \nabla^2 v_{p,q} = (\partial_x^2 + \partial_y^2)v_{p,q}.$$

- $\mathbb{T}^2$ & "fibre" eigenmodes:

$$\begin{aligned} v_{p,q}(x,y) &= e^{2\pi i(px+qy)}, \quad \mu_{p,q}^2 = 4\pi^2(p^2+q^2), \quad p,q \in \mathbb{Z}; \\ u_{k,\ell,n}(x,y,z) &= e^{2\pi ki(z+xy)} e^{2\pi \ell ix} \sum_{m\in\mathbb{Z}} e^{2\pi kmix} \Phi_n^{2\pi k}\left(y + m - \frac{\ell}{k}\right), \\ M_{k,n}^2 &= (2\pi k)^2 \left(1 + \frac{2n+1}{2\pi|k|}\right); \quad k \in \mathbb{Z}^*, \ell = 0, \ldots, |k-1|, n \in \mathbb{N}. \end{aligned}$$

- where $\Phi_n^{2\pi k}$ are Hermite functions (non-separable).
- **Non-separable**, precludes simple separation of variables.

Andriot et al (2016) *JHEP* **2016** 169

Eigenmodes of twisted/periodic topologies (a)

1. Möbius strip:

   (a). **Flat** i.e. $\Omega_{x,y} \in [0, L[\times [-\frac{W}{2}, \frac{W}{2}]$:

   - Exact eigenvalues:

$$\sigma(\Delta^{\Omega_{x,y}}) \supset \left\{ \left(\frac{n_x \pi}{L}\right)^2 + \left(\frac{n_y \pi}{W}\right)^2 \right\}_{\substack{n_x \in \mathbb{Z} \\ n_y \in \mathbb{N}\setminus\{0\} \\ n_x + n_y \text{ odd}}} ;$$

   (b). **Curved** i.e. $\Omega_{u,v} \in [0, 2\pi R] \times [-a, a]$:

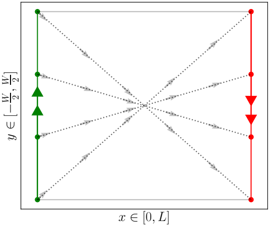
   - 3D embedding:

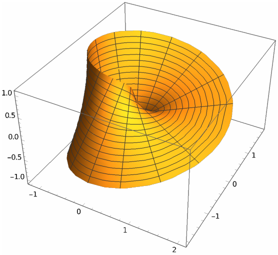
$$\begin{aligned} x(u,v) &= \left[R - v\cos\left(\frac{u}{2R}\right)\right]\cos\left(\frac{u}{R}\right), \\ y(u,v) &= \left[R - v\cos\left(\frac{u}{2R}\right)\right]\sin\left(\frac{u}{R}\right), \\ z(u,v) &= -v\sin\left(\frac{u}{2R}\right). \end{aligned}$$

   - Approx. eigenvalues:

$$\lim_{a\to 0} \sigma(\Delta^{\Omega_{u,v}}) \to \sigma(\Delta^{\Omega_{x,y}}).$$

$u(x,y) = u(x+L,-y)$;
$u(x,-\frac{W}{2}) = u(x,\frac{W}{2}) = 0$

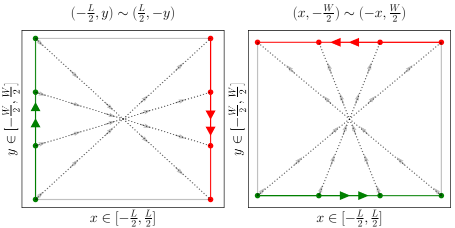




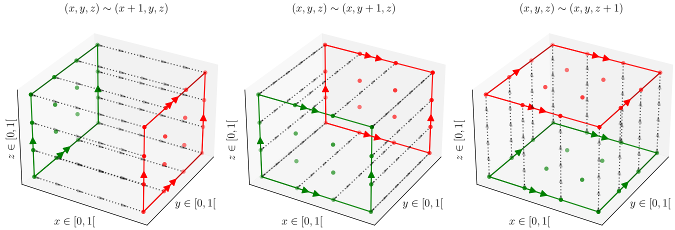
$$u(u,v) = u(u+2\pi R, -v);$$
$$u(u,-a) = u(u,a) = 0.$$

Eigenmodes of twisted/periodic topologies (b)

2. **flat** $R\mathbb{P}^2$: $\Omega_{x,y} := [-\frac{L}{2}, \frac{L}{2}]^2$; $\quad \sigma(\Delta^{\Omega_{x,y}}) \supset \left\{ \left(n_x\pi/L\right)^2 + \left(n_y\pi/W\right)^2 \right\}_{n_x,n_y\in\mathbb{Z}}$.*

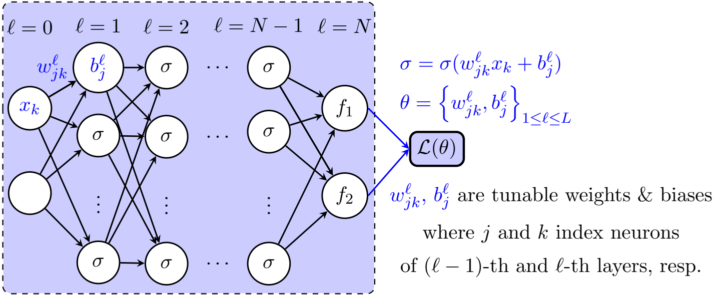


3. **flat** $\mathbb{T}^3$: $\Omega_{x,y,z} := [0,1]^3$; $\quad \sigma(\Delta^{\Omega_{x,y,z}}) \supset \left\{4\pi^2(n_x^2 + n_z^2 + n_z^2)\right\}_{n_x,n_y,n_z\in\mathbb{Z}}$.



* By inspection.

PINN architecture – generic



- FNN ansatz:

$$f(x) = \sigma^{\ell=L} \left[\sum w^{\ell=L} \sigma^{\ell=L} \left(\dots \sum w^{\ell=2} \sigma^{\ell=1} \left(\sum w^1 x + b^1 \right) + b^2 \dots \right) + b^L \right].$$

- Non-linear activation (σ): e.g. trig functions.
- PINN Loss ($\mathcal{L}$): $\mathcal{L}_{PDE} + \mathcal{L}_{IC/BC}$ for solving EIBVPs.

PINN optimisation algorithm – pseudo-code

- Initialise $\theta = \left\{ w_{jk}^{\ell}, b_j^{\ell} \right\}_{1 \leq \ell \leq L}$ randomly from e.g. $U(-\sigma, \sigma)$.
- **For each** epoch **in** training epochs:
  1. Input x_j (training points) + Evaluate $f(x_i)$ and $\mathcal{L}$.
  2. **Backpropagate:** compute $\frac{\partial \mathcal{L}}{\partial \theta} = \left\{ \frac{\partial \mathcal{L}}{\partial w_{jk}^{\ell}}, \frac{\partial \mathcal{L}}{\partial b_j^{\ell}} \right\}_{1 \leq \ell \leq L}$ using autodiff.*
  3. **Update θ:** $w \to w' = w - \frac{\partial \mathcal{L}}{\partial w}, \quad b \to b' = b - \frac{\partial \mathcal{L}}{\partial b}$ (e.g. ADAM optimiser).
- Increment eigenvalue approx e.g. $\hat{E}_{init} = 1$ (given $\hat{E} \in \mathbb{R}^{+}$).

- **Implementation:** Pytorch – an ML open-source library in Python.

PyTorch

* autodiff: exact numerical differentiation.

PINN implementation

- Loss function:

$$\mathcal{L}_{total} = \mathcal{L}_{PDE} + \mathcal{L}_{BC} + \mathcal{L}_{\substack{\text{extra}\\\text{terms}}}$$

- $\mathcal{L}_{BC}$ i.e. enforce twisted periodic boundary conditions, e.g. $\mathbb{T}^3$:

$$\mathcal{L}_{PBC} = \|u_{\substack{\text{left}\\\text{face}}} - u_{\substack{\text{right}\\\text{face}}}\|^2 + \text{et c.}$$

$$\mathcal{L}_{\substack{\text{extra}\\\text{terms}}} = \text{non-zero solutions} + \text{eigenvalue scanning} + \text{et c.}$$

- Alternatively, periodic input transforms in the architecture:

$$\text{input} = [\sin(2\pi x/L_x), \cos(2\pi x/L_x), \ldots]$$

- Standard hyperparameters e.g. ADAM optimizer, feed-forward NN architecture.

Numerical results – Möbius strip

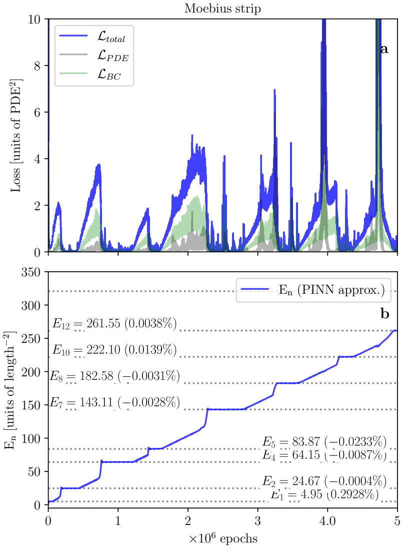
- e.g. Loss (equal weights):

$$\mathcal{L}_{\text{tot}} = \mathcal{L}_{PDE} + \mathcal{L}_{BC} + \mathcal{L}_{\text{extra}}$$

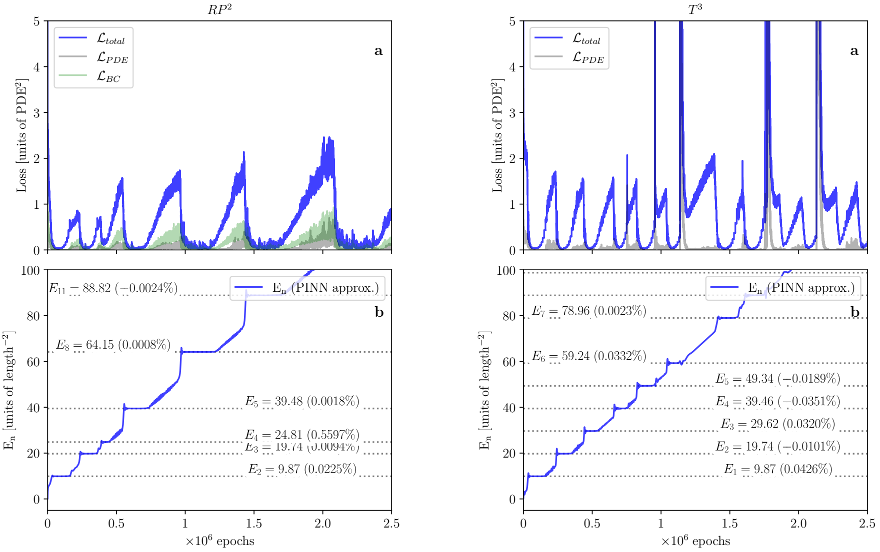
where:

$$\begin{aligned}
\mathcal{L}_{PDE} &= \|\Delta\hat{u}_n + \hat{E}_n\hat{u}\|^2; \\
\mathcal{L}_{BC} &= \|\underbrace{\hat{u}(x,y) - \hat{u}(x+1,-y)}_{\text{twisted PBC}}\|^2 \\
&\quad + \underbrace{\|\hat{u}(x,-0.5)\|^2 + \|\hat{u}(x,0.5)\|^2}_{\text{Dirichlet BC}}; \\
\mathcal{L}_{\text{extra}} &= \frac{1}{\|\hat{u}\|^2} + \frac{1}{\|\hat{E}\|^2} + \|e^{-\hat{E}_{\text{init}} + \hat{E}_{\text{step}}}\|\|^2.
\end{aligned}$$

- RMSE $< 0.5\%$.

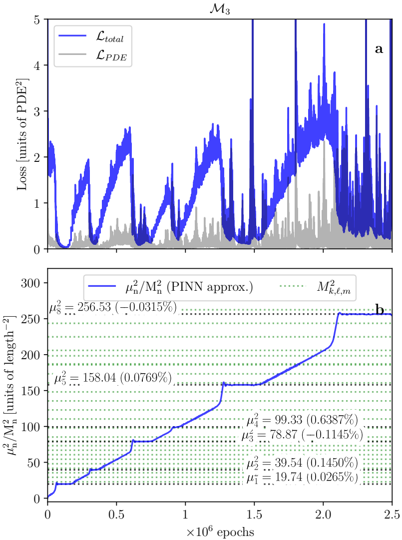


$\mathbb{RP}^2$ and $\mathbb{T}^3$



$\mathcal{M}_3$

- Default separation of variables favours learning $\mathbb{T}^2$ modes ($\mu^2_{p,q}$) vs. fibre modes ($M^2_{k,\ell,m}$).
- Overrides:
  1. Added NN hidden layers;
  2. Loss term weight tuning;
  3. Penalising $du/dz = 0$ (i.e. enforcing z-dependence).
  4. Non-separable ansatz enforcing BCs.
- Yet to test out Singular Value Decomposition as a loss term.



Summary & Outlook

- Solved Laplacian on elementary "twisted periodic" topology (Möbius strip, $R\mathbb{P}^2$ and $\mathbb{T}^3$, within flat spacetime) using PINNs.

- **pros:**
  - Exact vs. PINN approx MSE $< 0.5\%$;
  - Flexibility in setting up PDE, BCs (loss function/NN architecture);
  - Overcome the curse of dimensionality of mesh-based methods.

- **cons:**
  - Defaults to solving separable vs. non-separable functions;
  - Setting up optimal hyperparameters is by trail and error.
  - Sparse literature on the use of PINNs to solve eigenvalue problems.

- **Outlook:** Optimise PINNs to determine non-separable fibre eigenmodes of $\mathcal{M}_3$, consider propagation of SM fields on $\mathcal{M}_3$ & < 3 dimensional spaces.

Thank you