# Stable Evaluation of Lefschetz Thimble Intersection Numbers: Towards Real-Time Path Integrals


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# Motivation

- Oscillatory integrals such as real-time path integrals hard to evaluate due sign problem $\int Dx\ e^{\frac{iS}{\hbar}}$

  numerical instability caused by cancellations in highly oscillatory integrals as integrant keeps changing signs

- **Picard–Lefschetz** theory is powerful framework to manage such oscillatory instabilities

  → BUT: requires knowing so-called intersection numbers

- Methods proposed for up to two dimensional integrals but:

  → higher number of dimensions not well understood and numerically unstable

  → major obstacle to applying the method to realistic, complex problems

# Picard-Lefschetz Theory

- Real integration domain decomposed as a sum of integrals over Lefschetz-Thimbles

$$\int d^L x\, e^{\frac{I(x)}{\hbar}} = \sum_\sigma n_\sigma \int_{J_\sigma} d^L z\, e^{\frac{I(z)}{\hbar}}$$

- Lefschetz-Thimble are steepest-descent cycles in $\mathbb{C}^L$

downward flow

$$J_\sigma = \{z(0) \in \mathbb{C}^L \mid \frac{\partial z_i}{\partial u} = -\overline{\frac{\partial I}{\partial z_i}},\ z(u=-\infty) = z_\sigma\}$$

saddle point

- Along $J_\sigma$ : Im$[I(z)]$ remains constant, Re$[I(z)]$ decreases monotonically

→ integrals over thimbles are convergent and well-defined

- Intersection number $n_\sigma$ specifies contribution of each thimble to integral over original real domain: $n_\sigma = \langle \mathbb{R}^L, K_\sigma \rangle$

upward flow cycle

# Solving Boundary Value Problem

- Integrating upward flow equation: $$\frac{\partial z_i}{\partial u} = \overline{\frac{\partial I}{\partial z_i}}$$

- Single shooting method:
  - start with initial condition $z(0) = z_\sigma + \epsilon$
  - adjust $\epsilon$ to satisfy boundary condition at final point

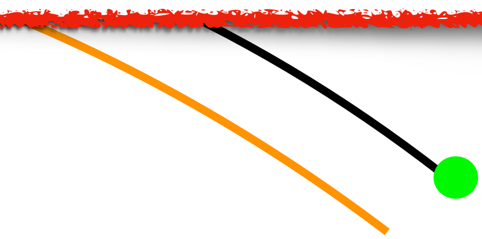
# Solving Boundary Value Problem

- Integrating upward flow equation: $$\frac{\partial z_i}{\partial u} = \overline{\frac{\partial I}{\partial z_i}}$$

- Sin

In systems characterised by strong sensitivity to initial conditions:

tiny change in $\epsilon$ → exponentially diverging trajectories as flow transverses regions of instability

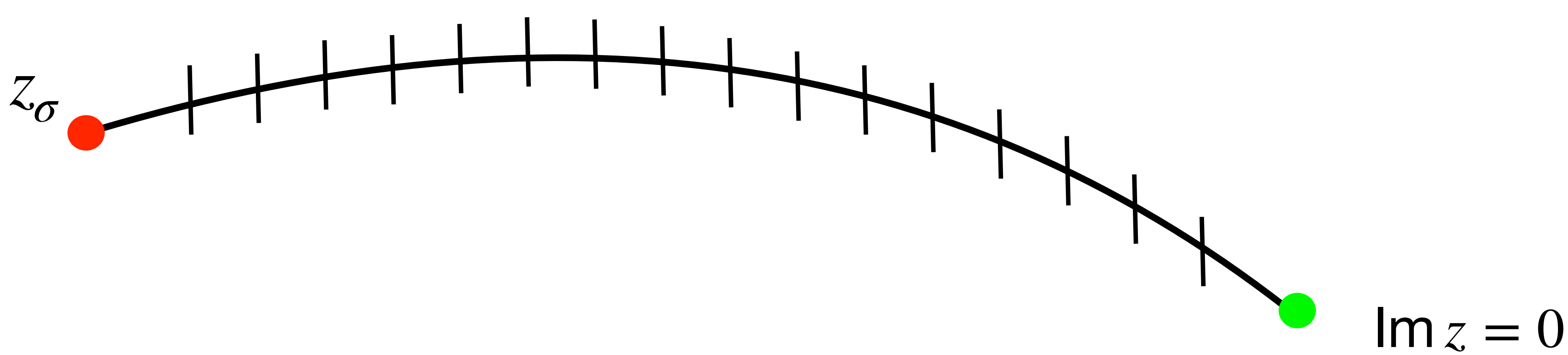


Im $z = 0$

# Solving Boundary Value Problem

- Integrating upward flow equation: $$\frac{\partial z_i}{\partial u} = \overline{\frac{\partial I}{\partial z_i}}$$

- Multiple shooting method:
  - → Domain divided into subintervals with approximately linear dependence on initial conditions
  - → Independent solutions for each interval
  - → Endpoints matched for continuity
  - → Boundary conditions enforced



# Solving Boundary Value Problem

- Integrating upward flow equation: $$\frac{\partial z_i}{\partial u} = \overline{\frac{\partial I}{\partial z_i}}$$

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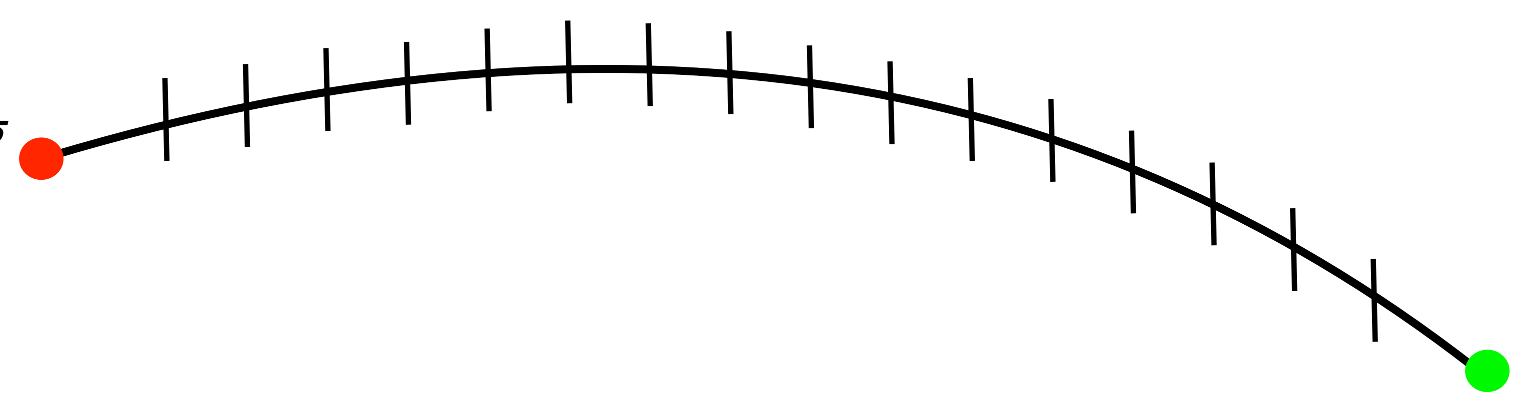
Limits perturbations to linear propagation, overcoming exponential sensitivity

This stabilization enhances robustness and convergence



# Multiple Shooting Method

- Normalized upward flow: $$\frac{\partial z_i}{\partial s} = \frac{\overline{\frac{\partial I}{\partial z_i}}}{\left|\frac{\partial I}{\partial z}\right|}$$
- Decompose complex variables: $Z = (\Re z_0 \cdots \Re z_{L-1} \Im z_0 \cdots \Im z_{L-1})$
- Fix: $N-1$ subintervals with step size $\delta s$
- Continuity condition: $R^{(k)} = Z^{(k)} - \Phi(Z^{(k-1)}; \delta s)$

$$\frac{\partial \Phi}{\partial s}(Z_{\text{init}}; s) = \frac{1}{\left|\frac{\partial I}{\partial z}(\Phi(Z_{\text{init}}; s))\right|} \begin{pmatrix} \Re \frac{\partial I}{\partial z}(\Phi(Z_{\text{init}}; s)) \\ -\Im \frac{\partial I}{\partial z}(\Phi(Z_{\text{init}}; s)) \end{pmatrix}$$

with $\quad \Phi(Z_{\text{init}}; 0) = Z_{\text{init}}$

# Multiple Shooting Method

- Around saddle point $Z_\sigma$ compute eigenvalues $\lambda_i > 0$ and eigenvectors $W_i^\pm$ of Hessian

$$H = \begin{pmatrix} \Re \frac{d^2 I}{dz^2} & -\Im \frac{d^2 I}{dz^2} \\ -\Im \frac{d^2 I}{dz^2} & -\Re \frac{d^2 I}{dz^2} \end{pmatrix}$$

- Boundary conditions:

→ $R_A^{(0)} = |Z(0) - Z_\sigma| - \delta r = 0$ fixing shift freedom along solution

→ $R_B^{(0)} = (W^-)^t (Z(0) - Z_\sigma) = 0$ selecting upward flow

→ $R_B^{(N)} = (0_{L\times L}\, 1_{L\times L}) Z(s_f) = 0$ endpoint on real plane

# Multiple Shooting Method

- $2NL + 1$ nonlinear equations for $2NL + 1$ variables

$$R = \begin{pmatrix} R_A^{(0)} \\ R_B^{(0)} \\ R^{(1)} \\ \vdots \\ R^{(N-1)} \\ R_B^{(N)} \end{pmatrix} = 0 \qquad\qquad X = \begin{pmatrix} Z^{(0)} \\ \vdots \\ Z^{(N-1)} \\ \delta s \end{pmatrix} = 0$$

- Efficiently solved by Newton's method

linear system $\frac{\partial R}{\partial X} \Delta X = - R$ $\qquad X \to X + \Delta X$

nearly block-diagonal

# Intersection Number

- Newton's method clear convergence behaviour:

  → if solution exists, rapid convergence of optimization sequence (typically 100 iterations until limited by numerical precision)

  → $n_\sigma = \pm 1$

  → if no solution exists, sequence oscillates or diverges

  → $n_\sigma = 0$

- Newton's method propagates tangent space of $K_\sigma$ at saddle point to tangent space at intersection point

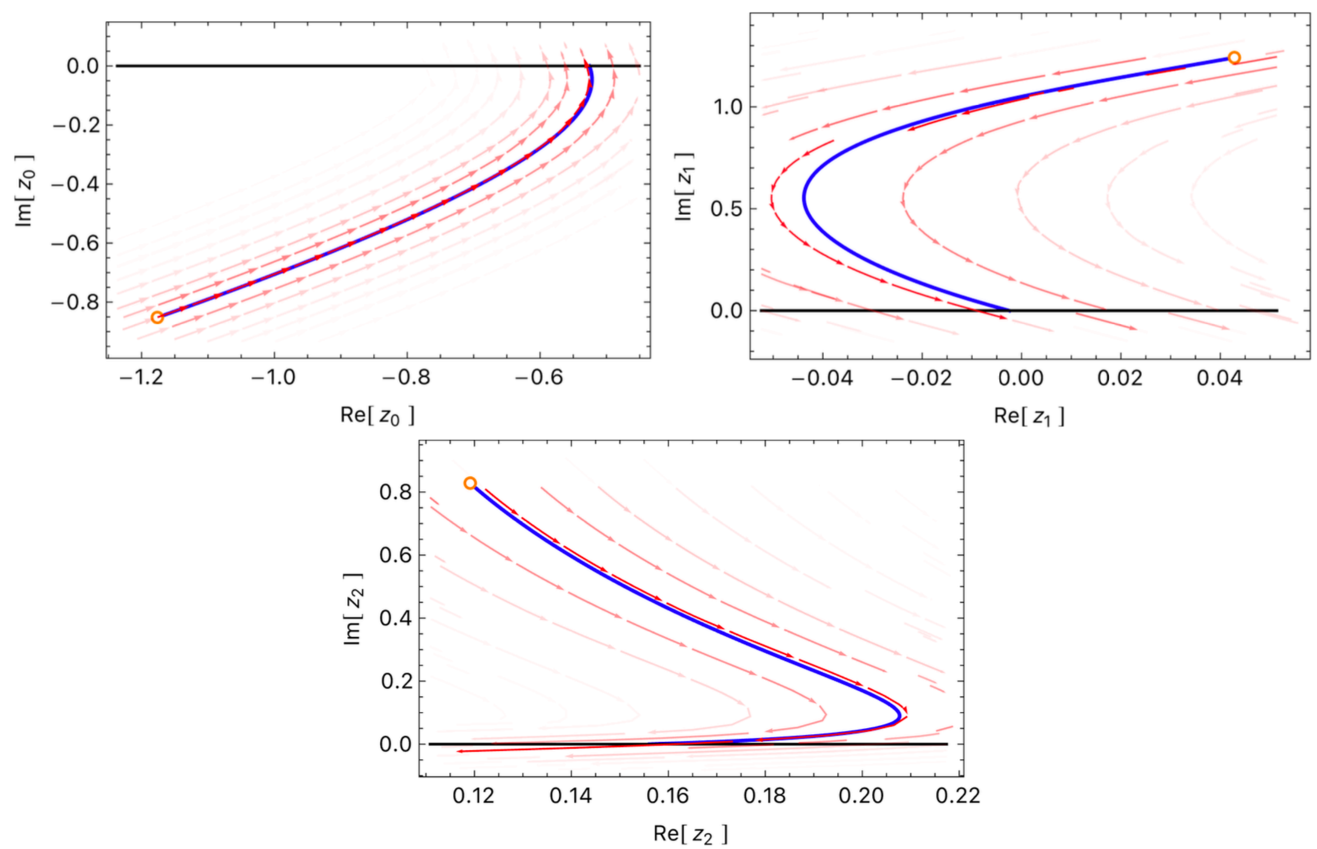
  → determining sign of $n_\sigma$ for given orientation of $J_\sigma$

# Example: Airy-Type Integral

✳ Three-variable example:

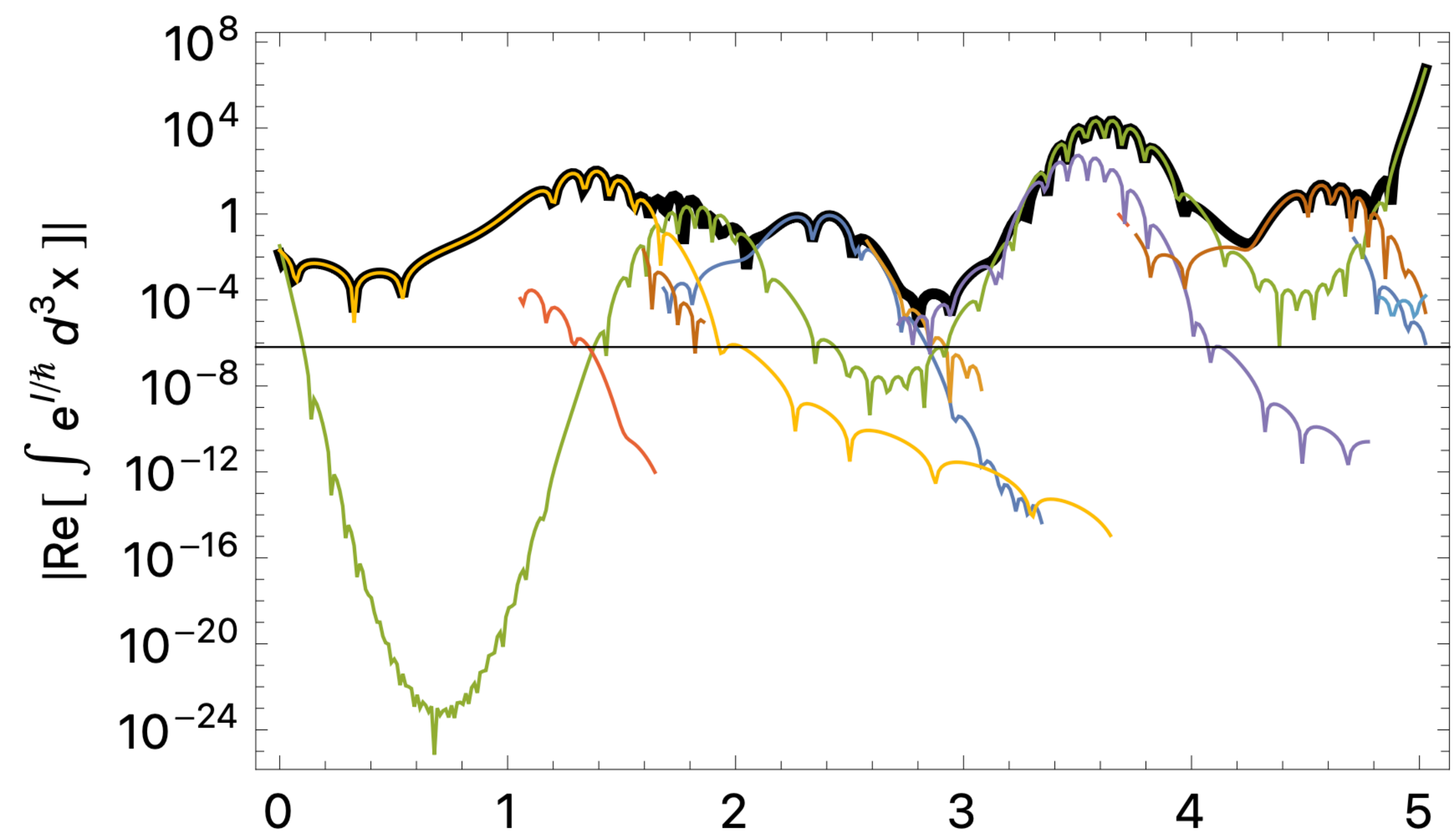
$$I(x) = i\left[\frac{x_0^3 + x_1^3 + x_3^3}{3} - x_0x_1 - x_0x_2 - x_1x_2 + c_0x_0 + c_1x_1 + c_2x_2\right]$$

✳ Upward flow for $c_n = 0.5e^{i(n+1)\alpha}$ with $\alpha = 3.01$



# Example: Airy-Type Integral

✳ Saddle point approximation $\int e^{I(x)/\hbar} d^L x = \sum_\sigma n_\sigma \, A_\sigma \, e^{I(z_\sigma)/\hbar} \left[1 + \mathcal{O}(\hbar)\right]$




$\alpha$

$c_n = 0.5 e^{i(n+1)\alpha}$

Stokes phenomenon!

# Example: Double Well

* Identifying which saddle point contributes to path-integral long-standing problem

* Discretize time duration $T$ of infinite-dimensional path integral into $L$ segments with lattice spacing $\Delta t = T/(L+1)$

$$I(x) = i\left[\frac{1}{2}\sum_{i=1}^{L-1}\left(\frac{x_i - x_{i-1}}{\Delta t}\right)^2 \Delta t + \frac{x_0^2 + x_{L-1}^2}{2\Delta t} - \frac{1}{2}\sum_{i=0}^{L-1}(x_i^2 - 1)^2 \Delta t - \Delta t\right] + \Delta I(x)$$

$$x_i = x((i+1)\Delta t) \qquad i = 1,\ldots,L \qquad x(0) = x(T) = 0$$

* Morsification term, break all symmetries so all saddle points generic

$$\Delta I(x) = ic\left[\sum_{i=0}^{L-1}\left(1 + \left(\frac{i+1}{L+1}\right)^2\right) x_i\right]\Delta t$$

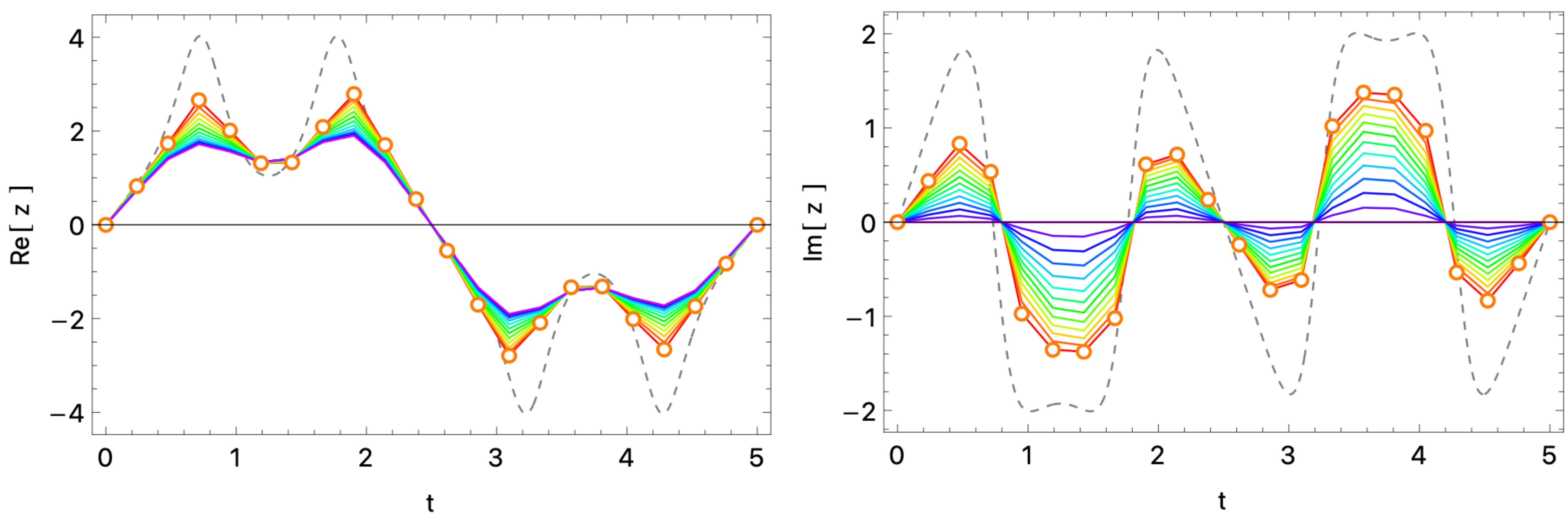
→ allowed to use Morse theory

# Example: Double Well

[Y. Tanizaki, T. Koike, 2014]

- Continuum case all saddle points labeled by two integers $(n, m)$

- Discretised model determine saddles numerically and solve upward flow from each one, using $T = 5, N = 300, \delta r = 0.01, c = 0.001 + 0.001i$




$(n, m) = (4,2)$ for $L = 20$

# Example: Double Well

✳ Cont

✳ Disc … d
flow … .001$i$


$(n, n$

Explicit determination of intersection numbers:
(sign of $n_\sigma$ depends on orientation of thimble, we fix
$\Re(A_\sigma/(2\pi i \Delta t)^{\frac{L+1}{2}}) > 0$ )

| $n$ | $m$ | $\mathcal{I}_\infty[z]$ | $\mathcal{I}(z)$ | $L$ | $n_\sigma$ |
|---|---|---|---|---|---|
| 2 | 1 | $-1.280 + 1.427i$ | $-0.775 + 1.271i$ | 12 | $+1$ |
| 1 | $-2$ | $-1.280 + 1.427i$ | $-0.764 + 1.257i$ | 12 | $+1$ |
| 3 | 2 | $-7.357 - 0.759i$ | – | – | 0 |
| 2 | $-3$ | $-7.357 - 0.759i$ | – | – | 0 |
| 4 | 1 | $-14.926 + 19.727i$ | $-5.783 + 17.860i$ | 16 | $-1$ |
| 1 | $-4$ | $-14.926 + 19.727i$ | $-5.783 + 17.862i$ | 16 | $-1$ |
| 4 | 2 | $-23.946 + 4.198i$ | $-15.311 + 6.545i$ | 20 | $-1$ |
| 2 | $-4$ | $-23.946 + 4.198i$ | $-15.314 + 6.549i$ | 20 | $-1$ |
| 4 | 3 | $-21.025 - 18.980i$ | – | – | 0 |
| 3 | $-4$ | $-21.025 - 18.980i$ | – | – | 0 |

# Conclusions

- ✳ Robust and efficient numerical method for computing intersection numbers of Lefschetz thimbles in multivariable systems
- ✳ Multiple shooting method to overcome sensitivity in initial conditions in upward flow equations
- ✳ Method demonstrated to be effective in systems with tens of variables, achieving rapid convergence and high reliability
- ✳ Broadly applicable to problems involving oscillatory integrals in physics and mathematics
- ✳ Efficient computation enables exploration of complex systems previously inaccessible to conventional methods

# Thank you!