Spinfoam numerics

How to calculate the amplitude and observables

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Overview of the spinfoam numerics

Spinfoam based on different formulations

Booster decomposition:
15j symbol + booster function

Sl2cfoam-next

2212.14396

Coherent states/intertwiners

Integral formulation

- Asymptotic expansion
- Real/complex critical points
- Lefschetz thimbles, Monte Carlo/ metroplis
- ...

Lattic QCD

1807.03066, 2202.04360

2012.11515

2007.01998, 2404.10563

Booster decomposition | Lefschetz thimbles | Asymptotic expansion

small spin (deep quantum)

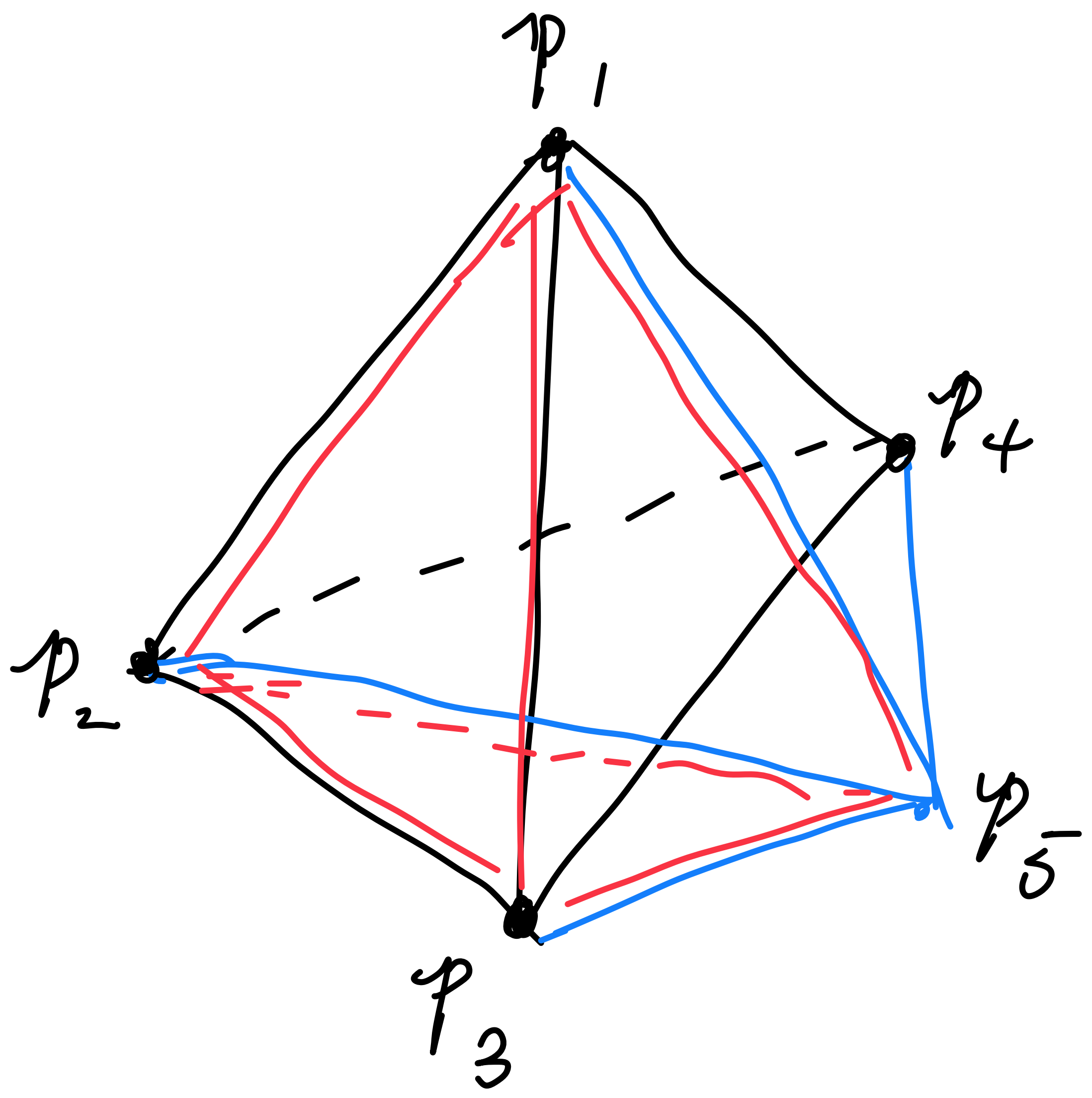
large spin

Spinfoam renomralization: 2211.09578

Structure

1. Introduction to EPRL and its extension
   1.1 Triangulation
   1.2 EPRL transition amplitude
   1.3 Booster function decomposition
   1.4 Integral representation
2. Introduction to (complex) saddle points and Lefschetz thimble methods
3. Numerical examples

Triangulation



4-simplex: triangulation of 4d manifold   generalization of triangles/tetrahedra

4d polytope as convex hull of 5 points

Each set of 4 points gives a tetrahedron

e.g. $[p_1, p_2, p_3, p_4]$ ...   5 tetrahedra e

Each set of 3 points gives a triangle

e.g. $[p_1, p_2, p_3]$ ...   10 triangles f

Each set of 2 points gives a segments

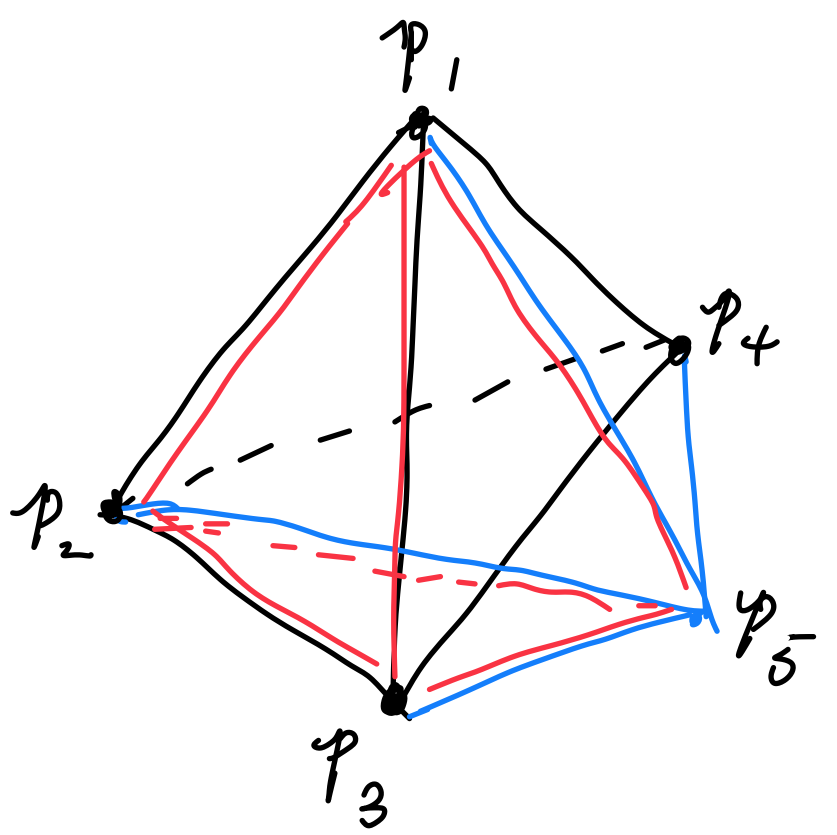
e.g. $[p_1, p_2]$ 10 segments

Can be described by 5 normals $\sum_i N_i V_i = 0 \Leftarrow V_i$ volume of tetrahedra.

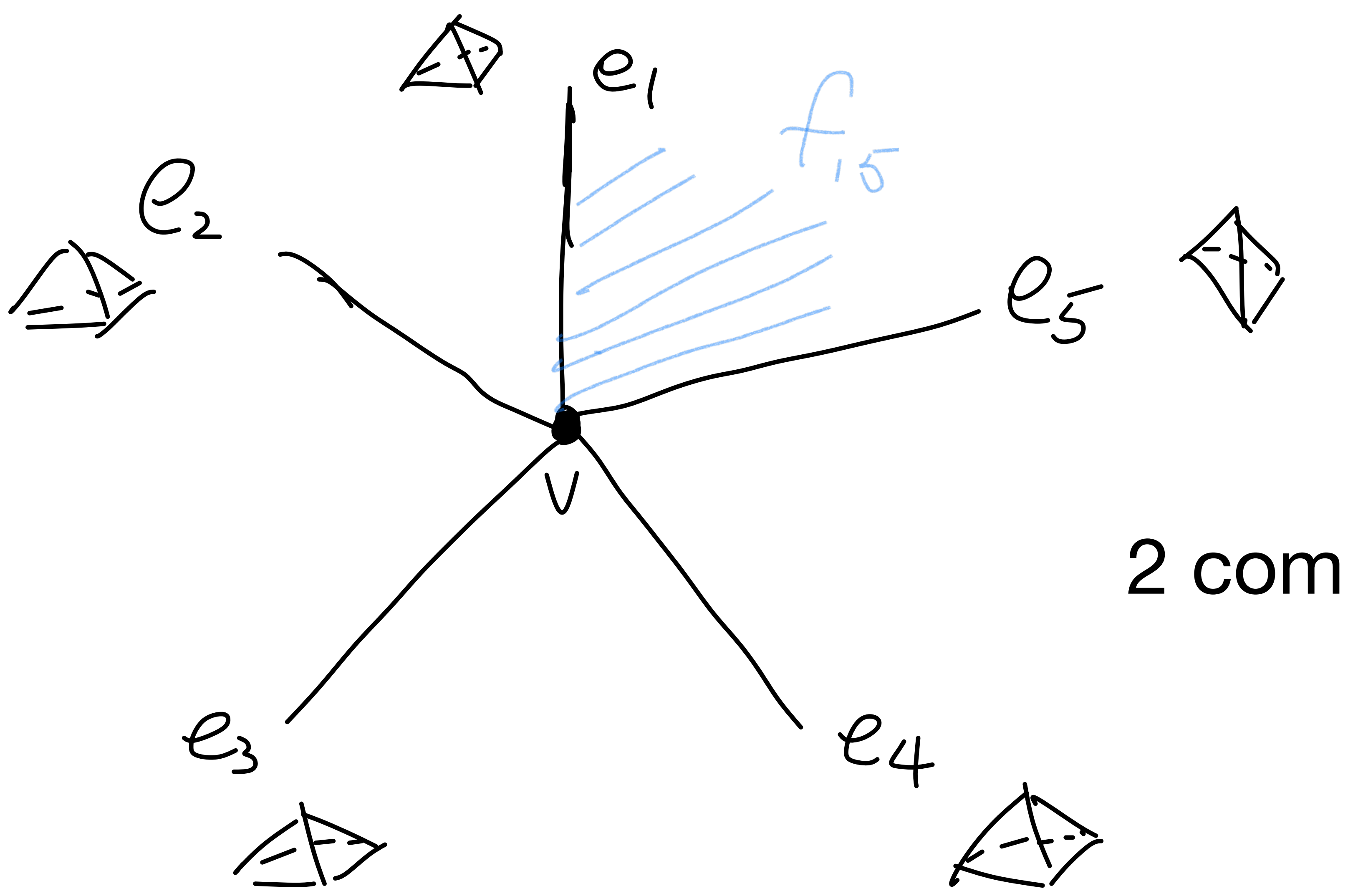
Can be described by 10 bivectors or 10 lengths.

$B_f = A_{ij} \frac{N_j \wedge N_i}{|N_j \wedge N_i|}$, A_{ij} area, describe the triangles.

Triangulation



dual graph



2 complex

group elements

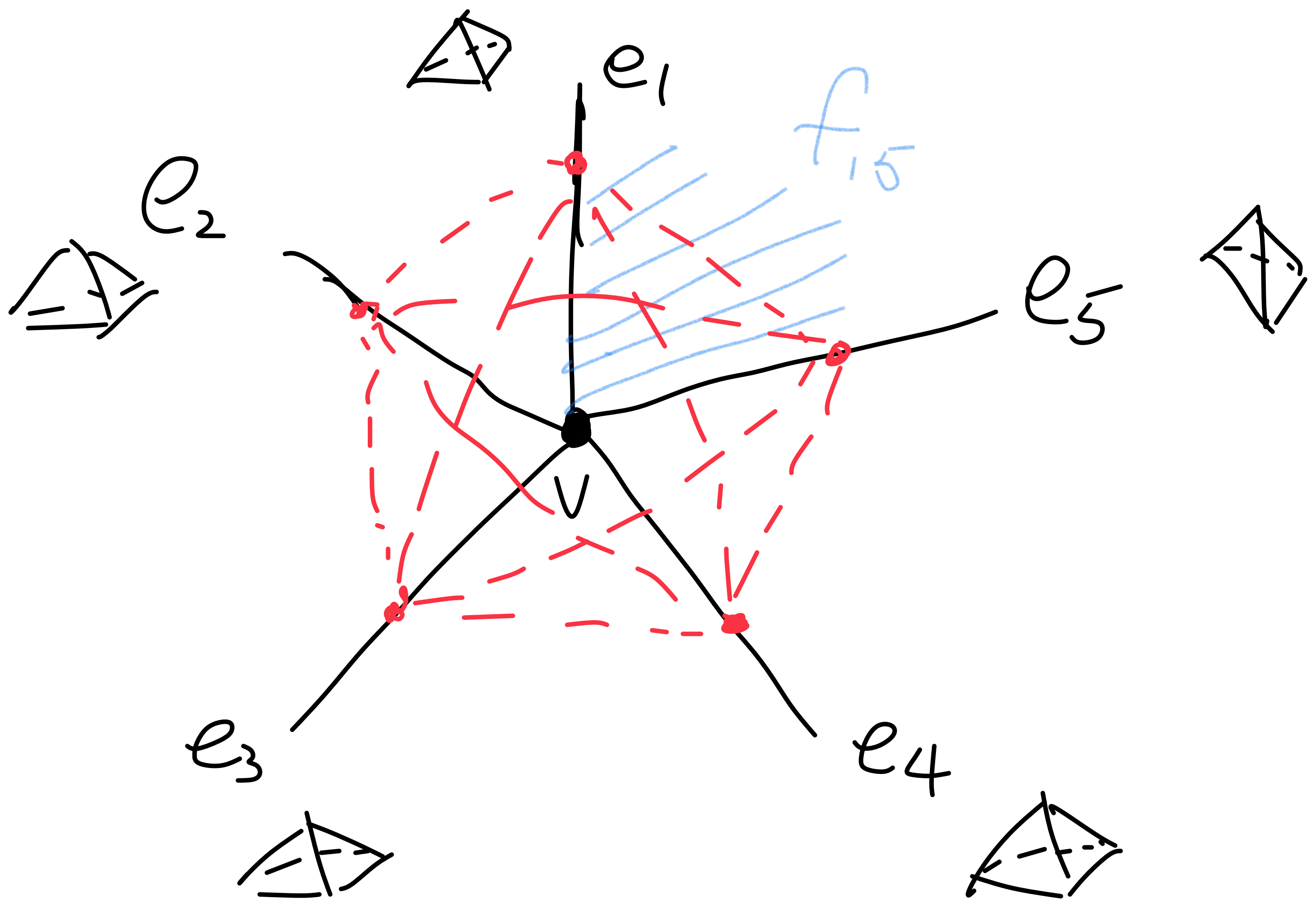
1 4-simplex ⟷ 1 vertex v

5 tetrahedra ⟷ 5 edges e_1, e_2, e_3, e_4, e_5

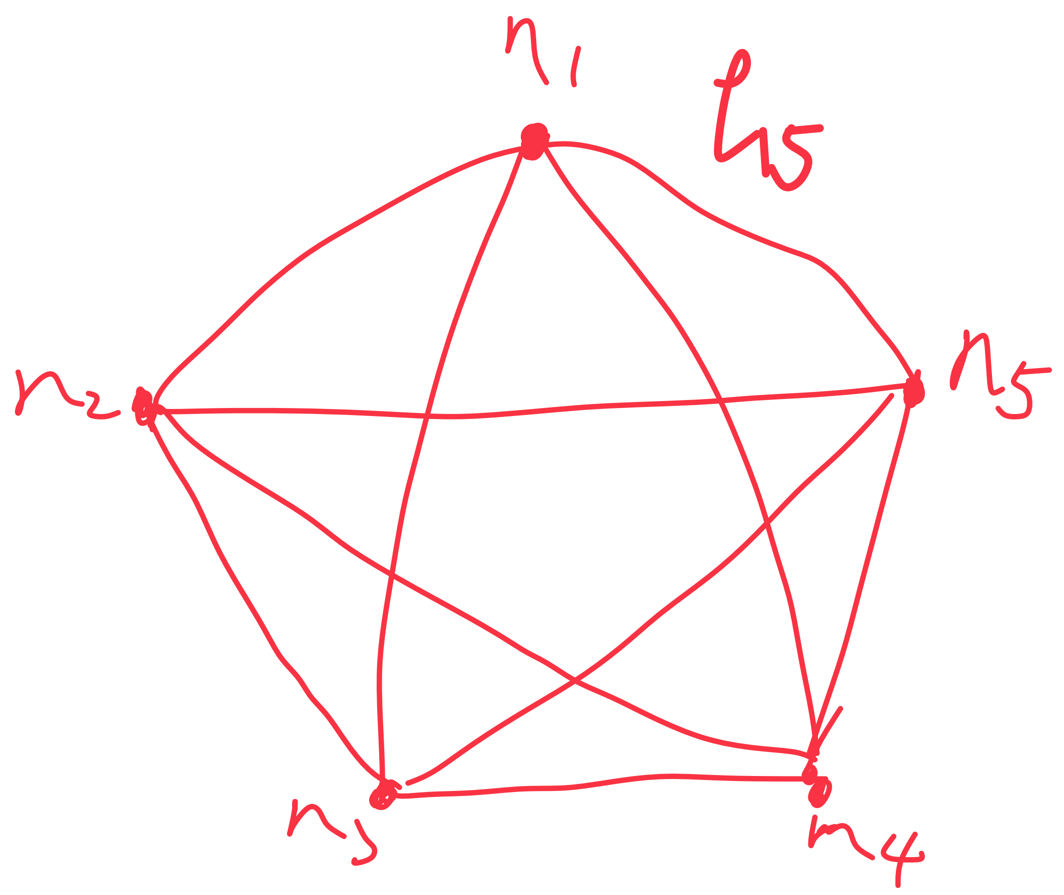
10 triangles ⟷ 10 faces $f_{15}, \ldots$

↖ reps labels. e.g. spin j in SU(2)

Triangulation



boundary graph



boundary spin-network states

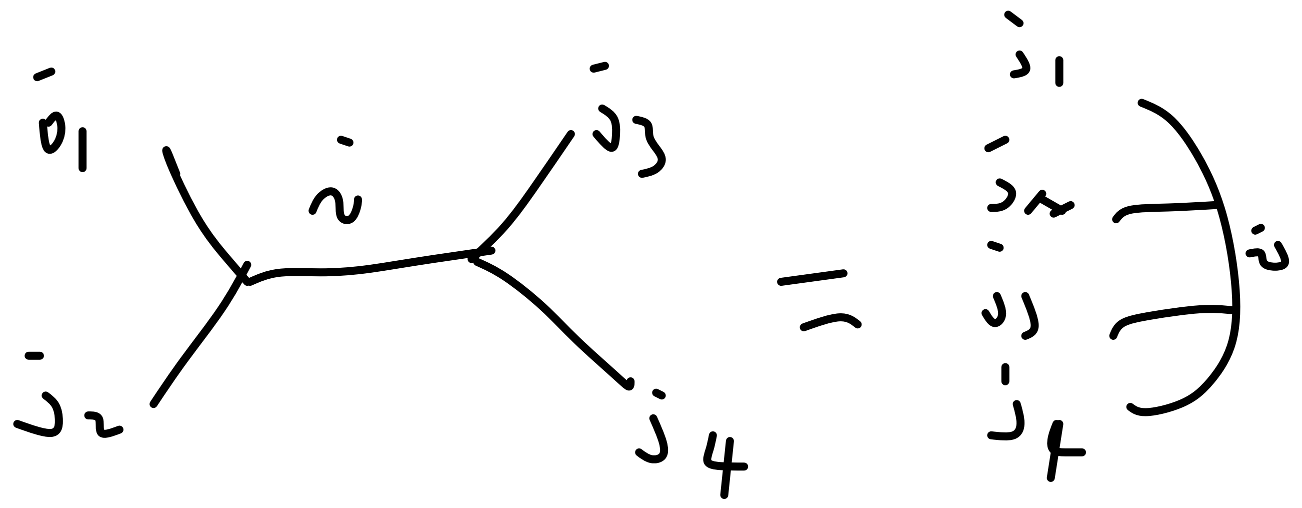
tetrahedra e

faces f

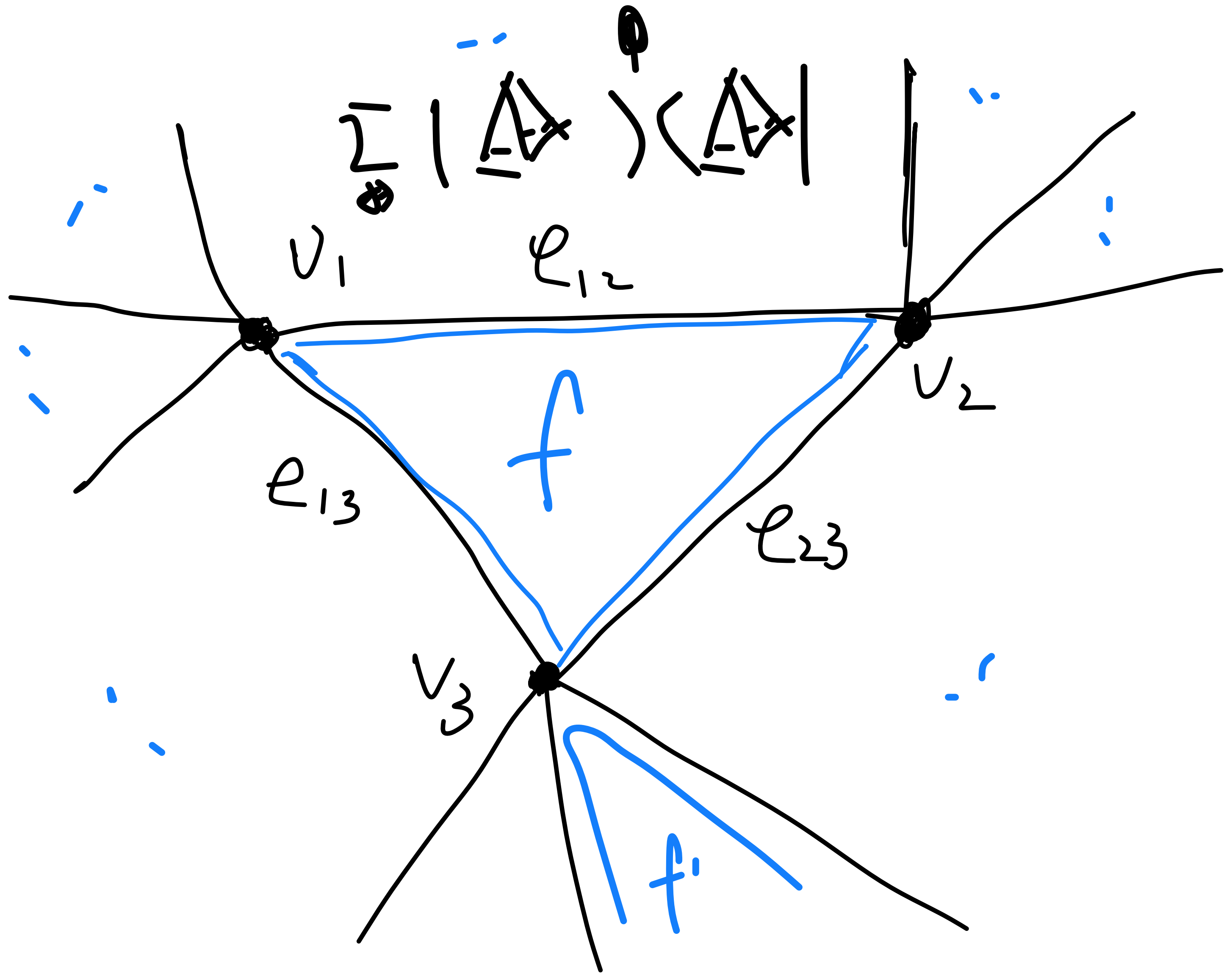
boundary nodes n

boundary links l

4 valent nodes: intertwiners



Triangulation



Full celluar decomposition:

Gluing single vertices via edges

Identifying and integrating states on the glued edge

Internal triangles: summing over reps labels

Spinfoam amplitude:

$$Z = \prod_f A_f \prod_e A_e \prod_v A_v$$

face amp. (A_f), edge amp (A_e), vertex amp (A_v)

EPRL model

SL(2,C) unitary irreps: principle series

SL(2,C) group $g = \begin{pmatrix} a, & b \\ c & d \end{pmatrix}$, $a, b, c, d \in \mathbb{C}$, $ad - bc = 1$.

generators $J^i = \frac{\sigma^i}{2}$, $K^i = \frac{i\sigma^i}{2}$ Casmirs $C_1 = 2(K^2 - J^2) = \frac{1}{2}(n^2 - \rho^2 - 4)$

$C_2 = 4\vec{J} \cdot \vec{K} = n\rho$, $\rho \in \mathbb{R}$.

irreps $\mathcal{H}^{(\rho, n)}$ $n \in \mathbb{Z}_+$

SU(2) decomposition $\mathcal{H}^{(\rho, n)} \simeq \bigoplus_{j \geq n/2}^{\infty} D^j$.

Naimark's canonical basis $J^2 |j m\rangle = j(j+1) |j m\rangle$, $J^3 |j m\rangle = m |j m\rangle$.

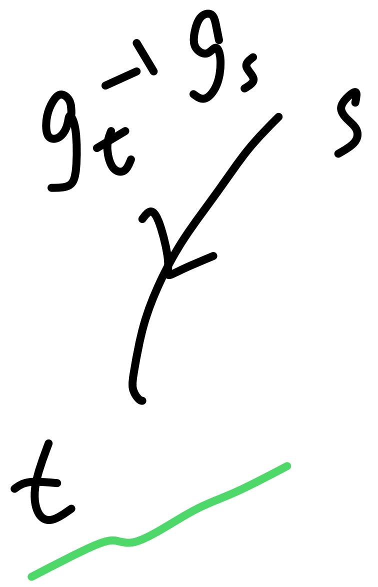
matrix element : $D^{(\rho, n)}_{j_1 m_1, j_2 m_2}$, $|\rho, n; j m\rangle$: $\mathbb{1}_{(\rho, n)} = \sum_{j = n/2}^{\infty} \sum_{m = -j}^{j} |\psi_{jm}\rangle\langle\psi_{jm}|$

EPRL model

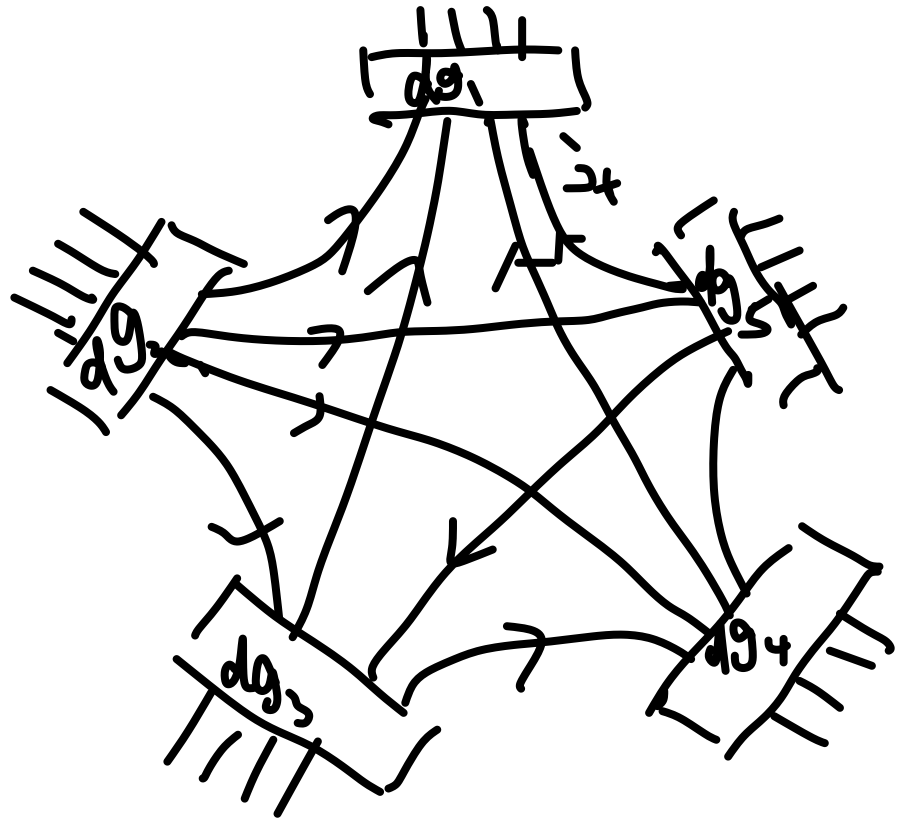
SL(2,C) BF theory + simplicity (weakly imposed)   **ArXiv: 1205.2019, 2310.20147**

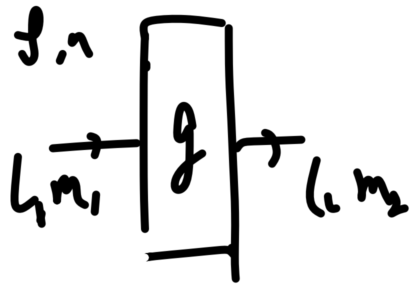
$$Z_v(\Delta) = \int \prod_e dg_e \prod_f \delta\Big(\underbrace{\prod_{e\in\partial f} \overleftarrow{g_e}}_{\text{loop holonomies}}\Big)$$

$$= \sum_{\{\tau_f\}} \int \prod_e dg_e \prod_f d_{\tau_f} \mathrm{Tr}\Big[\tau_f\Big(\prod_{e\in\partial f} \overleftarrow{g_e}\Big)\Big]$$

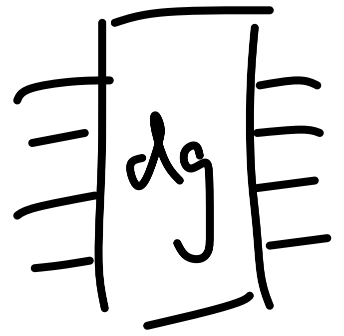


$=$





: $D^{(j,n)}_{l_2 m_2, l_1 m_1}(g)$,



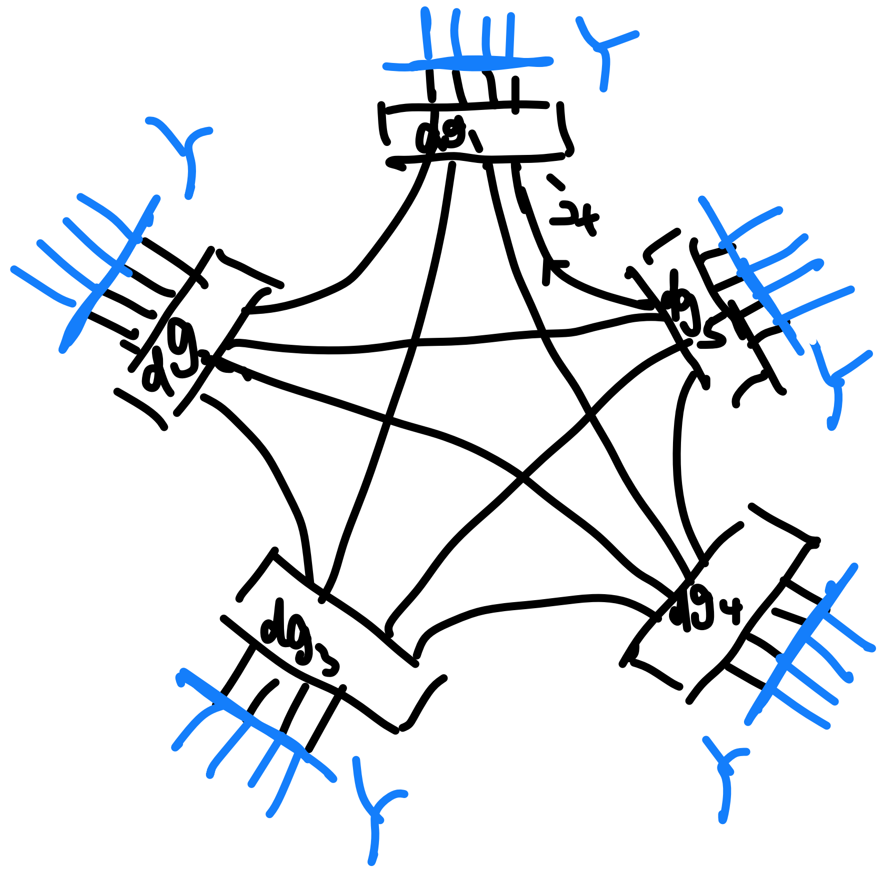
Proj into Inv. space.

Y-map :

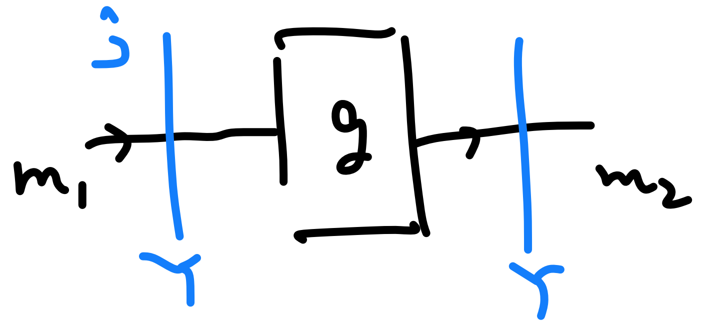
$$D^j \to \mathcal{H}^{(2\gamma j,\, 2j)} \simeq \bigoplus_{\ell \geq j} D^\ell$$

matrix element : $D^{(\gamma j,\, 2j)}_{jm_1,\, jm_2}$

$$Z_v^{EPRL} =$$

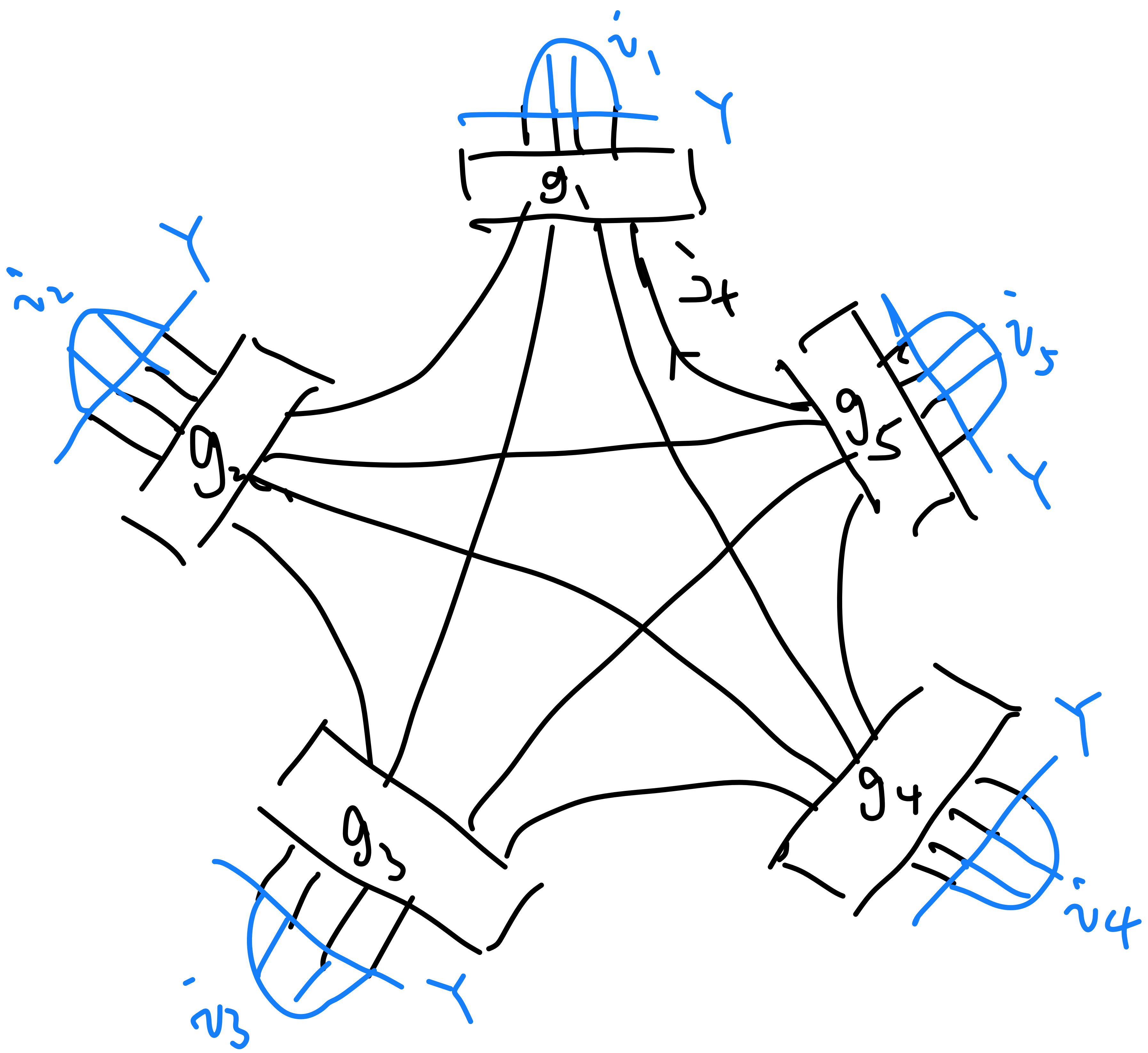


Y map :

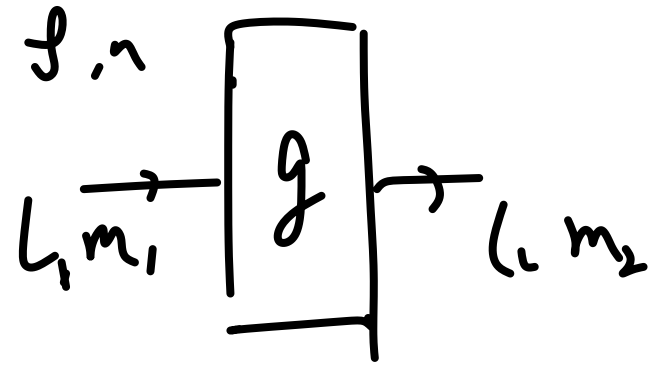


$D^{(2\gamma j,\, 2j)}_{jm_2,\, jm_1}(g)$.

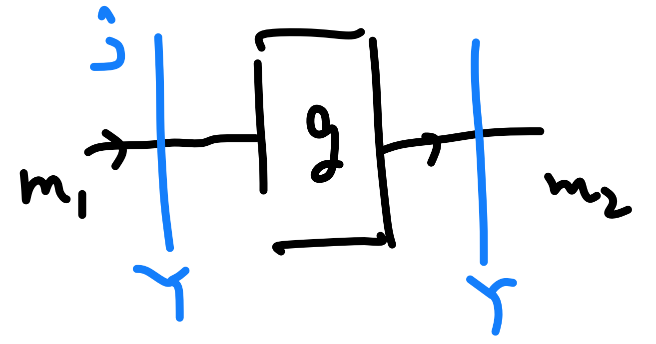
EPRL model



$A_v(j_f, i_e)$

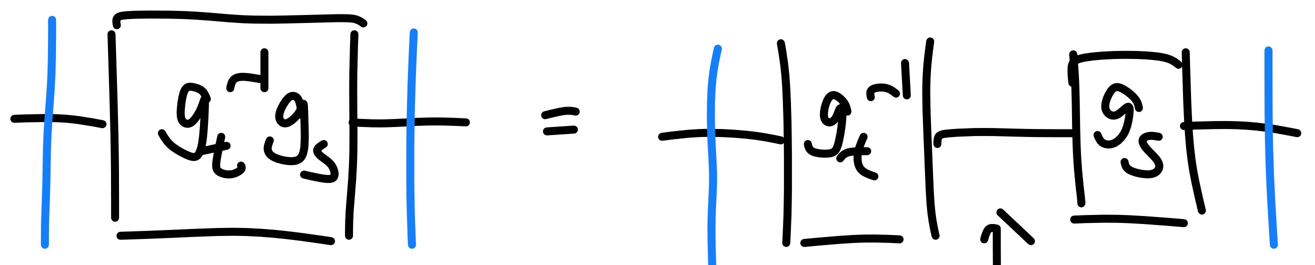


$D^{(\gamma,n)}_{l_2 m_2, l_1 m_1}(g)$



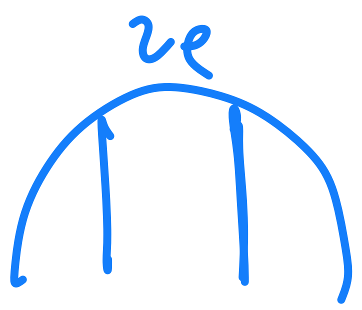
$D^{(2\gamma j, 2j)}_{j m_2, j m_1}(g)$.

$D^{(2\gamma j_f, 2j_f)}_{j_f m_t, j_f m_s}(g_t^{-1} g_s)$:



resolution of Identity in $\mathcal{H}^{(\rho,n)}$ $(\ell \geq j)$

Y map only on bdy.



$= \begin{pmatrix} j_i \\ m_i \end{pmatrix}^{(i)} = \sum_m (-1)^{i-m} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} \begin{pmatrix} j & j_3 & j_4 \\ -m & m_3 & m_4 \end{pmatrix}$ ← intertwiner

(3j symbol)

$u \in SU(2)$

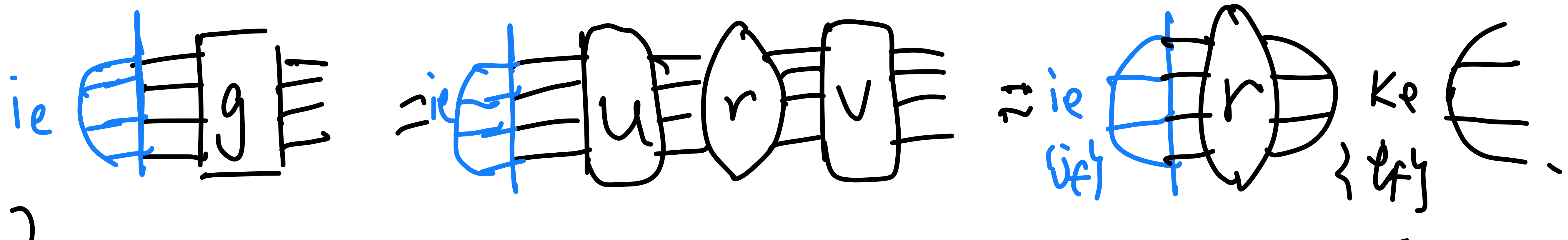
← SU(2) invariants

Booster decomposition

$$d^{(2rj,\,2j)}_{4\,j_f\,n}(r)$$

Decomposition of $SL(2,\mathbb{C})$ (cartan)

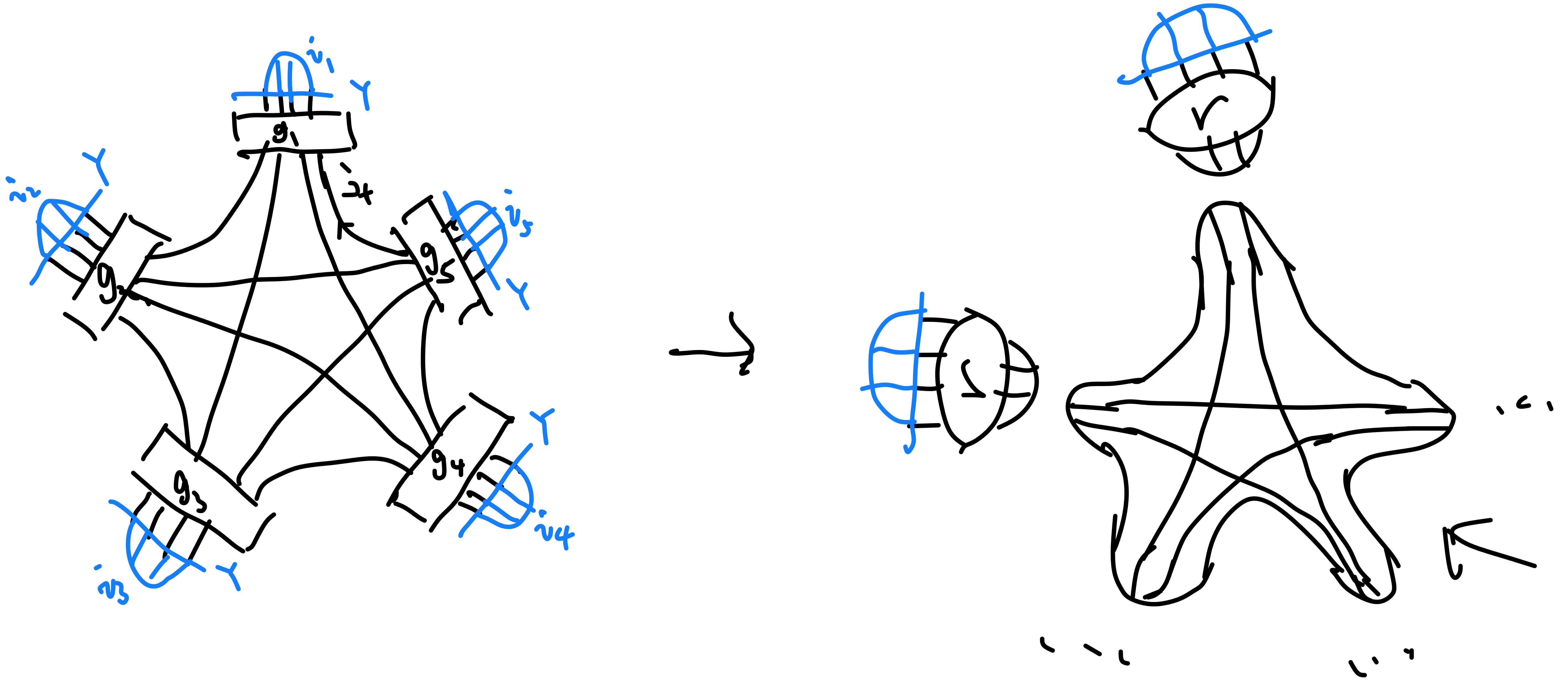
$$g = u\, e^{\frac{r}{2}\sigma_3}\, v^{-1}, \quad u, v \in SU(2)$$



$$B^r(j_f, l_f; i_e, k_e)$$

ArXiv: 1609.01632

→ 1d integral of dr.



$$A_v = \sum_{\{l_f, k_e\}} \{15j\}(l_f, k_e) \times B^r(j_f, l_f, i_e, k_e)$$

← {15j} symbol (SU(2) BF)

Integral representation

Again SL(2,C) representation theory

$\mathcal{H}^{(\rho,n)}$: $\Psi(z)$, $z = \begin{pmatrix} z_+ \\ z_- \end{pmatrix} \in \mathbb{C}^2$

- $\Psi(z)$ homogeneous functions : $\Psi : \mathbb{C}^2 \setminus \{0\} \to \mathbb{C}$

  $\forall \alpha \in \mathbb{C}$, $\Psi(\alpha z) = \alpha^{i\rho/2 + n/2 - 1} (\alpha^*)^{i\rho/2 - n/2 - 1} \Psi(z)$

- Action of $g \in SL(2,\mathbb{C})$:

  $$g \triangleright \Psi(z) = \Psi(g^T z)$$

- Scalar product :

  $$\langle \Psi_1 , \Psi_2 \rangle = \int_{\mathbb{C}P_1} \overline{\Psi_1(z)}\, \Psi_2(z)\, \omega_z$$

  invariant under $z \to \lambda z$

- $\omega_z = \frac{i}{2} (z_+ dz_- - z_- dz_+) \wedge (\bar{z}_+ d\bar{z}_- - \bar{z}_- d\bar{z}_+)$

$$\mathcal{H}_{(\rho,n)} = \{ \Psi : \langle \Psi , \Psi \rangle < \infty \}$$

Integral representation

SU(2) coherent states

$$u(z) = \frac{1}{\sqrt{\langle z, z\rangle}} \begin{pmatrix} z_+ , & z_- \\ -\bar{z}_- & \bar{z}_+ \end{pmatrix}$$

$\langle z, z'\rangle = \bar{z}_+ z'_+ + \bar{z}_- z'_-$

- $\Psi(z) = \frac{1}{\sqrt{\pi}} \langle z, z\rangle^{i\frac{\rho}{2}-1} \tilde{\Psi}_{jm}(z)$, $\tilde{\Psi}_{jm}(z) = \sqrt{2j+1}\, D^{j}_{\frac{n}{2}m}(u(z))$.
- Y maps : $D_j \longmapsto \mathcal{H}_{(2\gamma j, 2j)} \simeq \bigoplus_{k\geq j} D_k$, $\rho = 2\gamma j$, $n = 2j$
- SU(2) coherent states : $\Psi_{j\xi}(z) = v(\xi) \triangleright \Psi_{jj}(z)$, $v \in SU(2)$.

  └ highest weight state
- For highest weight states, we know

$$D^{j}_{jj}(u(z)) = \left(\langle \tfrac{1}{2}\tfrac{1}{2}|u(z)|\tfrac{1}{2}\tfrac{1}{2}\rangle\right)^{2j} = \langle z, z\rangle^{-j} \langle n_+, z\rangle^{2j} \quad n_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

→ e_3 axis geometrically

$$\Rightarrow \tilde{\Psi}_{j\xi}(z) = \tilde{\Psi}_{jj}(v(\xi)^T z) = \sqrt{2j+1} \langle z, z\rangle^{-j} \langle \xi, z\rangle^{2j}, \quad \xi = (v(\xi)^T)^{-1} n_+$$

rotation of e_3-axis

└ 3d normal vector of the triangle in each tetrahedron

Integral representation

action and measures

gauge fixing

we ignore $2j_f+1$ → face amp

$\langle \psi_{j_f \xi_{e'f}}, g_{e'}^{-1} g_e \psi_{j_f \xi_{ef}} \rangle$

$$A_v = \int \prod_e dg_{ve}\, \delta(g_{ve'}) \prod_f \int_{\mathbb{CP}_1} w_z\, \overline{g_{e'} \triangleright \psi_{j_f \xi_{e'f}}(z_{vf})}\, \big(g_e \triangleright \psi_{j_f \xi_{ef}}(z_{vf})\big)$$

$$= \int \prod_e dg_e \prod_f \int_{\mathbb{CP}_1} w_z\, \overline{\langle g_{e'}^T z_{vf}, g_{e'}^T z_{vf}\rangle^{i\gamma j_f - 1 - j_f} \langle \xi_{e'f}, g_{e'}^T z_{vf}\rangle^{2j_f}}$$
$$\times \langle g_e^T z_{vf}, g_e^T z_{vf}\rangle^{i\gamma j_f - 1 - j_f} \langle \xi_{ef}, g_e^T z_{vf}\rangle$$

$$= \int \prod_e dg_{ve} \prod_f \frac{w_z}{\langle z_{vef}, z_{vef}\rangle \langle z_{ve'f}, z_{ve'f}\rangle} \left(\frac{\langle z_{vef}, z_{vef}\rangle}{\langle z_{ve'f}, z_{ve'f}\rangle}\right)^{i\gamma j_f} \qquad z_{vef} := g_e^T z_{vf}$$

$[dx]$

$$\times \left(\frac{\langle z_{ve'f}, \xi_{e'f}\rangle \langle \xi_{ef}, z_{vef}\rangle}{\langle z_{ve'f}, z_{ve'f}\rangle \langle z_{vef}, z_{vef}\rangle}\right)^{2j_f}$$

$$= \int [dx]\, e^{S_v[x; j_f, \xi_f]} \qquad S_v = \sum_{(e,e')} (S_{vef} + S_{ve'f}), \qquad x = [g, z]$$

$k = 1$ for s.

$k = -1$ for t.

$$S_{vef} = j_f \left(\ln\left[\langle \xi_{ef}, z_{vef}\rangle^{\frac{\kappa_{vef}+1}{2}} \langle z_{vef}, \xi_{ef}\rangle^{\frac{1-\kappa_{vef}}{2}} \right] + (i\gamma \kappa_{vef} - 1) \ln\langle z_{vef}, z_{vef}\rangle \right)$$

Integral representation

$$A_v = \int [dx]\, e^{S_v[x;\, j_v, \xi_v]} \qquad S_v = \sum_{(e,e')} (S_{vef} + S_{ve'f}), \qquad X = [g, z]$$

$$S_{vef} = j_f \left(\ln\left[\langle \xi_{ef}, Z_{vef} \rangle^{\frac{\kappa_{vef}+1}{2}} \langle Z_{vef}, \xi_{ef} \rangle^{\frac{1-\kappa_{vef}}{2}} \right] + (i\gamma \kappa_{vef} - 1) \ln \langle Z_{vef}, Z_{vef} \rangle \right)$$

$$\kappa = \pm 1.$$

Beyond single vertex :

$$\sum_{j=0}^{j_{max}} f(j) \simeq \sum_{k \in \mathbb{Z}} \int_{\varepsilon}^{j_{max}+1-\varepsilon} dj\, f(j)\, e^{2\pi i k n}$$

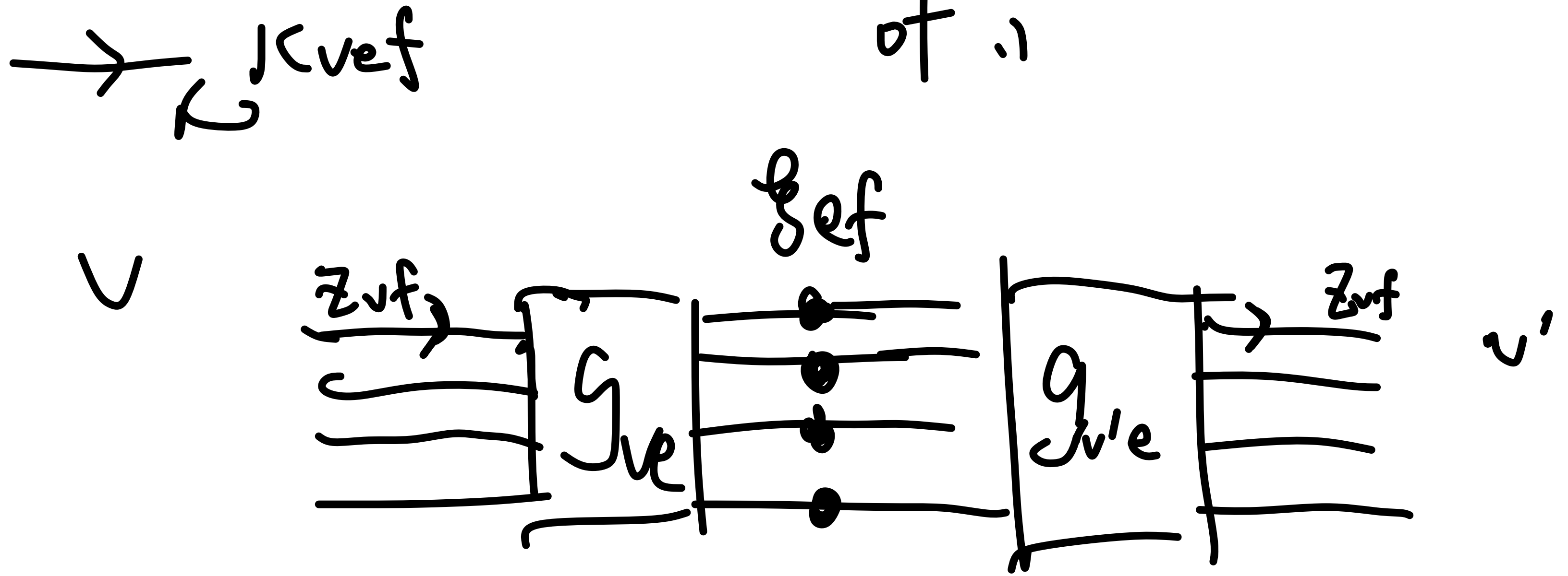
$$A = \prod_f A_f \sum_{j_f} \prod_{(e,f)} d\xi_{ef} \prod_v A_v$$

A_f ↓ polynomial of j

$$[dx] = \prod_{v,e} dg_{ve} \prod_{eh} d\xi_{eh} \prod_{(e,e')} \Omega .$$

(Ω ↙ dz_{vf}.)

$$X = [g_{ve}, z_{vf}, \xi_{eh}].$$



$$-\kappa_{ve'f} = \kappa_{vef} = -\kappa_{v'ef}$$

Gauge transformations

$S = \sum_v \sum_{(e,e')} (S_{vef} + S_{ve'f})$, $\quad S_{vef} = j_f \left(\ln\left[\langle \xi_{ef}, Z_{vef} \rangle^{\frac{\kappa_{vef}+1}{2}} \langle Z_{vef}, \xi_{ef} \rangle^{\frac{1-\kappa_{vef}}{2}} \right] + (i\gamma\kappa_{vef} - 1) \ln \langle Z_{vef}, Z_{vef} \rangle \right)$

$\kappa = \pm 1$

gauge trans. ⓪ $g_{ve} \to \pm g_{ve}$ discrete trans.

Contineous :

at each v : ① $g_{ve} \to \tilde{g}_v g_{ve}$, $\tilde{g}_v \in SL(2, \mathbb{C})$

$z_{vf} \to (\tilde{g}_v^{-1})^T z_{vf}$

For each z_{vf} ② $z_{vf} \to \lambda_{vf} z_{vf}$ $\leftarrow$ z in $\mathbb{CP}_1$

For internal e : ③ $\xi_{ef} \to e^{i\psi_{ef}} \xi_{ef}$, $\psi_{ef} \in \mathbb{R}$

④ $g_{ve'} \to g_{ve'} h_e^T$, $g_{ve} \to g_{ve} h_e^T$, $\xi_{ef} \to h_e \xi_{ef}$.

gauge fixing

2404.10563

Integral $A = \int_{\mathbb{R}^n} \mathrm{d}^n x f(x) \mathrm{e}^{-S(x)}$ with complex action $S(x)$

Sign-problem:

Not positive semi-definite
~~probability distribution~~

Saddle point approximation!

Perturbative (asymptotic) expansion

Saddle points

$$S_v = \sum_{(e,e')} (S_{vef} + S_{ve'f}), \quad S_{vef} = j_f \left(\ln\left[\langle \xi_{ef}, Z_{vef} \rangle^{\frac{\kappa_{vef}+1}{2}} \langle Z_{vef}, \xi_{ef} \rangle^{\frac{1-\kappa_{vef}}{2}} \right] + (i\gamma \kappa_{vef} - 1) \ln \langle Z_{vef}, Z_{vef} \rangle \right)$$

$\kappa = \pm 1.$

saddle point $\Leftrightarrow$ solutions of EoM.

Parallel transport eq.

Single vertex:

$Z_{vef} := g_{ve}^T z_{vf}. \Rightarrow g_{ve}^{T-1} Z_{vef} = g_{ve'}^{T-1} Z_{ve'f}$

$\delta_{z_{vf}} S \Rightarrow \tilde{Z}_{vef} g_{ve}^T = \tilde{Z}_{ve'f} g_{ve'}^T \Rightarrow g_{ve}^{T-1} B_{vef} g_{ve}^T = g_{ve'}^{T-1} B_{vef} g_{ve'}$

$B := (Z \otimes \tilde{Z}) - \frac{1}{2}\mathbb{1} = \frac{1}{2}(Z \otimes \tilde{Z} + (\tilde{Z} \otimes Z)^\dagger)$

$\delta_{g_{ve}} S \Rightarrow \forall_e \; \sum_f j_f B_{vef} = 0$ closure.

is a bivector, $B \in sl(2, \mathbb{C})$.

This hold for both real and complex saddle points.

For real critical points: $B_{vef} = \xi_{ef} \otimes \xi_{ef}^\dagger - \frac{1}{2}\mathbb{1}$, we have in addition $\forall e$,

ArXiv: 2104.06902

Saddle points

EoM: ① $g_{ve}^{T^{-1}} B_{vef}\, g_{ve}^{T} = g_{ve'}^{T^{-1}} B_{ve'f}\, g_{ve'}$ ② $\forall_e \sum_f j_f B_{vef} = 0$

For real critical points : $B_{vef} = \xi_{ef} \otimes \xi_{ef}^{\dagger} - \frac{1}{2}\mathbb{1} \equiv B_{ef}$ ⇐ Bivector from boundary tetrahedron

$v \in SU(2)$ $\quad v(\xi)^{T\dagger} \frac{\sigma_3}{2} v(\xi)^T = B_{ef} = N_0 \wedge \vec{n}_{ef}$. $\quad \vec{n}_{ef}$ 3d normal of triangles.

$N_0 = (1, 0, 0, 0)^T$

① + ② describe exactly a 4-simplex.

With $\quad B_f(v) := (g_{ve}^T)^{-1} B_{ef}\, g_{ve}^T = (g_{ve'}^T)^{-1} B_{e'f}\, g_{ve'}^T$

↑ 10 bivectors of 4-simplex triangle.

$N_e(v) := (g_{ve}^T)^{-1} N_0 \quad \to$ 5 normals of 4-simplex.

fix the 4-simplex by rescaling.

4 simplex geometry ⇄ (non-degenerate) real saddle points.

Saddle points

$\left((g_{ve}^T)^{-1} B_{ef}\, g_{ve}^T\right)^\dagger = \left((g_{ve'}^T)^{-1} B_{e'f}\, g_{ve'}^T\right)^\dagger$ also satisfied.

$B_{ef} = B_{ef}^\dagger$

$\Rightarrow \quad (g_{ve}^T)^\dagger B_{ef} (g_{ve}^T)^{-1\dagger} = (g_{ve'}^T)^\dagger B_{ef} (g_{ve'}^T)^{-1\dagger}$.

pairs of solutions $\{g_{ve}\}$, $\{g_{ve}^\dagger\}$.

It turns out they correspond to different orientations

Amp. at critical points :

Regge action

$$A_v \sim N_+ e^{i \sum_f j_f \Theta_{f(v)}} + N_- e^{-i \sum_f j_f \Theta_{f(v)}} \Leftarrow \text{Cosine prob.}$$

$\Theta_f := \operatorname{arccosh}(N_e \cdot N_{e'})$. $\Leftarrow$ dihedral angle.

Saddle points

$$A_v \sim N_+ e^{i\sum_f j_f \Theta_f} + N_- e^{-i\sum_f j_f \Theta_f}$$

For internal faces:

$$\delta_{j_f} S \Rightarrow \Theta_f \equiv \sum_v \Theta_f(v) = 0 \Leftarrow \text{"Flatness problem"}$$

Real saddles $\Longleftrightarrow$ Flat geometries

This can be resolved by complex critical points • Techniquelly difficult

EoM: ① $g_{ve}^{T^{-1}} B_{vef}\, g_{ve}^{T} = g_{ve'}^{T^{-1}} B_{ve'f}\, g_{ve'}$ ② $\forall_e \sum_f j_f B_{vef} = 0$ ③ $\delta_j S = 0$

No geometric notion as we do not have $\underbrace{\forall_e.\ N_e \cdot B_{vef} = 0}_{\text{part of the simplicity}}$

When we close to real critical points.
We can use Newton's method.

Lefschetz Thimble

Goal: computing the integral $A = \int_{\mathbb{R}^n} \mathrm{d}^n x f(x) \mathrm{e}^{-S(x)}$ non-perturbatively with complex action $S(x)$

Sign-problem: Not positive semi-definite ~~probability distribution~~

How we solve this in 1D?

Lefschetz Thimble

Goal: computing the integral $A = \int_{\mathbb{R}^n} \mathrm{d}^n x f(x) \mathrm{e}^{-S(x)}$ with complex action $S(x)$

Sign-problem: Not positive semi-definite ~~probability distribution~~

Complexify the action: $S(x) \to S(z)$

Lefschetz thimble

$$\mathscr{C} = \sum_\sigma n_\sigma \mathscr{J}_\sigma$$

Critical points: $\frac{\partial S(\vec{z})}{z_i}|_{\vec{z}=\vec{z}_\sigma} = 0$

σ all possible critical points in $\mathbb{C}^n$

Deformation of the integral curve → Picard-Lefschetz theory

$$\int_{\mathbb{R}^n} \mathrm{d}^n z f(\vec{z}) \mathrm{e}^{-S(\vec{z})} = \sum_\sigma n_\sigma \int_{\mathscr{J}_\sigma} \mathrm{d}^n z f(\vec{z}) \mathrm{e}^{-S(z)}$$

n_σ weight functions, usually hard to determine

E. Witten, Analytic Continuation Of Chern-Simons Theory

Lefschetz Thimble

Lefschetz thimble:

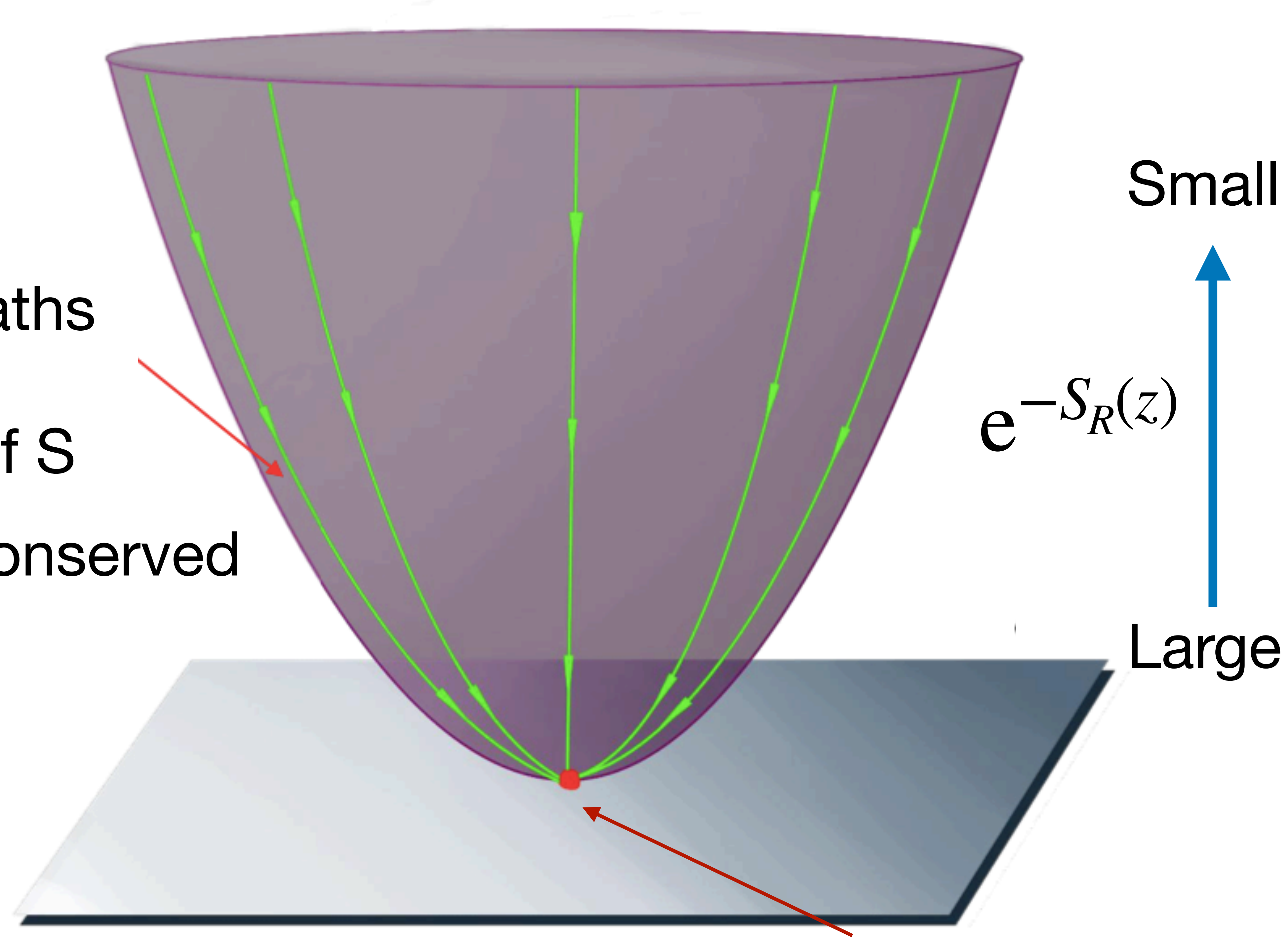
Union of steepest-decent paths falling to critical points

$$\frac{\mathrm{d}z^a}{\mathrm{d}t} = -\frac{\partial \overline{S(\vec{z})}}{\partial \overline{z^a}} \quad \Leftrightarrow \quad \begin{aligned} \frac{dz_i^R}{d\tau} &= -\frac{\partial S_R}{\partial z_i^R} = \frac{\partial S_I}{\partial z_i^I}, \\ \frac{dz_i^I}{d\tau} &= -\frac{\partial S_R}{\partial z_i^I} = -\frac{\partial S_I}{\partial z_i^R}, \end{aligned}$$

Gradient flow of real part, Hamiltonian flow of imaginary part of S

— Phase is conserved

$$\int_{\mathcal{J}_\sigma} \mathrm{d}^n z \hat{f}(\vec{z}) \mathrm{e}^{-S(\vec{z})} = \mathrm{e}^{-\mathrm{i}\, S_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n z f(\vec{z}) \mathrm{e}^{-S_R(\vec{z})}$$



Flow equation is first order:

Given asymptotic boundary conditions, any point on a thimble T lies on one and only one curve

Lefschetz Thimble

Picard-Lefschetz theory

$$\int_{\mathscr{C}} \mathrm{d}^n z \hat{f}(\vec{z}) \mathrm{e}^{-S(\vec{z})} = \sum_{\sigma} n_\sigma \int_{\mathscr{J}_\sigma} \mathrm{d}^n z \hat{f}(\vec{z}) \mathrm{e}^{-S(z)} \qquad \mathscr{C} = \sum_{\sigma} n_\sigma \mathscr{J}_\sigma$$

Suppose global minimum of $S_R(z)$ in $\mathscr{C}$ is given by $s_{\min} = \min_{z \in \mathscr{C}} S_R(z)$

Only σ s.t. $S_R(z_\sigma) \geq s_{\min}$ contribute: $n_\sigma = 0$ if $S_R(z_\sigma) < s_{\min}$

Contributions suppressed exponentially $\mathrm{e}^{s_{\min} - S_R(z_\sigma)}$

Suppose there is only one global minimum and is given by $z_{\sigma_{\min}}$

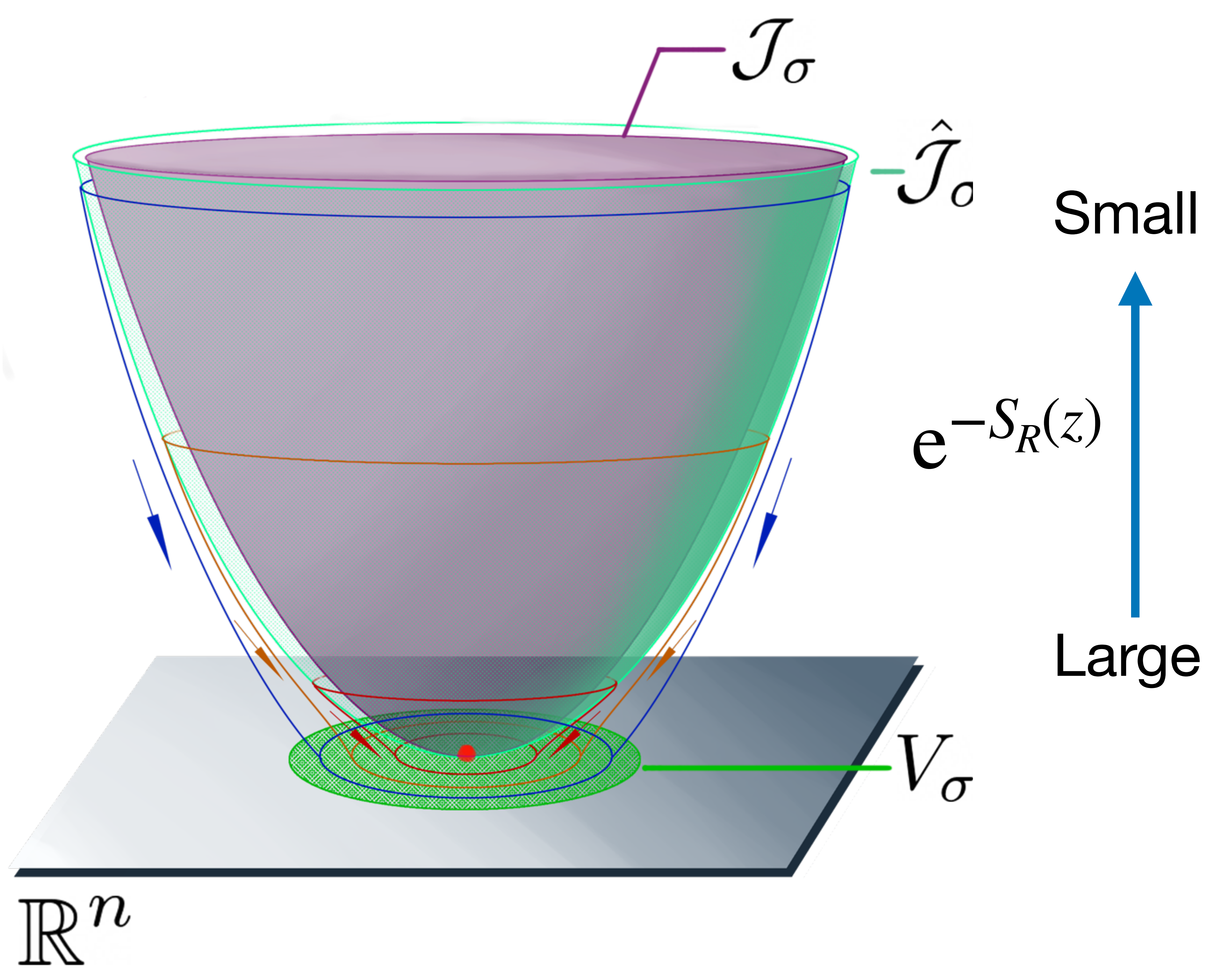
Only the thimble attached to global minimum dominate

$$\int_{\mathscr{C}} \mathrm{d}^n z \hat{f}(\vec{z}) \mathrm{e}^{-S(\vec{z})} \approx \mathrm{e}^{-\mathrm{i}\, S_I(z_{\sigma_{\min}})} \int_{\mathscr{J}_{\sigma_{\min}}} \mathrm{d}^n z f(\vec{z}) \boxed{\mathrm{e}^{-S_R(\vec{z})}} \rightarrow \text{positive semi-definite}$$

exclude: there are multiple thimbles close to the global minimum

How to obtain the Thimble?

Flow to z_σ need infinite time $t \to \infty$, practically we need approximation



Action decay exponentially

Only a subsets $\hat{\mathcal{J}}_\sigma$ on the thimble is relevant to the calculation

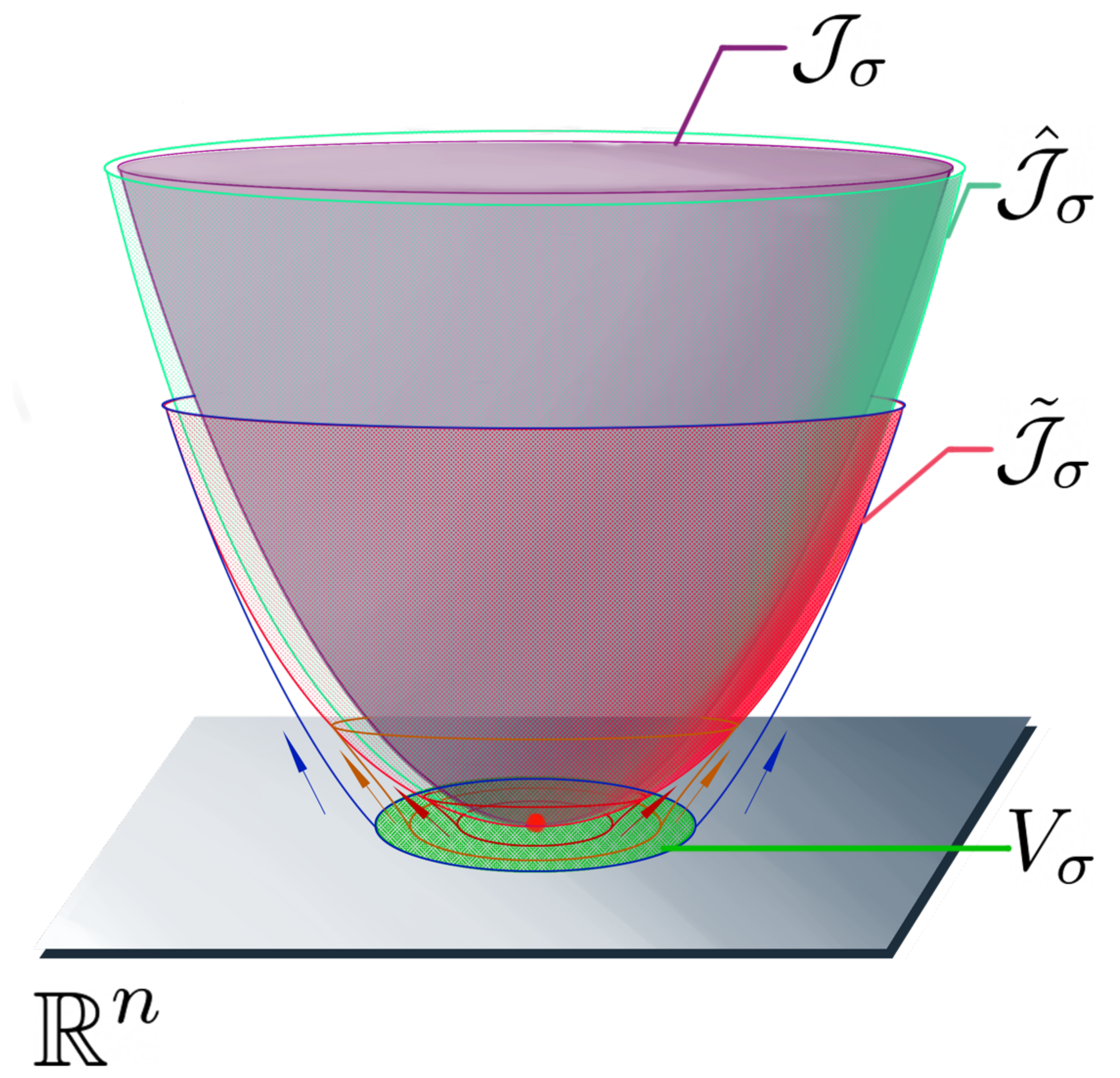
Under SD flow, points on $\hat{\mathcal{J}}_\sigma$ will arrive arbitrarily close to the critical point z_σ at some τ

near z_σ the thimble is well approximated by its tangent space

$\mathcal{J}_\sigma \longleftrightarrow V_\sigma$

thimble — tangent space of the critical point

How to obtain the Thimble?



In V_σ , phases are close to phases at z_σ

Small

$e^{-S_R(z)}$ ↑

Large

tangent space of the critical point — thimble

$V_\sigma \xleftrightarrow[\text{SD}]{\text{SA}} \mathcal{J}_\sigma$

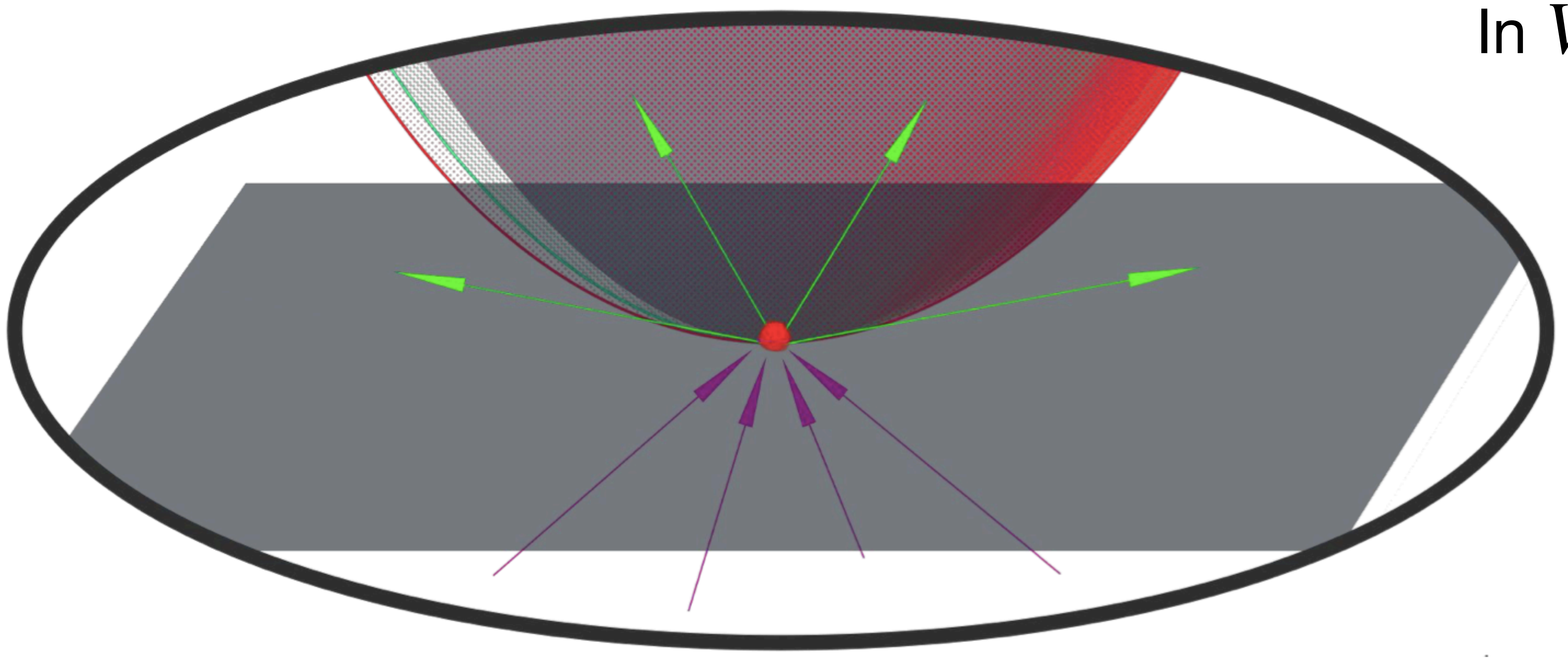
$\hat{z} \in V_\sigma \xmapsto{\text{SA}} z \in \mathcal{J}_\sigma$

SA flow $\quad \dfrac{dz^a}{dt} = + \dfrac{\partial \overline{S(\vec{z})}}{\partial \overline{z^a}}$

$\mathcal{J}_\sigma \xrightarrow{\text{Fix } V_\sigma} \hat{\mathcal{J}}_\sigma \xrightarrow{\text{Fix } T} \tilde{\mathcal{J}}_\sigma$

Approximation is better when V_σ is small and T is large

How to obtain the Thimble?



In V_σ, Action is well approximated by

$$S(z) = S(z_c) + \frac{1}{2}\omega_i \mathbf{H}_{ij}\omega_j$$

$$\mathbf{H} = H_{kl}(z_\sigma) = \frac{\partial^2 S}{\partial z_k \partial z_l}\Big|_{z=z_\sigma}$$

Linearized SA equation

$$\frac{\mathrm{d}\omega}{\mathrm{d}t} = \overline{\mathbf{H}\omega}$$

Real and imaginary part $\omega = \omega_{\mathbb{R}} + \mathrm{i}\omega_{\mathbb{I}}$

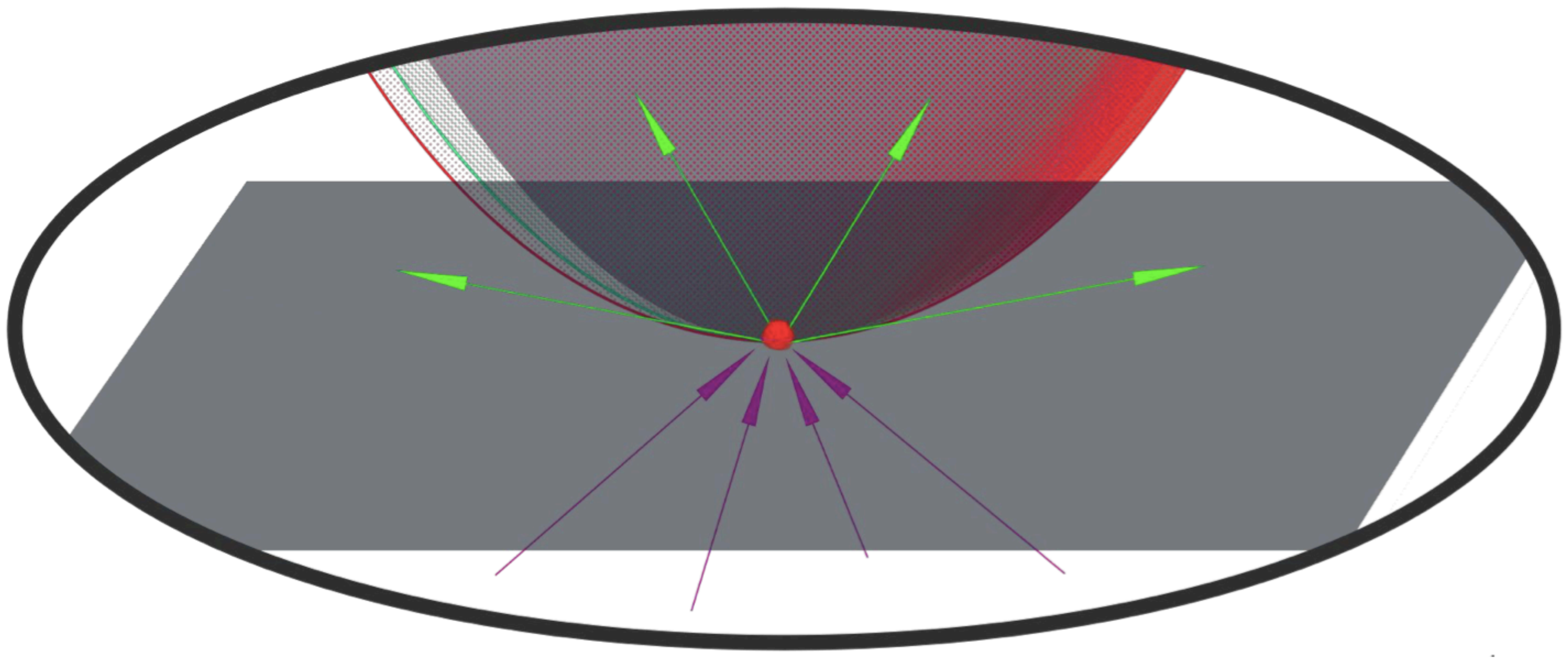
$\lambda > 0$ repulsive direction, $\lambda < 0$ attractive direction

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\omega_{\mathbb{R}}\\ \omega_{\mathbb{I}}\end{pmatrix} = \begin{pmatrix}\mathbf{H}_{\mathbb{R}} & -\mathbf{H}_{\mathbb{I}}\\ -\mathbf{H}_{\mathbb{I}} & -\mathbf{H}_{\mathbb{R}}\end{pmatrix}\begin{pmatrix}\omega_{\mathbb{R}}\\ \omega_{\mathbb{I}}\end{pmatrix} = \mathbb{H}\begin{pmatrix}\omega_{\mathbb{R}}\\ \omega_{\mathbb{I}}\end{pmatrix}$$

$\mathbb{H}$, real, symmetric matrix

Real eigenvalues appears pairs $(\lambda, -\lambda)$

How to obtain the Thimble?



the directions tangent to the thimble correspond to the eigenvectors with $\lambda > 0$

Complex eigen equation with eigenvector ρ

$$\overline{\mathbf{H}\rho} = \lambda\rho \qquad \rho = \rho_{\mathbb{R}} + \mathrm{i}\rho_{\mathbb{I}}$$

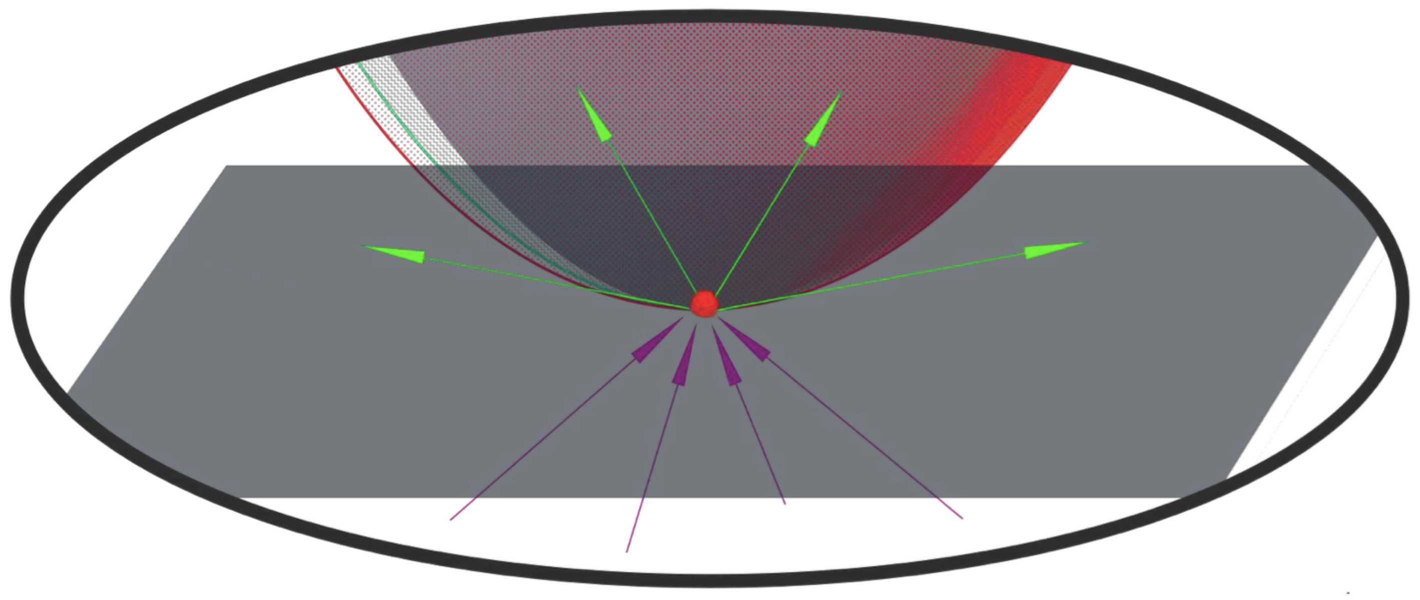
$$\begin{matrix} \mathbf{H}_{\mathbb{R}} & -\mathbf{H}_{\mathbb{I}} \\ -\mathbf{H}_{\mathbb{I}} & -\mathbf{H}_{\mathbb{R}} \end{matrix} \begin{matrix} \rho_{\mathbb{R}} \\ \rho_{\mathbb{I}} \end{matrix} = \lambda \begin{matrix} \rho_{\mathbb{R}} \\ \rho_{\mathbb{I}} \end{matrix}$$

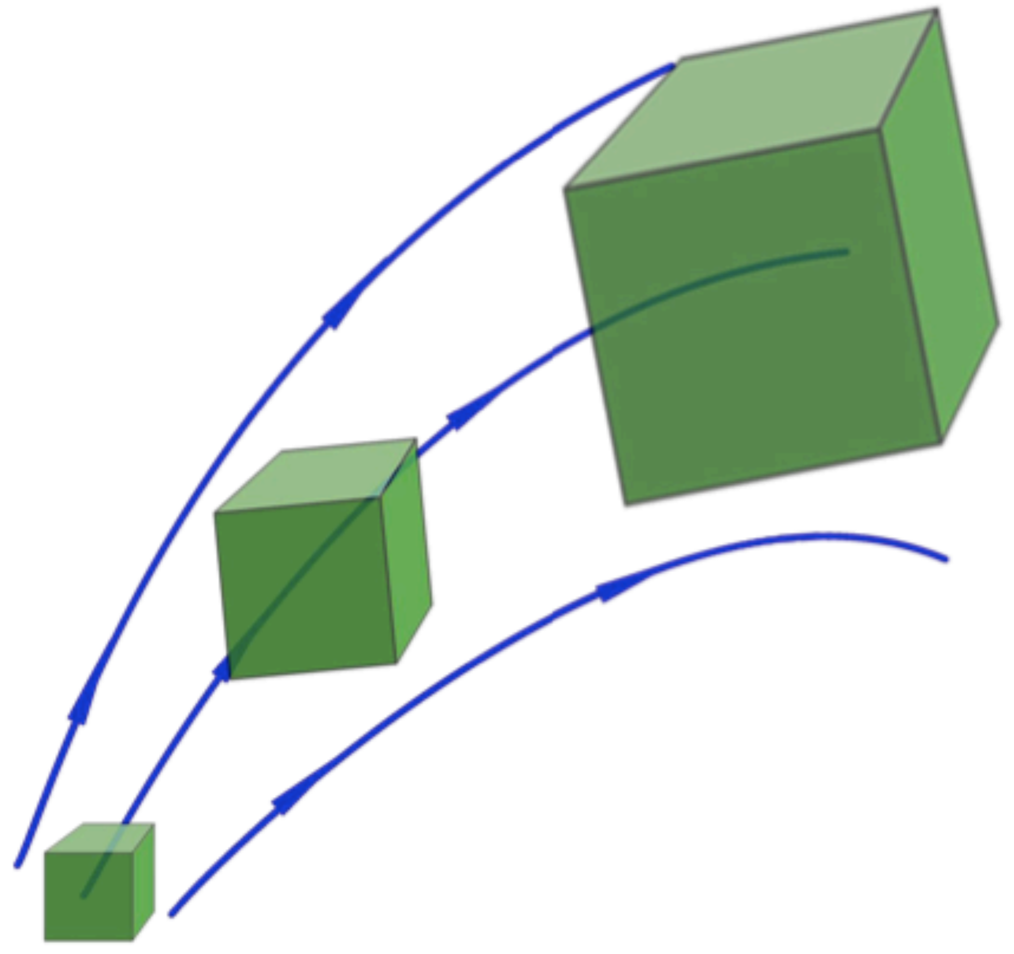
$\hat{V}_\sigma$ linear combinations of $\hat{\rho}$, eigenvector with $\lambda > 0$,

$$\hat{V}_\sigma = \{\tilde{z} \;\; \tilde{z} = \sum_{i=1}^{N} \hat{\rho}_i x^i + z_\sigma, \text{ each } x^i \in \mathbb{R} \text{ is small}\}$$

Now we have $$\int_{\tilde{\mathcal{J}}_\sigma} \mathrm{d}^n z\, \psi(z) = \int_{\hat{V}_\sigma} \mathrm{d}^n x\, \det\left(\frac{\partial z}{\partial x}(x)\right) \psi(z(x))$$

Flow of the Jacobian





Linearized SA equation again: $\frac{\mathrm{d}\delta z}{\mathrm{d}t} = \overline{H\delta z}$

$$\frac{\mathrm{d}J(x)}{\mathrm{d}t} = \overline{H(z(x))J(x)}, \quad J(0) = \frac{\partial \tilde{z}}{\partial x} = \vec{\rho}$$

Again first order ODE

can be solved numerically after we have the solution of SA equation

When ρ are real, we have the solution $J(t) = P\exp(\int \mathrm{d}t\overline{H(t)})$

And approximating solution in the Gaussian region $J(t) = P\exp(\int \mathrm{d}t\rho^{\dagger}\overline{H(t)}\bar{\rho}))$

The answer to our question

Goal: computing the integral $A = \int_{\mathbb{R}^n} \mathrm{d}^n x f(x) \mathrm{e}^{-S(x)}$ with complex action $S(x)$

Answer: $$\int_{\mathscr{C}} \mathrm{d}^n z \hat{f}(\vec{z}) \mathrm{e}^{-S(\vec{z})} \approx \mathrm{e}^{-\mathrm{i}\, S_I(z_{\sigma_{\min}})} \int_{V^\sigma} \mathrm{d}^n x \, \det(J(x)) \, f(\vec{z}(x)) \, \mathrm{e}^{-S_R(\vec{z}(x))} = \int_{\hat{V}_\sigma} \mathrm{d}^n x \, \hat{f} \, \mathrm{e}^{\mathrm{i}\theta_{res}} \, \mathrm{e}^{-S_{eff}}$$

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Monte Carlo method?

Still hard to get the normalisation factor for our probability distribution $\mathrm{e}^{-S_{eff}}$.

High - dimensional is not efficient (grow exponentially with dimension)

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$\mathrm{Re}(\hat{S}) - \log(\det(J)) \equiv S_{eff}$ $\quad \arg(\det(J)) - \mathrm{Im}(\hat{S}) \equiv \theta_{res}$

Monte Carlo method?

Still hard to get the normalisation factor for our probability distribution $\mathrm{e}^{-S_{eff}}$.

High - dimensional is not efficient (grow exponentially with dimension)

But for observables, we can use MCMC without knowing the normalization factor !

$$\langle f \rangle \simeq \frac{\int_{\tilde{\mathscr{J}}_\sigma} \mathrm{d}^n z \, \hat{f}(z) \, \mathrm{e}^{-\hat{S}(z)}}{\int_{\tilde{\mathscr{J}}_\sigma} \mathrm{d}^n z \, \mathrm{e}^{-\hat{S}(z)}} = \frac{\int_{\hat{V}_\sigma} \mathrm{d}^n x \, \hat{f} \, \mathrm{e}^{\mathrm{i}\theta_{res}} \, \mathrm{e}^{-S_{eff}}}{\int_{\hat{V}_\sigma} \mathrm{d}^n x \, \mathrm{e}^{-S_{eff}}} \times \frac{\int_{\hat{V}_\sigma} \mathrm{d}^n x \, \mathrm{e}^{-S_{eff}}}{\int_{\hat{V}_\sigma} \mathrm{d}^n x \, \mathrm{e}^{\mathrm{i}\theta_{res}} \, \mathrm{e}^{-S_{eff}}} = \frac{\langle \mathrm{e}^{\mathrm{i}\theta_{res}} \hat{f} \rangle_{eff}}{\langle \mathrm{e}^{\mathrm{i}\theta_{res}} \rangle_{eff}}$$

MCMC methods

Markov Chain: Markov property $P(X^{t+1} \;\; X^t, \cdots, X^1) = P(X^{t+1} \;\; X^t)$

transition Matrix $P(i,j) = P_{ij}^t = P(X_t = j \;\; X_{t-1} = i)$

Nice property: non-periodic Markov Chain $\lim_{t\to\infty} P_{ij}^t = \pi(j) = \sum_i \pi(i)P(i,j)$

target distribution $\pi(j)$ stationary distribution (equilibrium probabilities of being in states j)

π Is the only non-negative solution of $\pi P = \pi$

If we know π, how to get P such that we can finally sampling π using MCMC

Nice refs: https://github.com/rmcelreath/stat_rethinking_2022

Metropolis Hastings

Detailed balance condition (reversiable Markov Chains)

$$\pi(i)P(i,j) = \pi(j)P(j,i)$$

A sufficient but not necessary condition for π to be stationary distribution

P satisfying above relation is still unknown

We can introduce an extra acceptance rate $\alpha(i,j)$ s.t. $P(i,j) = \alpha(i,j)Q(i,j)$

$$\pi(i)Q(i,j)\alpha(i,j) = \pi(j)Q(j,i)\alpha(j,i) \longrightarrow \alpha(i,j) = \pi(j)Q(j,i),\ \ \alpha(j,i) = \pi(i)Q(i,j)$$

Acceptance rate may really small

Scale $\alpha(i,j)$ to increase acceptance rate :

$$\alpha(i,j) = \min \frac{\pi(j)Q(j,i)}{\pi(i)Q(i,j)},1$$

We can take Q to be symmetric $\alpha(i,j) = \min \frac{\pi(j)}{\pi(i)},1$

Metropolis Hastings

Algorithm

initial $x^{(0)}$
for iteration $i = 1, 2, \cdots N$ **do**
Propose candidate x^{cand} from $p(x|x^{(i-1)})$
Acceptance rate $\alpha \leftarrow \min\left\{1, \frac{\pi(x^{cand})}{\pi(x^{(i-1)})}\right\}$
$u \sim$Uniform$(u; 0, 1)$
if $u < \alpha$ **then**
$x^{(i)} \leftarrow x^{cand}$
else
$x^{(i)} \leftarrow x^{(i-1)}$
end if
end for

High dimensional: Gibbs sampling:

$$(x_1^{(1)}, x_2^{(1)}) \rightarrow (x_1^{(1)}, x_2^{(2)}) \rightarrow (x_1^{(2)}, x_2^{(2)}) \rightarrow \cdots \rightarrow (x_1^{(n_1+n_2-1)}, x_2^{(n_1+n_2-1)})$$

MCMC methods

In Lefschetz thimble spinfoam:

- high-dimensional:
  - single simplex 2*10+4*6+10 = 54
  - Multi-simplices: ~ 44*v - 3*t + f
- Probability distribution $e^{-S_{\mathrm{eff}}}$ is complicated
- $\partial_x S_{eff}$ is hard to compute
- Need to solve ODE in each update step: time - costing

In high dimensional problems, MH

- Calculation single step will cost a lot
- Acceptance rate may become low
- May take a very large number of updates to converge

Adaptive MH

Adjust proposal distribution s.t. acceptance rate stays around 0.3

Differential evolution Markov chain/
Differential Evolution Adaptive Metropolis

Parallel multiple chains + jump between chains to sample complicated π

Used by us in spinfoam propagator

Implemented with Mathematica

Julia conversion is undergoing

Vrugt et.al, DOI:10.1515/IJNSNS.2009.10.3.273

Summary of what we need to do

We can calculate:

$$\langle f\rangle \simeq \frac{\int_{\tilde{\mathcal{J}}_\sigma} d^n z\, \hat{f}(z)\, e^{-\hat{S}(z)}}{\int_{\tilde{\mathcal{J}}_\sigma} d^n z\, e^{-\hat{S}(z)}} = \frac{\int_{\hat{V}_\sigma} d^n x\, \hat{f}\, e^{i\theta_{res}}\, e^{-S_{eff}}}{\int_{\hat{V}_\sigma} d^n x\, e^{-S_{eff}}} \times \frac{\int_{\hat{V}_\sigma} d^n x\, e^{-S_{eff}}}{\int_{\hat{V}_\sigma} d^n x\, e^{i\theta_{res}}\, e^{-S_{eff}}} = \frac{\langle e^{i\theta_{res}}\hat{f}\rangle_{eff}}{\langle e^{i\theta_{res}}\rangle_{eff}}$$

We need:

Tangent space $\hat{V}_\sigma = \{\tilde{z}\ \ \tilde{z} = \sum_{i=1}^{N} \hat{\rho}_i x^i + z_\sigma,$ each $x^i \in \mathbb{R}$ is small$\}$

$$\begin{pmatrix} \mathbf{H}_\mathbb{R} & -\mathbf{H}_\mathbb{I} \\ -\mathbf{H}_\mathbb{I} & -\mathbf{H}_\mathbb{R} \end{pmatrix} \begin{pmatrix} \rho_\mathbb{R} \\ \rho_\mathbb{I} \end{pmatrix} = \lambda \begin{pmatrix} \rho_\mathbb{R} \\ \rho_\mathbb{I} \end{pmatrix}, \quad \lambda > 0$$

SA & Jacobian flow equation with fixed flow time T

$$\frac{dz^a}{dt} = +\frac{\partial \overline{S(\vec{z})}}{\partial \overline{z^a}} \qquad \frac{dJ(x)}{dt} = \overline{H(z(x))J(x)}, \quad J(0) = \frac{\partial \tilde{z}}{\partial x} = \hat{\rho}$$

Probability distribution $e^{-S_{eff}}/Z_0$ + MCMC

Special optimisations

Choose initial points for MC s.t. $0 < S_{eff} < 1$ is complicated

Do several test run's with different flow time T, chose the optimal one

Approximation is better when V_σ is small and T is large

But if T is too large, longer evaluation time + large errors from ODE (SA equations become stiff)

Burn-in optimazation

initial $t \leftarrow 1$, $L_m \leftarrow 0$, $p_m = 1/n_{cr}, m = 1, \cdots, n_{cr}$
while burn-in steps $t < K$ **do**
for chains $i = 1, \cdots, M$ **do**
$m \sim$ multinomial$(. ; p_1, \cdots, p_m)$
$CR \leftarrow m/n_{CR}$ and $L_m = L_m + 1$
Create a candidate
Accept/Reject the candidate
$\Delta_m \leftarrow \Delta_m + \sum_{j=1}^{d}((x_i^{(t)})^j - (x_i^{(t-1)})^j)^2/r_j^2$, where r denotes the standard deviation current locations of the chains.
end for
$p_m \leftarrow tN \cdot (\Delta_m/L_m)/\sum_{j=1}^{n_{CR}} \Delta_j$
$t \leftarrow t + 1$
end while

Next

Examples:

1. Real/complex critical points and Lefschetz thimble methods with Airy function
2. Real/complex critical points in EPRL vertex
3. Usage of sl2cfoam-next

Mainly Julia + Python (Sympy)