Application of the Lefschetz thimble formulation to the (0+1) dimensional Thirring model at finite density

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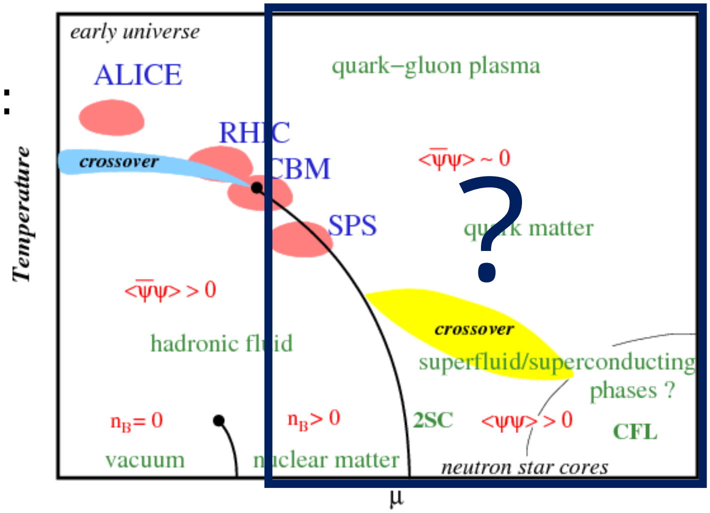
QCD and the sign problem

Exploring finite temperature and density QCD is the exciting topic, but is hard for lattice QCD because of the sign problem:

- **the action is complex because** $\det D(\mu) \in \mathbb{C}$ **at μ ≠ 0**
- **Importance sampling breaks down.**

It has been approached by various methods:

- SU(3) → SU(2)
- Imag chemical potential
- Taylor expansion
- Complex Langevin
- Histogram method
- Canonical approach
- …



Schaefer, Bernd-Jochen *et al.*
Prog.Part.Nucl.Phys. 62 (2009) 381

Our procject : Try to apply *the Lefschetz thimble method.*

[Cristoforetti et al. , 2012]
[Fujii et al. , 2013]

(0+1) dim. Thirring model on the lattice

Motivation

We apply the Lefschetz thimble formulation to a solvable model to learn lessons for investigating the (3+1) dim. QCD at finite density.

Thirring model **[Pawlowski et al. 2014]**

$$S_A = \sum_{n=0}^{L-1} \beta \mathcal{N}_f (1 - \cos A_n) - \sum_{i=1}^{\mathcal{N}_f} \log \det K_i$$

$$K_{i\,nm} = \frac{1}{2} \left[e^{\mu_i} e^{iA_n} \delta_{n+1,m} - e^{-\mu_i} e^{-iA_m} \delta_{n,m+1} \right] + m_i \delta_{n,m}$$

c.f. link variable

$$U(t) = \exp\left(iA(t)\right), \quad -\pi \le A(t) < \pi$$

$$Z = \pi^L e^{-L\beta} \left[2\cosh(L\mu)(I_1(\beta))^L + \left(m_+^L + m_-^L\right)(I_0(\beta))^L \right]$$

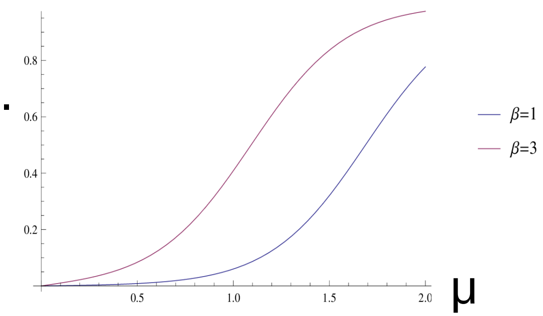
$I_0(x)$, $I_1(x)$: modified Bessel function

$m_\pm = m \pm \sqrt{m^2+1}$, $\beta = 1/(2g^2)$

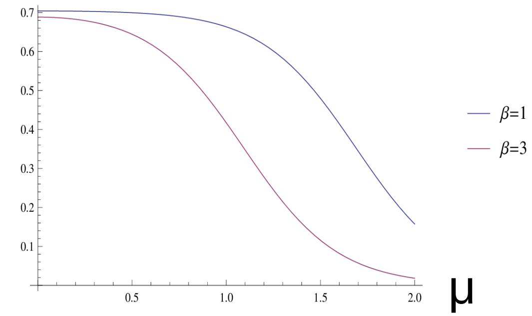
Similarity to lattice QCD at finite μ

- Compact variable
- Sign problem from fermion det.
- Behavior of <n> and <$\bar\chi\chi$>

<n>



<$\bar\chi\chi$>



Highlights in this work

The Lefschetz thimble method: $\mathcal{C}_{\mathbb{R}} = \sum_{\sigma \in \Sigma} n_\sigma \mathcal{J}_\sigma, \qquad n_\sigma = \langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_\sigma \rangle .$

Fermion determinant

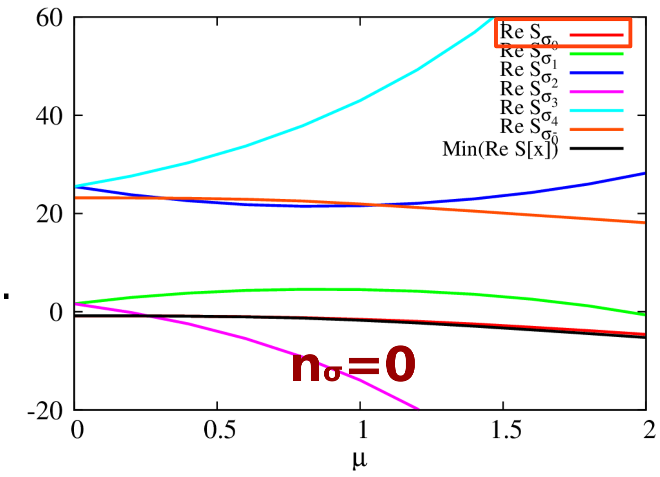
- The structure of thimbles is changed by the fermion determinant.

Change of intersection numbers due to the Stokes phenomenon

- In general it is hard to find the intersection numbers systematically.
- The Stokes phenomenon gives information of changing intersection numbers.
- We investigate the configuration space assuming that $z_n = \mathrm{const.}$.

Numerical simulation

- We perform numerical simulations on a particular thimble.
- We choose a thimble which is the most dominant.
- To what extent does it work ?



Talk plan

- Finding critical points, zero-points and thimbles
- Studying the Stokes phenomena
- Numerical results
- Summary

Critical points, thimbles and zero-points

- Extension of real variables to complex.

$$A_n \to z_n \in \mathbb{C} \qquad e^{iz_n}$$ … Non-compact variables

- We focus only on zero-mode solutions ($z_n = z \in \mathbb{C}$) and solve the complexified saddle point equation.

Critical points

$$\frac{\partial S_A}{\partial z} = 0, \quad \frac{\partial S_A}{\partial z} = \beta L \sin z - \frac{Li \sinh L(\mu + iz)}{\cosh L(\mu + iz) + \cosh L\hat{m}} \qquad \hat{m} = \sinh^{-1} m$$

Downward flows (thimbles) $\mathcal{J}_\sigma$

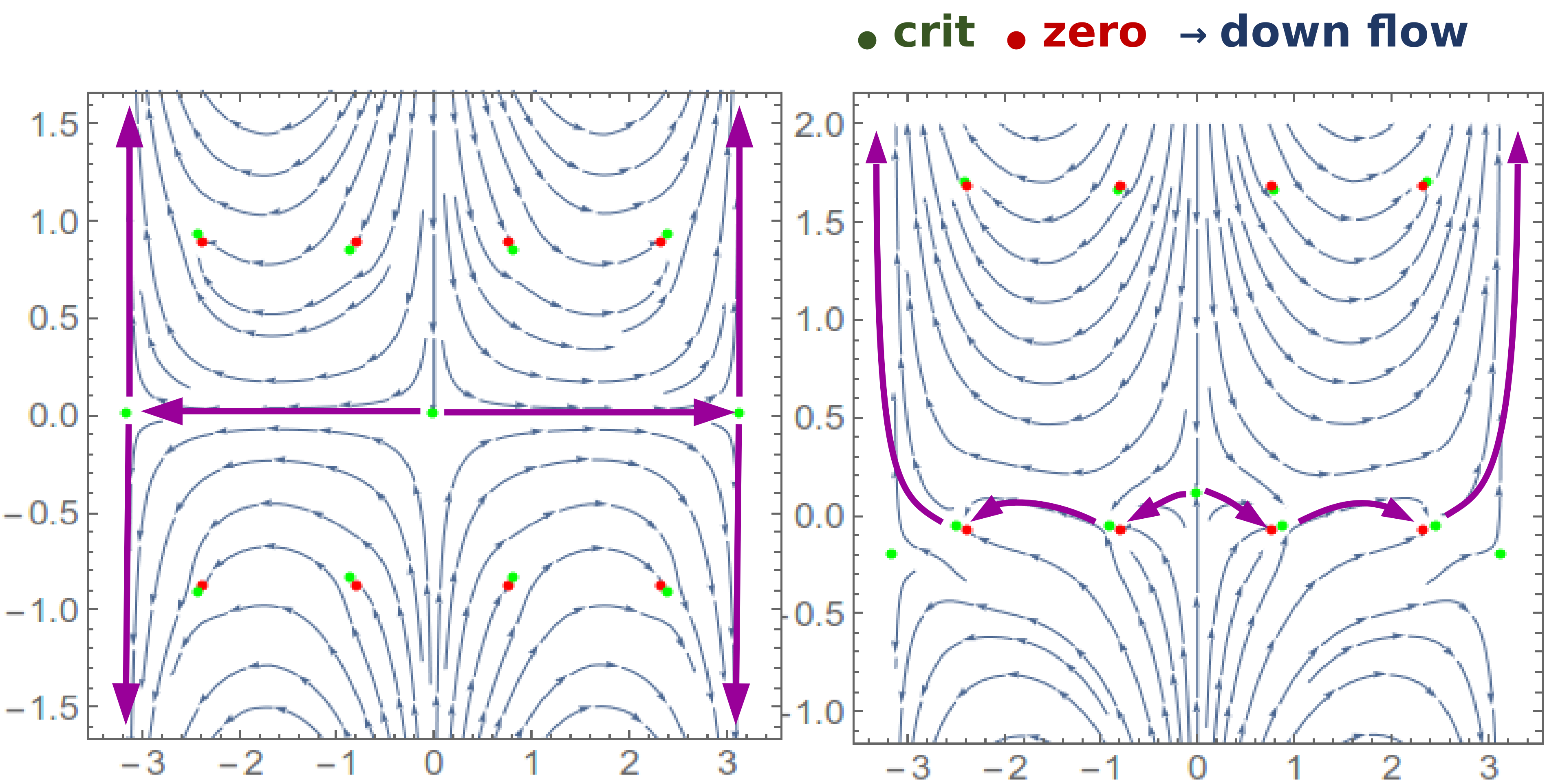
$$\frac{dz}{dt} = \frac{\partial \bar{S}_A[\bar{z}]}{\partial \bar{z}}$$

with the initial condition $z \to z_\sigma$ as $t \to -\infty$

Zero-points $\det K[z] = 0 \ (S_A = +\infty)$ ⇒ **end point of thimbles**

$$\cosh\left[L(\mu + iz)\right] + \cosh L\hat{m} = 0 \quad \Rightarrow \quad z_{\text{zero}} = i(\mu \mp \hat{m}) + \frac{2n+1}{L}\pi$$

$\mathcal{N}_f = 1, m = 1, \beta = 3, L = 4$



$\mu = 0.0$ $\mu = 0.8$

Intersection numbers

To count intersection numbers,
we obtain the upward cycles.

Upward cycles (dual flows) $\mathcal{K}_\sigma$

(Opposite direction to the downward flows)

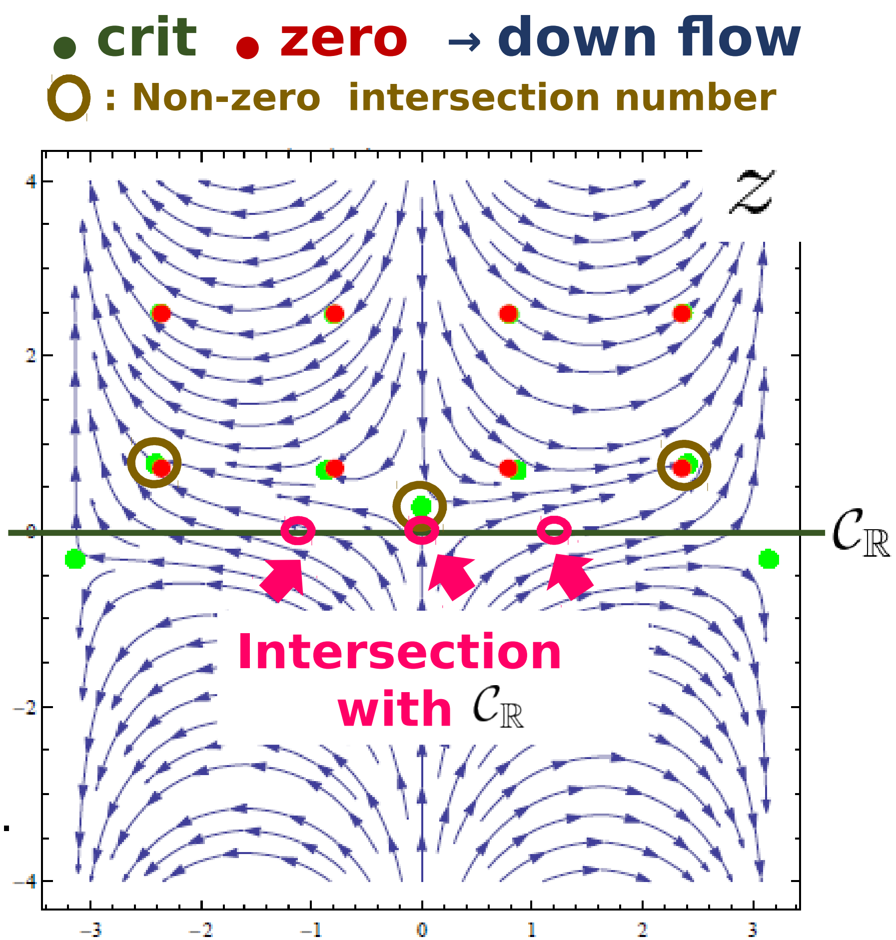
$$\frac{dz}{dt} = \frac{\partial \bar{S}_A[\bar{z}]}{\partial \bar{z}}$$

with the initial condition,

$$z \to z_\sigma \text{ as } t \to +\infty$$

A set of thimbles which contribute to
the partition function changes depending on μ.

We focus on *the Stokes phenomenon*.



Stokes phenomenon & intersection numbers

How to count intersection numbers ? In general it is hard systematically …
The Stokes phenomenon gives information of change of intersection numbers.

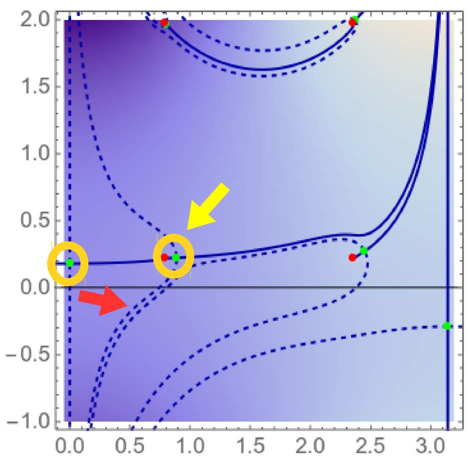
The Stokes phenomenon:

**When two critical points are connected by a flow,
we say that the Stokes phenomenon occurs.**

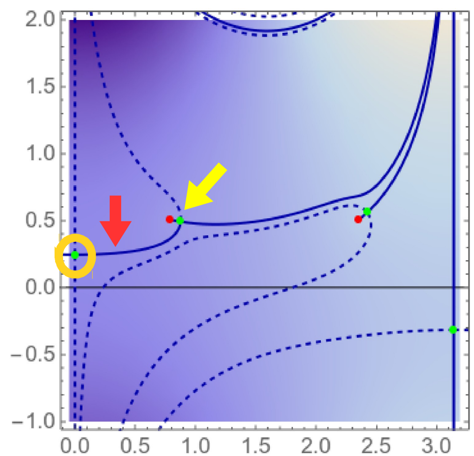
O : Non-zero intersection number

—— : Thimble

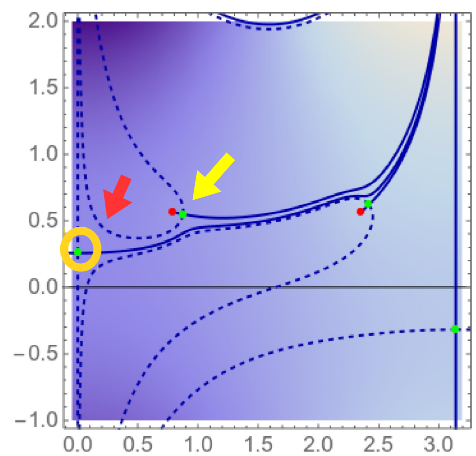
- - - : dual flow



$\mu < \mu^*$



$\mu = \mu^*$

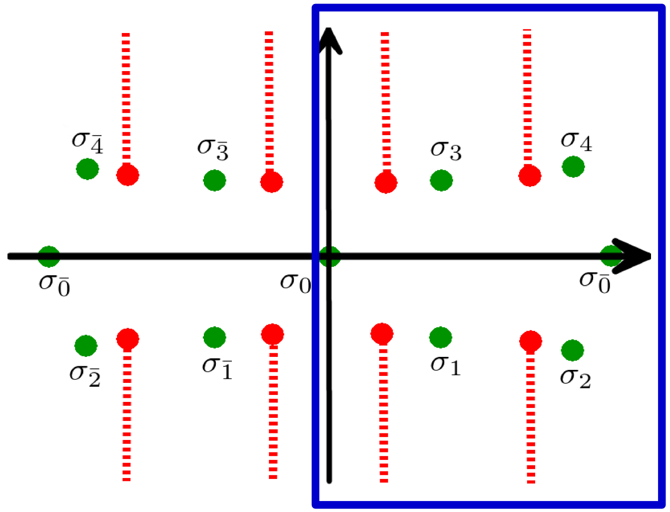


$\mu > \mu^*$

Stokes phenomenon

L=4, Nf=1, β=3, m=1

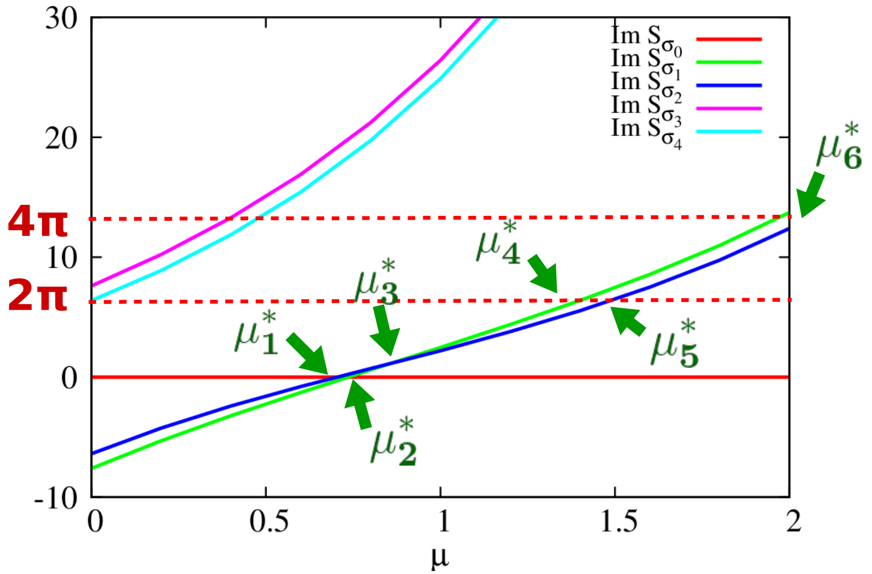
From the imaginary part of action on critical points, we can see where the Stokes phenomenon occurs.



Condition for the Stokes phenomenon

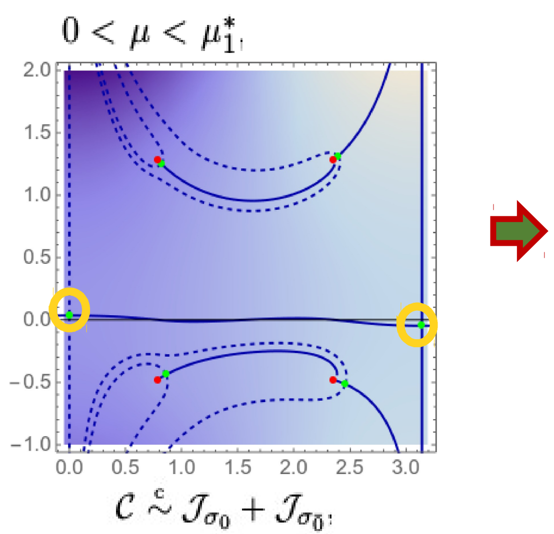
$$\mathrm{Im}S_\sigma = \mathrm{Im}S_{\sigma'} + \boxed{2\pi k} \qquad k \in \mathbb{Z}\ .$$

Branch from Dirac op. (log det D)



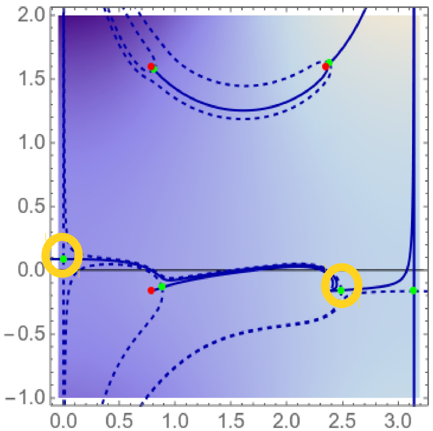
There are six μs at which the Stokes phenomenon occurs.

We construct the integration contour of the zero-mode partition function by thimbles.



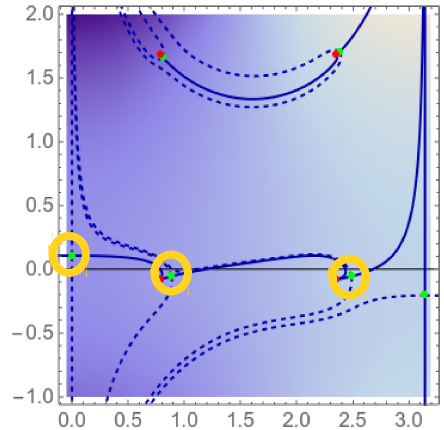
Stokes phenomenon   L=4, Nf=1, β=3, m=1

$\mu_1^* < \mu < \mu_2^*$



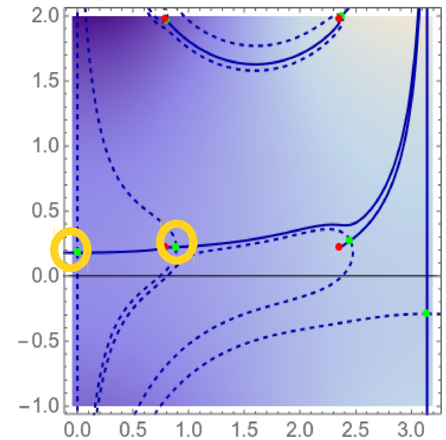
$\mathcal{C} \stackrel{c}{\sim} \mathcal{J}_{\sigma_0} + \mathcal{J}_{\sigma_2} + \mathcal{J}_{\sigma_{\bar{2}}}$

$\mu_2^* < \mu < \mu_3^*$.



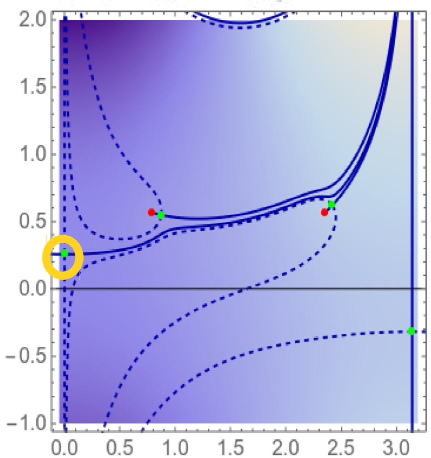
$\mathcal{C} \stackrel{c}{\sim} \mathcal{J}_{\sigma_0} + \mathcal{J}_{\sigma_1} + \mathcal{J}_{\sigma_{\bar{1}}} + \mathcal{J}_{\sigma_2} + \mathcal{J}_{\sigma_{\bar{2}}}$

$\mu_3^* < \mu < \mu_4^*$.



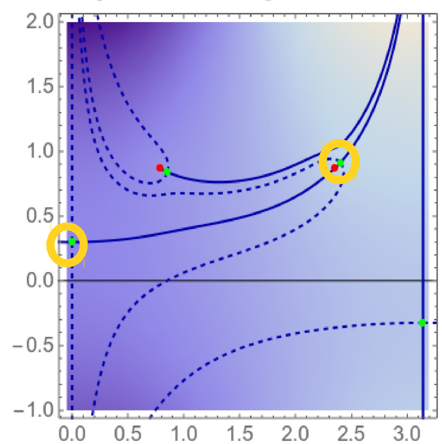
$\mathcal{C} \stackrel{c}{\sim} \mathcal{J}_{\sigma_0} + \mathcal{J}_{\sigma_1} + \mathcal{J}_{\sigma_{\bar{1}}}$

$\mu_4^* < \mu < \mu_5^*$



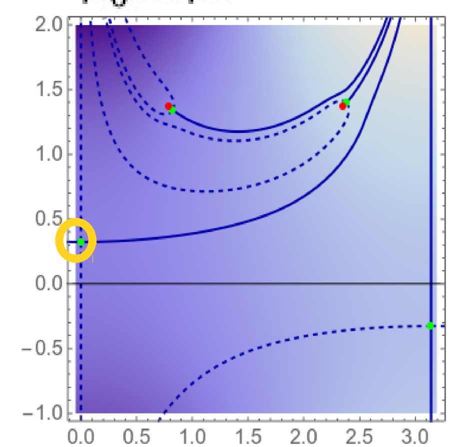
$\mathcal{C} \stackrel{c}{\sim} \mathcal{J}_{\sigma_0}$

$\mu_5^* < \mu < \mu_6^*$



$\mathcal{C} \stackrel{c}{\sim} \mathcal{J}_{\sigma_0} + \mathcal{J}_{\sigma_2} + \mathcal{J}_{\sigma_{\bar{2}}}$.

$\mu_6^* < \mu$.



$\mathcal{C} \stackrel{c}{\sim} \mathcal{J}_{\sigma_0}$

HMC simulation – details and results –

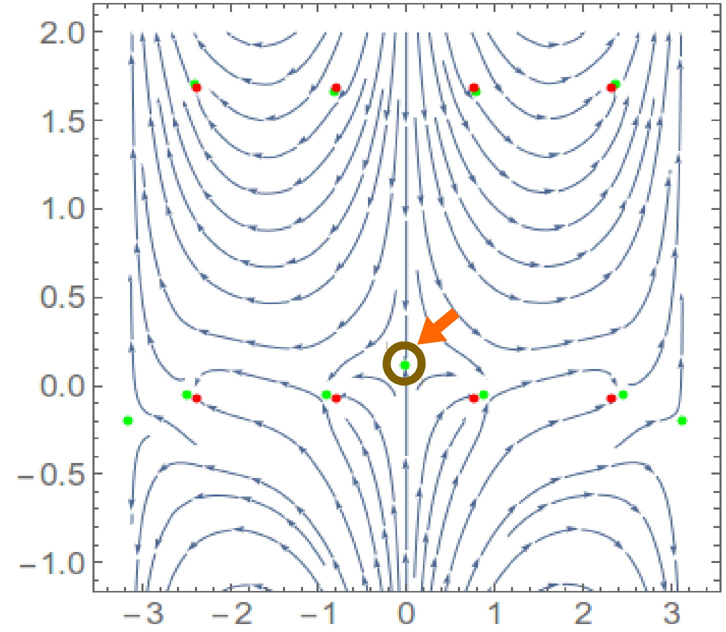
- We perform lattice simulations on a thimble $\mathcal{J}_0$, which in general ends at the zero of the fermion det.
- How can we reproduce the exact solution ?

- **Simulation parameters**

  Flavors $N_f = 1,$
  Mass $m = 1,$
  Lattice sites $L = 4, 8$
  Coupling $\beta = 1, 3$
  Chem pot $\mu = 0, 0.2, \cdots, 1.8, 2$

- **Number of confs and error estimate**

  Num of confs 1,000 confs
  Error estimate Jackknife method
  Bin size 10 confs / bin

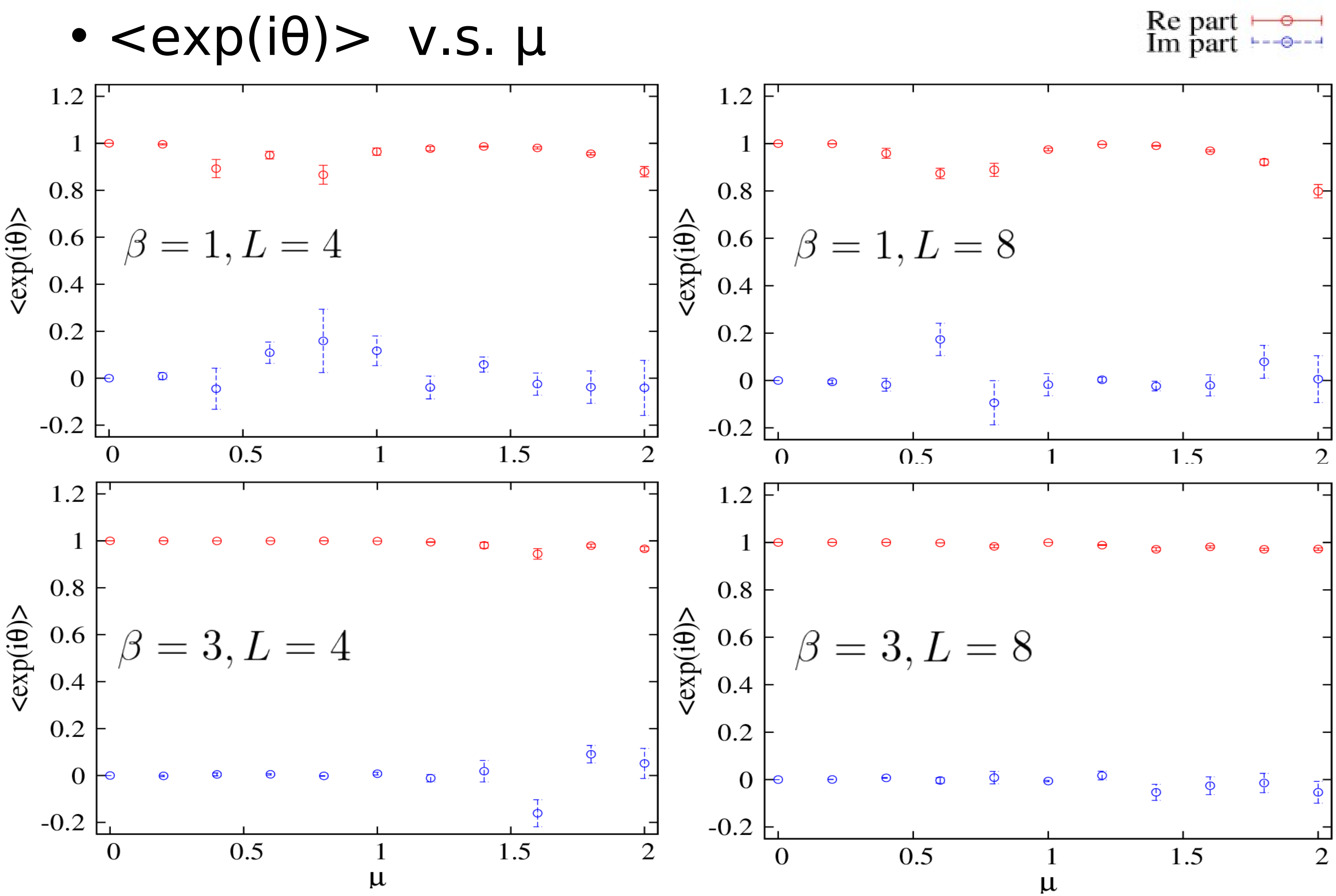


- **Improvements (cf.[Fujii et al. , 2013])**

  Scale parameter λ : $z_n \to \lambda z_n \quad \lambda \sim 0.1$
  Adaptive step in the 4th RK method : $\left\| \frac{\partial S}{\partial z_n} \right\| dt = \text{const.} \sim 0.005$

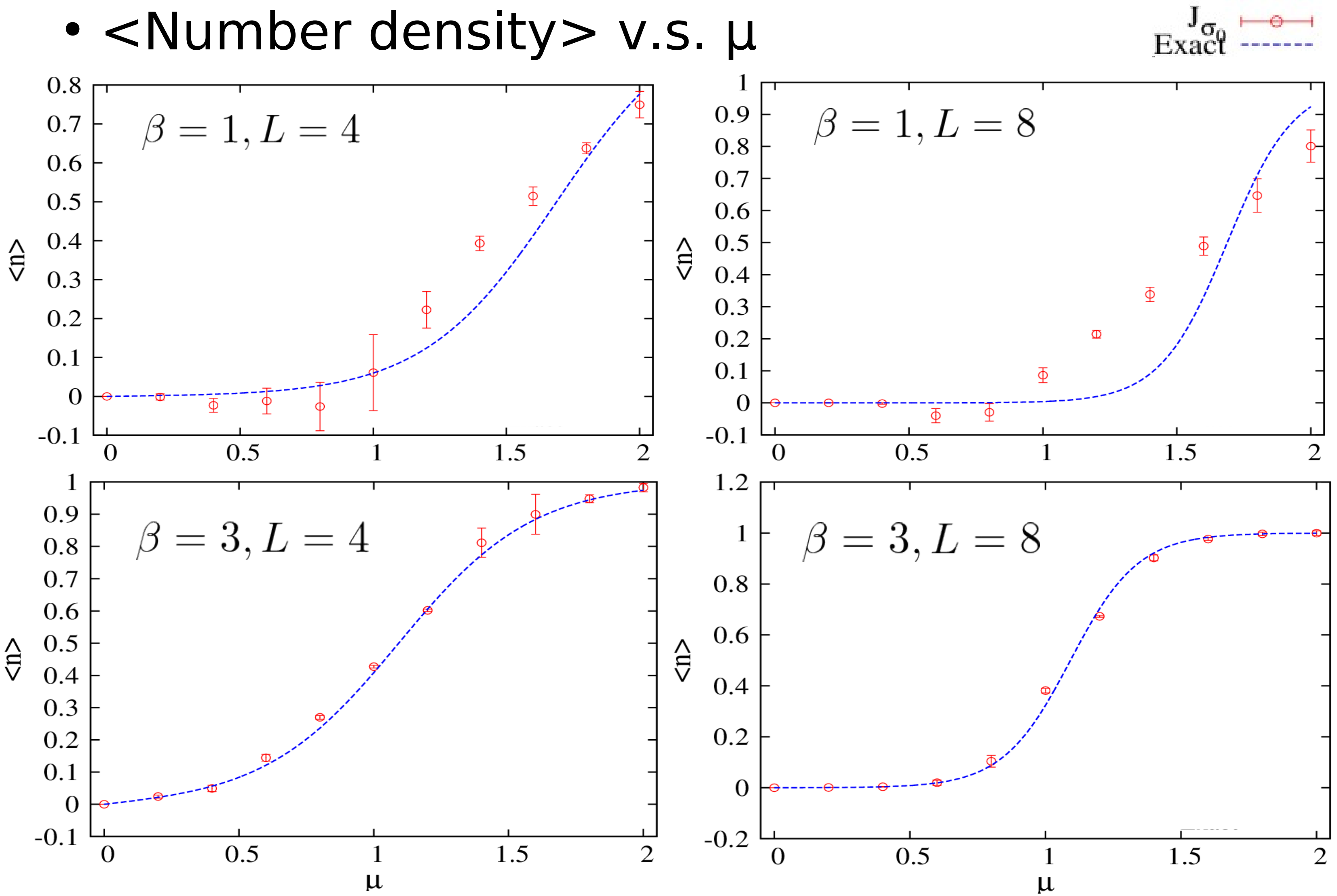
Results 1: Residual phase

- <exp(iθ)> v.s. μ



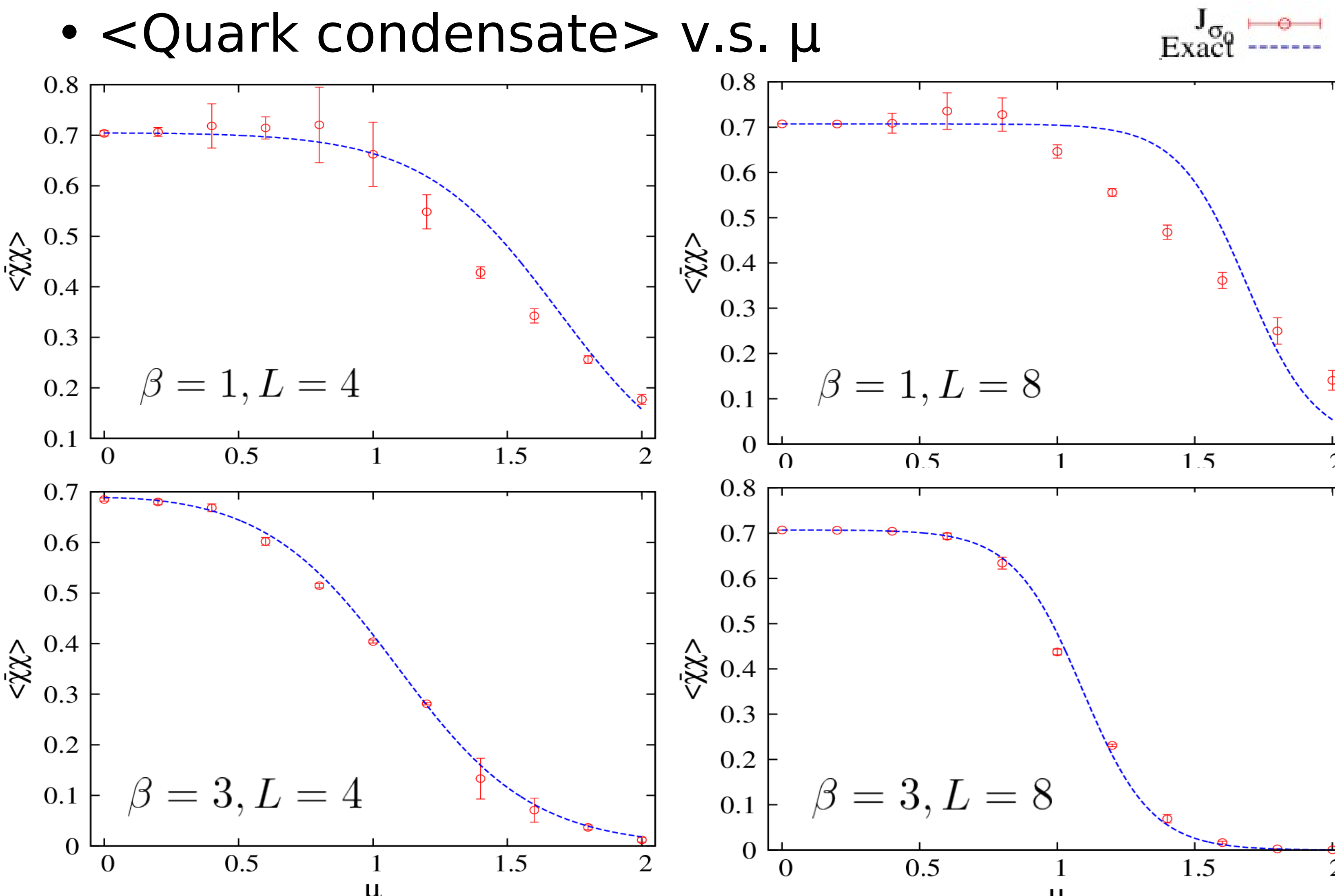
Results 2: Number density

- <Number density> v.s. μ

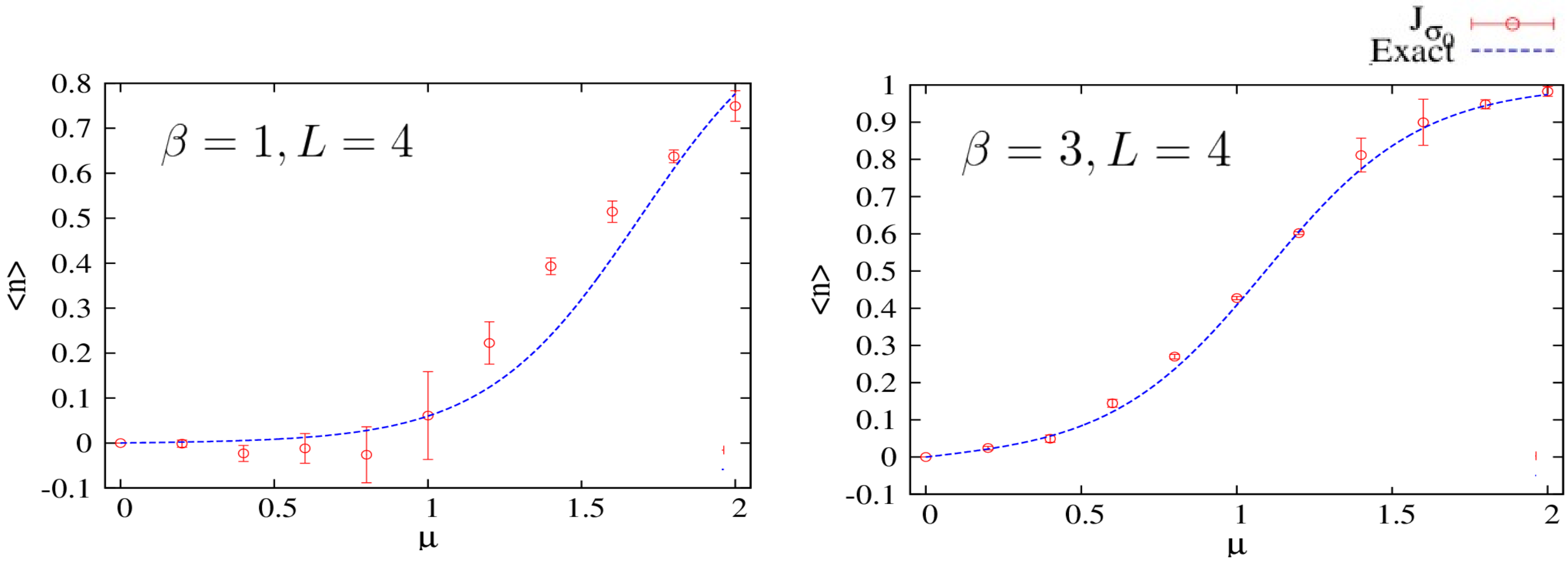


Results 3: Quark condensate

- <Quark condensate> v.s. μ



Simulation details and results



- At β=3, the numerical results are in good agreement with the exact solutions in the μ-range considerd.

- At β=1, we have observed some discrepancies between the numerical results and the exact one in the intermediate range of μ.

  ⇒ We need to consider other thimbles and its study is ongoing...

Summary

- We applied the Lefschetz thimble method to the (0+1) dimensional Thirring model at finite density.
- We investigated the Stokes phenomenon to identify the thimbles which contribute to the partition function, assuming that the complexified fields are constant.
- We performed the numerical simulation on a dominant thimble, which in general ends at the zero of the fermion det.
- At smaller β, we have observed some discrepancies between the numerical results and the exact one in the intermediate range of μ.
  We need to consider subdominant thimbles such as σ_1, σ_2, etc.
  The study is ongoing…

Future work:
1D QCD
(1+1) dim QEDμ + topological term
…
(3+1) dim QCDμ

Back up slides

QCD and the sign problem

If the phase fluctuation is sufficiently small, we can estimate observables by the rewighting method, decomposition of the complex weight to its absolute value and phase factor:

$$\langle A \rangle_\rho = \frac{\int D\sigma\ A[\sigma]\ \rho[\sigma]}{\int D\sigma\ \rho[\sigma]}.$$

$\rho[\sigma]$: Complex distribution function

decompose

$$\rho[\sigma] = p[\sigma]\ \exp(i\theta[\sigma])$$
$$p[\sigma] \in \mathbb{R}$$

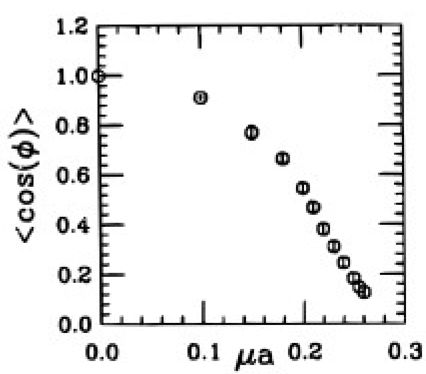
Rewight

$$\langle A \rangle_\rho = \frac{\int D\sigma A[\sigma] \exp(i\theta[\sigma])\ p[\sigma]}{\int D\sigma \exp(i\theta[\sigma])\ p[\sigma]} = \frac{\langle A[\sigma] \exp(i\theta[\sigma]) \rangle_p}{\langle \exp(i\theta[\sigma]) \rangle_p}$$

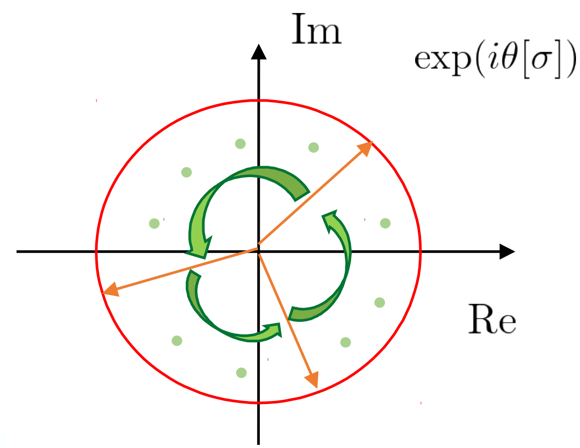
However,
MC does not work at large μ.

$$\mu \to \infty, \langle \mathcal{O} \rangle \to 0.$$

“Sign problem”



Toussaint-1990



Lefschetz thimbles **[Witten, 2010]**

- **Basic idea**

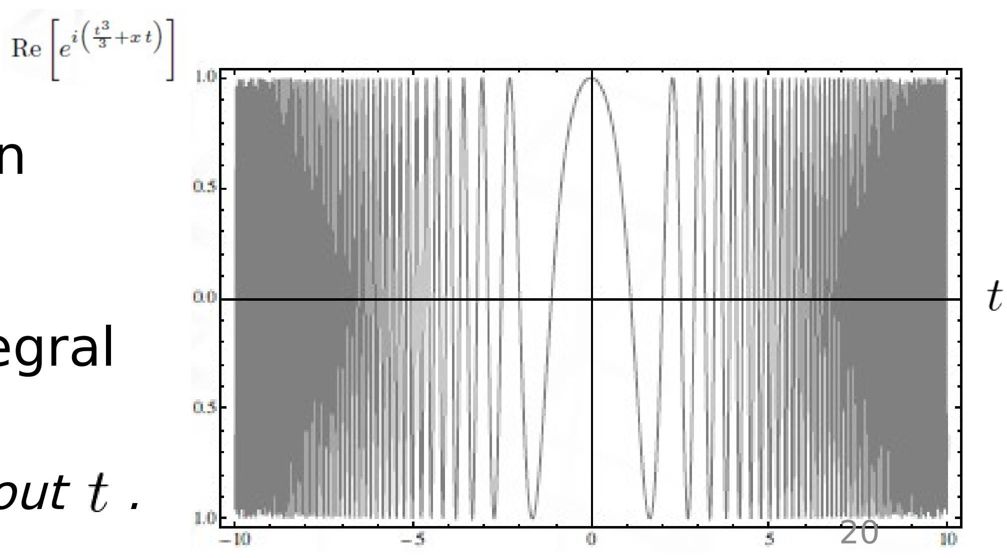
“Decomposition of a real integrate contour into particular contours called as Lefschets thimbles”

Example: Airy function

$$\mathrm{Ai}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\left(\frac{t^3}{3}+x\,t\right)}\mathrm{d}t$$

✓If x is **real**
⇒ well-defined function

✓If x is **complex**
⇒ highly oscillating integral



It is hard to directly integrate out t .

Lefschetz thimbles

[Witten, 2010]

$$Z_\lambda = \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(i\lambda(x^3/3 - x)\right)$$

Idea:

"the original integrate contour can be realized by linear combination with thimbles". **[Pham,1983]**

- *Extension of real variables to complex*

$$x \in \mathbb{R} \to x \in \mathbb{C}$$

- *Find critical points and thimbles defined by a Morse function*

$$h = \mathrm{Re}(\mathcal{I})$$
$$\mathcal{I} = i\lambda(x^3/3 - x)$$

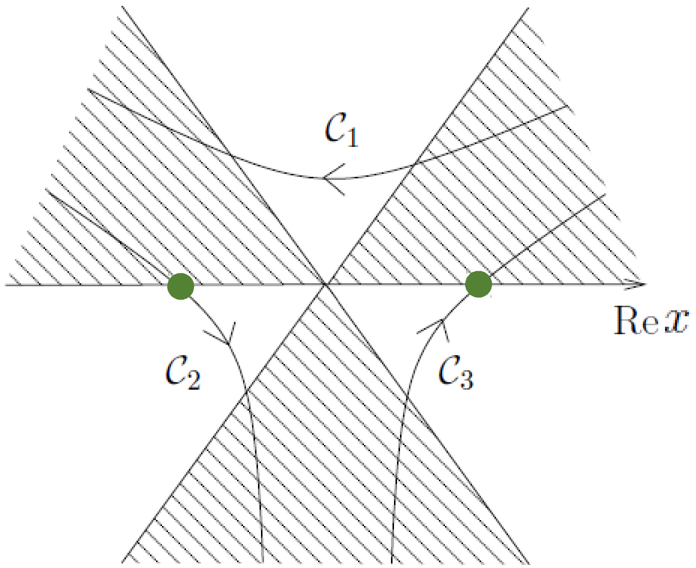
Crit point x_σ

$$\frac{d\mathcal{I}}{dx} = 0$$

Thimble $\mathcal{J}_\sigma$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\partial \overline{\mathcal{I}}}{\partial \overline{x}}$$

with $t \to -\infty,\ x \to x_\sigma$

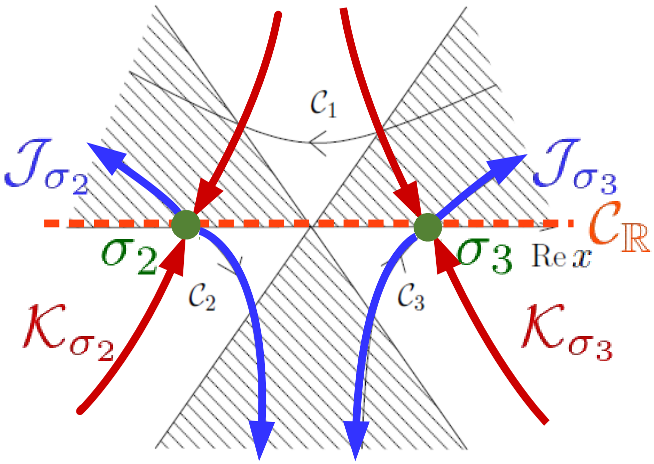


- *The integrate contour can obtained by the thimbles:*

$$Z_\lambda = \mathfrak{n}_+ Z_{+,\lambda} + \mathfrak{n}_- Z_{-,\lambda}.$$
$$\mathcal{C} = \mathfrak{n}_+ \mathcal{J}_+ + \mathfrak{n}_- \mathcal{J}_-.$$

Lefschetz thimbles

[Witten, 2010]



An original integration contour can be constructed by a inear combination with thimbles

- Extend real d.o.f. to complex.

$$\phi_R + i\phi_I \quad \phi_{R,I} \in \mathbb{R} \Rightarrow \tilde{\phi}_R + i\tilde{\phi}_I \quad \tilde{\phi}_{R,I} \in \mathbb{C}$$

- We find critical points and integration contours called as ***thimbles (downward flows)***

$\{z_\sigma\}$ $\quad \partial S[z]/\partial z_i|_{z=z_\sigma} = 0$ $\qquad$ $\mathcal{J}_\sigma$ $\quad g_i \equiv \frac{dz_i}{dt} = \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}_i}$

- Re S is non-decreasing func of t, and Im S is constant.

[Pham, 1983]

$$h \equiv -\mathrm{Re}S[z].$$

$$\frac{dh}{dt} = -\frac{1}{2}\left(\frac{dz_i}{dt}\frac{\partial S[z]}{\partial z_i} + \frac{d\bar{z}_i}{dt}\frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}_i}\right) = -\left|\frac{\partial S[z]}{\partial z_i}\right|^2 \le 0,$$

$$\frac{d\mathrm{Im}S[z]}{dt} = \frac{1}{2i}\left(\frac{dz_i}{dt}\frac{\partial S[z]}{\partial z_i} - \frac{d\bar{z}_i}{dt}\frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}_i}\right) = 0.$$

Integration contour :

$$\langle \mathcal{J}_\sigma, \mathcal{K}_\tau \rangle = \delta_{\sigma\tau}$$

$$\mathcal{C}_{\mathbb{R}} = \sum_{\sigma\in\Sigma} n_\sigma \mathcal{J}_\sigma, \qquad n_\sigma = \langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_\sigma \rangle\,.$$

Lefschetz thimbles **[Witten, 2010]**

From the procedure, the original partition function can be constructed by partition functions on thimbles:

$$Z = \sum_{\sigma} n_\sigma P_\sigma Z_\sigma, \qquad Z_\sigma = \int_{\mathcal{J}_\sigma} D[z] \; \exp\{-\mathrm{Re}(S[z] - S[z_\sigma])\}$$

$P_\sigma = \exp(-S_\sigma)$: **relative weight** $\qquad n_\sigma = \langle \mathcal{C}_{\mathbb{R}}, \mathcal{K}_\sigma \rangle$: **intersection number**

From this formula, expectation values can be obtained by

$$\boxed{\langle \mathcal{O}[z] \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} n_\sigma P_\sigma Z_\sigma \langle \mathcal{O}[z] \rangle_{\mathcal{J}_\sigma}} \qquad \langle \mathcal{O}[z] \rangle_{\mathcal{J}_\sigma} = \frac{1}{Z_\sigma} \int_{\mathcal{J}_\sigma} D[z] \; \exp\{-\mathrm{Re}(S[z] - S[z_\sigma])\} \; O[z].$$

Since Im S is always constant, the original phase fluctuation vanishes. However the residual phase occurs from the integration measure:

$$z \in \mathbb{C} \to \delta\xi \in \mathbb{R} \qquad \int_{\mathcal{J}_\sigma} D[z] = \int_{\mathcal{J}_\sigma} D[\delta\xi] e^{i\phi_z} \qquad \boxed{\langle \mathcal{O} \rangle_{\mathcal{J}_\sigma} = \frac{\langle e^{i\phi_z} \mathcal{O} \rangle_{\xi_\sigma}}{\langle e^{i\phi_z} \rangle_{\xi_\sigma}}}$$

⇒ We use the rewighting method to obtain observables on thimbles.

The Thirring model at finite density on lattice

- Continuum action in general dim

$$\mathcal{L} = \sum_{i=1}^{N_f} \bar{\psi}_i(\partial_\nu \gamma_\nu + m_i + \mu_i \gamma_4)\psi_i + \frac{g^2}{2N_f}\left(\sum_{i=1}^{N_f} \bar{\psi}_i \gamma_\nu \psi_i\right)^2$$

$$\mathcal{L} = \frac{N_f}{2g^2} A_\nu^2 + \sum_{i=1}^{N_f} \bar{\psi}_i(\nabla_\nu \gamma_\nu + m_i + \mu_i \gamma_4)\psi_i, \quad \nabla_\nu = \partial_\nu + iA_\nu$$

Boundary condition

$$\psi_i(t) = -\psi_i(t + 1/T),$$
$$\bar{\psi}_i(t) = -\bar{\psi}_i(t + 1/T).$$

- (0+1) dim lattice action with the KS fermion $(a = 1)$

$$\mathcal{L}_U = \frac{N_f \beta}{2}(2 - U(t) - U^{-1}(t)) + \sum_{i=1}^{N_f} \bar{\chi}_i(\tilde{\nabla}^{(i)} + m_i)\chi_i,$$

$$\tilde{\nabla}^{(i)}\chi_i(t) = \frac{1}{2}e^{+\mu_i}U(t)\chi_i(t+1) - \frac{1}{2}e^{-\mu_i}U^{-1}(t-1)\chi_i(t-1).$$

Compact (link-like) variable

$$U(t) = \exp(iA(t)).$$
$$-\pi \le A(t) < \pi$$

Effective action

$$\mathcal{L}_U = \frac{N_f \beta}{2}(2 - U(t) - U^{-1}(t)) - \sum_i \log\det \tilde{D}_i$$

$$\tilde{D}_i = \tilde{\nabla}^{(i)} + m_i.$$
$$\beta = 1/(2g^2)$$

The Thirring model at finite density on lattice

- Solving the partition function (L= even, Nf = 1)

$$Z_U = \int_{-\pi}^{\pi} DA \exp\left(-S_U\right)$$

$$\Rightarrow \quad \boxed{Z_U = \pi^L e^{-L\beta}\left[2\cosh(L\mu)(I_1(\beta))^L + (\mathcal{C}_+ + \mathcal{C}_-)(I_0(\beta))^L\right]}$$

$I_0(x),\ I_1(x)$: modified Bessel functions

$$\mathcal{C}_c = 1 + 4\kappa^2,\ \ \mathcal{C}_\pm = \frac{1}{(2\kappa)^L}\left(1 \pm \sqrt{\mathcal{C}_c}\right)^L \qquad \kappa = 1/2m$$

- Observables

Number density

$$\langle n \rangle \equiv \frac{1}{L}\frac{\partial \log Z}{\partial \mu} = \frac{2\sinh(L\mu)(I_1(\beta))^L}{2\cosh(L\mu)(I_1(\beta))^L + (\mathcal{C}_+ + \mathcal{C}_-)(I_0(\beta))^L},$$

Fermion condensate

$$\langle \bar{\chi}\chi \rangle \equiv \frac{1}{L}\frac{\partial \log Z}{\partial m} = \frac{2\kappa\sqrt{1/\mathcal{C}_c}(\mathcal{C}_+ - \mathcal{C}_-)(I_0(\beta))^L}{2\cosh(L\mu)(I_1(\beta))^L + (\mathcal{C}_+ + \mathcal{C}_-)(I_0(\beta))^L}$$

We will compare the exact solutions with our numerical results obtained by Lefschtez formulation.

Critical points and thimbles

- We firstly extend real variables to complex.

$$A \in \mathbb{R} \rightarrow \mathcal{A} \in \mathbb{C} \qquad U \rightarrow \mathcal{U} = \exp(i\mathcal{A}), \quad U^{-1} \rightarrow \mathcal{U}^{-1} = \exp(-i\mathcal{A})$$

- We focus on only on zero-mode solutions and solve the complexified saddle point equation.

Critical points

$$\frac{\partial S_{\mathcal{U}}}{\partial \mathcal{A}} = 0.$$

$$\Rightarrow \quad -\frac{i\mathcal{N}_f\beta}{2}(\mathcal{U} - \mathcal{U}^{-1}) - \sum_{i=1}^{\mathcal{N}_f} \mathrm{Tr}\left[\tilde{D}_i^{-1}\frac{\partial \tilde{D}_i}{\partial \mathcal{A}}\right] = 0,$$

Numerically obtained.

Zero-points

$$S_{\mathcal{U}} = \infty \Rightarrow \qquad \det \tilde{D} = 0$$

$$\Rightarrow \quad \mathcal{A}_{(\infty)} = \theta_n - \frac{i}{L}\mathrm{Log}\left[\frac{\mathfrak{D}}{2} \pm \sqrt{\left(\frac{\mathfrak{D}}{2}\right)^2 - 1}\right] + i\mu,$$

$$\theta_n = \frac{(2n+1)\pi}{L} \qquad n \in \mathbb{Z}_L = \{q \in \mathbb{Z} \mid -L/2 \leq q < L/2\}.$$

$$\mathfrak{D} = \mathcal{C}_+ + \mathcal{C}_- \qquad \mathcal{C}_c = 1 + 4\kappa^2, \;\; \mathcal{C}_\pm = \frac{1}{(2\kappa)^L}\left(1 \pm \sqrt{\mathcal{C}_c}\right)^L$$

Analytically obtained.

Flows and Intersection numbers

Downward flows (thimbles): $\mathcal{J}_\sigma$

$$\frac{d\mathcal{A}}{dt} = +\frac{\partial \bar{S}[\bar{\mathcal{A}}]}{\partial \bar{\mathcal{A}}}$$

with the initial condition,

$$t \to -\infty,\ \mathcal{A} \to \mathcal{A}_\sigma$$

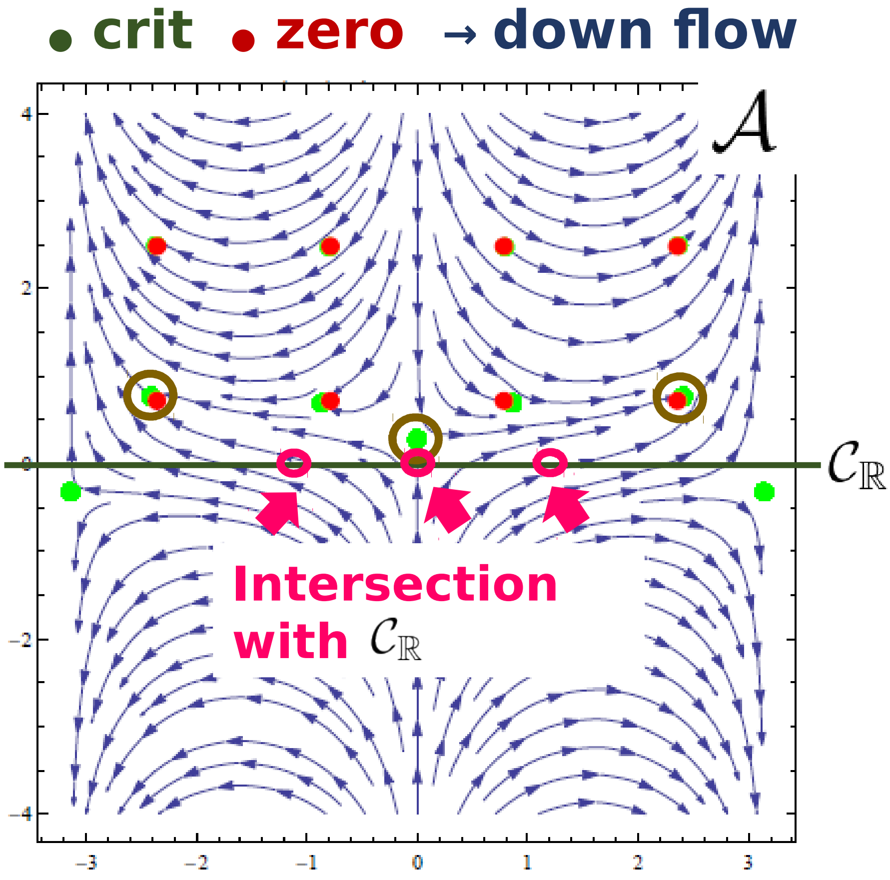
Upward flows (dual flow): $\mathcal{K}_\sigma$

(Opposite direction to the downward flow)

$$\frac{d\mathcal{A}}{dt} = +\frac{\partial \bar{S}[\bar{\mathcal{A}}]}{\partial \bar{\mathcal{A}}}$$

with the initial condition,

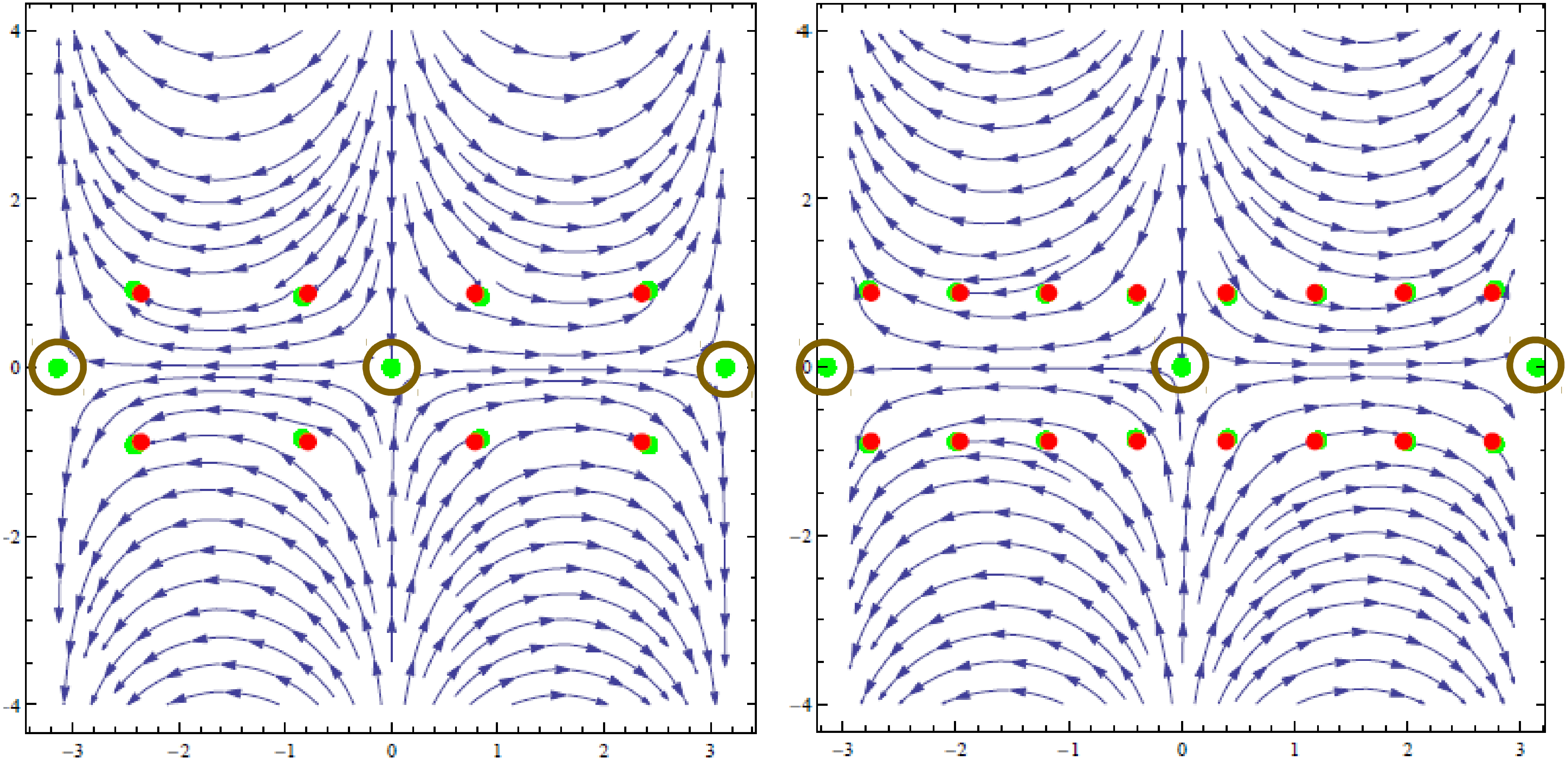
$$t \to \infty,\ \mathcal{A} \to \mathcal{A}_\sigma$$



Figs: configuration space

$\mathcal{N}_f = 1, m = 1, \beta = 3$ $\mu = 0.0$

O : **Non-zero intersection number**

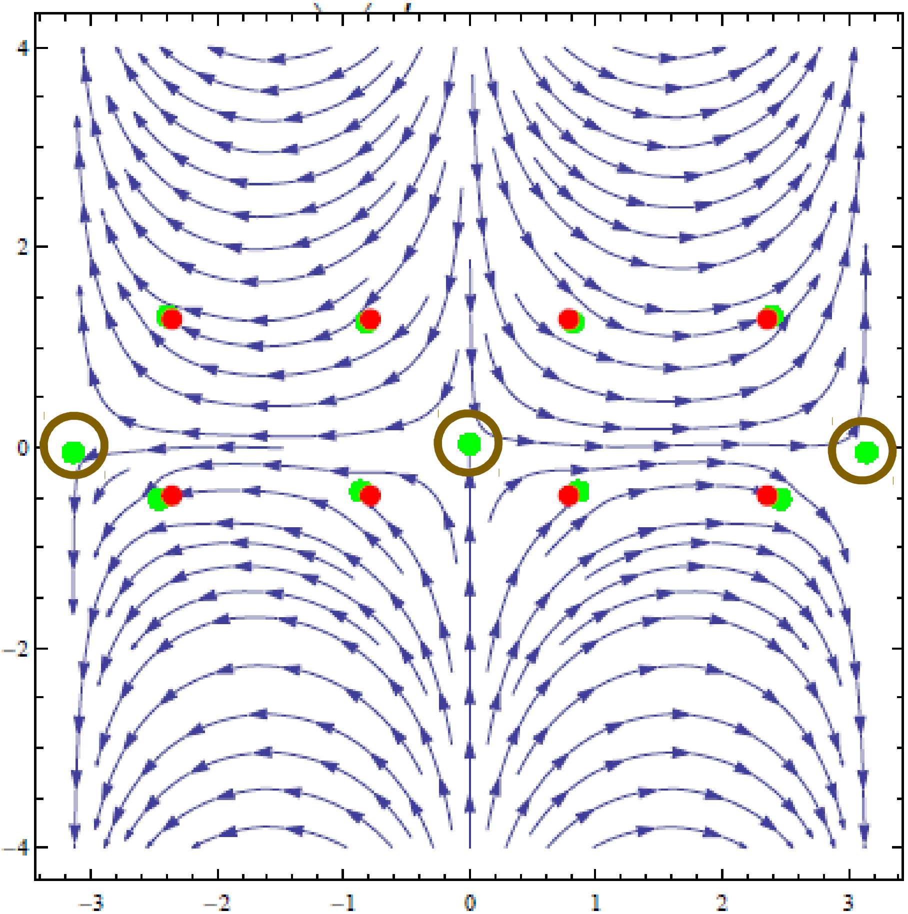


$L = 4$ $L = 8$

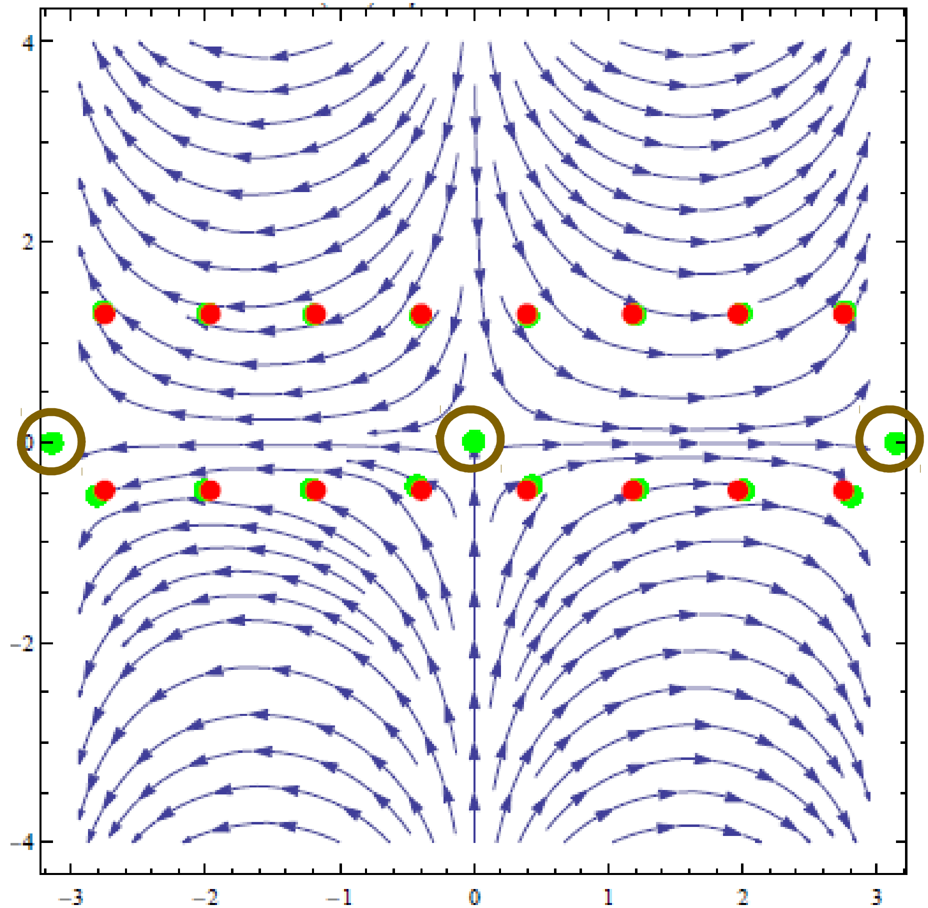
Figs: configuration space

$\mathcal{N}_f = 1, m = 1, \beta = 3$ $\mu = 0.4$

O : **Non-zero intersection number**



$L = 4$

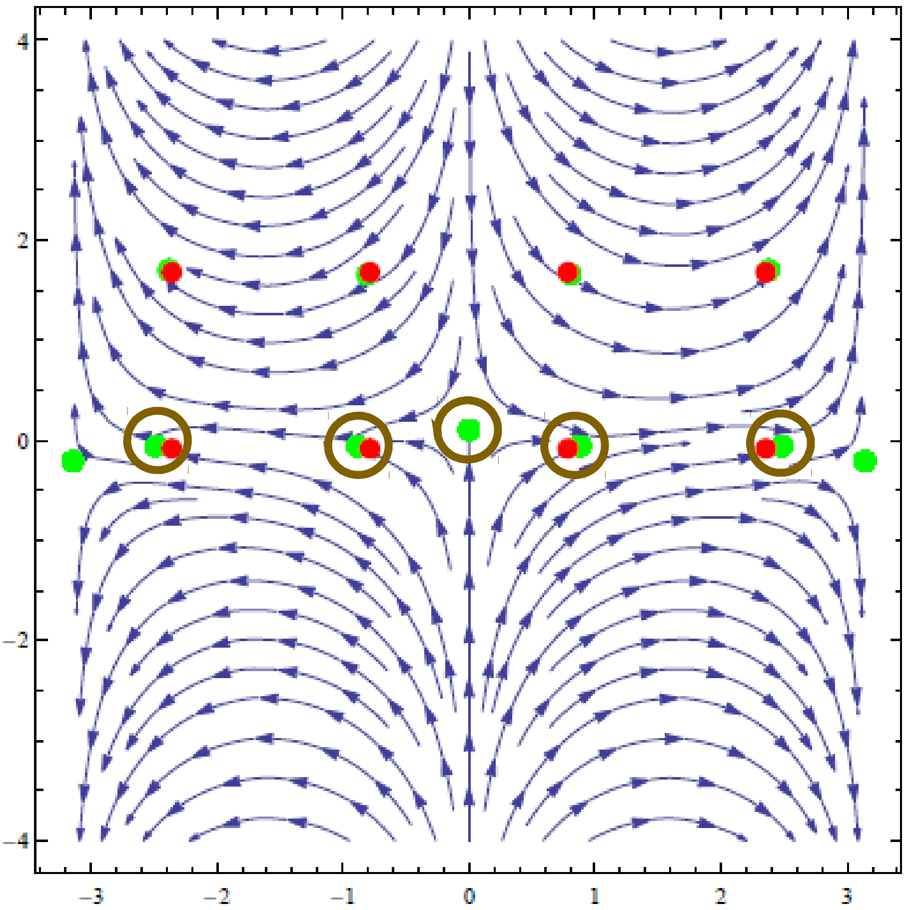


$L = 8$

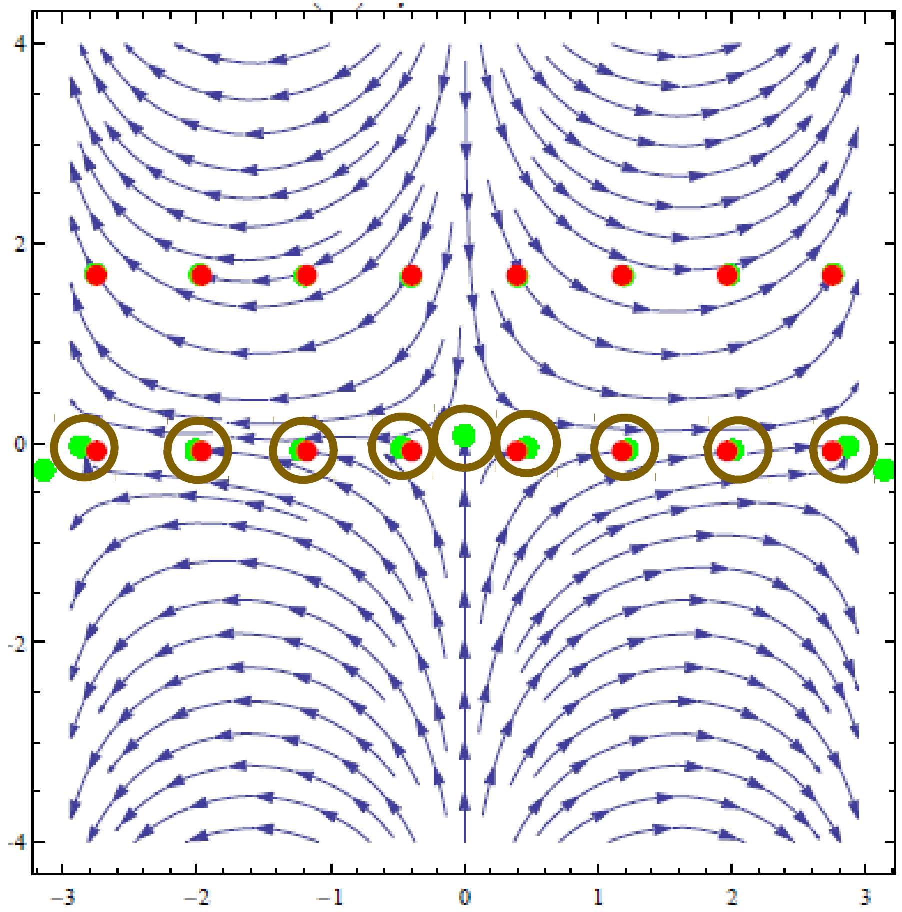
Figs: configuration space

$\mathcal{N}_f = 1, m = 1, \beta = 3$ $\mu = 0.8$

O : **Non-zero intersection number**



$L = 4$

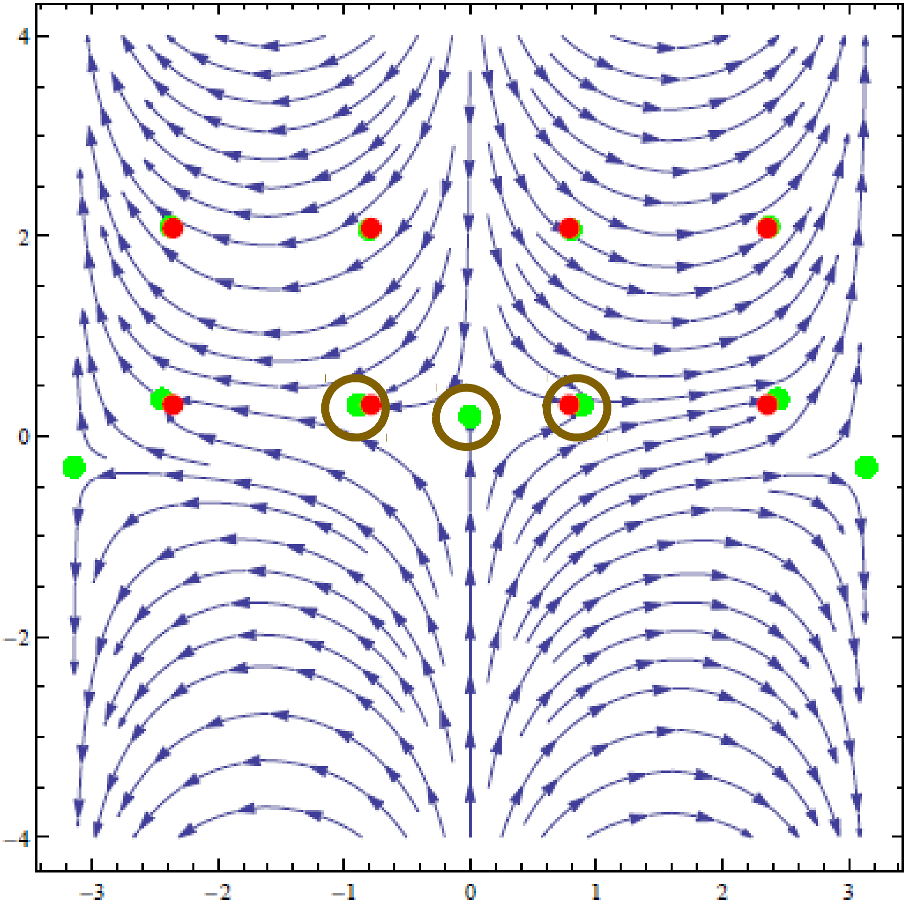


$L = 8$

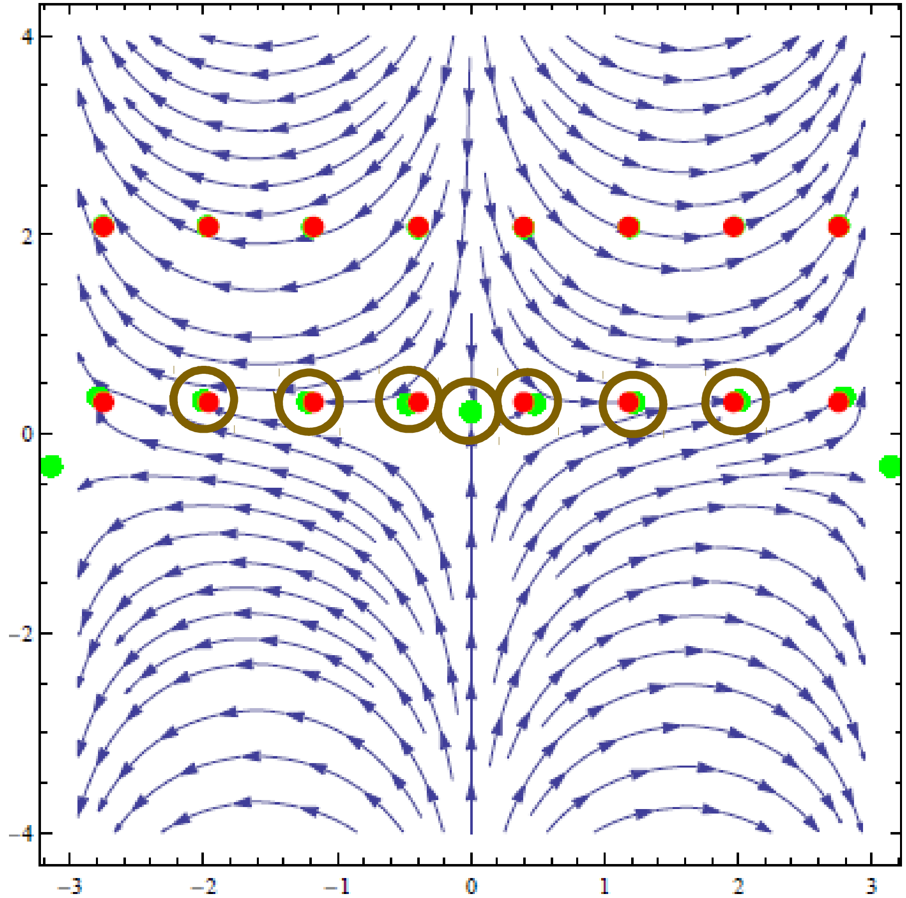
Figs: configuration space

$\mathcal{N}_f = 1, m = 1, \beta = 3$ $\mu = 1.2$

O : Non-zero intersection number



$L = 4$

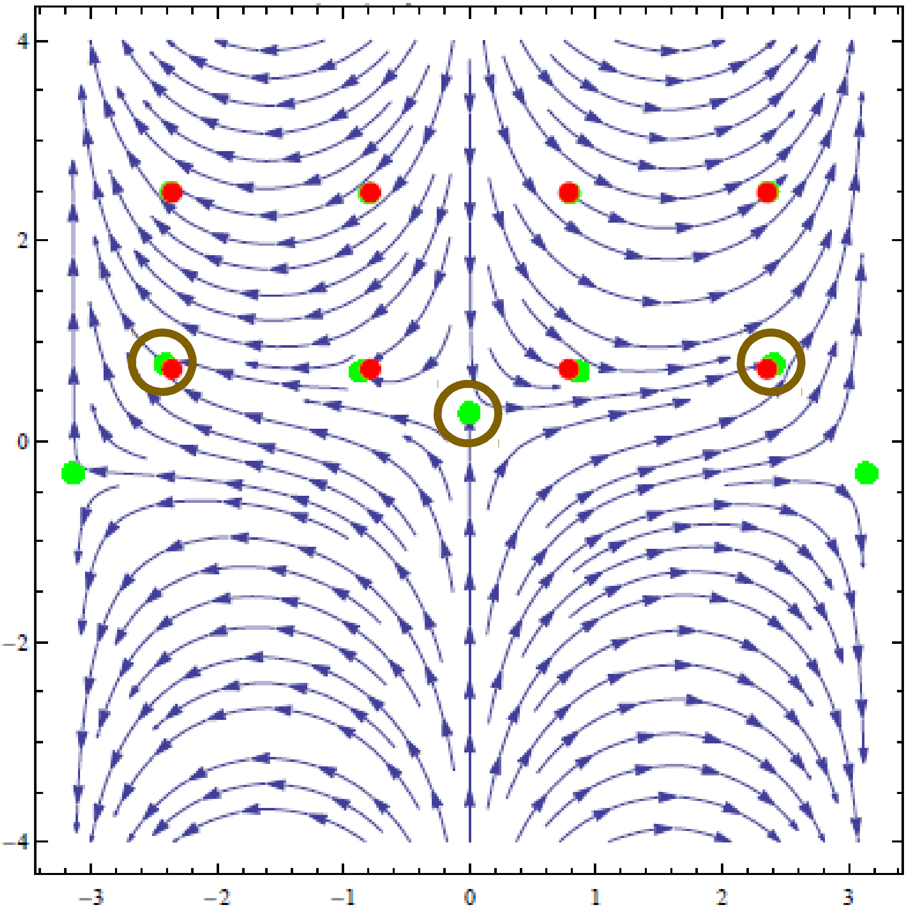


$L = 8$

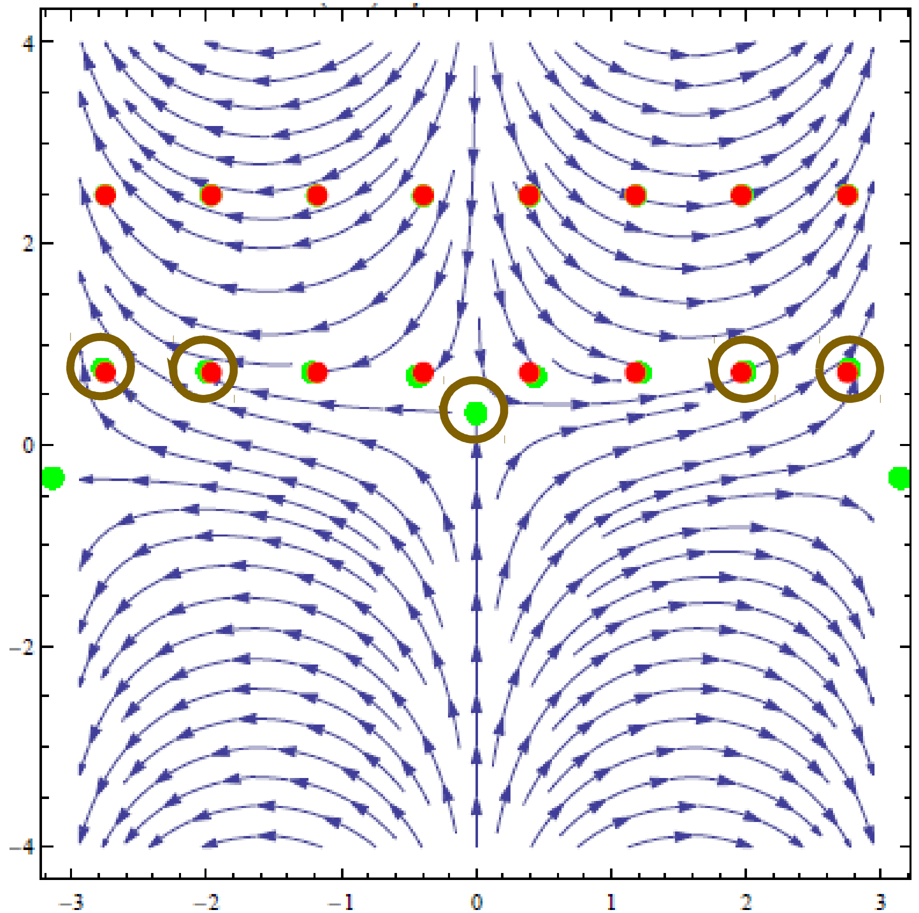
Figs: configuration space

$\mathcal{N}_f = 1, m = 1, \beta = 3$ $\mu = 1.6$

○ : Non-zero intersection number



$L = 4$

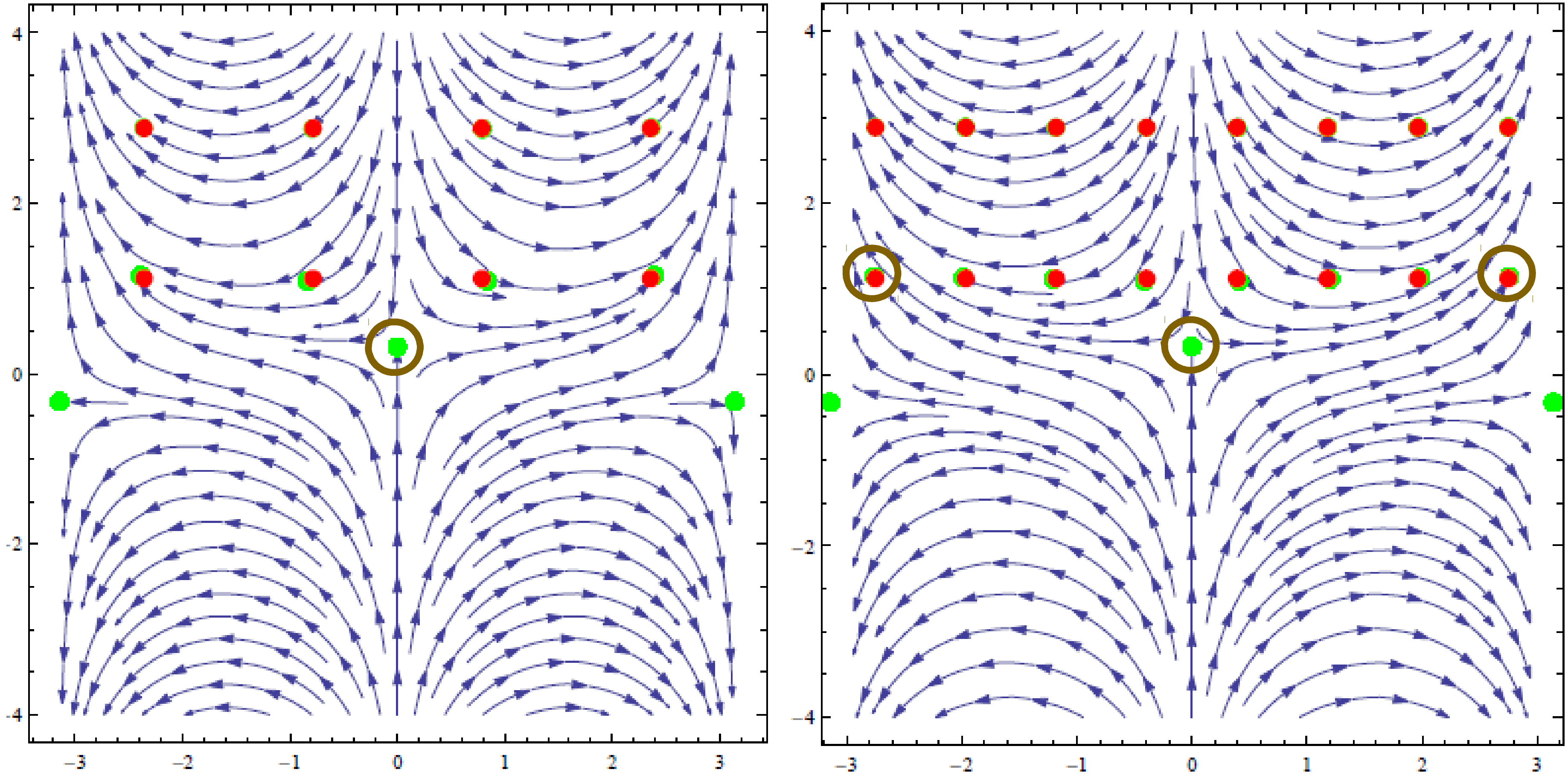


$L = 8$

Figs: configuration space

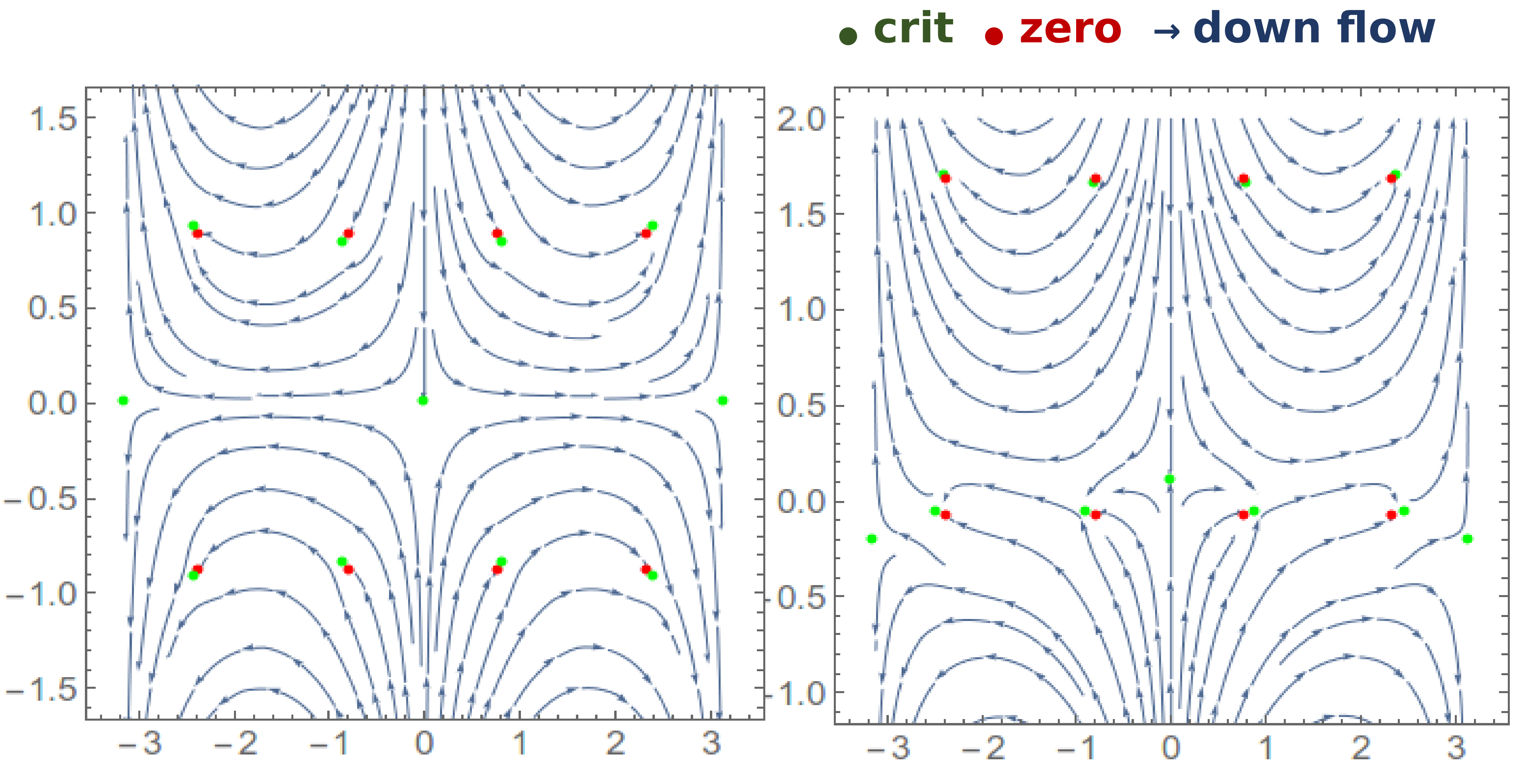
$\mathcal{N}_f = 1, m = 1, \beta = 3$ $\mu = 2.0$

○ : **Non-zero intersection number**



$L = 4$ $L = 8$

$$\mathcal{N}_f = 1, m = 1, \beta = 3, L = 4$$



$\mu = 0.0$ $\mu = 0.8$