Non-equilibrium QCD dynamics on the lattice

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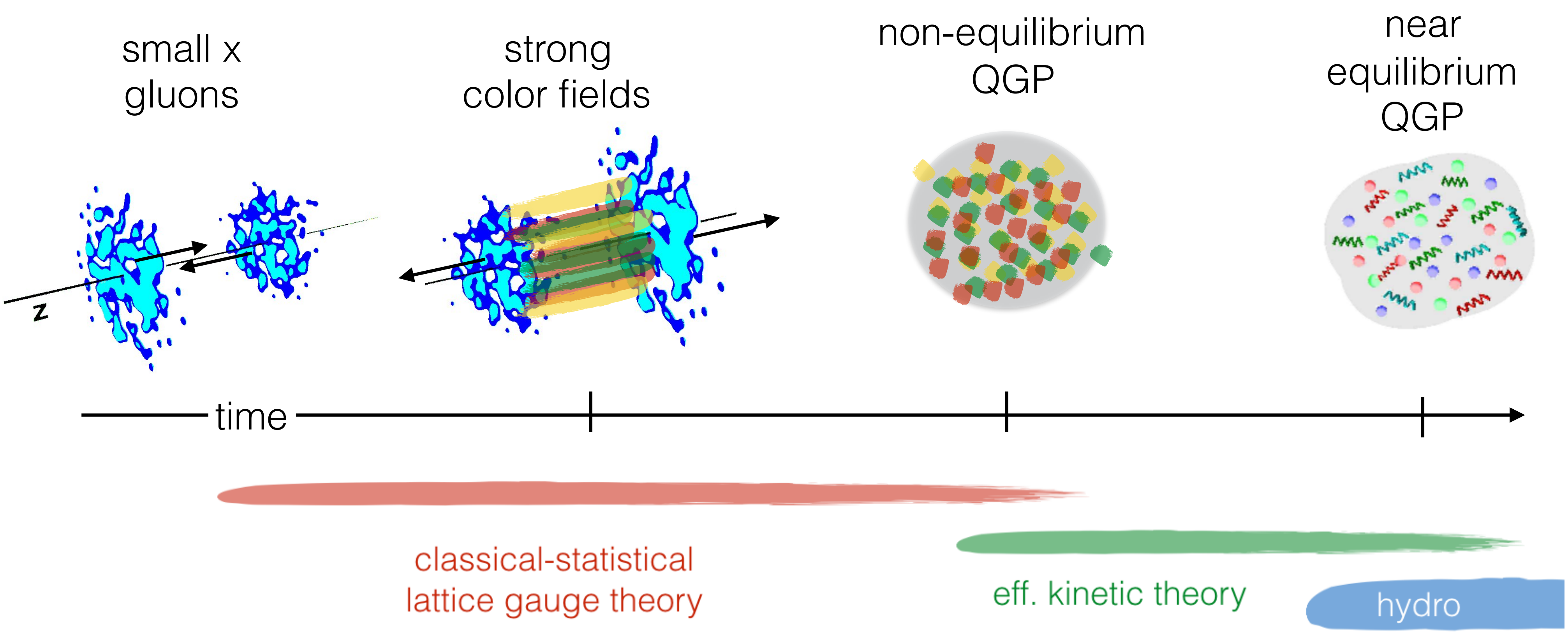
CRC-TR 211
Strong-interaction matter under extreme conditions

Early time dynamics of heavy-ion collisions

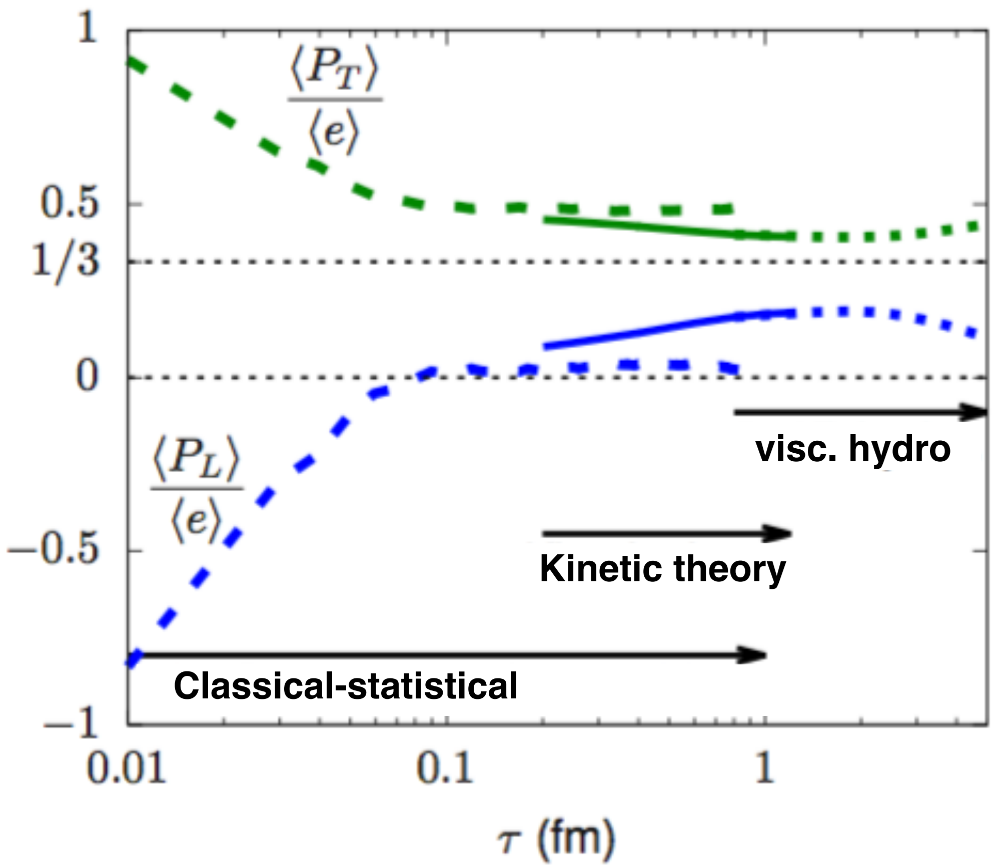
Different degrees of freedom relevant at different at different stages of the evolution



Need combination of non-equilibrium methods
to describe early time dynamics & approach to equilibrium

Early time dynamics of heavy-ion collisions

Evolution of energy momentum tensor in central Pb+Pb event



Based on combination of non-equilibrium methods can describe the space-time dynamics of HIC from beginning to end on event-by-event basis

-> Overlap in the range of validity ensures consistent matching

Kurkela, Mazeliauskas, Paquet, SS, Teaney arXiv:1805.01604; arXiv:1805.00961

Dynamical fermions

So far discussed classical-statistical approximation of boson fields

criterion for validity $n(t,p) \gg 1$ (strong Bose enhancement)

Not only interested in bosonic fields but also need to describe non-equilibrium dynamics of fermions

Pauli blocking $n(t,p) \leq 1$

However for theories of interest fermions appear quadratically in the action, can be integrated out exactly

$$\int_{\varphi_0^+}^{\varphi_0^-} D\varphi D\bar{\Psi} D\Psi \; e^{i\left[S_{\mathcal{C}}^B[\varphi]+\int_{xy,\mathcal{C}} \bar{\Psi}(x) i D^{-1}[\varphi](x,y)\Psi(y)\right]} \longrightarrow \int_{\varphi_0^+}^{\varphi_0^-} D\varphi \; e^{iS_{\mathcal{C}}^B[\varphi]+\mathrm{tr}\log D_{\mathcal{C}}^{-1}[\varphi]}$$

expand tr log D^{-1} in powers of classical and quantum fields

$$\int_{\varphi_0^{cl}}^{\varphi_0^{cl}} D\varphi_{cl} \; e^{\mathrm{tr}\log D_{\mathcal{C}}^{-1}[\varphi_{\mathrm{cl}}]} \int D\chi \;\; e^{i\int_{x,\mathcal{C}}\left(\frac{\delta S^B[\varphi_{cl}]}{\delta\varphi_{cl}} - D[\varphi_{\mathrm{cl}}]\frac{\delta i D^{-1}[\varphi_{cl}]}{\delta\varphi_{cl}}\right)\chi + h.o.}$$

Evolution of fermion in classical field bg

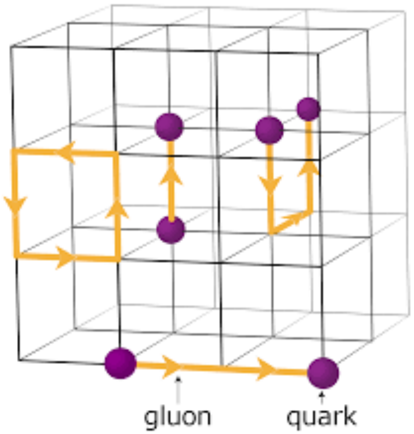
Backreaction of fermions via average current

Aarts,Smit NPB 555 (1999) 355-394

Berges,Kasper, Hebenstreit PRD90 (2014) no.2, 025016

Dynamical fermions

- Discretize theory on 3D spatial lattice using the Hamiltonian lattice formalism



- Solve operator Dirac equation in the presence of classical SU(N) and U(1) gauge fields

$$i\gamma^0 \partial_t \hat{\psi} = (-i\not{D}_W^s + m)\hat{\psi}$$

- Compute expectation values of fermion currents

$$j_v^\mu(x) = \langle \hat{\bar{\psi}}(x)\gamma^\mu \hat{\psi}(x)\rangle$$

- Solve classical Yang-Mills equations in the presence of fermonic currents

$$D_\mu F^{\mu\nu} = j_v^\nu$$

Mueller,SS, Sharma PRL 117 (2016) no.14, 142301
Mace, Mueller, SS, Sharma PRD95 (2017) no.3, 036023

Dynamical fermions

Solving the operator Dirac equation can be achieved by expanding the fermion field in operator basis at initial time

$$\hat{\psi}(x,t) = \sum_{p,\lambda} \hat{b}_{p,\lambda}(t=0)\phi_u^{p,\lambda}(x,t) + \hat{d}^{\dagger}_{p,\lambda}(t=0)\phi_v^{p,\lambda}(x,t)$$

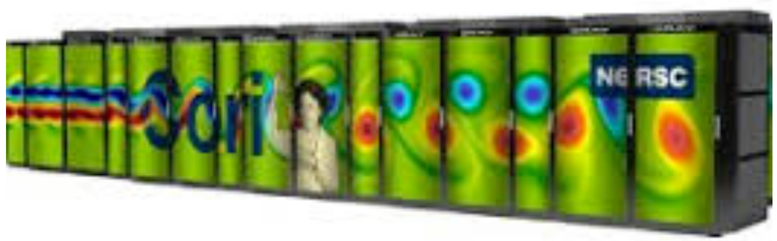
and solving the Dirac equation for evolution of $4N_cN^3$ wave-functions

Numerical cost:

gauge fields $\sim N_c^3 N^3$

$\sim 10^2$ CPU hours

gauge fields + fermions $\sim N_c^2 N^6$



$\sim 10^6$ CPU hours

Chiral magnetic effect:

New kind of conductivity for systems with chiral fermions and chirality imbalance

$$\vec{j}_V \propto n_5 \vec{B}$$

n_5: axial charge imbalance

B: magnetic field

Several possible manifestations of this effect from high-energy QCD to Dirac/Weyl semi-metals

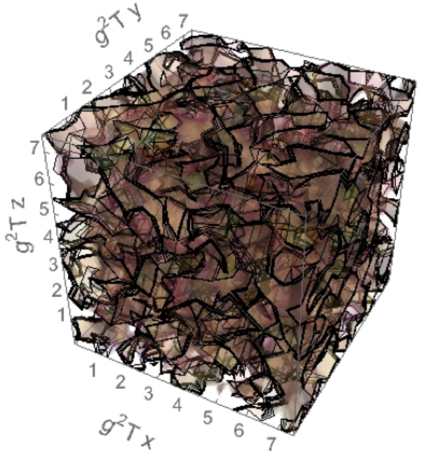
Fukushima, Kharzeev, Warringa PRD 78 (2008) 074033

Example: Sphaleron transitions & Chiral transport

Magnetic field: Spectators in off-central heavy-ion collisions create a strong magnetic field eB ~ m_π^2 (although presumably only for a very short time)

Axial charge density: Expect space-time dependent fluctuations due to axial anomaly

$\vec{E} \cdot \vec{B}$

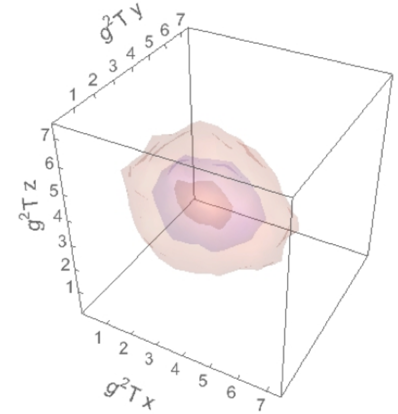


$$\partial_\mu j^\mu_{5,f} = 2m_f \bar{q}\gamma_5 q - \frac{g^2}{16\pi^2} F^a_{\mu\nu}\tilde{F}^{\mu\nu}_a - \frac{e^2}{8\pi^2} F_{\mu\nu}\tilde{F}^{\mu\nu}$$

axial current $j^\mu_5 = (n_5, \vec{j}_5)$

quark mass

field-strength fluctuations $\propto \vec{E} \cdot \vec{B}$



- space-time dependent fluctuations of $\vec{E} \cdot \vec{B}$
- topological sphaleron transitions

Mace,SS,Venugopalan PRD93 (2016) no.7, 074036

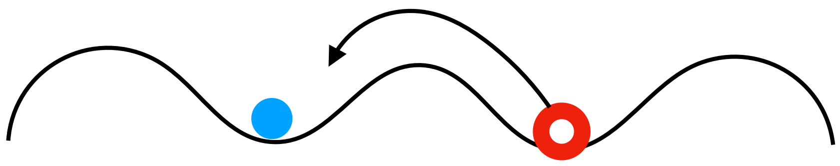
Example: Sphaleron transitions & Chiral transport

Classical (3D) vacuum configurations physically equivalent and connected by gauge transformation

$$G : T_3 \rightarrow SU(N_c)$$

$$\pi_3(SU(N_c)) \simeq Z$$

which can have topologically non-trivial properties



Sphaleron transitions:

real-time transition between topologically distinct sectors

Vacuum to vacuum transitions give rise to integer change of the Chern-Simons number

$$\Delta N_{CS} = \frac{g^2}{8\pi^2} \int d^4x \; \vec{E}_a \vec{B}_a$$

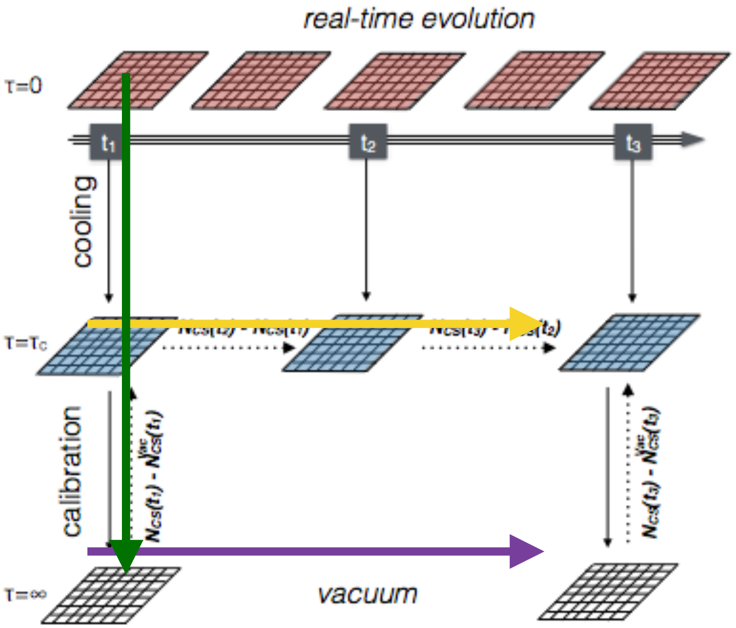
Generally $\Delta N_{CS}(t)$ is not integer valued and can be non-zero also in abelian gauge theories (e.g. parallel E,B)

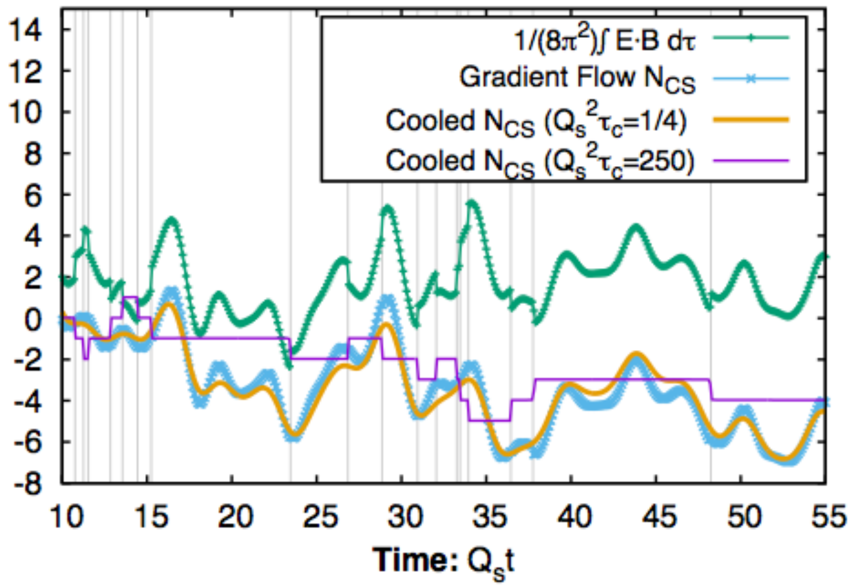
see e.g. F. Lenz https://arxiv.org/abs/hep-th/0403286
Mace,SS,Venugopalan PRD93 (2016) no.7, 074036

Example: Sphaleron transitions & Chiral transport

Definition of Chern-Simons number on the lattice can be problematic due to UV fluctuations

Generally strategy is to use cooling to define ΔN_{CS}



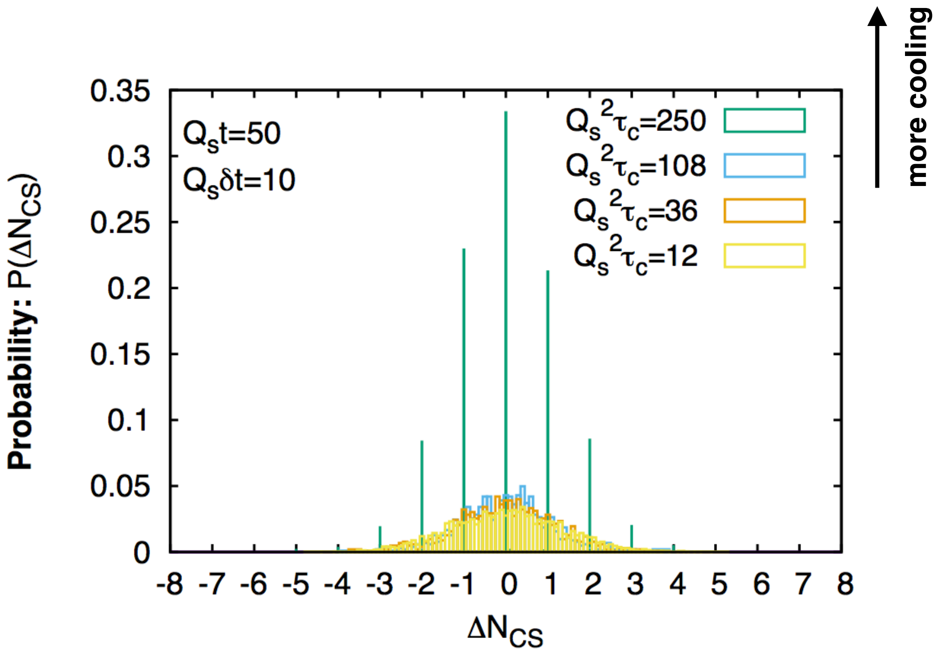


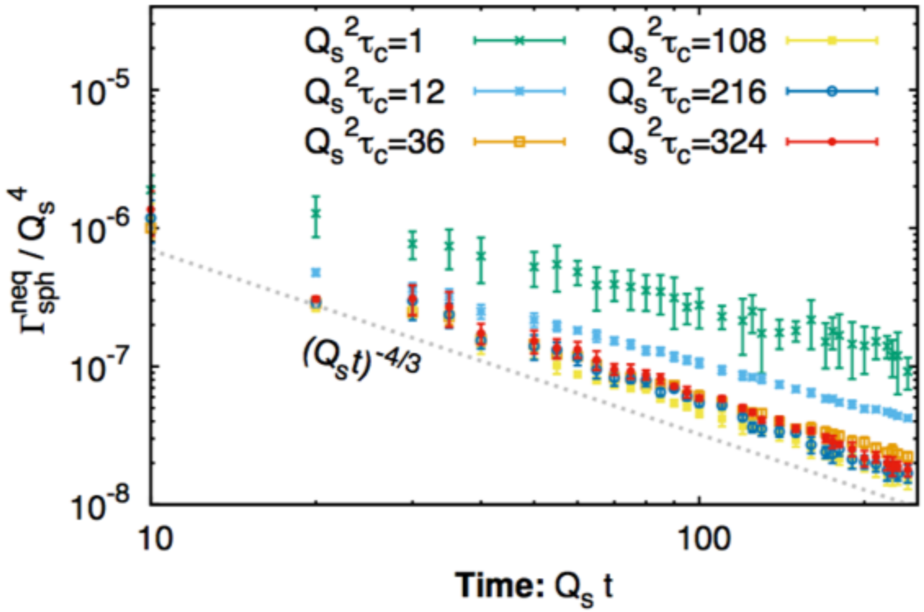
If only interested in topological information, can also measure winding number of gauge transformation to minimal Coulomb gauge

Mace,SS,Venugopalan PRD93 (2016) no.7, 074036
see also papers by G.D. Moore

Example: Sphaleron transitions & Chiral transport

Histograms of Chern-Simons number difference





Enhancement of the sphaleron transition rate in out-of-equilibrium plasma

Mace,SS,Venugopalan PRD93 (2016) no.7, 074036

Example: Sphaleron transitions & Chiral transport

Very challenging to simulate dynamical fermions on top of noisy gauge field background

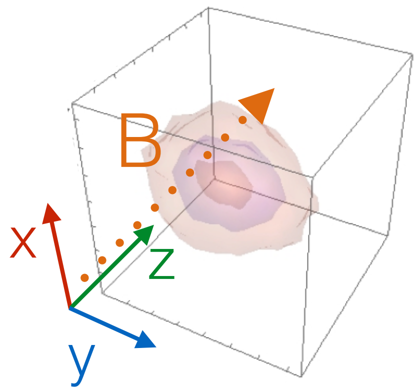
no fundamental problem
just need very large lattices

$\vec{E} \cdot \vec{B}$

Will consider a clean theoretical setup

SU(N): Single sphaleron transition
U(1): constant magnetic field

Neglect back-reaction of fermions on dynamical gauge field in this study



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Discretization of fermions & axial anomaly

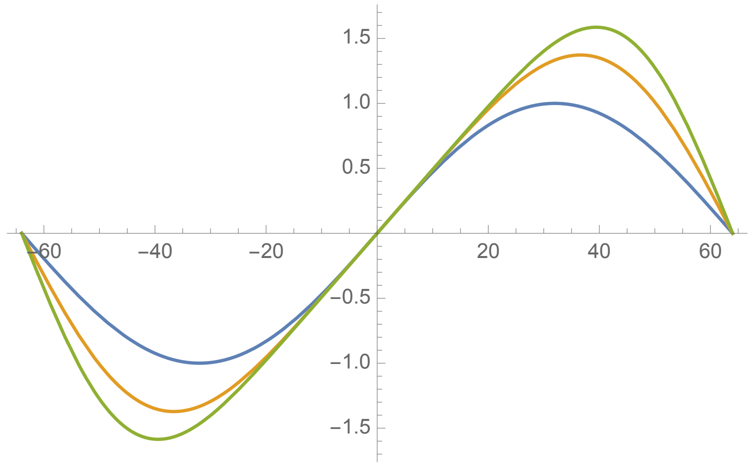
Definition of chiral properties (axial charge) of fermions on the lattice generally a tricky issue

Naive fermion discretization:

$$-i \not{D}^s_W \hat{\psi}_{\mathbf{x}} = -i \sum_{n,i} \frac{C_n}{2a_i} \left[\gamma^i U_{\mathbf{x},+ni} \hat{\psi}_{\mathbf{x}+n\mathbf{i}} - \gamma^i U_{\mathbf{x},-ni} \hat{\psi}_{\mathbf{x}-n\mathbf{i}} \right]$$

Cancellation of axial anomaly due to Fermion doublers

$$\partial_\mu j^\mu_5(x) = 2m < \bar{\psi}(x) i\gamma_5 \psi(x) >$$



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Wilson fermions: Explicit symmetry breaking term added to the Hamiltonian to decouple doublers (c.f. Aarts,Smit)

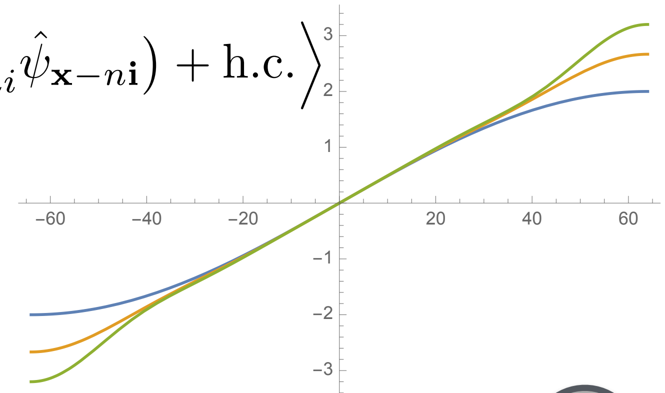
$$-i\not{D}^s_W\hat{\psi}_{\mathbf{x}} = \sum_{n,i}\frac{C_n}{2a_i}\Big[\Big(-i\gamma^i - nr_w\Big)U_{\mathbf{x},+ni}\hat{\psi}_{\mathbf{x}+n\mathbf{i}} + 2nr_w\hat{\psi}_{\mathbf{x}} - \Big(-i\gamma^i + nr_w\Big)U_{\mathbf{x},-ni}\hat{\psi}_{\mathbf{x}-n\mathbf{i}}\Big]$$

$$\partial_\mu j^\mu_5(x) = 2m < \bar{\psi}(x) i\gamma_5 \psi(x) > + r_W < W(x) >$$

$$W(x) = \sum_{n,i}\frac{n\cdot C_n}{2}\langle \hat{\psi}^\dagger_{\mathbf{x}} i\gamma_5\gamma_0 \big(U_{\mathbf{x},+ni}\hat{\psi}_{\mathbf{x}+n\mathbf{i}} - 2\hat{\psi}_{\mathbf{x}} + U^\dagger_{\mathbf{x}-n\mathbf{i},+ni}\hat{\psi}_{\mathbf{x}-n\mathbf{i}}\big) + \text{h.c.}\rangle$$

cont. limit

$$\rightarrow -\frac{g^2}{8\pi^2}\mathrm{Tr}F_{\mu\nu}F^{\mu\nu}$$



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Example: Sphaleron transitions & Chiral transport

Non-trivial cross check of axial charge production (B=0)

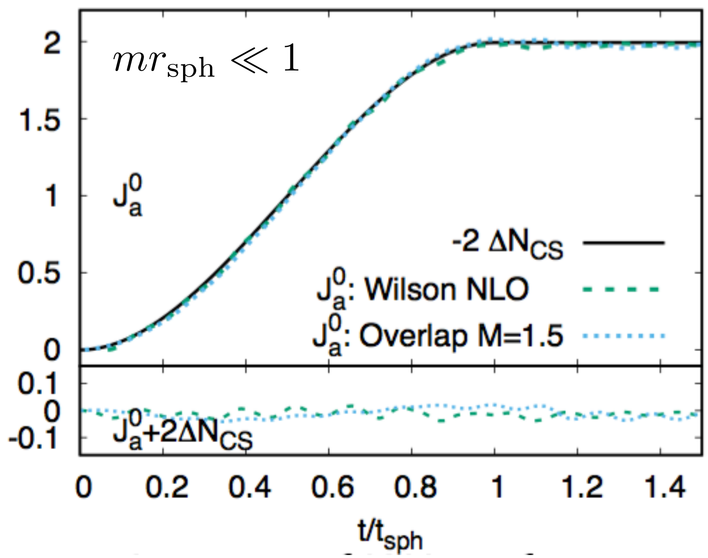
Over the coarse of the sphaleron transition Chern-Simons number

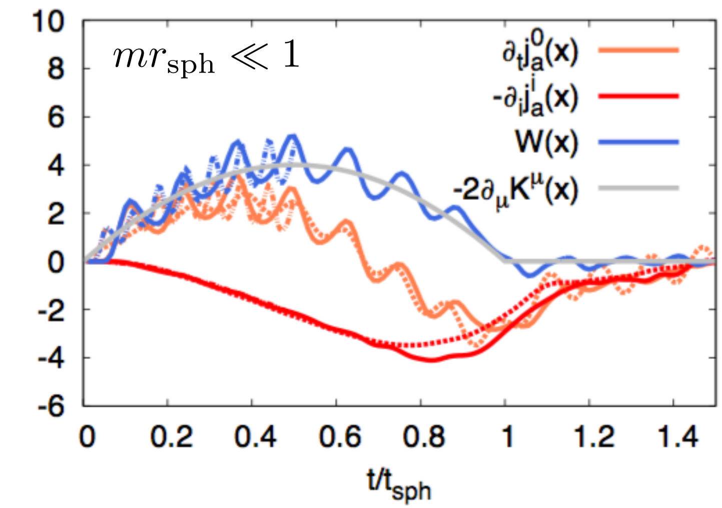
$$\Delta N_{CS} = \frac{g^2}{8\pi^2} \int d^4x \; \vec{E}_a \vec{B}_a$$

changes by an integer amount leading to an imbalance of axial charge

$$\Delta J_5^0 = -2\Delta N_{CS} + 2m_f \int d^4x \langle \bar{\psi} i \gamma_5 \psi \rangle$$

Excellent agreement for (almost) massless fermions from simulations with improved Wilson fermions and Overlap fermions





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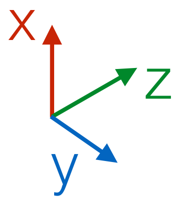
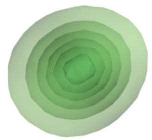
Example: Sphaleron transitions & Chiral transport

Axial charge j_5^0



Sphaleron transition induces local imbalance of axial charge density

Vector current j_V^z



Non-zero magnetic field B_z leads to vector current j_V^z in z-direction

Vector charge j_V^0

Vector current j_V^z leads to separation of electric charges j_V^0 along the z-direction

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Example: Sphaleron transitions & Chiral transport

Axial charge j_5^0

Sphaleron transition induces local imbalance of axial charge density

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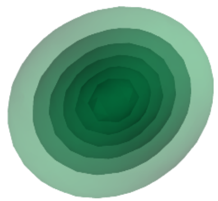

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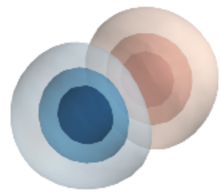

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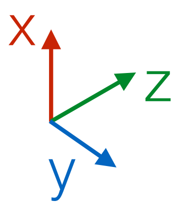
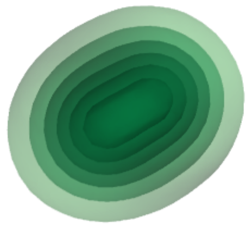
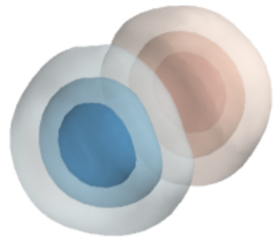
Example: Sphaleron transitions & Chiral transport

Axial charge j_5^0	Vector current j_V^z	Vector charge j_V^0







Sphaleron transition induces local imbalance of axial charge density

Non-zero magnetic field B_z leads to vector current j_V^z in z-direction

Vector current j_V^z leads to separation of electric charges j_V^0 along the z-direction

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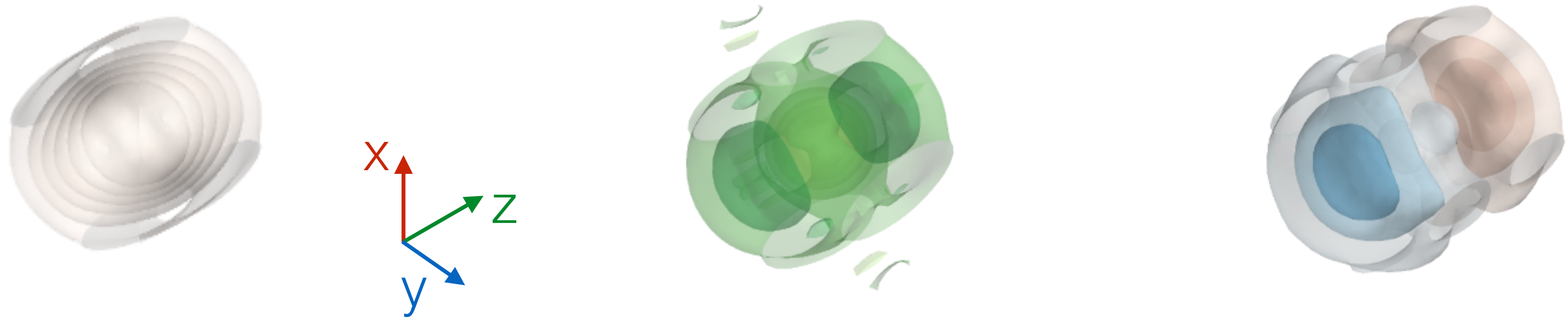
Example: Sphaleron transitions & Chiral transport

Vector charge imbalance j_V^0 generates an axial current j_5^z
so that axial charge also flows along the B-field direction

Axial charge j_5^0 Vector current j_V^z Vector charge j_V^0



Emergence of a Chiral Magnetic Shock-wave of vector charge and axial charge propagating along B-field direction

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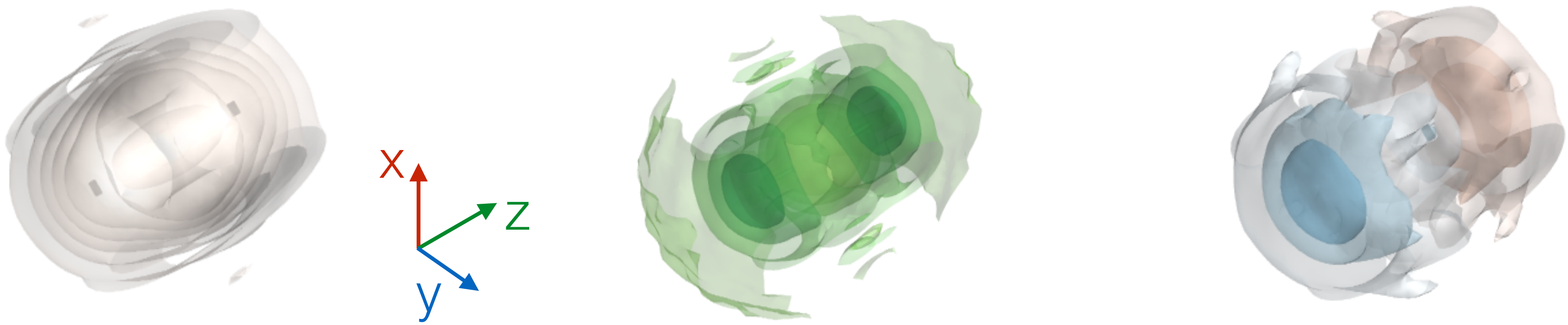
Example: Sphaleron transitions & Chiral transport

Vector charge imbalance j_V^0 generates an axial current j_5^z
so that axial charge also flows along the B-field direction

Axial charge j_5^0 Vector current j_V^z Vector charge j_V^0



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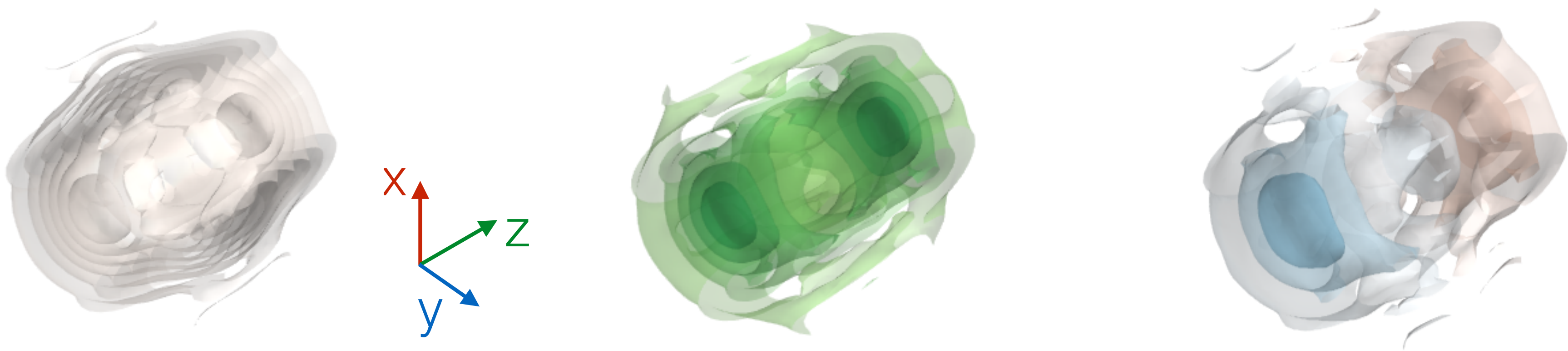
Example: Sphaleron transitions & Chiral transport

Vector charge imbalance j_V^0 generates an axial current j_5^z so that axial charge also flows along the B-field direction

Axial charge j_5^0 | Vector current j_V^z | Vector charge j_V^0



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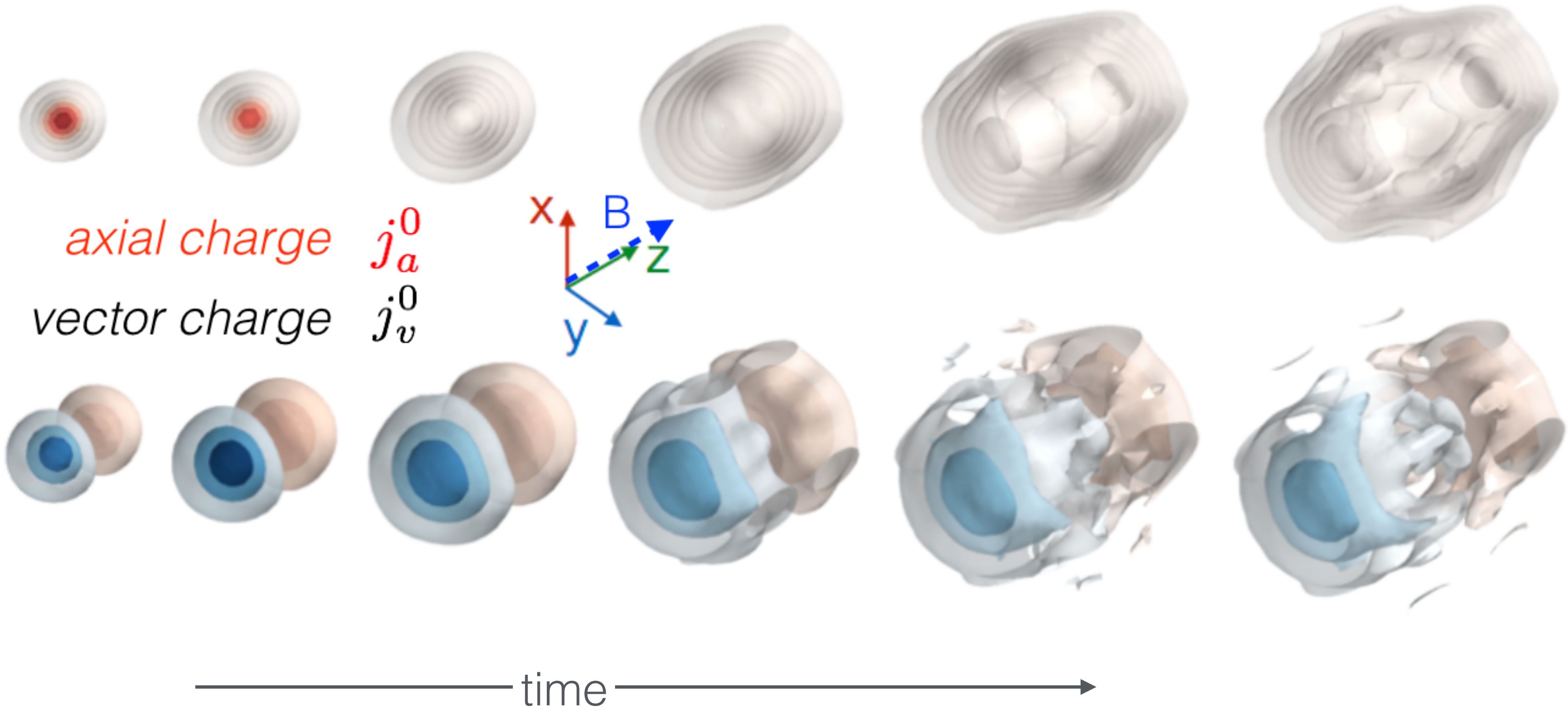
Example: Sphaleron transitions & Chiral transport



Clear separation of electric charge j_V^0 along the B-field direction

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Example: Sphaleron transitions & Chiral transport

Comparison with anomalous hydro
(light quarks $mr_{\rm sph} \ll 1$)

$$\partial_\mu j_a^\mu = S(x)\ , \qquad \partial_\mu j_v^\mu = 0$$

$$j^\mu_{v/a} = n_{v/a} u^\mu + \sigma^B_{v/a} B^\mu$$

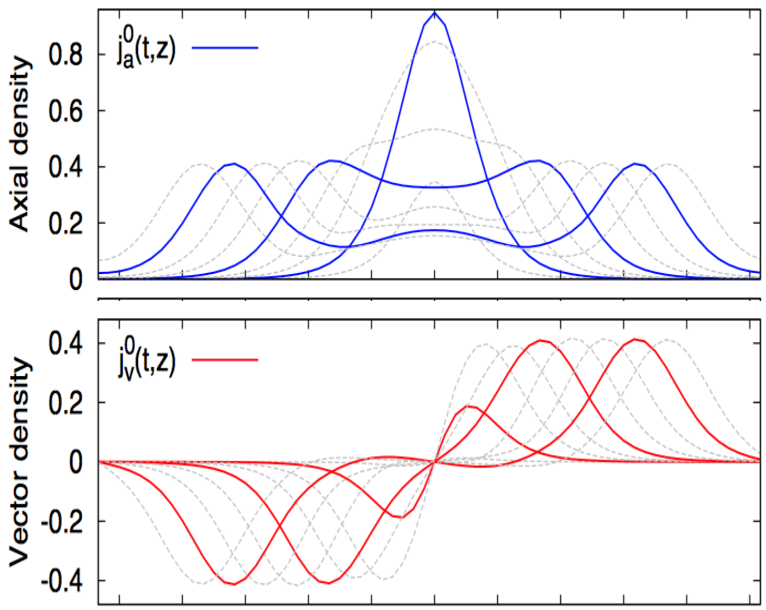
Strong field limit ($B \gg r_{\rm sph}^{-2}, m^2$)

$$\partial_t \begin{pmatrix} j_v^0(t,z) \\ j_a^0(t,z) \end{pmatrix} = -\partial_z \begin{pmatrix} j_a^0(t,z) \\ j_v^0(t,z) \end{pmatrix} + \begin{pmatrix} 0 \\ S(t,z) \end{pmatrix}$$

Chiral magnetic shock-wave

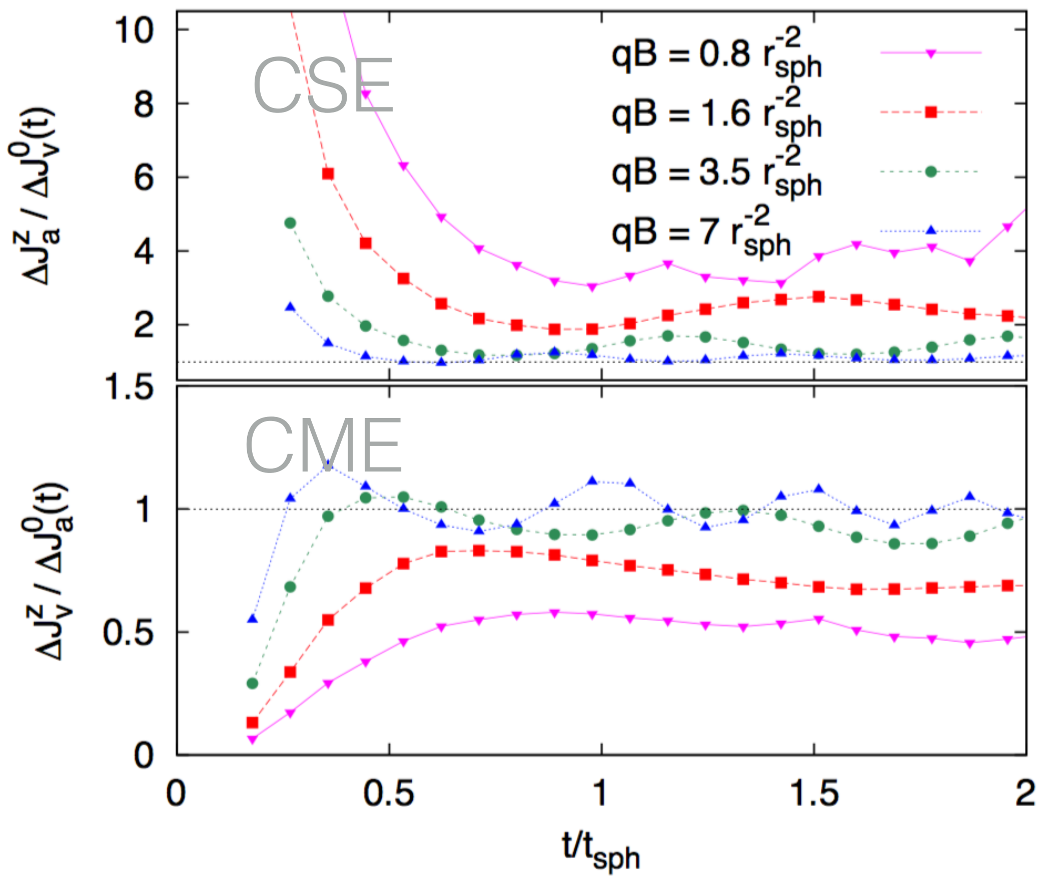
$$j^0_{v/a}(t > t_{\rm sph}, z) = \frac{1}{2}\int_0^{t_{\rm sph}} dt' \left[S(t', z - c(t-t')) \mp S(t', z + c(t-t')) \right]$$

Simulation results for light quarks



-> Evolution for light quarks and strong magnetic fields
well described by anomalous hydrodynamics at late times

Example: Sphaleron transitions & Chiral transport



Check of constitutive relations:

Verify ratios vector/axial currents and axial/vector charge

$$C_{\mathrm{CME}}(t) = \frac{\Delta J_v^z(t)}{\Delta J_a^0(t)}\,, \qquad C_{\mathrm{CSE}}(t) = \frac{\Delta J_a^z(t)}{\Delta J_v^0(t)}\,.$$

In the strong field limit related to thermodynamic constitutive relations

$$C_{CME} = 1\,, \qquad C_{CSE} = 1\,.$$

equal to time independent constants.

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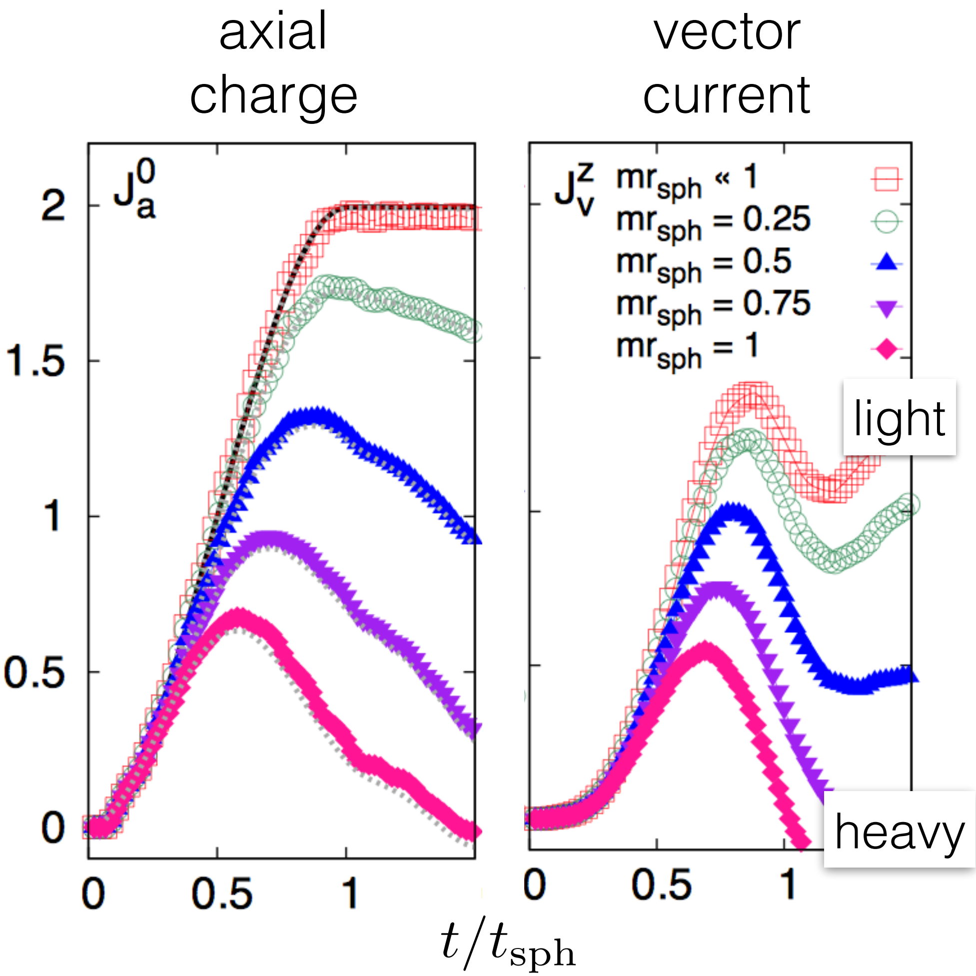
Example: Sphaleron transitions & Chiral transport



Quark mass dependence:

Explicit violation of axial charge conservation for finite quark mass

$$\partial_\mu j_a^\mu(x) = 2m\langle\hat{\bar{\psi}}(x)i\gamma_5\hat{\psi}(x)\rangle + S(x)$$

leads to damping of axial charge

Since chiral magnetic effect current is proportional to axial charge density it will also be reduced

$$\vec{j}_v \propto j_a^0 \vec{B}$$

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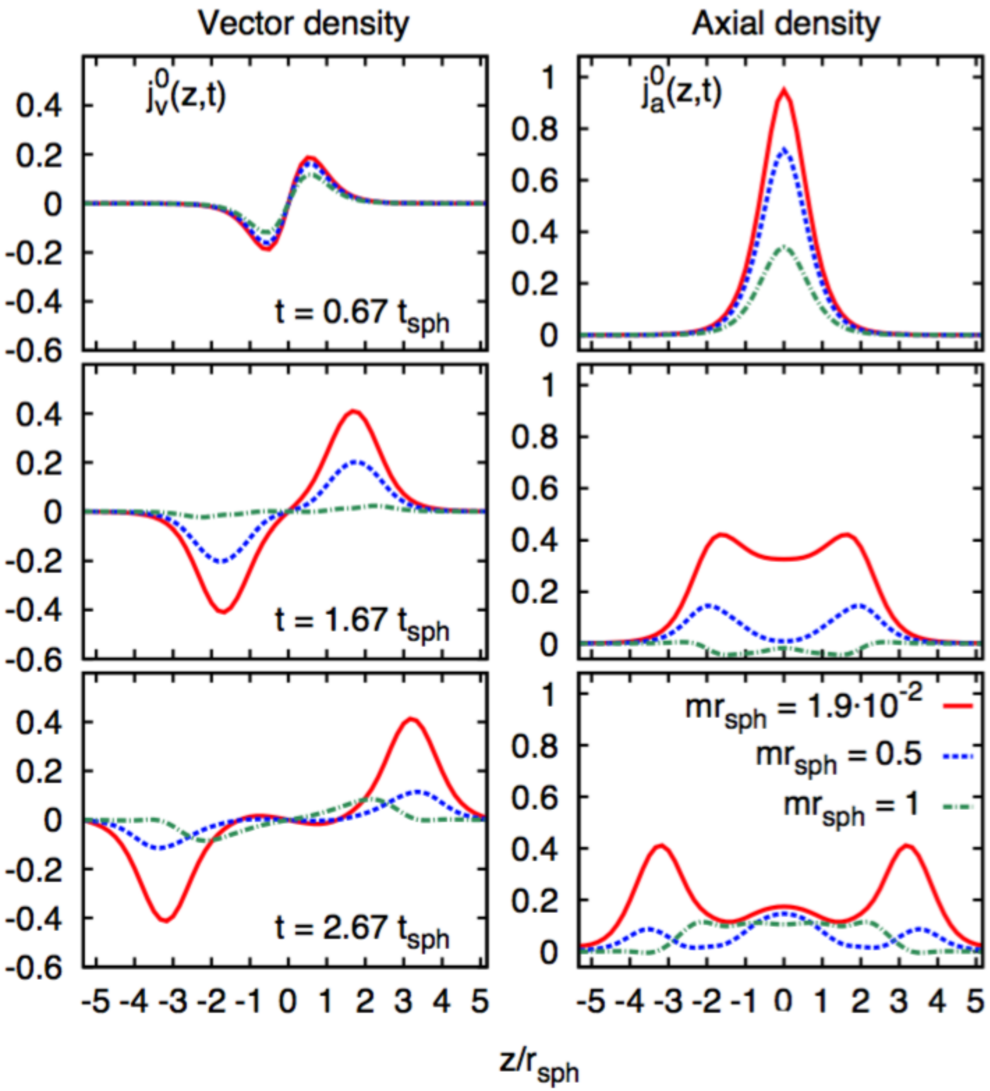
Example: Sphaleron transitions & Chiral transport



Light quarks ($\mathbf{mt_{sph} \ll 1}$ ***)***

Chiral magnetic wave leads to non-dissipative transport of axial and vector charges

Heavy quarks ($\mathbf{mt_{sph} \sim 1}$ ***)***

Dissipation of axial charge leads to significant reduction of charge separation

Mueller,SS, Sharma PRL 117 (2016) no.14, 142301
Mace, Mueller, SS, Sharma PRD95 (2017) no.3, 036023

Quo vadis non-equilibrium QFT?

We want to describe non-equilibrium QFT to study
Heavy-Ion collisions, Cosmology, Cold Atom experiments, …

$$Z[J,R,\hat{\rho}_0] = \underbrace{\int [d\varphi_0^+][d\varphi_0^-]\langle\varphi_0^+|\hat{\rho}_0|\varphi_0^-\rangle}_{\text{initial state}} \underbrace{\int_{\varphi_0^+}^{\varphi_0^-} D\varphi\ e^{\frac{i}{\hbar}\left[S_{\mathcal{C}}[\varphi]+\int_{x_{\mathcal{C}}} J(x)\varphi(x)+\frac{1}{2}\int_{x_{\mathcal{C}},y_{\mathcal{C}}}\varphi(x)R(x,y)\varphi(y)\right]}}_{\text{non-equilibrium dynamics}}$$

Discussed different non-equilibrium methods based on expansion

- semi-classical expansions ($\hbar$), weak-coupling expansions (λ), …

No exact answers; generally need multiple methods to describe physics

Natural question: Can we do better?

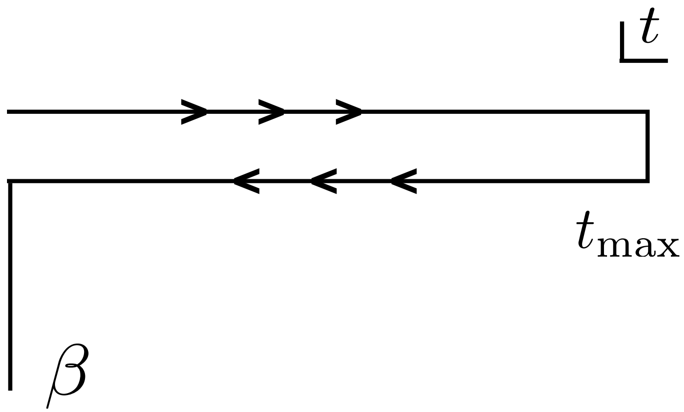
Complexifiaction: real-time stochastic quantization (Complex Langevin), deformed integration contours (Lefsheftz thimbles,…)

Hamiltonian simulation: Variational diagonalization (DMRG,TNS), Quantum computing/simulation of Hamiltonian dynamics

Sign problem for real-time dynamics

Consider for definiteness real-time dynamics in thermal equilibrium

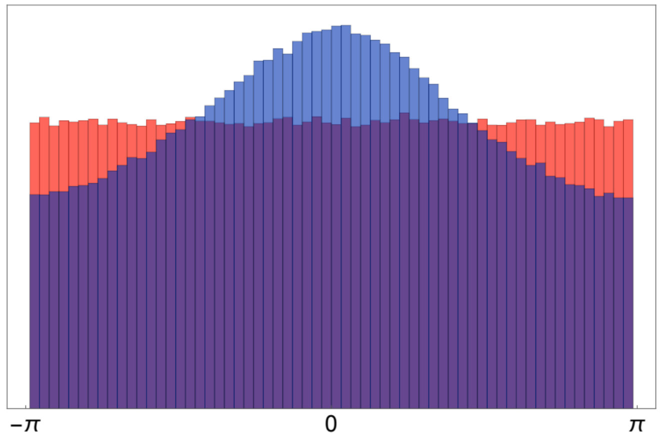
$$Z[J] = \int_{\rm pbc} D\varphi \; e^{i\left(S_{\mathcal{C}_\beta}[\varphi] + \int_{\mathcal{C}_\beta} J(x)\varphi(x)\right)}$$



Euclidean part of the contour:
action weight is real (<0)

Minkowski part of the contour:
action weight is purely imaginary (up to ie)

Strong oscillations of the phase factor prohibit direct importance sampling



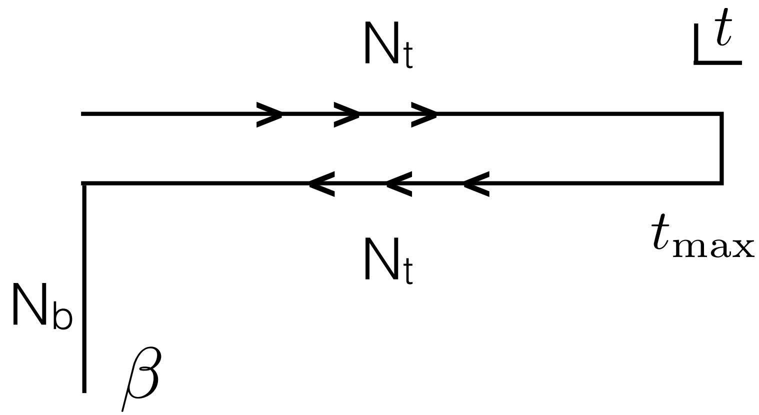
Alexandru et al. PRL 117 (2016) no.8, 081602

Complexification: Holomorphic gradient flow/Lefshetz thimbles

Discretize space on N_s sites and time path in N_t and N_b pieces

Need to perform $X=N_s^d \times (2N_t + N_b)$ dimensional integral over real variables

$\phi(x_i,t_i)$



Basic idea is to consider a deformation of the integration from real domain R^X to a X-dimensional manifold embedded in C^X where the sign problem is mild

calculate observables via reweighting

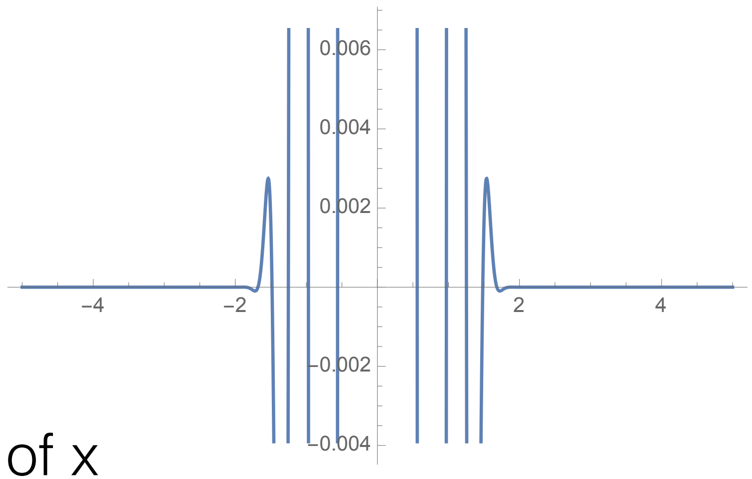
generate field configurations with probability $\propto e^{Re(iS_{\mathcal{C}_\beta}[\varphi])}$

$$\langle O \rangle = \frac{\langle O[\varphi]\, e^{iImS_{\mathcal{C}_\beta}} \rangle}{\langle e^{iImS_{\mathcal{C}_\beta}} \rangle}$$

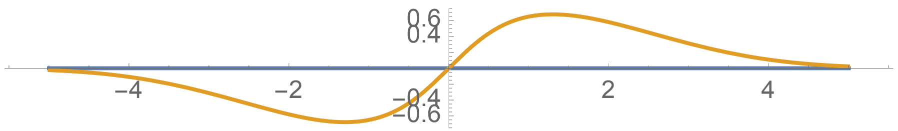
Complexification: Holomorphic gradient flow/Lefshetz thimbles

Consider one dimensional integral

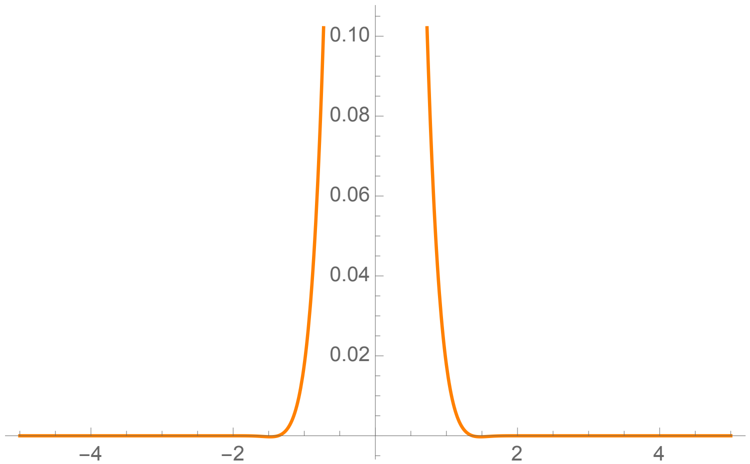
$$Z = \int_{\mathcal{R}} dx\; e^{5ix^2 - x^4}$$



Since action is holomorphic function of x can use Cauchy theorem to deform integration contour



$$Z = \int_{\mathcal{M}} dx\; e^{ix^2 - x^4}$$



Complexification: Holomorphic gradient flow/Lefshetz thimbles

General strategy

$$\int_{R^X} e^{iS[\varphi]} = \int_{\mathcal{M}} e^{iS[\varphi_{\mathcal{M}}]} = \int_{R^X} J[\varphi] e^{iS[\varphi_{\mathcal{M}}[\varphi]]} \qquad J[\varphi] = \det \frac{\partial \varphi_M}{\partial \varphi}$$

Need to find suitable integration manifolds M and parametrize them

Lefshetz thimbles: Stationary phase contours attached to a critical point*

$$\left.\frac{\partial S}{\partial \varphi}\right|_{\varphi_c} = 0 \; , \qquad Im(S[\varphi]) = Im(S[\varphi_c])$$

Holomorphic Gradient flow:
Generated by flow equation**

$$\partial_\tau \varphi = \overline{\frac{\partial S}{\partial \varphi}} \qquad \partial_\tau S[\varphi] = \frac{\partial S}{\partial \varphi} \overline{\frac{\partial S}{\partial \varphi}} \geq 0$$

Sign Optimized Manifolds:
Explicit parametrization or Neural networks***

*see e.g http://ribf.riken.jp/~tanizaki/thesis/yuya_phd.pdf

** Bedaque EPJ Web Conf. 175 (2018) 01020

***Ohnishi, Mori, Kashiwa arXiv:1812.11506

Complexification: Holomorphic gradient flow/Lefshetz thimbles

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Need to find suitable integration manifolds M and parametrize them

Lefshetz thimbles: stationary phase contours
(+ mathematically clean, -efficient parametrization & sampling)

Holomorphic Gradient flow: generated by flow equation
(+ mathematically clean, - numerical cost, efficient sampling)

Sign Optimized Manifolds: Explicit parametrization
(+ numerically cheap, - need physical insight)

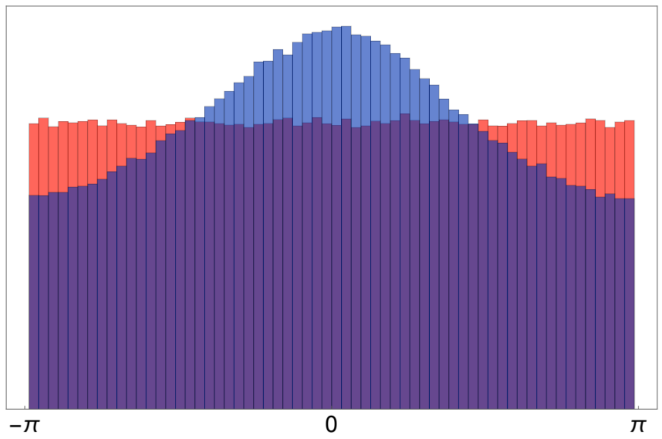
Challenge is to efficiently find suitable manifolds & perform efficient Monte-Carlo sampling in presence of large action barriers

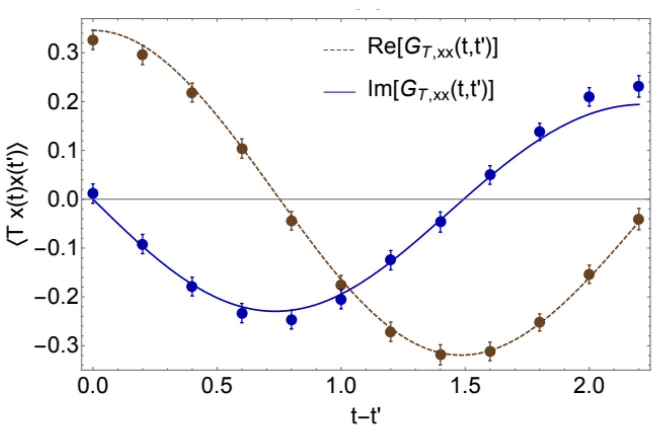
Complexification: Holomorphic gradient flow/Lefshetz thimbles

Simulation results based on Holomorphic gradient flow simulations

0+1D Φ^4

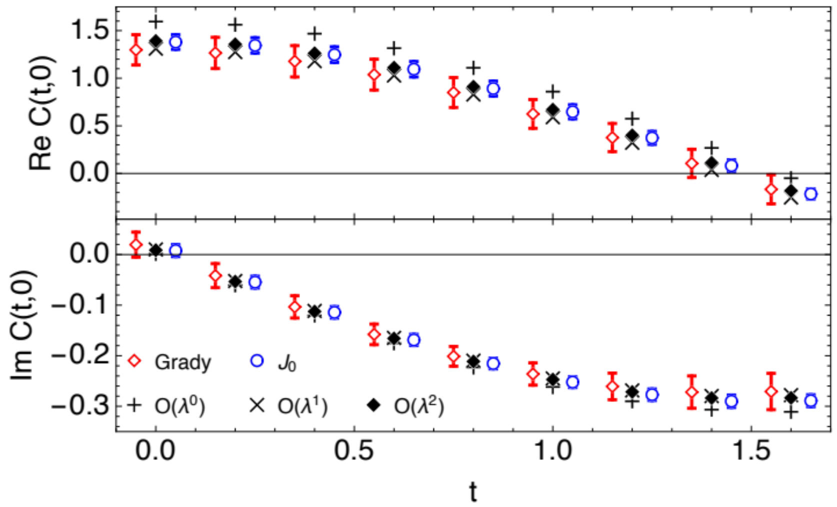
Nt = 8, Nβ = 2, and Nx = 8





1+1D Φ^4

Nt = 8, Nβ = 2, and Nx = 8



Alexandru et al. PRD 95 (2017) no.11, 114501

Alexandru et al. PRL 117 (2016) no.8, 081602

Hamiltonian simulation

Basic idea is to perform Hamiltonian evolution of the system

$$|\underbrace{000001}_{N_{\text{qubits}}}\rangle$$

Digital quantum computing

Quantum computer with universal set of instructions allows for any operation to be performed on spin system

Natural to perform time evolution by applying e^{iHt}

Need to map Hamiltonian of theory on set of spin 1/2s

Discretize theory on lattice & discretize field space

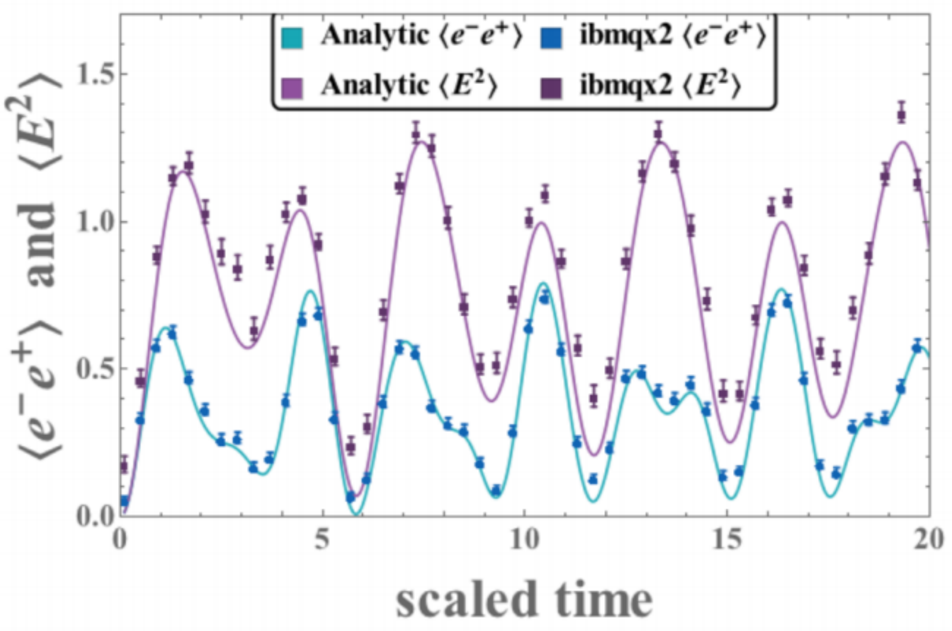
$$\hat{\phi}_{\mathbf{x}} \approx \sum_{i=1}^{N} \phi_{i,\mathbf{x}} |\phi_{i,\mathbf{x}} >< \phi_{i,\mathbf{x}}|$$

need to take limits N->∞ in addition to usual continuum and infinite volume limits

see e.g. Jordan, Lee, Preskill, Science 336, 1130-1133 (2012)
Preskill arXiv:1811.10085

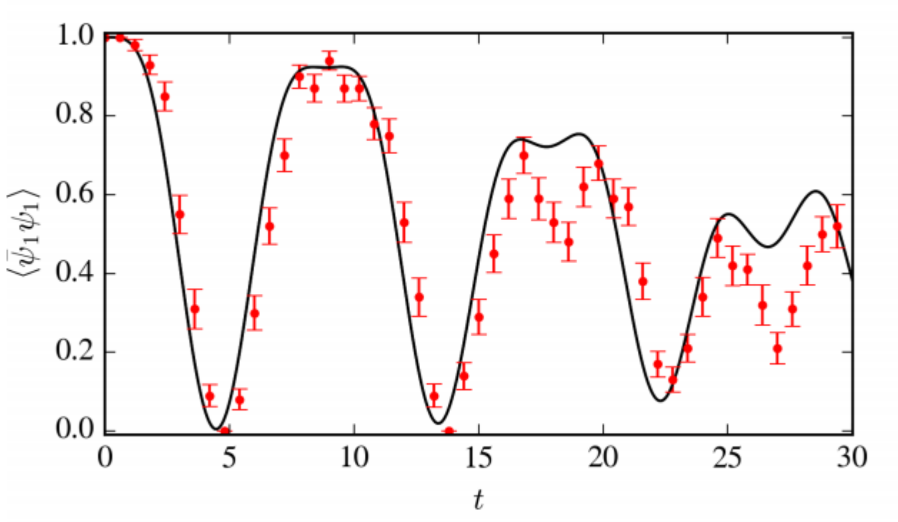
Examples of digital quantum computing

Schwinger model*
(2 sites; 3 quits; 8192 meas)



*Klco et al. PRA98 (2018) no.3, 032331

Z_2 gauge theory
(4 sites; 8 quits; 100 meas)



NuQS Collaboration
arXiv:1903.08807

Digital quantum computing

$$|\underbrace{000001}_{N_{\text{qubits}}}\rangle$$

Conceptual Challenges:

Discretization of (non-abelian) gauge theories & reducing redundancies in the calculation

Computational Challenges:

Building and operating a large-scale quantum computer

Errors induced due to loss imperfect isolation

Near term: NISQ era Noisy IntermediateScale Quantum

~50-100s of qubits ~1000 two-qubit operations

see Preskill arXiv:1811.10085 and references therein

Epilogue

Description of real-time/out-of-equilibrium dynamics in QCD remains a formidable challenge

Number of different approaches with different ranges of validity

Exciting non-equilibrium phenomena discovered with available methods

Currently no first principles methods available

Non-equilibrium QCD remains a largely unexplored area

Great opportunities for young scientists to have an impact!

Comments/Questions/Complaints/Feedback

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Thank you!!!