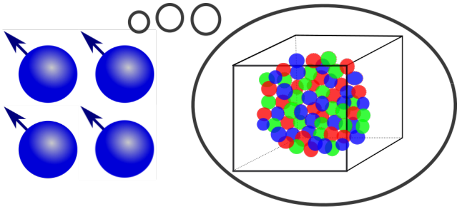
Toward first-principles calculation of shear viscosity - classical and quantum approaches



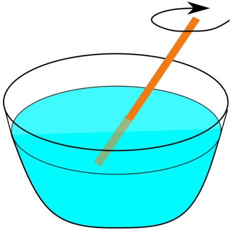
Yukari Yamauchi

arXiv:2101.05755 with S. Lawrence
arXiv:2104.02024 with T. Cohen, H. Lamm, S. Lawrence
and two projects in progress

26 October 2021, Fermi National Accelerator Laboratory

UNIVERSITY OF MARYLAND

What is Shear Viscosity? - Intuitively



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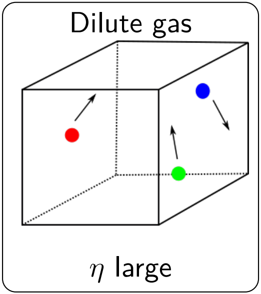
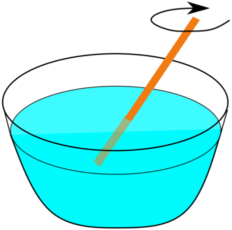
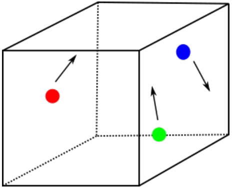


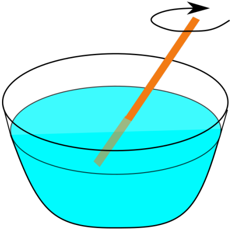


What is Shear Viscosity? - Intuitively

Dilute gas



η large



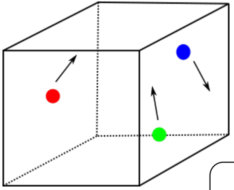
$\mathcal{N} = 4$ SYM

strong g, large N

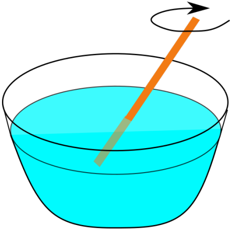
$$\frac{\eta}{s} = \frac{1}{4\pi}$$

What is Shear Viscosity? - Intuitively

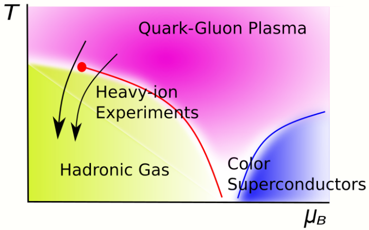
Dilute gas



η large



QCD



η small

$\mathcal{N} = 4$ SYM

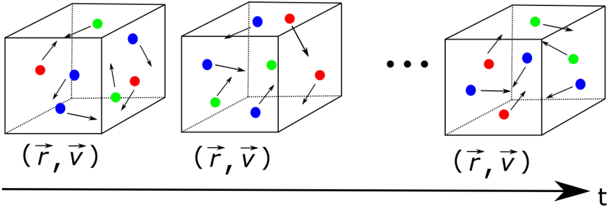
strong g, large N

$$\frac{\eta}{s} = \frac{1}{4\pi}$$

What is shear viscosity? - Theoretically

Low energy constant in the hydrodynamic description of an underlying theory

The underlying theory of molecule dynamics



The hydrodynamic description of this system via $\vec{u}$ (velocity field)

Navier-Stokes Equation: $\rho \frac{\partial \vec{u}}{\partial t} + \rho(\vec{u} \cdot \nabla)\vec{u} = \rho \vec{a} - \nabla p + \eta \nabla^2 \vec{u}$

(ρ: mass density, $\vec{a}$: external force, p: pressure)

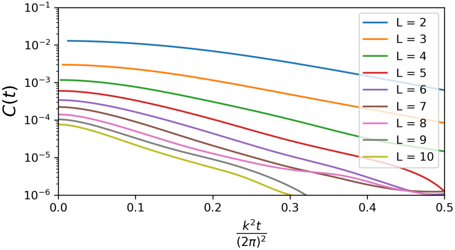
Shear viscosity η is obtained from $(\vec{r}(t), \vec{v}(t))$ by

$$C(k,t) = \langle u(k,t) u(k,0) \rangle \sim e^{-\frac{\eta k^2}{\rho} t} \quad \text{with} \quad u(k,t) = \sum_{j=1}^{N} \vec{v}^j(t) e^{-i\vec{k}\cdot\vec{r}^j(t)}$$

Shear Viscosity from Molecule Dynamics[1]

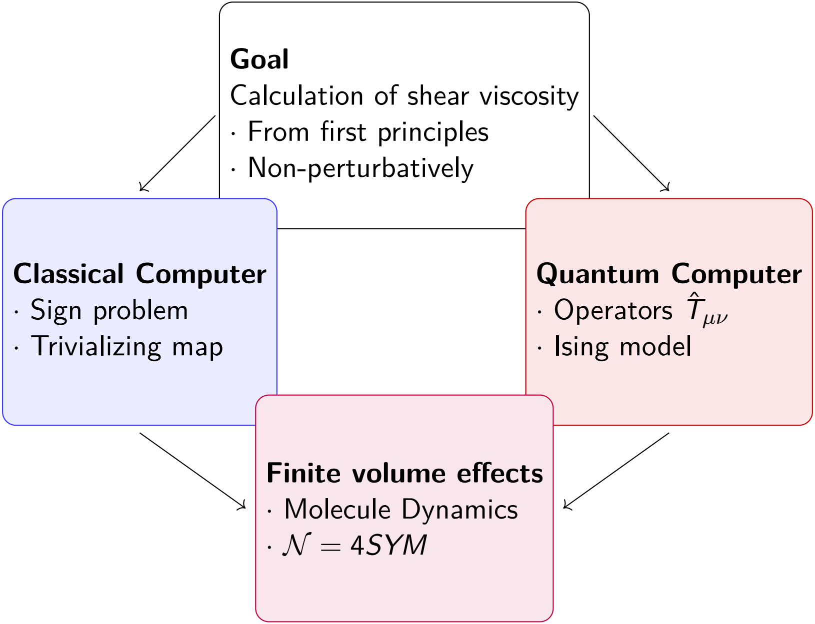
1. Prepare a box (volume L^3) of particles in thermal equilibrium $|F(r)| = e^{-2r}$, repulsive force
2. Measure transverse velocity field $\vec{u}(\vec{k}, 0)$
3. Time-evolve the system via molecular dynamics simulation
4. Measure $\vec{u}(\vec{k}, t)$ and compute $\vec{u}(\vec{k}, t)\vec{u}(\vec{k}, 0)$

$$C(k, t) = \langle \vec{u}(\vec{k}, t)\vec{u}(\vec{k}, 0)\rangle \sim e^{-\frac{\eta k^2}{\rho} t} \quad (\rho : \text{mass density})$$



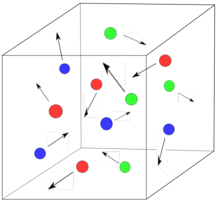
[1] B.Palmer, Phys.Rev.E 49(1994)359, B.Hess, J.Chem.Phys.116,209(2002)

Roadmap


Goal
Calculation of shear viscosity
· From first principles
· Non-perturbatively
Classical Computer
· Sign problem
· Trivializing map
Quantum Computer
· Operators $\hat{T}_{\mu\nu}$
· Ising model
Finite volume effects
· Molecule Dynamics
· $\mathcal{N} = 4 SYM$

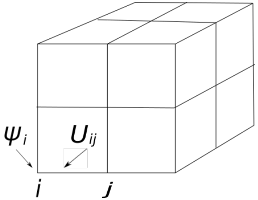
Shear Viscosity of QFT

Non-relativistic gas of particles



$\rightarrow$

QCD on a lattice



$(\vec{r}_i, \vec{v}_i)$ for N particles

$\vec{F} = m\vec{a}$

measure u

ψ_i on each site, U_{ij} on each link

S_{QCD}

measure T_{01}

From T_{01} correlator:

$$\int_V d\vec{x}\; e^{i\vec{k}\cdot\vec{x}} \langle\phi(\beta)|\,[T_{01}(t,\vec{x}), T_{01}(0,0)]\,|\phi(\beta)\rangle \sim e^{-\frac{\eta(\beta)k^2}{\epsilon}t}$$

(ϵ: energy density)

From T_{12} correlator:

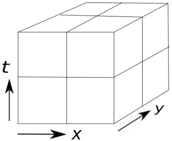
$$\eta(\beta) = \frac{1}{T}\int_V dx \int_0^\infty dt\; \langle\phi(\beta)|\,[T_{12}(x,t), T_{12}(0,0)]\,|\phi(\beta)\rangle$$

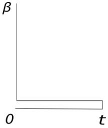
Sign Problem

Goal: compute $\langle\phi(\beta)|\,[T_{\mu\nu}(t,\vec{x}),\,T_{\mu\nu}(0,0)]\,|\phi(\beta)\rangle$

Method: Non-perturbative calculation on a lattice

$$\langle\mathcal{O}(t,\vec{x})\rangle = \frac{1}{Z}\int\mathcal{D}[\psi,U]e^{-S}\mathcal{O}(t,\vec{x})$$



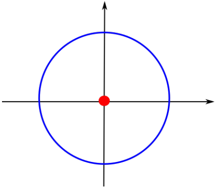


The action S is complex $\rightarrow$ define "quenched distribution" $e^{-\operatorname{Re}S}$

$$\langle\mathcal{O}(t,\vec{x})\rangle = \frac{\frac{\int\mathcal{D}[\psi,A]e^{-\operatorname{Re}S}e^{-i\operatorname{Im}S}\mathcal{O}(t,\vec{x})}{\int\mathcal{D}[\psi,A]e^{-\operatorname{Re}S}}}{\frac{\int\mathcal{D}[\psi,A]e^{-\operatorname{Re}S}e^{-i\operatorname{Im}S}}{\int\mathcal{D}[\psi,A]e^{-\operatorname{Re}S}}} = \frac{\left\langle e^{-i\operatorname{Im}S}\mathcal{O}\right\rangle_{e^{-\operatorname{Re}S}}}{\left\langle e^{-i\operatorname{Im}S}\right\rangle_{e^{-\operatorname{Re}S}}}$$

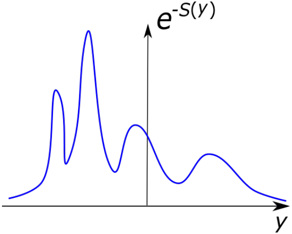
Especially the **"average sign"** is challenging:

$$\langle\sigma\rangle = \left\langle e^{-i\operatorname{Im}S}\right\rangle_{e^{-\operatorname{Re}S}} \propto a^V,\quad a\leq 1$$



Trivializing Map[2]

Some distribution

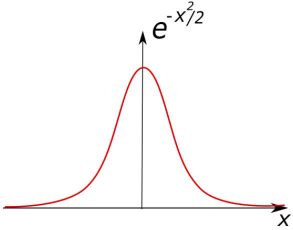


Map

$\leftrightarrow$

$y(x)$

Simple Gaussian distribution



Trivializing map:

$$dy\ e^{-S(y)} = dx\ \frac{dy(x)}{dx}\ e^{-S(y(x))} = dx\ \mathcal{N} e^{-x^2/2}$$

Expectation values:

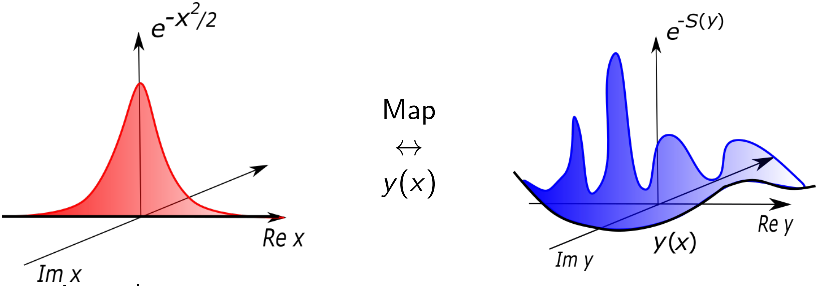
$$\langle \mathcal{O} \rangle = \frac{\int dy\ e^{-S(y)} \mathcal{O}(y)}{\int dy\ e^{-S(y)}} = \frac{\int dx\ e^{-x^2/2} \mathcal{O}(y(x))}{\int dx\ e^{-x^2/2}}$$

[2] M. Albergo et.el. Phys. Rev. D 100, 034515(2019)
K. A. Nicoli, et.el. Phys. Rev. E 101, 023304(2020)

Complex Trivializing Map

Application to complex actions:

$$dx\, \mathcal{N} e^{-x^2/2} = dx\, \frac{dy(x)}{dx}\, e^{-S(y(x))} = dy\, e^{-S(y)}$$



Expectation values:

$$\frac{\int_{\mathbb{R}} dx\; e^{-x^2/2} \mathcal{O}(y(x))}{\int_{\mathbb{R}} dx\; e^{-x^2/2}} = \frac{\int_{y(\mathbb{R})} dy\; e^{-S(y)} \mathcal{O}(y)}{\int_{y(\mathbb{R})} dy\; e^{-S(y)}} \stackrel{?}{=} \langle \mathcal{O} \rangle$$

Contour of integration changes!

Constraints on Trivializing Map[3]

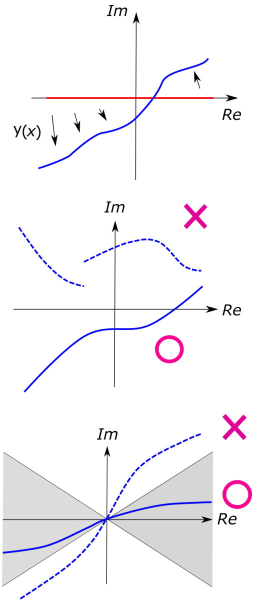
Trivializing maps give the correct $\langle \mathcal{O} \rangle$

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathbb{R}} dy\ e^{-S(y)} \mathcal{O}(y)}{\int_{\mathbb{R}} dy\ e^{-S(y)}} = \frac{\int_{y(\mathbb{R})} dy\ e^{-S(y)} \mathcal{O}(y)}{\int_{y(\mathbb{R})} dy\ e^{-S(y)}}$$

when:

- The induced contour (—) is a continuous manifold
- The induced contour (—) is in "asymptotically safe" region
- Both $e^{-S(y)}$ and $e^{-S(y)}\mathcal{O}(y)$ are holomorphic functions in the region between (—) and (—)

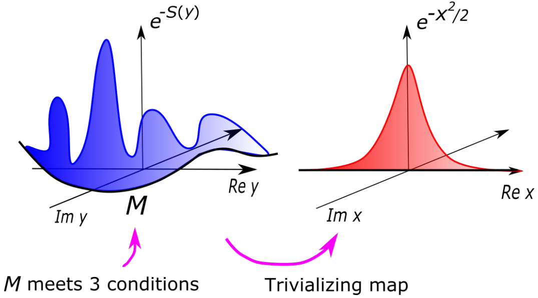
→ **Cauchy's integral theorem!**



[3] A. Alexandru et.el., Phys. Rev. D. 98, 034506(2018)

Trivializing Map and the Generalized Thimble Method

$\mathcal{M}$ is of exactly the sort used in the generalized thimble method



"Average sign" on the manifold $\mathcal{M}$ is

$$\langle \sigma \rangle = \frac{\int_{\mathcal{M}} dy \; e^{-S(y)}}{\int_{\mathcal{M}} dy \; e^{-\operatorname{Re} S(y)}} = \frac{\int_{\mathbb{R}} dx \; e^{-x^2/2}}{\int_{\mathbb{R}} dx \; e^{-x^2/2}} = 1$$

So the manifold $\mathcal{M}$ has no sign problems.

Trivializing maps exist $\leftrightarrow$ Perfect manifolds exist

Do they exist? If so, can we find them? If so can use them?

Existence of Trivializing Maps

Type of action: action S which is finite except at infinity

When with **NO** sign problems

Fact: Trivialiaing maps exist. $(\mathbb{R}^N \to \mathbb{R}^N)$

Conjecture:
Trivializing maps are analytic functions of the parameters of the action.

Example: Scalar field theory $S(y; M, \Lambda) = y_i\, M_{ij}\, y_j + \lambda\, \Lambda_i\, y_i^4$
The map:

$$\frac{dy(x)}{dx}\; e^{-S(y(x))} = \mathcal{N} e^{-x^2/2}$$

Perturbative map in weak λ:

$$y_i(x; M, \Lambda) = x_i - \lambda \left(\sum_j \tfrac{1}{2} M_{ij}^{-1} \Lambda_j x_j^3 + \tfrac{3}{4} M_{ij}^{-1} M_{jj}^{-1} \Lambda_j x_j \right)$$

(analytic in M, Λ except at $M = 0$)

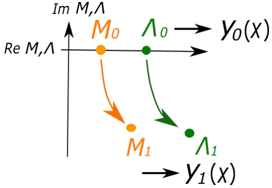
Perturbative map in strong λ is analytic in M, Λ except at $\Lambda = 0$

Existence of Perfect Manifolds[4]

Conjecture:
Trivializing maps are analytic functions of the parameters of the action, when $M, \Lambda \in \mathcal{R}$.

Conjecture implies:

Perfect manifolds exists for $M, \Lambda \in \mathcal{C}$



Caveat:

When manifolds intersect with singularity of S,
Trivializing maps are not guaranteed to exist

For actions without singularities at finite field values, perfect manifolds exist with $M, \Lambda \in \mathcal{C}$

Great, but can we find them? If so can use them?

[4] S. Lawrence and YY, arXiv:2101.05755

Example with ϕ^4 Scalar Field Theory

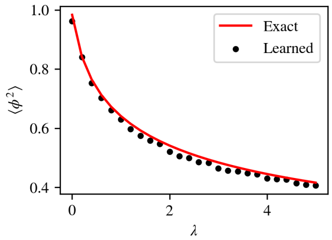
To estimate $\langle \mathcal{O} \rangle_S$ for the action S, let us define $S' = S + \alpha\, \mathcal{O}$.

A perturbing map $\vec{y}(x)$ from $S'(x + \alpha\, \vec{y}(x))$ to $S(x)$ satisfies

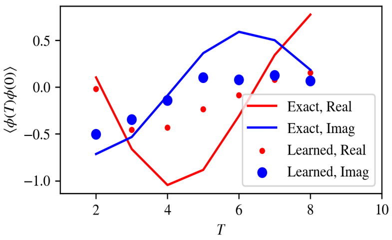
$$\nabla \cdot \vec{y}(x) - \vec{y}(x) \cdot \nabla S(x) - \mathcal{O}(x) + \langle \mathcal{O} \rangle_S = 0$$

Solve the ODE for $\vec{y}(x)$ and $\langle \mathcal{O} \rangle_S$ via machine learning:

$$C(w, \langle \mathcal{O} \rangle_S) = \sum_x |\nabla \cdot \vec{y}_w(x) - \vec{y}_w(x) \cdot \nabla S(x) - \mathcal{O}(x) + \langle \mathcal{O} \rangle_S|^2$$

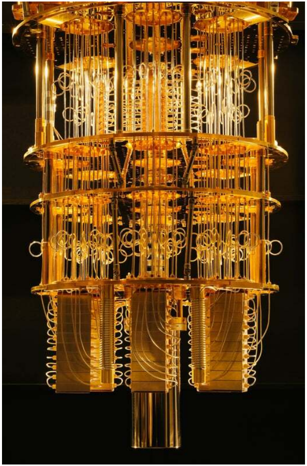


$0 + 1\mathrm{d},\ m = 0.5,\ N_\beta = 10,\ N_T = 0$

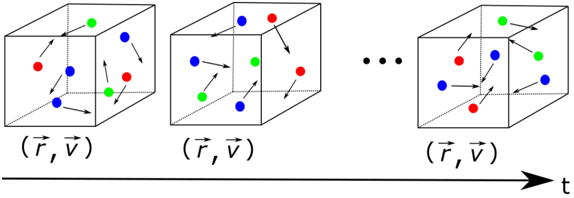


$0 + 1\mathrm{d},\ m = 0.5, \lambda = 0.5, N_\beta = 2$

Anywhere without Sign Problems...?

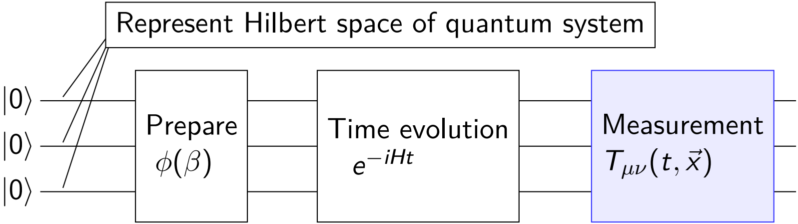


Quantum Computing - No Sign Problem



$$C(k,t) = \langle \vec{u}(\vec{k},t)\vec{u}(\vec{k},0)\rangle \sim e^{-\frac{\eta k^2}{\rho}t}$$

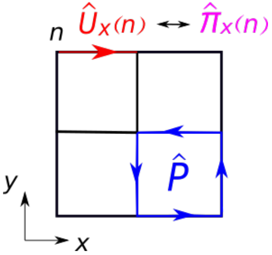
Quantum computer can simulate quantum system naturally



$$\langle\phi(\beta)|\,[T_{01}(t,\vec{x}),\, T_{01}(0,0)]\,|\phi(\beta)\rangle \;\; (\vec{x} \to \vec{k}) \;\; e^{-\frac{\eta k^2}{\epsilon}t}$$

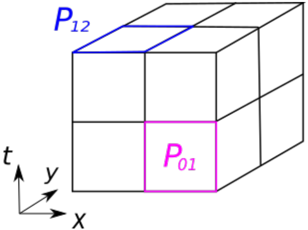
Operator $T_{\mu\nu}$ for Gauge Theories

Hamiltonian:



$$\hat{H}_{\rm KS} = \frac{g^2}{2a}\sum_{n,i}\hat{\pi}_i(n)^2 - \frac{1}{2g^2 a}\sum_{n,i<j}\mathrm{Re\,Tr}[\hat{P}_{ij}(n)]$$

Action:



$$S_{\rm W} = \frac{a}{g^2 a_0}\sum_{n,t,i}\mathrm{Re\,Tr}[1 - P_{0i}(n,t)] - \frac{a_0}{g^2 a}\sum_{n,t,i<j}\mathrm{Re\,Tr}[1 - P_{ij}(n,t)]$$

Hamiltonian and Action are connected by the Trotterization[5]:

$$\mathrm{Tr}[e^{-i\,H_{KS}\,t}] = \int \mathcal{D}[\vec{U}]\; e^{iS_{\rm W}[U]}$$

We can derive $T_{\mu\nu}$ **operators** by adding $T_{\mu\nu}$ at $t = t_0$

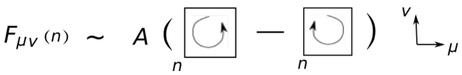
$$\int \mathcal{D}[\vec{U}]\; e^{i(S_{\rm W} + \epsilon T_{\mu\nu}\delta(t-t_0))} = \mathrm{Tr}[e^{-i\,H'\,t}],\ \text{with}\ \hat{H}'(t_0) = H_{KS} - \epsilon\,\hat{T}_{\mu\nu}/a_0$$

[5] M. Creutz, Phys.Rev.D 15, 1128

$\hat{T}_{12}$ for $SU(3)$ LGT - Action to Hamiltonian

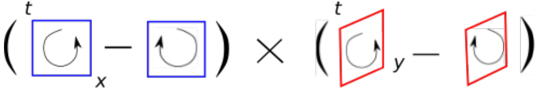
$$T_{12} = \mathrm{Tr}\left[-F_{10}F_{20} + F_{13}F_{23}\right] \text{ (in the continuum)}$$

1. $F_{\mu\nu}$ on a lattice in the action formulation:



2. Let us add T_{12} at site n to the action:

$$S' = S_{\mathrm{W}} + \epsilon\left(\mathrm{Tr}\left[-F_{10}(n)F_{20}(n) + F_{13}(n)F_{23}(n)\right]\right)$$



The relation between S' and H' tells us:

$$H' = H_{KS} + \epsilon\left(\frac{g^2}{a^4 a_0}\hat{\pi}_1^a\hat{\pi}_2^a + \frac{1}{4g^2a^4a_0}(\hat{P}_{13} - \hat{P}_{13}^\dagger)(\hat{P}_{23} - \hat{P}_{23}^\dagger)\right)(n)$$

3. Read off $\hat{T}_{12}$

$$\hat{T}_{12} = -\frac{g^2}{a^4}\mathrm{Tr}\left[\hat{\pi}_1(n)\hat{\pi}_2(n)\right] - \frac{1}{4g^2a^4}\mathrm{Tr}\left[(\hat{P}_{13} - \hat{P}_{13}^\dagger)(\hat{P}_{23} - \hat{P}_{23}^\dagger)\right](n)$$

$T_{\mu\nu}$ operators up to $O(a^2)$[6]

All operators needed for $T_{\mu\nu} = \frac{1}{4}\delta_{\mu\nu}\,\mathrm{Tr}[F_{\rho\sigma}F_{\rho\sigma}] - \mathrm{Tr}[F_{\mu\alpha}F_{\nu\alpha}]$

Operator	$O(a)$	$O(a^2)$
$\mathrm{Tr}\,F_{0i}F_{0i}(n)$	$\frac{g^2}{a^4}\,\mathrm{Tr}\left[\pi^2_{n,i}\right]$	$\sum_{x=0,1}\frac{g^2}{2a^4}\,\mathrm{Tr}\left[\pi^2_{n-x\hat{\imath},i}\right]$
$\mathrm{Tr}\,F_{0i}F_{0j}(n)$	$\frac{g^2}{a^4}\,\mathrm{Tr}\left[\pi_{n,i}\pi_{n,j}\right]$	$\frac{g^2}{4a^4}\Big(\mathrm{Tr}\left[\hat{\pi}_{n,i}\hat{\pi}_{n,j}\right] + \mathrm{Tr}\left[\hat{\pi}_{n,i}\hat{U}^\dagger_{n-\hat{\jmath},j}\hat{\pi}_{n-\hat{\jmath},j}\hat{U}_{n-\hat{\jmath},j}\right] + \mathrm{Tr}\left[\hat{U}^\dagger_{n-\hat{\imath},i}\hat{\pi}_{n-\hat{\imath}}\hat{U}_{n-\hat{\imath},i}\hat{\pi}_{n,j}\right] + \mathrm{Tr}\left[\hat{U}^\dagger_{n-\hat{\imath},i}\hat{\pi}_{n-\hat{\imath},i}\hat{U}_{n-\hat{\imath},i}\hat{U}^\dagger_{n-\hat{\jmath},j}\hat{\pi}_{n-\hat{\jmath},j}\hat{U}_{n-\hat{\jmath},j}\right]\Big)$
$\mathrm{Tr}\,F_{0j}F_{ij}(n)$	$-\frac{1}{a^4}\,\mathrm{Tr}\left[\hat{\pi}_{n,j}\,\mathrm{Im}\,\hat{P}_{ij}(n)\right]$	$-\frac{1}{2a^4}\Big(\mathrm{Tr}\left[\hat{\pi}_{n,j}\,\mathrm{Im}\,\hat{C}_{ij}(n)\right] + \mathrm{Tr}\left[\hat{U}^\dagger_{n-\hat{\jmath},j}\hat{\pi}_{n-\hat{\jmath},j}\hat{U}_{n-\hat{\jmath},j}\,\mathrm{Im}\,\hat{C}_{ij}(n)\right]\Big)$
$\mathrm{Tr}\,F_{ij}F_{ij}(n)$	$\frac{2}{g^2a^4}\,\mathrm{Re}\,\mathrm{Tr}\left[1-\hat{P}_{ij}(n)\right]$	$\sum_{x=0,1}\sum_{y=0,1}\frac{1}{2g^2a^4}\,\mathrm{Re}\,\mathrm{Tr}\left[1-\hat{P}_{ij}(n-x\hat{\imath}-y\hat{\jmath})\right]$
$\mathrm{Tr}\,F_{ij}F_{kj}(n)$	$\mathrm{Tr}[\hat{F}^N_{ij}(n)\hat{F}^N_{kj}(n)]$	$\mathrm{Tr}[\hat{F}^C_{ij}(n)\hat{F}^C_{kj}(n)]$

$O(a^2)$ operators are important especially in the near term

How do we implement them using primitive gates?

[6] T. Cohen, H. Lamm, S. Lawrence, and YY, arXiv:2104.02024

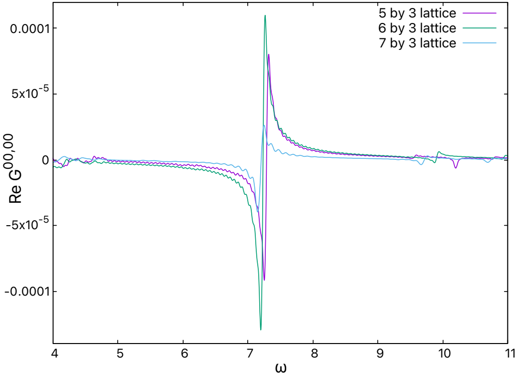
Shear Viscosity of Ising Model[7]

Shear viscosity of Ising model in $2+1$d via T_{00} correlators:

$$\langle T^{00} T^{00} \rangle(\omega, k) = \frac{k^2(\epsilon+P)}{\omega^2 - c_s^2 k^2 + i\omega k^2 \gamma_s} \text{ with } \gamma_s = \frac{4\eta}{3(\epsilon+P)} + \frac{\zeta}{\epsilon+P}$$

(ϵ: energy density, P: pressure, c_s: speed of sound, ζ: bulk viscosity)

Model: $H = -\sum_{i,j} \sigma_z(i)\sigma_z(j) - \mu \sum_i \sigma_x(i)$



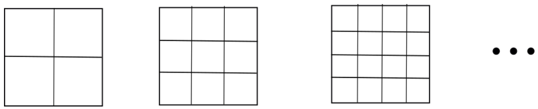
Time extent: 100
$dt = 0.001$ for 5×3,
$dt = 0.001$ for 6×3,
$dt = 0.005$ for 7×3,
$\mu = 1.1$, $\beta = 1$
$k = \frac{\pi}{L_x}$

[7] work in progress

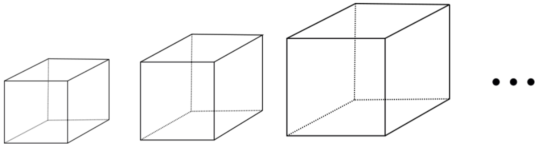
Taking Limits

Whether classical or quantum, after lattice calculations,

limits need to be taken



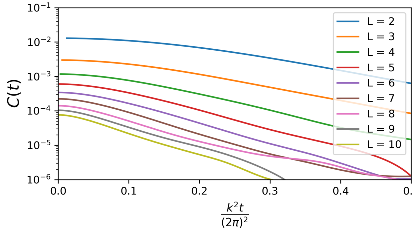
AND

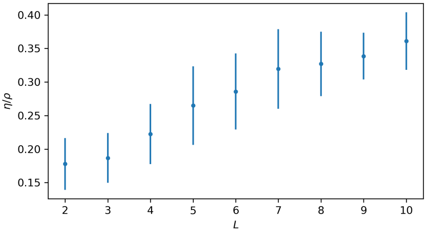


Finite volume effects on shear viscosity

For example... Molecule dynamics again:

$$C(k,t) = \langle \vec{u}(\vec{k},t)\vec{u}(\vec{k},0)\rangle \sim e^{-\frac{\eta k^2}{\rho}t} \quad (\rho : \text{mass density})$$





Finite volume effects exist and are not small for this system

Shear Viscosity of $\mathcal{N} = 4$ SYM

$G^{\mu\nu,\mu\nu}(\omega, k)$: correlator of $T_{\mu\nu}$ in momentum space

To extract viscosity, need $G^{\mu\nu,\mu\nu}(\omega, k)$ for small (ω, k)[8]

T_{xy}: $G^{12,12}(\omega, k) = -i\eta\omega + O(\omega^2, k^2)$

$\rightarrow \eta = i \lim_{\omega\rightarrow 0} \frac{\partial G^{12,12}(\omega, k=0)}{\partial\omega}$

$\mathcal{N} = 4$ SYM $\rightarrow G^{12,12}(\omega, k) = -\frac{is}{4\pi}\omega$

T_{tx}: $G^{01,01}(\omega, k) = \frac{k^2\eta}{i\omega - \frac{\eta}{\epsilon+p}k^2}$

$\mathcal{N} = 4$ SYM

$\rightarrow G^{01,01}(\omega, k) = \frac{N^2\pi T^3 k^2(1+O(\omega,k^2))}{8(i\omega - \frac{k^2}{4\pi T} + O(\omega^2, \omega k^2))}$

For $\mathcal{N} = 4$ SYM, $\frac{\eta}{s} = \frac{1}{4\pi}$

N = 4 SYM
Stroung coupling
& large *N*

[8] G. Policastro et al., Phys.Rev.Lett 87(2001)081601

Shear Viscosity in a Finite-size Box[9]

Finite-size box $\rightarrow$ smallest k may not be zero

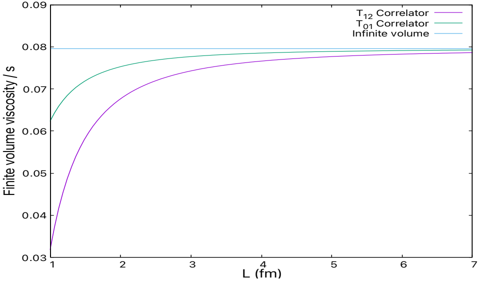
$$G^{12,12}(\omega,k) = s\left(-\frac{i}{4\pi}\omega - \frac{1}{8\pi^2 T}k^2 + \frac{i\ln(2)}{8\pi^3 T^2}\omega k^2 + O(\omega^2,\omega^2 k^2)\right)$$

$$\rightarrow \frac{\eta}{s} = \frac{1}{4\pi} - \frac{\ln(2)}{8\pi T^2 L^2} \quad \left(k \sim \frac{\pi}{L}\right)$$

$$G^{01,01}(\omega,k) = \frac{N^2\pi T^3}{8}\frac{k^2+O(\omega k^2,k^4)}{i\omega(1+\frac{\log 2}{16\pi^2 T^2}k^2) - \frac{k^2}{4\pi T}(1-\frac{k^2}{8\pi^2 T^2})}$$

$$\rightarrow \frac{\eta}{s} = \frac{1}{4\pi}\frac{1-\frac{1}{8T^2L^2}}{1+\frac{\ln(2)}{16T^2L^2}}$$

For $T = 150$ MeV



[9] T. Cohen, S. Lawrence, and YY, in preparation

Future Work

Goal
Calculation of shear viscosity
· From first principles
· Non-perturbatively

Classical Computer
Search manifolds via
· Machine learning
· Any clever algorithm?

Quantum Computer
· Concrete algorithm for quantum refrigerator
· Ising model viscosity
· What about $SU(3)$?

Finite volume effects
· More QCD-like model?
· Efficient algorithms?

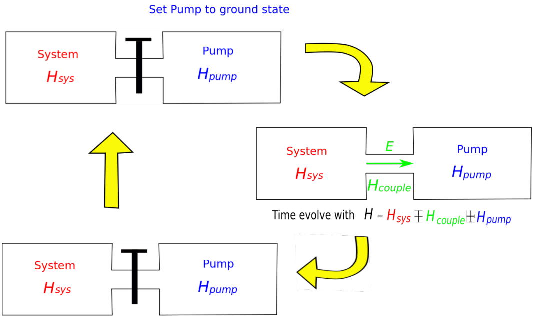
Thank you!

Thermal State Preparation - Naive Idea[10]

Goal: Prepare a state with temperature around crossover

Fact: High energy physical states are easily prepared

Tool: Quantum refrigerator



$$E_i > E_1 > E_2 > \cdots > E_N > E_f$$

Start from hot gas of free gluons → Lower E via "active cooling" → thermalize

- Don't need a large heat bath → Save qubit costs!
- The number of cycle $\propto \log\left(\frac{E_i}{E_f}\right)$

[10] R. Kosloff and A. Levy, Annual Review of Physical Chemistry 65, 365 (2014)