(Lattice) QCD at nonzero baryon number

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QCD phase diagram

extreme conditions: high temperature and/or density



no first-principle determination at finite density :

lattice QCD and the sign problem

Lattice QCD at nonzero chemical potential

QCD action (schematically)

$$S = S_{\rm YM} + \int d^4x \, \bar{\psi} M \psi$$

QCD partition function

$$Z = \int DU D\bar{\psi} D\psi \, e^{-S} = \int DU \, e^{-S_{\rm YM}} \det M(\mu)$$

fermion determinant is complex

$$\left[\det M(\mu)\right]^* = \det M(-\mu^*) \in \mathbb{C}$$

no positive weight in path integral

 \Rightarrow sign problem

Outline

chemical potential continuum/lattice

remarks about sign/overlap/Silver Blaze problems

complex Langevin dynamics & Lefschetz thimbles

(towards) QCD

for review and references (and exercises!), see

Introductory lectures on lattice QCD at nonzero baryon number

J. Phys. Conf. Ser. 706 (2016) 022004 [arXiv:1512.05145 [hep-lat]]

Chemical potential

- \checkmark phase diagram: introduce chemical potential μ
- couples to conserved charge (baryon number)

$$n \sim \psi^{\dagger} \psi = \bar{\psi} \gamma_4 \psi = j_4$$

• temporal component of current $j_{\nu} = \bar{\psi} \gamma_{\nu} \psi$

on the lattice: fermion hopping terms $j_{\nu} \sim \kappa \bar{\psi}_x \gamma_{\nu} \psi_{x+\nu}$ modify temporal hopping terms:

- **s** forward hopping: κe^{μ}
- backward hopping: $\kappa e^{-\mu}$

⇒ exactly conserved (Noether) charge at *finite* lattice spacing
Hasenfratz & Karsch 83

Chemical potential on the lattice

chemical potential introduces an imbalance between forward and backward hopping

- forward hopping (quark)
 ⇒ favoured as $e^{\mu n_{\tau}}$
- **s** backward hopping (anti-quark) $\Rightarrow \quad \text{disfavoured as } e^{-\mu n_{\tau}}$
- closed worldline



 μ dependence only remains when worldline wraps around time direction

$$e^{\mu N_{\tau}} = e^{\mu/T} \qquad \qquad e^{-\mu N_{\tau}} = e^{-\mu/T}$$

Chemical potential on the lattice

suggestion:

• μ is effectively a boundary condition

make explicit:

• field redefinition
$$\psi_x = e^{-\mu\tau}\psi'_x$$
 $\bar{\psi}_x = e^{\mu\tau}\bar{\psi}'_x$

- μ dependence drops from all terms $\bar{\psi}_x e^{\mu} \psi_{x+4}$ etc (and also from spatial terms)
- but appears as a boundary condition

$$\psi_{N_{\tau}} = -\psi_0 \quad \Rightarrow \quad \psi'_{N_{\tau}} = -e^{\mu N_{\tau}} \psi'_0$$

wrapping around the temporal direction

Chemical potential on the lattice

imbalance leads to fundamental issue: sign problem! at $\mu = 0$: quark matrix M

 $\det M^{\dagger} = \det \left(\gamma_5 M \gamma_5\right) = \det M = (\det M)^*$

 \checkmark real determinant " γ_5 hermiticity"

at $\mu \neq 0$:

det $M^{\dagger}(\mu) = \det \gamma_5 M(-\mu^*) \gamma_5 = \det M(-\mu^*) = [\det M(\mu)]^*$

- complex determinant
- no real weight: numerical methods break down

note: real determinant for imaginary chemical potential Roberge & Weiss 86, Lombardo 00, de Forcrand & Philipsen 03-12

Dubna, August 2017 – p. 8

Sign problem

sign problem not specific for QCD

- appears generically in theories with imbalance
- in both fermionic and bosonic theories
 i.e. not due to anti-commuting nature of fermions
- also in condensed-matter models, e.g. Hubbard model away from half-filling

understanding of sign problem relevant across physics

generic solution to sign problem not expected: NP hard

Troyer & Wiese 04

more and more solutions to specific theories available

Towards the Silver Blaze problem

consider massive particle with mass m at low temperature:

- µ is the change in free energy when a particle carrying the corresponding quantum number is added
 i.e. energy cost for adding one particle
- if $\mu < m$: not enough energy to create a particle \Rightarrow no change in groundstate
- if $\mu > m$: plenty of energy available \Rightarrow nonzero density

onset at $\mu = \mu_c(=m)$ at zero temperature generic principle of statistical mechanics

 \Rightarrow demonstrate for free fermions

Free fermions: onset at low temperature

standard thermal field theory: free fermion gas

$$\ln Z = 2V \int \frac{d^3 p}{(2\pi)^3} \left[\beta \omega_{\mathbf{p}} + \ln \left(1 + e^{-\beta(\omega_{\mathbf{p}} - \mu)} \right) + \ln \left(1 + e^{-\beta(\omega_{\mathbf{p}} + \mu)} \right) \right]$$

J density: $\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + m^2}$

$$\langle n \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial \mu} = 2 \int_{\mathbf{p}} \left[\frac{1}{e^{\beta(\omega_{\mathbf{p}} - \mu)} + 1} - \frac{1}{e^{\beta(\omega_{\mathbf{p}} + \mu)} + 1} \right]$$

■ low-temperature limit: $T \to 0, \beta \to \infty$ case 1:

$$\mu < m : \langle n \rangle \sim 2 \int_{\mathbf{p}} \left[e^{-\beta(\omega_{\mathbf{p}} - \mu)} - e^{-\beta(\omega_{\mathbf{p}} + \mu)} \right] \to 0$$

(anti)particles thermally excited but Boltzmann suppressed

Free fermions: onset at low temperature

Fermi-Dirac distribution become step function at T = 0

$$\mu > m : \langle n \rangle \sim 2 \int_{\mathbf{p}} \Theta(\mu - \omega_{\mathbf{p}}) = \frac{\left(\mu^2 - m^2\right)^{3/2}}{3\pi^2} \Theta(\mu - m)$$

filled Fermi sphere: nonzero density onset at $\mu = \mu_c = m$ no μ dependence below onset Silver Blaze region

How hard is the sign problem?

partition function: $Z = \int DU D \bar{\psi} D \psi e^{-S} = \int DU e^{-S_B} \det M$ complex weight due to complex determinant

$$[\det M(\mu)]^* = \det M(-\mu^*)$$

write det $M = |\det M|e^{i\varphi}$ and absorb phase in observable

$$\begin{split} \langle O \rangle_{\text{full}} &= \frac{\int DU \, e^{-S_B} \det M \, O}{\int DU \, e^{-S_B} \det M} = \frac{\int DU \, e^{-S_B} |\det M| \, e^{i\varphi} O}{\int DU \, e^{-S_B} |\det M| \, e^{i\varphi}} \\ &= \frac{\langle e^{i\varphi} O \rangle_{\text{pq}}}{\langle e^{i\varphi} \rangle_{\text{pq}}} \end{split}$$

expectation values are taken wrt phase-quenched weight well-defined in principle ...

Sign and overlap problems

• what is average phase factor $\langle e^{i\varphi} \rangle_{pq}$?

$$\langle e^{i\varphi} \rangle_{\mathrm{pq}} = \frac{\int DU \, e^{-S_B} |\det M| \, e^{i\varphi}}{\int DU \, e^{-S_B} |\det M|} = \frac{Z_{\mathrm{full}}}{Z_{\mathrm{pq}}} = e^{-\Omega \Delta f} \to 0$$

■ ratio of two partition functions! note: $Z_{\text{full}} \leq Z_{\text{pq}}$

$$Z = e^{-F/T} = e^{-\Omega f} \qquad \qquad \Omega = N_\tau N_s^3$$

• average phase factor $\rightarrow 0$ in thermodynamic limit! (unless $f = f_{pq}$)

this is the overlap problem: sampling with the 'wrong' weight exponentially hard

Origin of overlap problem

phase-quenched physics is different!

consider two flavours: $\left[\det D(\mu)\right]^2$ vs $\left|\det D(\mu)\right|^2$

• recall
$$D^{\dagger}(\mu) = \gamma_5 D(-\mu^*) \gamma_5$$

• then
$$|\det D(\mu)|^2 = \det D(-\mu) \det D(\mu)$$

 \Rightarrow isospin chemical potential! up/down quark: $\pm \mu$

- Iightest particle with nonzero isospin: pion
- Iightest particle with nonzero baryon number: nucleon

Onset, phase-quenching and Silver Blaze

full QCD with quark chemical potential:

onset when $\mu = [lightest baryon mass - binding energy]/3 nuclear matter$

phase-quenched QCD with isospin chemical potential:

onset when μ equals [pion mass]/2 (nonzero isospin) pion condensation

Onset, phase-quenching and Silver Blaze

full QCD with quark chemical potential:

s onset when $\mu = [lightest baryon mass - binding energy]/3 nuclear matter$

phase-quenched QCD with isospin chemical potential:

In onset when μ equals [pion mass]/2 (nonzero isospin) pion condensation

 $0 < \mu < m_{\pi}/2$ full = phase-quenched at T = 0no severe sign problem, but no interesting physics

 $m_{\pi}/2 < \mu \lesssim m_B/3$ severe sign problem strong cancelations required to cancel μ dependence of phase-quenched theory

Onset, phase-quenching and Silver Blaze



- perform lattice simulations in phase-quenched theory
- extract full QCD results
- \Rightarrow requires severe cancelations of the μ dependence in region $m_{\pi}/2 < \mu \lesssim m_B/3$
- \Rightarrow Silver Blaze problem: get cancelations right

most straightforward numerical methods will fail this test!

Complex measure

complex weight

$$\det M(\mu) = |\det M(\mu)|e^{i\theta}$$

cancelation between configurations with 'positive' and 'negative' weight



take the complexity seriously!

Complex integrals

consider simple integral

$$Z(a,b) = \int_{-\infty}^{\infty} dx \, e^{-S(x)} \qquad S(x) = ax^2 + ibx$$

- complete the square/saddle point approximation: into complex plane
- Iesson: don't be real(istic), be more imaginative

radically different approach:

- complexify all degrees of freedom $x \to z = x + iy$
- enlarged complexified space
- new directions to explore

Complexified field space

dominant configurations in the path integral?



• real and positive distribution P(x, y): complex Langevin

Parisi 83, Klauder 83

deformation of integration contour: Lefschetz thimbles

Airy 1838, Witten 10





GA, 1308.4811

GA, Bongiovanni, Seiler, Sexty, 1407.2090

GA, Giudice, Seiler, 1306.3075

main idea:

generate field configurations using stochastic process

$$\dot{z} = -\partial_z S + \eta$$
 $\langle \eta(t)\eta(t') \rangle = 2\delta(t-t')$

- reach equilibrium distribution à la Brownian motion
- no importance sampling required

Langevin drift $K = -\partial_z S$ derived from complex weight: explore complexified configurations

- one degree of freedom: $z \to x + iy$
- real scalar field: $\phi(x) \rightarrow \phi_{\rm R}(x) + i\phi_{\rm I}(x)$
- gauge link U: $SU(3) \Rightarrow SL(3,\mathbb{C})$

rely on holomorphicity

Langevin dynamics:

zero-dimensional example complex action S(z)

associated Fokker-Planck equation (FPE)

 $\dot{P}(x,y;t) = [\partial_x(\partial_x + \operatorname{Re}\partial_z S(z)) + \partial_y \operatorname{Im}\partial_z S(z)]P(x,y;t)$

(equilibrium) distribution in complex plane: P(x, y)
 observables

$$\langle O(x+iy)\rangle = \frac{\int dx dy P(x,y)O(x+iy)}{\int dx dy P(x,y)}$$

P(x, y) real and non-negative: no sign problem
 criteria for correctness

applicability for holomorphic actions:

- check criteria a posteriori
- gauge cooling essential
- dynamical stabilisation

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GA, Seiler & Stamatescu 09
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Seiler, Sexty & Stamatescu 12
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Attanasio & Jäger 17
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successful applications to various models, including with phase transitions and severe sign problems

but success not guaranteed (criteria)

open question: meromorphic drift

- with weight det M: drift contains $Tr M^{-1}$
- poles: problems *may* appear Mollgaard & Splittorff 13
- analysis

GA, Seiler, Sexty & Stamatescu 17

Nagata, Nishimura & Shimasaki 16, ...

Lefschetz thimbles

generalised saddle point integration/steepest descent:

extend definition of path integral

- Chern-Simons theories
- mathematical foundation in Morse theory

formulation:

- find *all* stationary points z_k of holomorphic action S(z)
- paths of steepest descent: stable thimbles \mathcal{J}_k
- paths of steepest ascent: unstable thimbles \mathcal{K}_k
- Im S(z) constant along thimble k

integrate over stable thimbles, with proper weighting

Lefschetz thimbles

generalised saddle point integration/steepest descent:

integrate over stable thimbles

$$Z = \sum_{k} m_{k} e^{-i \operatorname{Im} S(z_{k})} \int_{\mathcal{J}_{k}} dz \, e^{-\operatorname{Re} S(z)}$$
$$= \sum_{k} m_{k} e^{-i \operatorname{Im} S(z_{k})} \int ds \, z'(s) e^{-\operatorname{Re} S(z(s))}$$

- ✓ intersection numbers: $m_k = \langle C, \mathcal{K}_k \rangle$ (C = original contour, $\mathcal{K}_k =$ unstable thimble)
- residual sign problem: complex Jacobian J(s) = z'(s)
- global sign problem: phases $e^{-i \text{Im}S(z_k)}$

two approaches in the complex plane:

Langevin

$$\langle O(z) \rangle = \frac{\int dx dy P(x, y) O(x + iy)}{\int dx dy P(x, y)}$$



$$\langle O(z) \rangle = \frac{\sum_{k} m_{k} e^{-i \operatorname{Im} S(z_{k})} \int_{\mathcal{J}_{k}} dz \, e^{-\operatorname{Re} S(z)} O(z)}{\sum_{k} m_{k} e^{-i \operatorname{Im} S(z_{k})} \int_{\mathcal{J}_{k}} dz \, e^{-\operatorname{Re} S(z)}}$$

- two- versus one-dimensional
- real versus residual/global phases

relation? validity? \Rightarrow simple models

Quartic model

$$Z = \int_{-\infty}^{\infty} dx \, e^{-S} \qquad \qquad S(x) = \frac{\sigma}{2}x^2 + \frac{\lambda}{4}x^4$$

complex mass parameter $\sigma = A + iB$, $\lambda \in \mathbb{R}$

Often used toy model Ambjorn & Yang 85, Klauder & Petersen 85, Okamoto et al 89, Duncan & Niedermaier 12

essentially analytical proof for CL GA, Giudice, Seiler 13

- CL gives correct result for all observables $\langle x^n \rangle$ provided that A > 0 and $A^2 > B^2/3$
- **•** based on properties of the distribution P(x, y)
- follows from classical flow or directly from FPE

Quartic model



- determine where drift $K_{I} = -\text{Im}\partial_{z}S(z)$ vanishes (blue lines)
- at the extrema: impenetrable barrier (for real noise)
- distribution localised between dashed lines

Quartic model

- numerical solution of FPE for P(x, y)
- distribution is localised in a strip around real axis
- ▶ P(x,y) = 0 when $|y| > y_-$ with $y_- = 0.303$ for $\sigma = 1 + i$



Lefschetz thimbles for quartic model

critical points:

 $z_0 = 0$ $z_{\pm} = \pm i \sqrt{\sigma/\lambda}$

thimbles can be computed analytically

> $ImS(z_0) = 0$ $ImS(z_{\pm}) = -AB/2\lambda$



- **•** for A > 0: only 1 thimble contributes
- integrating along thimble gives correct result, with inclusion of complex Jacobian

Quartic model: thimbles

compare thimble and FP distribution P(x, y)



• thimble and P(x, y) follow each other

Quartic model: thimbles

compare thimble and FP distribution P(x, y)



- thimble and P(x, y) follow each other
- however, weight distribution quite different

intriguing result: complex Langevin process finds the thimble – is this generic?

compare evolution equations in more detail

complex Langevin (CL) dynamics

$$\dot{x} = -\operatorname{Re} \partial_z S(z) + \eta$$
 $\dot{y} = -\operatorname{Im} \partial_z S(z)$

• Lefshetz thimble dynamics, with $z(t \rightarrow \infty) = z_k$

$$\dot{x} = -\operatorname{Re}\partial_z S(z)$$
 $\dot{y} = +\operatorname{Im}\partial_z S(z)$

 \Rightarrow change in sign for y drift

- stable and unstable fixed points
- unstable runaways as $y \to \pm \infty$
- saddle points
- \checkmark stable thimbles coming from $y \to \pm \infty$

Langevin:

thimbles:

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deform quartic model with linear term, break symmetry



- one stable/two unstable fixed points for CL
- $y \to -\infty$ classical runaway trajectory
- two contributing thimbles (global phase problem) due to Stokes' phenomenon

histogram of P(x, y) collected during CL simulation





- thimbles: both saddle points contribute
- CL: unstable fixed point avoided
- no role for second thimble in Langevin
- \Rightarrow distributions manifestly different

Langevin and Lefschetz

exploring the complex plane: thimbles and Langevin

- Iocation of distributions related but not identical
- weight distributions typically different
- repulsive fixed points in Langevin dynamics avoided
- thimbles end on zeroes of measure/poles of drift

(Towards) QCD

Complex Langevin dynamics

Aarts, Stamatescu, 0807.1597
Seiler, Sexty, Stamatescu, 1211.3709
Sexty, 1307.7748
GA, Seiler, Sexty, Stamatescu, 1408.3770
GA, Attanasio, Jäger, Sexty, 1606.05561

QCD phase structure

Columbia plot: order of thermal transition at $\mu = 0$



QCD with heavy quarks

heavy quark corner of Columbia plot

- first order transition to deconfined phase
- Polyakov loop order parameter
- quark determinant simplifies considerably
- hopping expansion (LO): only straight quark world lines
- fermion determinant

$$\det M = \prod_{\mathbf{x}} \det \left(1 + h e^{\mu/T} \mathcal{P}_{\mathbf{x}} \right)^2 \left(1 + h e^{-\mu/T} \mathcal{P}_{\mathbf{x}}^{-1} \right)^2$$

 $\mathcal{P}_{\mathbf{x}} =$ untraced Polyakov loop $h = (2\kappa)^{N_{\tau}}$

determine phase diagram in heavy quark sector

widely used limit of QCD to test methods

SU(N) gauge theory: complexification to $SL(N, \mathbb{C})$

Iinks $U \in SU(N)$: complex Langevin update

 $U(n+1) = R(n) U(n) \qquad \qquad R = \exp\left[i\lambda_a\left(\epsilon K_a + \sqrt{\epsilon\eta_a}\right)\right]$

Gell-Mann matrices λ_a ($a = 1, \ldots N^2 - 1$)

• drift:
$$K_a = -D_a(S_{YM} + S_F)$$
 $S_F = -\ln \det M$

SU(N) gauge theory: complexification to $SL(N, \mathbb{C})$

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Gell-Mann matrices λ_a ($a = 1, \ldots N^2 - 1$)

- drift: $K_a = -D_a(S_{YM} + S_F)$ $S_F = -\ln \det M$
- complex action: $K^{\dagger} \neq K \Leftrightarrow U \in SL(N, \mathbb{C})$
- deviation from SU(N): unitarity norms

$$\frac{1}{N} \operatorname{Tr} \left(U U^{\dagger} - \mathbb{1} \right) \ge 0 \qquad \qquad \frac{1}{N} \operatorname{Tr} \left(U U^{\dagger} - \mathbb{1} \right)^2 \ge 0$$







heavy dense QCD, 4^4 lattice with $\beta = 5.6$, $\kappa = 0.12$, $N_f = 3$

GA & Stamatescu 0807.1597

controlled evolution: stay close to SU(N) submanifold when

- small chemical potential μ
- small non-unitary initial conditions
- in presence of roundoff errors

controlled evolution: stay close to SU(N) submanifold when

- small chemical potential μ
- small non-unitary initial conditions
- in presence of roundoff errors

in practice this is not the case

 \Rightarrow unitary submanifold is unstable!

- process will not stay close to SU(N)
- distributions not localised
- wrong results in practice, non-analytic around $\mu^2 \sim 0$
- \Rightarrow controlled by gauge cooling, dynamical stabilisation, ...

QCD with heavy quarks

expectations for phase diagram two transitions:

- full Wilson gauge action is included
- thermal deconfinement transition (as in pure glue)

$$\det M = \prod_{\mathbf{x}} \det \left(1 + h e^{\mu/T} \mathcal{P}_{\mathbf{x}} \right)^2 \det \left(1 + h e^{-\mu/T} \mathcal{P}_{\mathbf{x}}^{-1} \right)^2$$

•
$$\mu$$
-driven transition: $2\kappa e^{\mu} \ge 1$

• critical chemical potential for onset at $\mu_c^0 = -\ln(2\kappa)$

determine phase diagram by direct simulation in $T - \mu$ plane

QCD with static quarks or heavy dense QCD (HDQCD) simulation details

- I lattice coupling/spacing: $\beta = 5.8$ $a \sim 0.15$ fm
- hopping parameter: $\kappa = 0.04$ $\mu_c^0 = -\ln(2\kappa) = 2.53$
- \checkmark spatial volume $6^3, 8^3, 10^3$
- $N_{\tau} = 2 \ 3 \ 4 \ 5 \ 6 \ 7 \ 8 \ 9 \ 10 \ 11 \ 12 \ 13 \ 14 \ 15 \ 16 \ 18 \ 20 \ 24 \ 28$
- $T \sim 48 \dots 671 \text{ MeV}$
- direct simulation in $T \mu$ plane (~ 880 parameter combinations)

observables: Polyakov loop, quark density



- $\langle P \rangle = 0$ at low T, μ : confinement
- $\langle P \rangle \neq 0$ at high T, μ : deconfinement
- $\mu > \mu_c^0$ at T = 0: saturation, lattice artefact, unphysical



•
$$\langle n \rangle = 0$$
 at $\mu = 0$

- \checkmark $\langle n \rangle$ rises slowly at high T, onset at low T
- $\mu > \mu_c^0$ at T = 0: saturation, lattice artefact, unphysical

attempt to determine the phase boundary Polyakov loop susceptibility $\chi_P \sim \langle P^2 \rangle - \langle P \rangle^2$



signal not very clear

better estimate of boundary: Binder cumulant *B* for order parameter *O*

$$B = 1 - \frac{\langle O^4 \rangle}{3 \langle O^2 \rangle^2}$$

then

$$\langle O \rangle = 0 \Leftrightarrow B = 0$$
 $\langle O \rangle \neq 0 \Leftrightarrow B = \frac{2}{3}$

(assume Gaussian fluctuations)



- $B \sim 0 \text{ at low } T, \mu$
- $B \sim 2/3 \text{ at high } T, \mu$

Binder cumulant: phase boundary



- determine boundary by B = 1/3
- fixed lattice spacing: less resolution at higher temperature $T \sim 1/N_{\tau}$

Heavy dense QCD phase diagram



- simple fits up to μ^4 (2 parameters) are sufficient
- no sign for nonanalyticity at T = 0 from data yet

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Heavy dense QCD phase diagram

possible to determine and parametrise boundary

many things to improve

- fixed lattice spacing
- affects thermal transition
- order of transition
- vary κ : critical endpoints



extension to (more) dynamical quarks

- HDQCD is starting point of systematic hopping parameter expansion Philipsen et al 10-16
- all-orders expansion GA, Seiler, Sexty, Stamatescu 14
- **full QCD** Sexty 13, Kogut & Sinclair 15-Nagata, Nishimura, Shimasaki 15-, Bloch 16-

Complex Langevin dynamics: Full QCD

implementation of hopping parameter expansion to high order $\mathcal{O}(\kappa^{50})$ and comparison with full QCD



- convergence of hopping expansion
- agreement between expansion and full QCD

Summary

theories with sign problem:

- rich topic with diverse solutions
- some theories solvable in more than one way
- some not all (yet!)

into the complex plane:

- complex action leads naturally to complexification
- complex Langevin dynamics
- Lefschetz thimbles/holomorphic flow
- no fully satisfactory solution yet

lots of work to do!

Where is Swansea?



in Wales, United Kingdom about three hours from London by direct train

Swansea University



university campus next to the beach

Swansea and the Gower peninsula



many beautiful beaches, and even occasional sunshine!