The density of states approach for the simulation of finite density quantum field theories

DISCRETE 2014, 4 December 2014 King’s College London

Kurt Langfeld

School of Comp. and Mathematics
Mathematical Sciences Research Centre
Plymouth University, UK

with:
B. Lucini, Swansea
R. Pellegrini, Edinburgh
A. Rago, Plymouth
L. Bongiovanni, Swansea
Evolution of the Universe:

Big Bang

Unified Forces

Inflationary Expansion

Forces Separate

Nucleons Form

Atoms Form

Stars Are Born

Today

Time:
- $10^{-43}$ s
- $10^{-35}$ s
- $10^{-10}$ s
- $10^{-6}$ s
- 300,000 Years
- 10$^9$ Years
- 15·10$^9$ Years

Energy:
- $10^{17}$ TeV
- $10^{13}$ TeV
- 1 TeV
- 150 MeV
- 1 eV
- 4 meV
- 0.7 meV

NIC, FZ–Juelich
Evolution of the Universe:

QCD physics

Evolution of the Universe:

Big Bang

Unified Forces

Inflationary Expansion

Forces Separate

Nucleons Form

Atoms Form

Stars Are Born

Today

Time:

$10^{-43}$ s

$10^{-35}$ s

$10^{-10}$ s

$10^{-6}$ s

300,000 Years

$10^9$ Years

$15 \cdot 10^9$ Years

Energy:

$10^{17}$ TeV

$10^{13}$ TeV

1 TeV

150 MeV

1 eV

4 meV

0.7 meV

NIC, FZ–Juelich
Phases of QCD:

- compact stars
- quark gluon plasma
- superconductor
- confinement
- colour density
- temperature
- nuclear matter
- early universe
- LHC
- RHIC

The density of states approach for the simulation of finite density quantum field theories – p. 4/31
Phases of QCD:

The density of states approach for the simulation of finite density quantum field theories – p. 5/31
What did we know in 2003?

First principle calculations: Lattice gauge simulations

The density of states approach for the simulation of finite density quantum field theories – p. 6/31
What do we know NOW?

First principle calculations: **Lattice gauge simulations**

The density of states approach for the simulation of finite density quantum field theories – p. 7/31
What do we NOT know?

- Density of compact stars
- Temperature
- Colour confinement
- Nuclear matter
- Quarkyonic "chiral spirals"
- Fermi Einstein condensation

References:
- McLarren, Pisarski 2010
- Fukushima, 2009
- Langfeld, Wipf 2011
What is the problem?

- Quantum Field Theory:
  \[ Z = \int D\phi \exp\{\beta S_R[\phi]\} \]

  infinite dimension integral
  Monte-Carlo simulation (importance sampling!)
  \[ \exp\{\beta S_R[\phi]\} \]: probabilistic weight
What is the problem?

- Quantum Field Theory:
  \[ Z = \int \mathcal{D}\phi \exp\{\beta S_R[\phi]\} \]
  infinite dimension integral
  Monte-Carlo simulation (importance sampling!)
  \(\exp\{\beta S_R[\phi]\}\): probabilistic weight

- QFT at finite densities:
  \[ Z = \int \mathcal{D}\phi \exp\{\beta S_R[\phi] + i\mu S_I[\phi]\} \]
  \(\mu\): chemical potential
  \(S_I\): imaginary part of the action
  complex!
Promising “solutions”

Re-weighting approach: [Fodor, Katz, since 2000]
(eventually restricted to high $T$)
Promising “solutions”

- **Re-weighting approach**: [Fodor, Katz, since 2000]
  (eventually restricted to high $T$)

- **Complex Langevin simulations**
  [Parisi, 1983] [Karsch, Wyld, 1985] [Ambjorn, Yang, 1986]
  recently [Aarts, Seiler, Stamatescu, 2009 -- present]
Promising “solutions”

- Re-weighting approach: [Fodor, Katz, since 2000] (eventually restricted to high $T$)

- Complex Langevin simulations

- Strong coupling expansion
  Nuclear Physics [deForcrand, Fromm, 2010] [Philipsen et al, 2011]
**Promising “solutions”**

- **Re-weighting approach:** [Fodor, Katz, since 2000]  
  (eventually restricted to high $T$)

- **Complex Langevin simulations**  
  [Parisi, 1983] [Karsch, Wyld, 1985] [Ambjorn, Yang, 1986]  
  recently [Aarts, Seiler, Stamatescu, 2009 -- present]

- **Strong coupling expansion**  
  Nuclear Physics [deForcrand, Fromm, 2010] [Philipsen et al, 2011]

- **The LLR-algorithm**  
  [Langfeld, Lucini, Rago, 2012]
Promising “solutions”

- **Re-weighting approach:** [Fodor, Katz, since 2000] (eventually restricted to high $T$)
- **Complex Langevin simulations**
- **Strong coupling expansion**
  Nuclear Physics [deForcrand, Fromm, 2010] [Philipsen et al, 2011]
- **The LLR-algorithm**
  [Langfeld, Lucini, Rago, 2012]
- **Worm algorithms**
  [Prokof’ev, Svistuno, 2001] [Chandrasekharan 2010] [Gattringer, Evertz, 2011]
The sign problem revisited

model QFT: \[ Z = \int \mathcal{D}\phi \exp\{\beta S_R[\phi] + i\mu S_I[\phi]\} \]

\( \mu \): chemical potential
\( S_I \): imaginary part of the action
\( S_R \): real part of the action
The sign problem revisited

- model QFT:

\[ Z = \int \mathcal{D}\phi \exp\{\beta S_R[\phi] + i\mu S_I[\phi]\} \]

\( \mu \): chemical potential
\( S_I \): imaginary part of the action
\( S_R \): real part of the action

- generalised density of states:

\[ P_\beta(s) = \int \mathcal{D}\phi \delta\left(s - S_I[\phi]\right) \exp\{\beta S_R[\phi]\} \]

partition function from a Fourier transformation:

\[ Z = \int ds \, P_\beta(s) \exp\{i\mu s\} \]
The sign problem revisited

problem:

\[ S_I[\phi] \text{ is an extensive quantity} \]

\[ S_I[\phi] = V s_I, \quad \langle s_I \rangle \sim \mathcal{O}(1), \quad V : \text{ volume}. \]
The sign problem revisited

- problem:
  \[ S_I[\phi] \text{ is an extensive quantity} \]
  \[ S_I[\phi] = V s_I, \quad \langle s_I \rangle \sim \mathcal{O}(1), \quad V : \text{ volume.} \]

- Example: \( P_\beta(s) = \exp\left\{-\frac{s^2}{V}\right\} \) \( (s \sim V: \text{ground state}) \)

partition function from a Fourier transformation:

\[
Z = \int ds \ e^{-s^2/V} \ \exp\{i \mu s\} \ \propto \ \exp\left\{-\frac{\mu^2}{4} V\right\}
\]
The sign problem revisited

- problem:
  \[ S_I[\phi] \] is an extensive quantity
  \[ S_I[\phi] = V s_I, \quad \langle s_I \rangle \sim \mathcal{O}(1), \quad V : \text{ volume}. \]

- Example: \[ P_\beta(s) = \exp\left\{-\frac{s^2}{V}\right\} \quad (s \sim V: \text{ ground state}) \]

partition function from a Fourier transformation:

\[
Z = \int ds \, e^{-s^2/V} \exp\{i \mu s\} \propto \exp\left\{-\frac{\mu^2}{4} V\right\}
\]

\[ \Rightarrow P_\beta(s) \sim \mathcal{O}(1), \text{ only known numerically} \]

\[ \Rightarrow \text{need to produce an exponentially small signal} \]
We need a numerical method to calculate $P_\beta(s)$ with exponential error suppression over the whole action range ?!
The LLR approach ($\mu = 0$)

- How do we calculate $\rho(E)$ numerically?
The LLR approach \((\mu = 0)\)

- How do we calculate \(\rho(E)\) numerically?
- Observation:
  \(\log \rho(E)\) is a remarkable smooth function of \(E\)!

Here: density for the real part of the SU(2) action

SU(2), \(10^4\) lattice:
\(E_{\text{max}} = 60,000\):
Choose a piecewiese linear ansatz:

\[ \rho(E) = \rho(E_0) \exp\left\{ a(E_0) (E - E_0) \right\}, \quad E_0 < E < E_0 + \delta E \]

need to find the \( a(E_0) \)!
The LLR approach \((\mu = 0)\)

- Choose a piecewiese linear ansatz:

\[
\rho(E) = \rho(E_0) \exp\left\{ a(E_0) (E - E_0) \right\}, \quad E_0 < E < E_0 + \delta E
\]

need to find the \(a(E_0)\)!

- The LLR algorithm:
  \(\triangle\) derive non-linear equation for \(a(E_0)\)
  \(\triangle\) uses MC expectation values (truncation + reweighting)
  \(\triangle\) use Robbins Monroe\(^*\) to find \(a(E_0)\)

* [Pellegrini, Langfeld, Lucini, Rago, arXiv:1411.0655, Lattice 2013]
preliminary results for SU(3):
The density of states - compact U(1)

- study phase transition in U(1):

\[ \Delta \text{ weakly first order} \]


\[ \Delta \rho(E) = \rho(E) \exp\{\beta E\} \]

[Langfeld, Lucini, Pellegrini, Rago, in preparation]
study phase transition in U(1):

△ weakly first order


△ \( P_\beta(E) = \rho(E) \exp\{\beta E\} \)

[Langfeld, Lucini, Pellegrini, Rago, in preparation]
Solving sign-problems

Can we use the modified WL method to simulate finite density systems?
Consider a theory with complex action:

\[
Z(\mu) = \int \mathcal{D}\phi \exp\{i\mu S_I[\phi]\} \exp\{S_R[\phi, \mu]\}
\]
Overlap and Sign Problems

Consider a theory with complex action:

\[ Z(\mu) = \int D\phi \exp\{i\mu S_I[\phi]\} \exp\{S_R[\phi, \mu]\} \]

**sign problem:** complex/negative integrand \(\Rightarrow\) no importance sampling with respect to the action
Consider a theory with complex action:

\[ Z(\mu) = \int \mathcal{D}\phi \exp\{i\mu S_I[\phi]\} \exp\{S_R[\phi, \mu]\} \]

**sign problem:** complex/negative integrand \(\Rightarrow\) no importance sampling with respect to the action

Let us *drop* it:

\[ Z_{\text{mod}}(\mu) = \int \mathcal{D}\phi \exp\{S_R[\phi, \mu]\} \]
Consider a theory with complex action:

\[ Z(\mu) = \int \mathcal{D}\phi \exp\{i\mu S_I[\phi]\} \exp\{S_R[\phi, \mu]\} \]

- sign problem: complex/negative integrand \(\Rightarrow\) no importance sampling with respect to the action

Let us drop it:

\[ Z_{\text{mod}}(\mu) = \int \mathcal{D}\phi \exp\{S_R[\phi, \mu]\} \]

How big is the error?

\(\Rightarrow\) apparently small for small chemical potential \(\mu\)
Quantifying the problem:

We have: $Z(\mu), \ Z_{\text{mod}}(\mu) > 0$

$$O(\mu) := \frac{Z(\mu)}{Z_{\text{mod}}(\mu)}, \quad Z(\mu) = O(\mu) Z_{\text{mod}}(\mu)$$
Quantifying the problem:

We have: \( Z(\mu), \ Z_{\text{mod}}(\mu) > 0 \)

\[
O(\mu) := \frac{Z(\mu)}{Z_{\text{mod}}(\mu)} \, , \quad Z(\mu) = O(\mu) \ Z_{\text{mod}}(\mu)
\]

Density:

\[
\rho(\mu) = \Delta \rho(\mu) + \rho_{\text{mod}}(\mu) \, ,
\]

\[
\rho = \frac{1}{V} \frac{d}{d\mu} \ln Z(\mu): \quad \text{full density}
\]

\[
\Delta \rho = \frac{1}{V} \frac{d}{d\mu} \ln O(\mu): \quad \text{overlap contribution}
\]

\[
\rho_{\text{mod}} = \frac{1}{V} \frac{d}{d\mu} \ln Z_{\text{mod}}(\mu): \quad \text{easy to calculate}
\]
The Z3 Polyakov spin model:

**Theory** - degrees of freedom: \( z(x) \in Z_3 \)

\[
S[z] = \tau \sum_{x,\nu} [z_x z_{x+\nu}^* + cc] + \sum_x [\eta z_x + \bar{\eta} z_x^*]
\]

\( \tau \): “temperature”

\[
\eta = \kappa \exp(\mu)
\]

\[
\bar{\eta} = \kappa \exp(-\mu)
\]

⇒ solvable by a **worm** algorithm

[Delago Mercado, Evertz, Gattringer, PRL 106 (2011) 222001 ]
The Z3 Polyakov spin model:

**Theory** - degrees of freedom: $z(x) \in \mathbb{Z}_3$

$$S[z] = \tau \sum_{x,\nu} [z_x z_{x+\nu}^* + cc] + \sum_x [\eta z_x + \bar{\eta} z_x^*]$$

- $\tau$: "temperature"
- $\eta = \kappa \exp(\mu)$
- $\bar{\eta} = \kappa \exp(-\mu)$

⇒ solvable by a worm algorithm

[Delago Mercado, Evertz, PRL 106 (2011) 222001]

⇒ close to QCD

⇒ my choice here!
The Z3 Polyakov spin model:

**Results** *(answer from the dual theory)*

$24^3$, $\tau=0.1$, $\kappa=0.01$, $\Delta \mu = 0.01$

- **full theory**
- **no sign term**

The density of states approach for the simulation of finite density quantum field theories – p. 22/31
The Z3 Polyakov spin model:

Results (answer from the dual theory)

\[ \ln Z(\mu) \]

- full theory
- no sign term

\[ O(\mu) \]

\[ 24^3, \tau=0.1, \kappa=0.01, \Delta \mu = 0.01 \]
The Z3 Polyakov spin model:

Introduce - generalised density-of-states:

\[ P(s) = \int \mathcal{D}z \, \delta(s - \Delta N) \exp\{S_R[z, \mu]\} . \]

Symmetries: \( P(s) = P(-s) \)
The Z3 Polyakov spin model:

- **Introduce** - generalized density-of-states:

\[ P(s) = \int Dz \, \delta(s - \Delta N) \exp\{S_R[z, \mu]\} . \]

Symmetries: \( P(s) = P(-s) \)

- **Partition function**:

\[ Z(\mu) = \int ds \, P(s) \cos\left(\sqrt{3} \sinh(\mu) \, s\right) . \]
The Z3 Polyakov spin model:

- **Introduce** - generalised density-of-states:

\[
P(s) = \int \mathcal{D}z \, \delta(s - \Delta N) \, \exp\{S_R[z, \mu]\}.
\]

Symmetries: \( P(s) = P(-s) \)

- **Partition function**:

\[
Z(\mu) = \int ds \, P(s) \, \cos\left(\sqrt{3} \, \sinh(\mu) \, s\right).
\]

- **Overlap factor**:

\[
O(\mu) = \int ds \, P(s) \, \cos\left(\sqrt{3} \, \sinh(\mu) \, s\right) / \int ds \, P(s)
\]

[no need to calculate the normalisation of \( P \)]
**Results:** histogram versus density-of-states method
The Z3 Polyakov spin model:

- **Results:** histogram versus density-of-states method
Can we do oscillating integrals?

- Generalised **density of states**
  (Wang-Landau, LLR $\Rightarrow$ exponential error suppression)
Can we do oscillating integrals?

- Generalised **density of states**
  
  (Wang-Landau, LLR ⇒ *exponential* error suppression)

**Promising attempts:**
Can we do oscillating integrals?

- Generalised **density of states**
  (Wang-Landau, LLR ⇒ *exponential* error suppression)

**Promising attempts:**

**M1:** Fit a Polynomial: \( \ln P(s) = \sum_{i \text{ even}}^{p} c_i s^i \), for \( p = 2, 4, 6, 8.. \)

Calculate the Fourier transform semi-analytically
Can we do oscillating integrals?

- Generalised **density of states**
  (Wang-Landau, LLR ⇒ *exponential* error suppression)

**Promising attempts:**

**M1:** Fit a Polynomial: \( \ln P(s) = \sum_{i \text{ even}}^p c_i s^i \), for \( p = 2, 4, 6, 8.. \)
Calculate the Fourier transform semi-analytically

**M2:** Expand in Hermite functions \( H_n(s) \): \( P(s) = \sum_n c_n H_n(s) \)
Use \( \text{FT}[H_n] = H_n \): \( \text{FT}[P] = \sum_n c_n H_n(\mu) \)
Can we do oscillating integrals?

- **Generalised density of states** (Wang-Landau, LLR ⇒ exponential error suppression)

**Promising attempts:**

**M1:** Fit a Polynomial: \[ \ln P(s) = \sum_{i \text{ even}}^p c_i s^i , \text{ for } p = 2, 4, 6, 8.. \]

Calculate the Fourier transform semi-analytically

**M2:** Expand in Hermite functions \( H_n(s) \): \[ P(s) = \sum_n c_n H_n(s) \]

Use \( \text{FT}[H_n] = H_n \): \[ \text{FT}[P] = \sum_n c_n H_n(\mu) \]

**M3:** Grasp the asymptotic: \[ P(s) = \bar{P}(s) P_{\text{asy}}(s) \]

\[ \text{FT}[P](\mu) = \int dx \text{FT}[\bar{P}](x) \text{FT}[P_{\text{asy}}](\mu - x) \]

\( \text{FT}[P_{\text{asy}}] \): known analytically
Can we do oscillating integrals?

Bootstrap error analysis:
1. Choose a set of $a(s_0), s_0 = 1 \ldots s_{max} \approx 5000$
2. Fit a Polynomial: $\ln P(s) = \sum_{i \text{ even}}^{p} c_i s^i$, for $p = 2, 4, 6, 8..$
3. Get an answer for $O(\mu)$

Repeat steps 1-3 many times and produce the bootstrap average & standard deviation for $O(\mu)$. 

The density of states approach for the simulation of finite density quantum field theories – p. 27/31
The Z3 Polyakov spin model:

- Results for the overlap:

![Graph showing results for the overlap.]

\[ \mathcal{O}(\mu) \]

\[ DS \text{ L=24} \]

[use quad precision]

[Langfeld, Lucini
Phys. Rev. D90
(2014) 9, 094502 ]
The Z3 Polyakov spin model:

Results for the overlap:

[use quad precision]

[Langfeld, Lucini
Phys. Rev. D90 (2014) 9, 094502]
The Z3 Polyakov spin model:

Results for the overlap:

[use quad precision]

[Langfeld, Lucini
Phys. Rev. D90
(2014) 9, 094502 ]
Conclusions

Simulating Quantum Field Theory at finite densities:
many promising recent attempts:

‘‘Complex Langevin’’, ‘‘strong coupling expansions’’, ‘‘worm algorithms’’
Simulating Quantum Field Theory at finite densities: many promising recent attempts: ‘‘Complex Langevin’’, ‘‘strong coupling expansions’’, ‘‘worm algorithms’’

**LLR:** recursive calculation of the (generalised) density of states works well! \([U(1), SU(2), SU(3), \ldots] \)


⇒ made to solve overlap problems, exponential error suppression
Conclusions

- **Simulating Quantum Field Theory at finite densities:**
  - many promising recent attempts:
    - ‘Complex Langevin’, ‘strong coupling expansions’, ‘worm algorithms’
  - **LLR:** recursive calculation of the (generalised) density of states works well! [U(1), SU(2), SU(3),...]
    - made to solve overlap problems, exponential error suppression

- **Progress with highly oscillating integrals:**
  - showcase: *Z3 spin model in 2+1 dimensions*:
    - using LLR + cumulant expansion of the density-of-states
    - solves a strong sign problem (without re-formulation)