Lattice QCD with Chemical Potential

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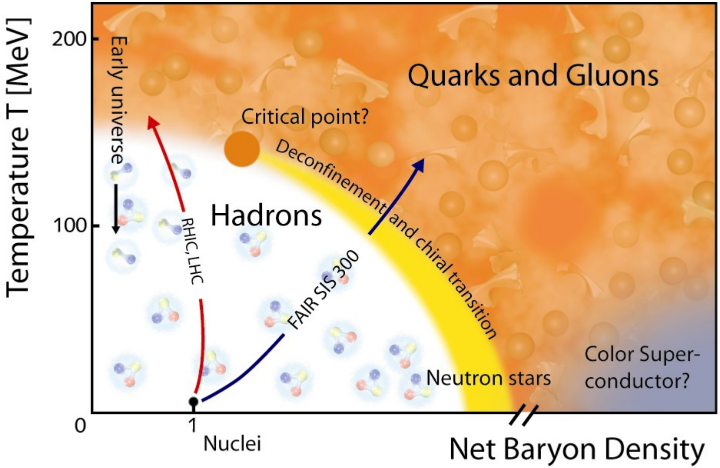
CONTENTS

Interest in high temperatures and high matter densities

- Better understanding of quark-gluon matter shortly after Big Bang
- Neutron stars: High densities and temperatures
- Heavy ion collisions: Matter under extreme conditions

THE QCD PHASE DIAGRAM



THE QCD PHASE DIAGRAM

- Transition from a confined to a deconfined phase
- For zero baryon density at about 170 $MeV \longrightarrow$ crossover
- Increasing baryon density $\rightsquigarrow$ crossover turns into a first order phase transition
- For $m_u = m_d$: Critical endpoint of the first order transition line is of second order
- For $m_u = m_d = m_s$: The first order line extends until the point $\mu = 0$

QCD ON A SPACE-TIME LATTICE

- The lattice is defined as:

$$\Lambda = \{\mathbf{x} = a \cdot \mathbf{n} | \mathbf{n} = (n_1, n_2, n_3, n_4)\}$$
$$n_i = 0, \ldots, \ N-1, \ i = 1,2,3 \ ; \ n_4 = 0, \ldots, N_T - 1$$

- Continuum free fermion action:

$$S_F^0[\psi, \overline{\psi}] = \int d^4x \, \overline{\psi}(x)[\gamma_\mu \partial_\mu + m]\psi(x)$$

- Discretisation prescription:

$$\begin{aligned} \psi(\mathbf{x}), \overline{\psi}(\mathbf{x}) \quad &\longrightarrow \quad \psi(\mathbf{n}), \overline{\psi}(\mathbf{n}) \\ \int d^4x \ \ldots \quad &\longrightarrow \quad a^4 \sum_{\mathbf{n} \in \Lambda} \ldots \\ \partial_\mu \, \psi(\mathbf{x}) \quad &\longrightarrow \quad \frac{\psi(\mathbf{n}+\hat{\mu}) - \psi(\mathbf{n}-\hat{\mu})}{2a} + \mathcal{O}(a^2) \end{aligned}$$

INTRODUCTION OF GAUGE FIELDS

- Invariance of the action under local rotation $\Omega(n) \in SU(3)$:

$$\psi'(n) \longrightarrow \Omega(n)\psi(n) \quad , \quad \overline{\psi}'(n) \longrightarrow \overline{\psi}(n)\Omega(n)^\dagger$$

- Discretised derivative term in the action:

$$\overline{\psi}'(n)\psi'(n+\hat{\mu}) \longrightarrow \overline{\psi}(n)\Omega(n)^\dagger\Omega(n+\hat{\mu})\psi(n+\hat{\mu})$$

- Requires introduction of gauge fields:

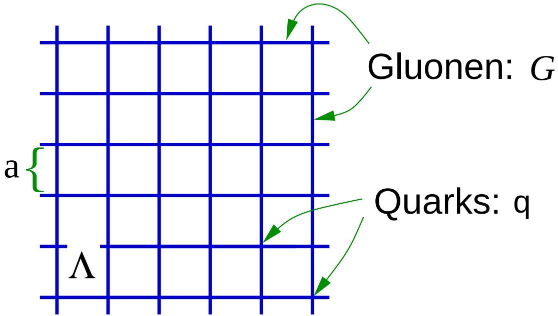
$$\overline{\psi}'(n)U'_\mu(n)\psi'(n+\hat{\mu}) \longrightarrow \overline{\psi}(n)\Omega(n)^\dagger U'_\mu(n)\Omega(n+\hat{\mu})\psi(n+\hat{\mu})$$

- Define gauge transformation:

$$U'_\mu(n) = \Omega(n)U_\mu(n)\Omega(n+\hat{\mu})^\dagger$$

- $U_\mu(n)$ link variable: connects n and $n+\hat{\mu}$

QCD ON A SPACE-TIME LATTICE



THE LATTICE ACTION

$$S[U,\overline{\psi},\psi] = S_F[U,\overline{\psi},\psi] + S_G[U]$$

- Fermion action S_F:

$$S_F[U,\overline{\psi},\psi] = \sum_{f=1}^{N_f} a^4 \sum_{n,m\in\Lambda} \overline{\psi}^{(f)}(n) D^{(f)}(n,m) \psi^{(f)}(m)$$

- Dirac matrix:

$$\begin{aligned} D^{(f)}(n,m)_{\alpha\beta,ab} &= \left(\frac{4}{a} + m^{(f)}\right) \delta_{\alpha\beta}\delta_{ab}\delta_{nm} - \\ &\quad \frac{1}{2a} \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{1} - \gamma_\mu)_{\alpha\beta}\, U_\mu(n)_{ab}\, \delta_{n+\hat{\mu},m} \end{aligned}$$

THE LATTICE ACTION

- Gauge action S_U:

$$S_G[U] = \frac{2}{g^2} \sum_{n \in \Lambda} \sum_{\mu < \nu} \mathrm{Re}\mathrm{Tr}[\mathbb{1} - U_{\mu\nu}(n)]$$

- Plaquette $U_{\mu\nu}(n)$:

$$U_{\mu\nu}(n) = U_\mu(n) U_\nu(n+\hat{\mu}) U_\mu(n+\hat{\nu})^\dagger U_\nu(n)^\dagger$$

- Partition function:

$$Z = \int \mathcal{D}[\overline{\psi}, \psi] \mathcal{D}[U] \; e^{-S_G[U] - S_F[\overline{\psi}, \psi]}$$

- Integrate out fermion fields:

$$Z = \int \mathcal{D}[U] \; e^{-S_G[U]} \det[D]$$

THE LATTICE ACTION

- Gauge action S_U:

$$S_G[U] = \frac{2}{g^2} \sum_{n \in \Lambda} \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{Tr}[\mathbb{1} - U_{\mu\nu}(n)]$$

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- Integrate out fermion fields:

$$Z = \int \mathcal{D}[U]\; e^{-S_G[U]} \det[D]$$

LATTICE SIMULATION

- Evaluation of Z with Monte Carlo techniques is possible
- $\det D \in \mathbb{R}$
- $\Longrightarrow$ real Boltzmann weight
- Generate configurations according to the weight factor $P[U]$:

$$P[U] = e^{-S_G[U]} \det[U]$$

Introduction of chemical potential

- Grand-canonical ensemble:

$$Z_{GC}(\mu) = \mathrm{Tr}[e^{-(H-\mu N_q)/T}]$$

- Path integral formulation:

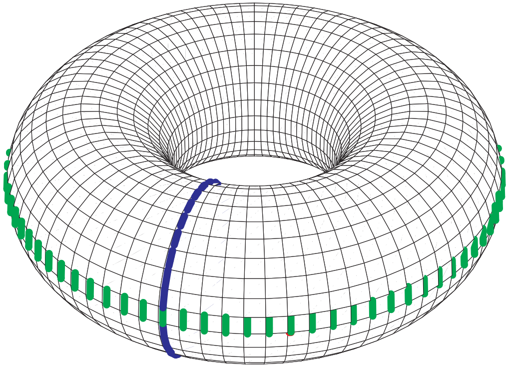
$$Z_{GC}(\mu) = \int \mathcal{D}[U,\overline{\psi},\psi]\; e^{-S[U,\overline{\psi},\psi]}$$

- The Dirac matrix with chemical potential:

$$\begin{aligned} D(n,m)_{\alpha\beta,ab} &= \left(\frac{4}{a}+m\right)\delta_{\alpha\beta}\delta_{ab}\delta_{nm} - \\ &\quad \frac{1}{2a}\sum_{\mu=\pm 1}^{\pm 4} f(\mu)\,(\mathbb{1}-\gamma_\mu)_{\alpha\beta}\; U_\mu(n)_{ab}\;\delta_{n+\hat{\mu},m} \end{aligned}$$

$$f(\mu) = \begin{cases} 1 & : \quad \hat{\mu} = 1,2,3,-1,-2,-3 \\ e^{a\mu} & : \quad \hat{\mu} = 4 \\ e^{-a\mu} & : \quad \hat{\mu} = -4 \end{cases}$$

INTRODUCTION OF CHEMICAL POTENTIAL



- At each temporal hop the Dirac matrix picks up a factor e^{μ}
- N_T temporal lattice points
- Move chemical potential at the temporal boundary of the lattice $\Longrightarrow e^{\mu N_T}$

γ_5-Hermiticity

- Introduction of μ causes a severe technical problem
- $\Longrightarrow$ Dirac operator is no longer γ_5-hermitian
- γ_5-hermiticity:

$$\gamma_5 D \gamma_5 = D^\dagger$$

- Including the chemical potential:

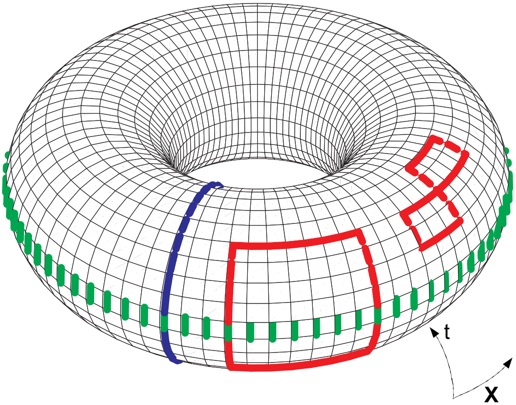
$$\gamma_5 D(\mu) \gamma_5 = D^\dagger(-\mu)$$

- Hence the fermion determinant is complex:

$$\det[D(\mu)] \neq \det[D(\mu)]^*$$

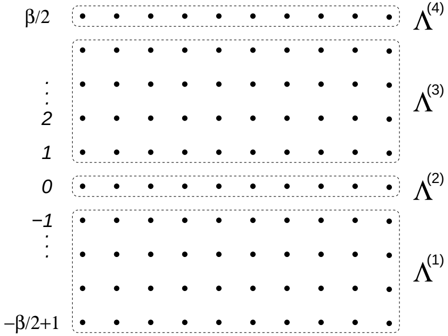
$\longrightarrow$ fermion sign problem
$\longrightarrow$ Standard Monte Carlo techniques fail

FERMION DETERMINANT



- Write fermion determinant as a sum of loops
- Only the loops that wind around time cause a problem!
- There are forward and backward winding loops $\Longrightarrow$ complex number

LATTICE DECOMPOSITION



$$\begin{aligned}
\Lambda^{(1)} &= \{(\vec{x}, x_4) \mid \vec{x} \in \Lambda_s,\ x_4 = -\beta/2+1,\ \ldots\ -1\} \\
\Lambda^{(2)} &= \{(\vec{x}, x_4) \mid \vec{x} \in \Lambda_s,\ x_4 = 0\} \\
\Lambda^{(3)} &= \{(\vec{x}, x_4) \mid \vec{x} \in \Lambda_s,\ x_4 = 1,\ \ldots\ \beta/2-1\} \\
\Lambda^{(4)} &= \{(\vec{x}, x_4) \mid \vec{x} \in \Lambda_s,\ x_4 = \beta/2\}
\end{aligned}$$

THE DIRAC OPERATORS

$$\begin{aligned} D^{(1)}(x,y) &= \delta_{\vec{x},\vec{y}}\,\delta_{x_4,y_4} \\ &\quad - \kappa \sum_{j=\pm 1}^{\pm 3} \frac{1 \mp \gamma_{|j|}}{2}\, U_j(\vec{x},x_4)\,\delta_{\vec{x}+\hat{j},\vec{y}}\,\delta_{x_4,y_4} \\ &\quad - \kappa \sum_{n_4=-\frac{\beta}{2}+1}^{-2} \frac{1-\gamma_4}{2}\, U_4(\vec{x},n_4)\,\delta_{\vec{x},\vec{y}}\,\delta_{x_4,n_4}\,\delta_{y_4,n_4+1} \\ &\quad - \kappa \sum_{n_4=-\frac{\beta}{2}+2}^{-1} \frac{1+\gamma_4}{2}\, U_4(\vec{x},n_4-1)^{\dagger}\,\delta_{\vec{x},\vec{y}}\,\delta_{x_4,n_4}\,\delta_{y_4,n_4-1} \end{aligned}$$

$$\begin{aligned} D^{(2)}(x,y) &= \delta_{\vec{x},\vec{y}}\,\delta_{x_4,0}\,\delta_{y_4,0} \\ &\quad - \kappa \sum_{j=\pm 1}^{\pm 3} \frac{1 \mp \gamma_{|j|}}{2}\, U_j(\vec{x},x_4)\,\delta_{\vec{x}+\hat{j},\vec{y}}\,\delta_{x_4,0}\,\delta_{y_4,0} \end{aligned}$$

THE LINKING OPERATORS

- Terms that connect $\Lambda^{(i)}$ only hop in time direction:

$$D^{(1,2)}(x,y) \;=\; -\,\kappa \frac{1-\gamma_4}{2}\, U_4(\vec{x},-1)\, \delta_{\vec{x},\vec{y}}\, \delta_{x_4,-1}\, \delta_{y_4,0}$$

$$D^{(2,1)}(x,y) \;=\; -\,\kappa \frac{1+\gamma_4}{2}\, U_4(\vec{x},-1)^{\dagger}\, \delta_{\vec{x},\vec{y}}\, \delta_{x_4,0}\, \delta_{y_4,-1}$$

- In $D^{(4,1)}$ and $D^{(1,4)}$ the chemical potential μ is coupled:

$$D^{(4,1)} \;=\; e^{\mu\beta}\, D_0^{(4,1)}\;,\;\; D^{(1,4)} \;=\; e^{-\mu\beta}\, D_0^{(1,4)}$$

$$D_0^{(4,1)}(x,y) = \kappa \frac{1-\gamma_4}{2}\, U_4(\vec{x},\beta/2)\, \delta_{\vec{x},\vec{y}}\, \delta_{x_4,\frac{\beta}{2}}\, \delta_{y_4,-\frac{\beta}{2}+1}$$

$$D_0^{(1,4)}(x,y) = \kappa \frac{1+\gamma_4}{2}\, U_4(\vec{x},\beta/2)^{\dagger}\, \delta_{\vec{x},\vec{y}}\, \delta_{x_4,-\frac{\beta}{2}+1}\, \delta_{y_4,\frac{\beta}{2}}$$

FACTORISATION OF THE DETERMINANT

- Rewrite the fermion determinant:

$$\det[D] = \int \mathcal{D}[\overline{\psi}, \psi]\; e^{-\overline{\psi} D \psi}$$

- Use the partition of the lattice into domains
- Integrate out the Grassmann variables $\overline{\psi}^{(i)}, \psi^{(i)}$ in each domain $\Lambda^{(i)}$
- Result:

$$\det[D] = A_0 W$$

$$\begin{aligned} A_0 &= \det\left[D^{(1)}\right] \det\left[D^{(3)}\right] \det\left[\widetilde{D}^{(2)}\right] \det\left[\widetilde{D}^{(4)}\right] \\ W &= \det\left[1 - \widetilde{S}^{(4)}\left[e^{\mu\beta}\widetilde{D}_1^{(4,2)} + \widetilde{D}_3^{(4,2)}\right]\right. \\ &\qquad \left. \times \widetilde{S}^{(2)}\left[e^{-\mu\beta}\widetilde{D}_1^{(2,4)} + \widetilde{D}_3^{(2,4)}\right]\right] \end{aligned}$$

FACTORISATION OF THE DETERMINANT

- Abbreviations:

$$
\begin{aligned}
S^{(1)} &= \left(D^{(1)}\right)^{-1}, \quad S^{(3)} = \left(D^{(3)}\right)^{-1} \\
\widetilde{D}^{(2)} &= D^{(2)} - D^{(2,1)} S^{(1)} D^{(1,2)} - D^{(2,3)} S^{(3)} D^{(3,2)} \\
\widetilde{D}^{(4)} &= D^{(4)} - D_0^{(4,1)} S^{(1)} D_0^{(1,4)} - D^{(4,3)} S^{(3)} D^{(3,4)} \\
\widetilde{S}^{(2)} &= \left(\widetilde{D}^{(2)}\right)^{-1}, \quad \widetilde{S}^{(4)} = \left(\widetilde{D}^{(4)}\right)^{-1} \\
\widetilde{D}_1^{(4,2)} &= D_0^{(4,1)} S^{(1)} D^{(1,2)} \\
\widetilde{D}_3^{(4,2)} &= D^{(4,3)} S^{(3)} D^{(3,2)} \\
\widetilde{D}_1^{(2,4)} &= D^{(2,1)} S^{(1)} D_0^{(1,4)} \\
\widetilde{D}_3^{(2,4)} &= D^{(2,3)} S^{(3)} D^{(3,4)}
\end{aligned}
$$

- Large hopping terms: γ_5 - hermiticity:

$$
\begin{aligned}
D_1^{(2,4)\,\dagger} &= \gamma_5\, D_1^{(4,2)}\, \gamma_5 \\
D_3^{(2,4)\,\dagger} &= \gamma_5\, D_3^{(4,2)}\, \gamma_5
\end{aligned}
$$

PROPERTIES

- γ_5-hermiticity:

$$
\begin{aligned}
D^{(i)\,\dagger} &= \gamma_5\, D^{(i)}\, \gamma_5 \quad , \quad i = 1,2,3,4 \\
D^{(i,j)\,\dagger} &= \gamma_5\, D^{(j,i)}\, \gamma_5 \quad , \quad (i,j) = (1,2),(2,3),(3,4) \\
D_0^{(4,1)\,\dagger} &= \gamma_5\, D_0^{(1,4)}\, \gamma_5
\end{aligned}
$$

- The first four subdeterminants are real
- Complex phase only in the last determinant factor
- Dimensionally reduced fermion sign problem!

DECOMPOSITION INTO WINDING SECTORS

- Expand W according to its number of loops
- Trace-log formula:

$$\det[\mathbb{1} - M] = \exp(\mathrm{Tr}[\ln(\mathbb{1} - M)]) = \exp\Big(- \sum_{n=1}^{\infty} \frac{1}{n} \mathrm{Tr}[M^n] \Big)$$

- Introduce:

$$\begin{aligned} H_0 &= \widetilde{S}^{(4)} D_1^{(4,2)} \widetilde{S}^{(2)} D_1^{(2,4)} + \widetilde{S}^{(4)} D_3^{(4,2)} \widetilde{S}^{(2)} D_3^{(2,4)} \\ H_{+1} &= \widetilde{S}^{(4)} D_1^{(4,2)} \widetilde{S}^{(2)} D_3^{(2,4)} \\ H_{-1} &= \widetilde{S}^{(4)} D_3^{(4,2)} \widetilde{S}^{(2)} D_1^{(2,4)} \end{aligned}$$

- Dimensionally reduction:

$$W = \det\left[\mathbb{1} - H_0 - e^{\mu\beta} H_{+1} - e^{-\mu\beta} H_{-1}\right]$$

Decomposition into winding sectors

- Use Trace-log formula:

$$\begin{aligned} W &= \det\left[\mathbb{1} - H_0 - e^{\mu\beta} H_{+1} - e^{-\mu\beta} H_{-1}\right] \\ &= \exp\left(-\sum_{n=1}^{\infty} \frac{1}{n} \mathrm{Tr}\left[H_0 + e^{\mu\beta} H_{+1} + e^{-\mu\beta} H_{-1}\right]^n\right) \\ &= \exp\left(-\sum_{q\in\mathbb{Z}} e^{\mu\beta q} \sum_{n=1}^{\infty} \frac{1}{n} \sum_{k_1+\ldots+k_n=q} \mathrm{Tr}\left[H_{k_1} H_{k_2} \ldots H_{k_n}\right]\right) \end{aligned}$$

- Rewrite W as a product over the winding number q:

$$W = \prod_{q\in\mathbb{Z}} W^{(q)}$$

- Relation between opposite winding numbers:

$$W^{(-q)}(\mu) = W^{(q)}(-\mu)^*$$

NUMERICAL ANALYSIS

- Contributions in each winding sector:

$$W^{(q)} = \exp\left(-e^{\mu q \beta}\, T^{(q)}\right)$$

$$T^{(q)} = \sum_{n=1}^{\infty} T_n^{(q)}$$

$$T_n^{(q)} = \frac{1}{n} \sum_{k_1+\ldots+k_n=q} \mathrm{Tr}\left[H_{k_1} H_{k_2} \ldots H_{k_n}\right]$$

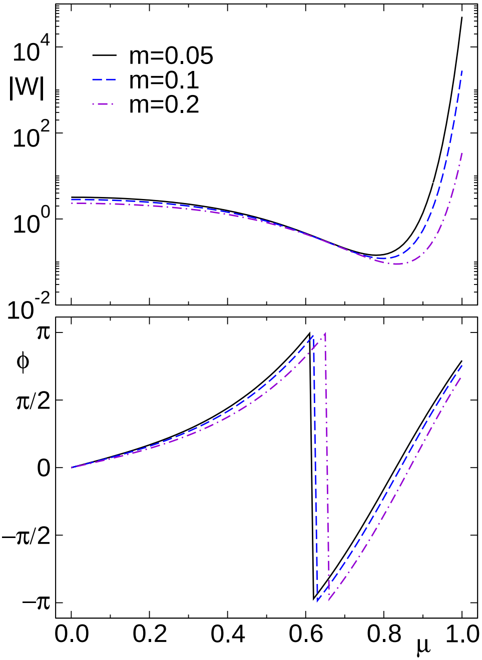
- List of a few terms:

$$T_1^{(0)} = \mathrm{Tr}\, H_0 \;,\; T_2^{(0)} = \mathrm{Tr}\, H_{+1} H_{-1} + \frac{1}{2}\mathrm{Tr}\, H_0^2$$

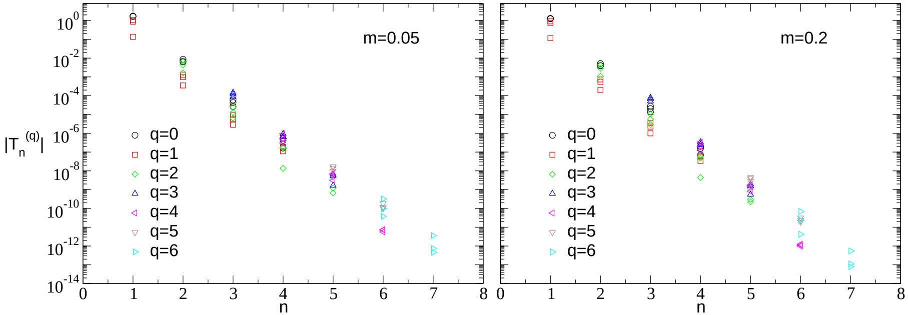
$$T_1^{(1)} = \mathrm{Tr}\, H_{+1} \;\;,\; T_2^{(1)} = \mathrm{Tr}\, H_{+1} H_0$$

$$T_1^{(2)} = 0 \;,\;\; T_2^{(2)} = \frac{1}{2}\mathrm{Tr}\, H_{+1}^2$$

- Property: $T_n^{(-q)} = T_n^{(q)\,*}$


m=0.05
m=0.1
m=0.2
|W|
10^4
10^2
10^0
10^-2
π
φ
π/2
0
−π/2
−π
0.0
0.2
0.4
0.6
0.8
1.0
μ

$T_n^{(q)}$ vs. n



m=0.05
m=0.2
|T_n^(q)|
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
10^-12
10^-14
q=0
q=1
q=2
q=3
q=4
q=5
q=6
n
0
1
2
3
4
5
6
7
8

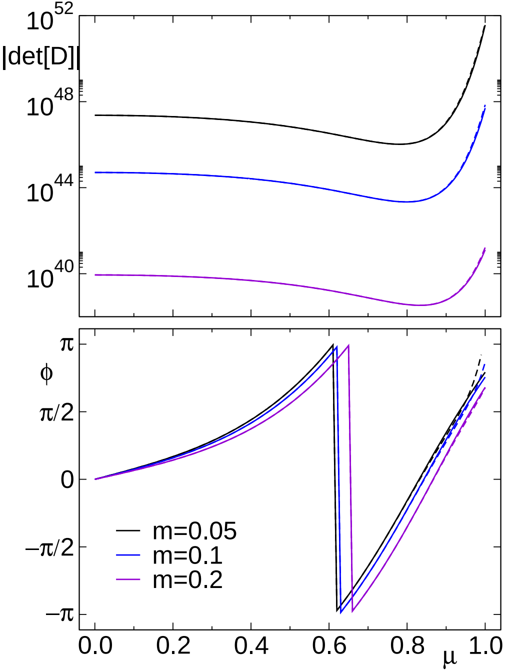
TRUNCATION SCHEME

- $T^{(q)}$ given by infinite sums
- Exponential decrease suggests a truncation of the sums:

$$
\begin{aligned}
\widehat{T}^{(0)} &= \sum_{n=1}^{1+\Delta} T_n^{(0)} \\
\widehat{T}^{(q)} &= \sum_{n=|q|}^{|q|+\Delta} T_n^{(q)} \quad \text{for} \;\; q \neq 0
\end{aligned}
$$

- Choice: $\Delta = 1$

$$
\begin{aligned}
\widehat{T}^{(0)} &= \mathrm{Tr}\,[H_0] + \frac{1}{2}\,\mathrm{Tr}\,[(H_0)^2] + \mathrm{Tr}\,[H_{+1} H_{-1}] \\
\widehat{T}^{(q)} &= \frac{1}{q}\,\mathrm{Tr}\,[(H_{+1})^q] + \mathrm{Tr}\,[(H_{+1})^q H_0]\,, \;\; q > 0
\end{aligned}
$$



10^{52}
|det[D]|
10^{48}
10^{44}
10^{40}
π
φ
π/2
0
–π/2
–π
m=0.05
m=0.1
m=0.2
0.0
0.2
0.4
0.6
0.8
1.0
μ

Canonical Approach

- Grand-canonical partition function:

$$Z_{GC}(\mu) = \int \mathcal{D}[U]\, e^{-S_G[U]} \det[D(\mu)]$$

- Fixed quark number:

$$Z_{GC}(\mu) = \sum_Q e^{\mu Q \beta} Z_C^{(Q)} = \sum_B e^{3\mu B\beta} Z_C^{(3B)}$$

- Determine the canonical partition functions $Z_C^{(Q)}$ with the winding decomposition formula!

$D^{(Q)}$ from the Fourier transformation method

- Fourier transformation:

$$Z_C^{(Q)} = \frac{1}{2\pi} \int d\varphi e^{-iQ\varphi} \; Z_{GC}(\mu = i\varphi/T)$$

- Insert Z_{GC}:

$$Z_C^{(Q)} \;=\; \int \mathcal{D}[U]\, e^{-S_G[U]}\, D^{(Q)}$$

- Projected determinants $D^{(Q)}$:

$$D^{(Q)} \;=\; \int_{-\pi}^{\pi} \frac{d\varphi}{2\pi}\, e^{-iQ\varphi}\, \det[D(\mu = i\varphi/T)]$$

- Use factorisation formula for the determinant:

$$D^{(Q)} = \frac{A_0}{2\pi}\int_{-\pi}^{\pi} d\varphi\, e^{-iQ\varphi}\, \det[1 - H_0 - e^{i\varphi} H_{+1} - e^{-i\varphi} H_{-1}]$$

$D^{(Q)}$ from the Fourier transformation method

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- Insert Z_{GC}:

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- Use factorisation formula for the determinant:

$$D^{(Q)} = \frac{A_0}{2\pi} \int_{-\pi}^{\pi} d\varphi \, e^{-iQ\varphi} \det[1 - H_0 - e^{i\varphi} H_{+1} - e^{-i\varphi} H_{-1}]$$

$D^{(Q)}$ FROM A POWER SERIES EXPANSION

- Fugacity expansion:

$$\det[D(\mu)] = \sum_Q e^{\mu Q \beta} D^{(Q)}$$

- Rewriting the determinant:

$$\det[D(\mu)] = A_0 W^{(0)} \prod_{q=1}^{\infty} \exp\left(-e^{\mu q \beta} T^{(q)} - e^{-\mu q \beta} T^{(q)*}\right)$$

- Expand the exponential functions, order with respect to $e^{\pm\mu\beta}$:

$$\begin{aligned} D^{(0)} &= A_0 W_0 \left(1 + \sum_{q=1}^{\infty} |T^{(q)}|^2 + \frac{1}{4} \sum_{q=1}^{\infty} |T^{(q)}|^4 \ldots\right) \\ D^{(1)} &= A_0 W_0 \left(-T^{(1)} + \sum_{q=1}^{\infty} T^{(q+1)} T^{(q)*} + \ldots\right) \\ \ldots \end{aligned}$$

Free Energy

- Free Energy of a single quark:

$$\frac{Z^{(Q=1)}}{Z^{(Q=0)}} = \frac{\langle \det[Q=1] \rangle}{\langle \det[Q=0] \rangle} = e^{-\beta F^{(1)}}$$

- Confinement/Deconfinement:

$$\frac{Z^{(Q=1)}}{Z^{(Q=0)}} = \begin{cases} 0 & : \quad T < T_c \implies F^{(1)} = \infty \\ \neq 0 & : \quad T > T_c \implies F^{(1)} < \infty \end{cases}$$

SUMMARY

- We investigated the fermion action with chemical potential
- Found the fermion determinant in a sector with fixed quark number $\longrightarrow$ Canonical approach
- Idea:
  - Partition of the lattice
  - Fermion determinant expressed in terms of subdeterminants
  - Only last subdeterminant part contains the chemical potential!!
  - Apply a winding number decomposition

Summary

- Idea allows two ways of calculating the projected determinant at a fixed quark number
- Advantage of our idea:
  - Factorisation of the determinant dimensionally reduces the part which depends on μ
  - Can precalculate important terms, e.g., $D^{(Q)}$ from a power series expansion is numerically cheap
- Study of free energy $\Longrightarrow$ phase transitions
- Application: Simulations with fixed quark number are possible