Introduction to Lattice QCD

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References

1. C. Gattringer and C.B. Lang, “Quantum Chromodynamics on the lattice”, Springer
2. H.J. Rothe, “Introduction to Lattice Gauge Theories”, 4th Ed., World Scientific Lecture Notes in Physics, vol. 82
3. I. Montvay and G. Muenster, “Quantum Fields on a Lattice”, Cambridge Monographs on Mathematical Physics
4. M. Creutz, “Quarks, Gluons and Lattices”, Cambridge University Press

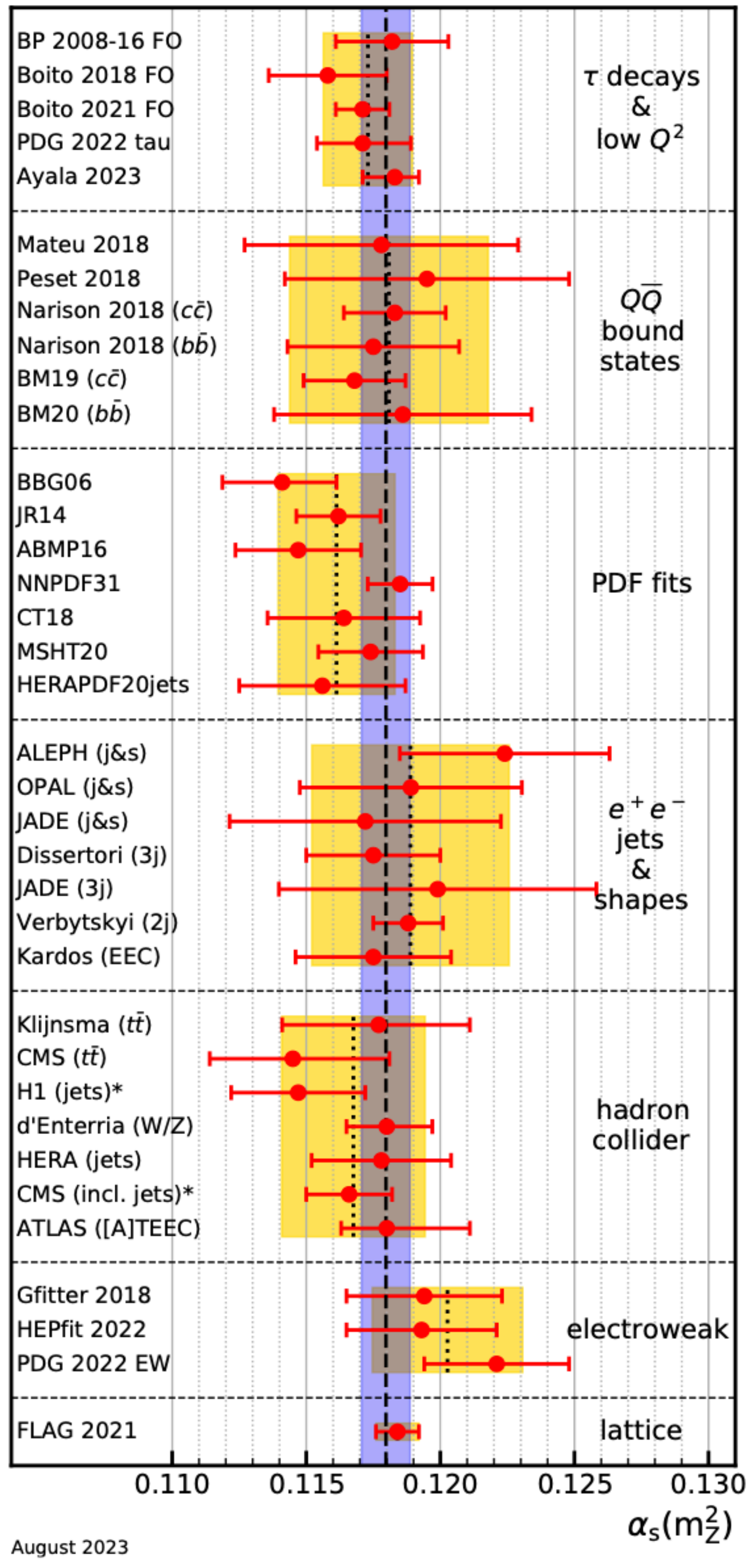
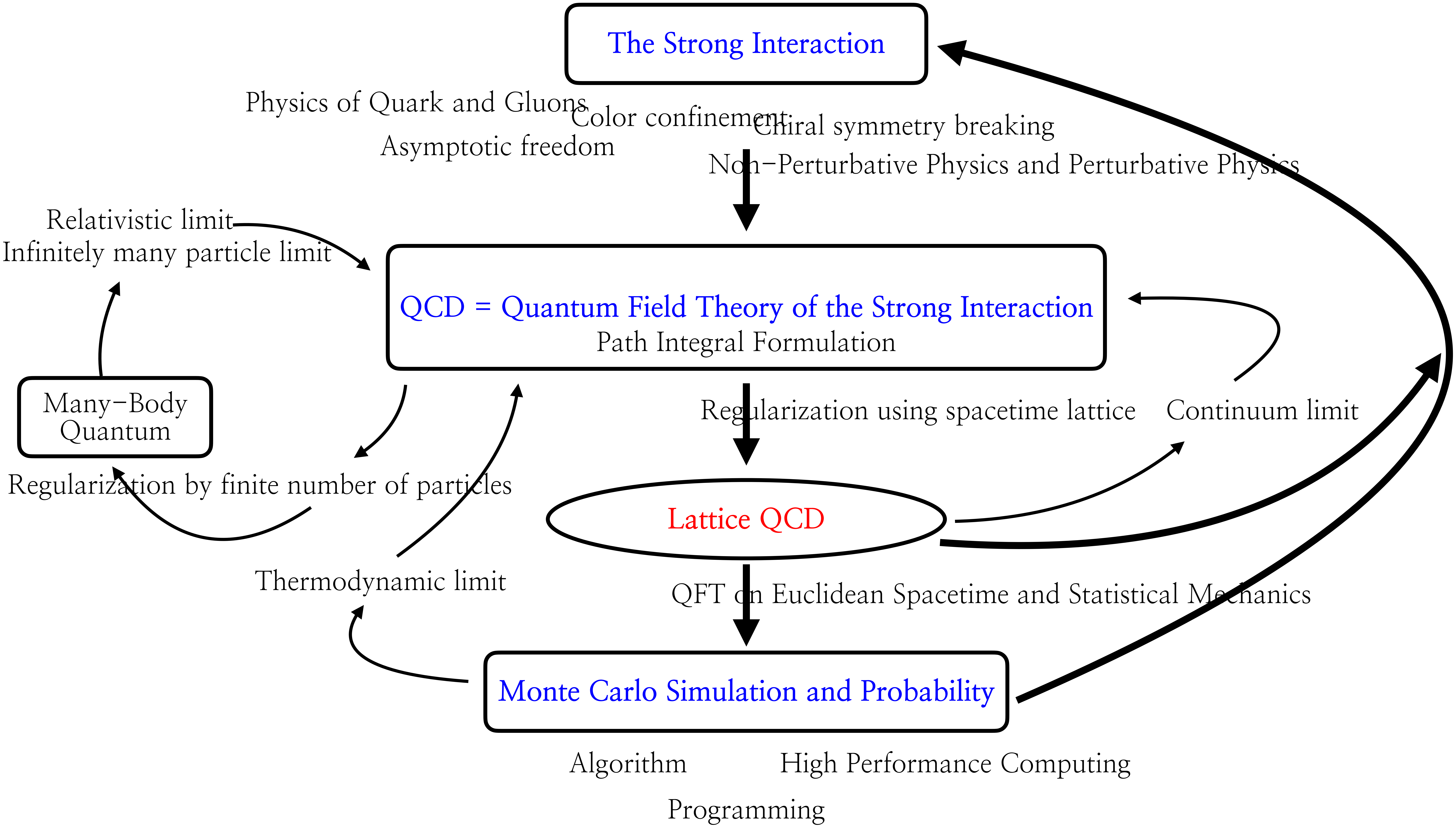


Figure 9.2: Summary of determinations of $\alpha_s(m_Z^2)$ with uncertainty in the seven sub-fields as discussed in the text. The yellow (light shaded) bands and dotted lines indicate the pre-average values of each sub-field. The dashed line and blue (dark shaded) band represent the final world average value of $\alpha_s(m_Z^2)$. The "*" symbol within the "hadron colliders" sub-field indicates a determination including a simultaneous fit of PDFs.

A lattice QCD project

1. Lattice field theory formulation
2. Monte Carlo simulation of quark–gluon fields
3. Calculation of observables
4. Lattice perturbation theory


The Strong Interaction
Physics of Quark and Gluons
Color confinement
Chiral symmetry breaking
Asymptotic freedom
Non−Perturbative Physics and Perturbative Physics
Relativistic limit
Infinitely many particle limit
QCD = Quantum Field Theory of the Strong Interaction
Path Integral Formulation
Many−Body
Quantum
Regularization using spacetime lattice
Continuum limit
Regularization by finite number of particles
Lattice QCD
Thermodynamic limit
QFT on Euclidean Spacetime and Statistical Mechanics
Monte Carlo Simulation and Probability
Algorithm
High Performance Computing
Programming

Contents

1. Short introduction to path integral formulation of quantum mechanics
2. QCD on spacetime lattice
3. Path integral formulation of quantum field theory on Euclidean spacetime and statistical mechanics
4. Monte Carlo method and algorithm

Short introduction to path integral

- Schroedinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \hat{H}\psi(\mathbf{x},t)$$

- Schroedinger picture:

$$\psi(\mathbf{x},t) = <\mathbf{x}|\psi(t)>$$

$$= <\mathbf{x}|e^{-i\frac{\hat{H}}{\hbar}(t-t')}|\psi(t')>$$

$$= <\mathbf{x}|e^{-i\frac{\hat{H}}{\hbar}(t-t')}\int d^3x'|\mathbf{x}'><\mathbf{x}'|\psi(t')> \text{ using } I = \int d^3x'|\mathbf{x}><\mathbf{x}|$$

$$= \int d^3x' G(\mathbf{x},t;\mathbf{x}',t') <\mathbf{x}'|\psi(t')> \text{ using } G(\mathbf{x},t;\mathbf{x},t') = <\mathbf{x}|e^{-i\frac{\hat{H}}{\hbar}(t-t')}|\mathbf{x}'>$$

Short introduction to path integral

- Green's function (1-d):

$$G(x,t;x',t') = <x|e^{-i\frac{\hat{H}}{\hbar}(t-t')}|x'> \; = <x|e^{-i\frac{\hat{H}}{\hbar}N\epsilon}|x'> \text{ with } (t-t') = N\epsilon, \text{ or } \epsilon = \frac{t-t'}{N}$$

$$= <x|e^{-i\frac{\hat{H}}{\hbar}\epsilon}e^{-i\frac{\hat{H}}{\hbar}\epsilon}\cdots e^{-i\frac{\hat{H}}{\hbar}\epsilon}|x'> \; = \int dx_{N-1} <x|e^{-i\frac{\hat{H}}{\hbar}\epsilon}|x_{N-1}> <x_{N-1}|e^{-i\frac{\hat{H}}{\hbar}\epsilon}\cdots e^{-i\frac{\hat{H}}{\hbar}\epsilon}|x'>$$

$$= \int dx_{N-1} G(x,t;x_{N-1},t-\epsilon) <x_{N-1}|e^{-i\frac{\hat{H}}{\hbar}\epsilon}\cdots e^{-i\frac{\hat{H}}{\hbar}\epsilon}|x'> \text{ with } G(x,t;x_{N-1},t-\epsilon) = <x|e^{-i\frac{\hat{H}}{\hbar}\epsilon}|x_{N-1}>$$

$$= \int dx_{N-1} G(x,t;x_{N-1},t_{N-1}) <x_{N-1}|e^{-i\frac{\hat{H}}{\hbar}\epsilon}\cdots e^{-i\frac{\hat{H}}{\hbar}\epsilon}|x'>$$

$$= \int dx_{N-1} \int dx_{N-2} G(x,t;x_{N-1},t_{N-1}) G(x_{N-1},t_{N-1};x_{N-2},t_{N-2}) <x_{N-2}|e^{-i\frac{\hat{H}}{\hbar}\epsilon}\cdots e^{-i\frac{\hat{H}}{\hbar}\epsilon}|x'>$$

$$= \int\cdots\int \prod_{i=1}^{N-1} dx_i \; G(x,t;x_{N-1},t_{N-1}) \; G(x_{N-1},t_{N-1};x_{N-2},t_{N-2}) \;\cdots\; G(x_1,t_1;x',t')$$

Short introduction to path integral

$$G(x_i, t_i; x_{i-1}, t_{i-1}) = < x_i | e^{-i\frac{\hat{H}}{\hbar}\epsilon} | x_{i-1} >$$

$$= < x_i | e^{-\frac{i\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)} | x_{i-1} > \text{ for } \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

$$= < x_i | e^{-\frac{i\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m}\right)} e^{-\frac{i\epsilon}{\hbar}V(\hat{x})} e^{\mathcal{O}(\epsilon^2)} | x_{i-1} > \simeq < x_i | e^{-\frac{i\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m}\right)} e^{-\frac{i\epsilon}{\hbar}V(x)} | x_{i-1} >$$

$$= < x_i | e^{-\frac{i\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m}\right)} \int \frac{dp}{2\pi\hbar} | p_i > < p_i | x_{i-1} > e^{-\frac{i\epsilon}{\hbar}V(x_{i-1})} \text{ with } I = \int \frac{dp}{2\pi\hbar} | p_i > < p_i |$$

$$= \int \frac{dp}{2\pi\hbar} < x_i | p_i > < p_i | x_{i-1} > e^{-\frac{i\epsilon}{\hbar}\left[\frac{p_i^2}{2m} + V(x_{i-1})\right]} = \int \frac{dp}{2\pi\hbar} e^{ix_i p_i - ix_{i-1}p_i} e^{-\frac{i\epsilon}{\hbar}\left[\frac{p_i^2}{2m} + V(x_{i-1})\right]}$$

$$= \int \frac{dp}{2\pi\hbar} e^{-\frac{i\epsilon}{\hbar}\left[-i\frac{p_i(x_i - x_{i-1})}{\epsilon} + \frac{p_i^2}{2m} + V(x_{i-1})\right]} \simeq e^{\frac{i\epsilon}{\hbar}\left[\frac{1}{2}m\left(\frac{x_i - x_{i-1}}{\epsilon}\right)^2 - V(x_{i-1})\right]} = e^{\frac{i}{\hbar}\epsilon L\left[x_{i-1}, \dot{x}_{i-1}\right]}$$

Short introduction to path integral

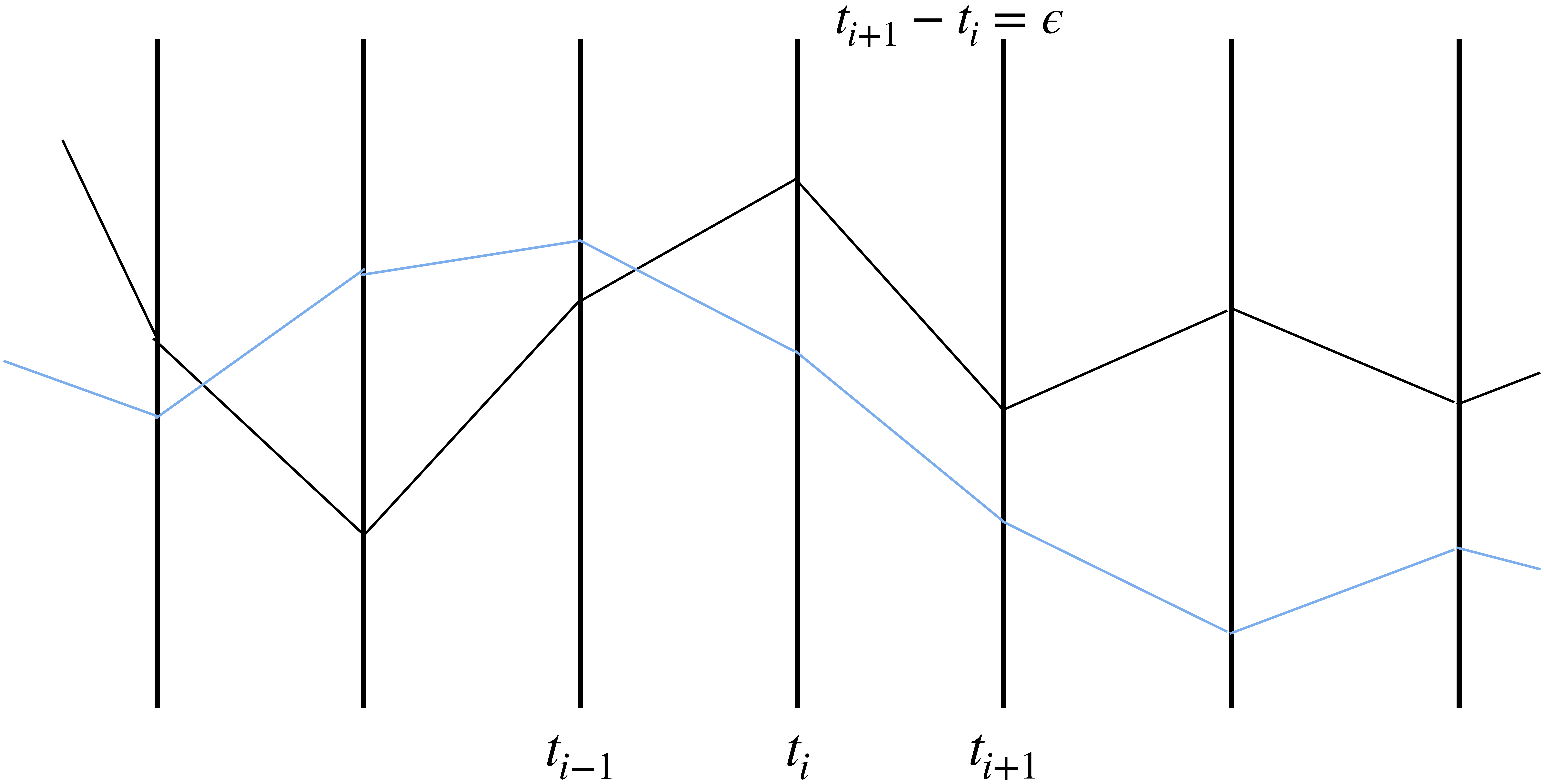
- Green's function (1-d):

$$G(x,t;x',t') = < x | e^{-i\frac{\hat{H}}{\hbar}(t-t')} | x' >$$

$$= \int \cdots \int \prod_{i=1}^{N-1} dx_i \, G(x,t;x_{N-1},t_{N-1}) \, G(x_{N-1},t_{N-1};x_{N-2},t_{N-2}) \, \cdots \, G(x_1,t_1;x',t')$$

$$\simeq \int \cdots \int \prod_{i=1}^{N-1} dx_i \, \exp\left(\frac{i}{\hbar}\int dt \, L[x,\dot{x}]\right) \equiv \int [\mathscr{D}x] \exp\left(\frac{i}{\hbar} S[x,\dot{x}]\right)$$

Sum over paths



Short introduction to path integral with "Euclidean time"

- Wick rotation: $t \to -i\tau$

$$G(x,t;x',t') = < x|e^{-i\frac{\hat{H}}{\hbar}(t-t')}|x' > \equiv \int [\mathscr{D}x]\ \exp\left(\frac{i}{\hbar}S[x,\dot{x}]\right)$$

$$\to G_E(x,\tau;x',\tau') = \int [\mathscr{D}x]\ \exp\left(-\frac{1}{\hbar}S_E\left[x,\frac{dx}{d\tau}\right]\right)$$

Monte Carlo approach to Quantum Mechanics

- M. Creutz, B. Freedman, "Statistical approach to quantum mechanics", Annals. Phys. 132 (1981) 427
- M.J. Westbroek, P.R. King, D.D. Vedensky, S. Durr, "Users' guide to Monte Carlo methods for evaluating path integrals", Am. J. Phys. 86 (2018) 293
- partition function for statistical mechanics and path integral quantum mechanics in Euclidean time:

$$Z = \sum_n e^{-\frac{E_n}{k_B T}} = \mathrm{Tr}\exp\left(-\frac{H}{k_B T}\right) = \int dx < x|\exp\left(-\frac{H}{k_B T}\right)|x >$$

$$G_E(x, \tau; x', \tau') = \int [\mathscr{D}x] \ \exp\left(-\frac{1}{\hbar} S_E\left[x, \frac{dx}{d\tau}\right]\right)$$

- With the boundary conditions

What to calculate in the path integral with "Euclidean time"?

Heisenberg picture： $\hat{Q}(\tau_i) = e^{H\tau_i}\hat{Q}(0)e^{-H\tau_i}$

$$< x, \tau | \hat{Q}(\tau_1)\hat{Q}(\tau_2)\cdots\hat{Q}(\tau_j) | x', \tau' > \equiv < x | e^{-H\tau}\hat{Q}(\tau_1)\hat{Q}(\tau_2)\cdots\hat{Q}(\tau_j)e^{H\tau'} | x' >$$

$$e^{H\tau'} | x' > = \sum_n e^{H\tau'} | n > < n | x' > = \sum_n e^{E_n\tau'}\Psi_n(x')^\dagger$$

$$< x | e^{-H\tau} = \sum_m < x | m > < m | e^{-H\tau} = \sum_m e^{-E_m\tau}\Psi_m(x)$$

$$= \sum_{n,m} e^{-E_m\tau}e^{E_n\tau'}\Psi_m(x)\Psi_n(x')^\dagger < m | \hat{Q}(\tau_1)\hat{Q}(\tau_2)\cdots\hat{Q}(\tau_j) | n >$$

$$\rightarrow \; e^{-E_0(\tau-\tau')}\Psi_0(x)\Psi_0(x')^\dagger < 0 | \hat{Q}(\tau_1)\hat{Q}(\tau_2)\cdots\hat{Q}(\tau_j) | 0 >$$

What to calculate in the path integral with "Euclidean time"?

$$< x, \tau \,|\, \hat{Q}(\tau_1)\hat{Q}(\tau_2)\cdots\hat{Q}(\tau_j) \,|\, x', \tau' > \;\rightarrow\; e^{-E_0(\tau-\tau')}\Psi_0(x)\Psi_0(x')^\dagger < 0 \,|\, \hat{Q}(\tau_1)\hat{Q}(\tau_2)\cdots\hat{Q}(\tau_j) \,|\, 0 >$$

$$< x, t \,|\, x', t' > \;\rightarrow\; e^{-E_0(\tau-\tau')}\Psi_0(x)\Psi_0(x')^\dagger$$

$$\frac{< x, \tau \,|\, \hat{Q}(\tau_1)\hat{Q}(\tau_2)\cdots\hat{Q}(\tau_j) \,|\, x', \tau' >}{< x, \tau \,|\, x', \tau' >} \rightarrow < 0 \,|\, \hat{Q}(\tau_1)\hat{Q}(\tau_2)\cdots\hat{Q}(\tau_j) \,|\, 0 >$$

In quantum field theory, we are interested in "propagator"

$$\frac{\int [\mathscr{D}x] x(\tau_1)x(\tau_2)\cdots x(\tau_j)\; e^{-\frac{S_E}{\hbar}}}{\int [\mathscr{D}x]\; e^{-\frac{S_E}{\hbar}}}$$

In path integral, "propagator" is a ratio of two integrals

QCD, a Quantum Field Theory

1. QFT of quarks and gluons
2. QFT has divergences (IR and UV)
3. QFT needs regularization to tame divergences
4. Pauli–Villars regularization, dimensional regularization, spacetime discretization and so on
5. Quantum states and Hamiltonian for a quantum theory

Consistent QFT: Renormalizability

Quantum Field Theory

↓

Regularization

↓

Renormalized Quantum Field Theory

Anomaly and regulator

1. Classical symmetry can be broken by quantum correction (e.g., Adler–Bell–Jackiw chiral anomaly of Quantum Electrodynamics)
2. Regulator to tame divergences is related to quantum correction
3. QCD is a “vector” gauge theory, not a chiral gauge theory

Quantum ChromoDynamics (QCD)

- Quantum ChromoDynamics: gauge theory of quark field and gluon field

$$\mathscr{L}_{QCD} = \bar{\psi}^{i}_{a,f}\left[i\gamma^{\mu}_{ab}\left(\partial_{\mu} + ig(A_{\mu}))_{ij}\right) - m_f\right]\psi^{j}_{b,f} - \frac{1}{4}\mathrm{Tr}\left(F_{\mu\nu}F^{\mu\nu}\right),\quad A_{\mu} = A_{\mu}{}^{c}T^{c},\ \ F_{\mu\nu} = \partial_{\mu}A^{c}_{\nu}T^{c} - \partial_{\nu}A^{c}_{\mu}T^{c} + ig\left[A_{\mu}, A_{\nu}\right]^{c}T^{c}$$

T^c : Gell−Mann matrices

- The Strong interaction as a "color" gauge theory: compare with Quantum ElectroDynamics

$$\mathscr{L}_{QED} = \bar{\psi}_{a,f}\left[i\gamma^{\mu}_{ab}\left(\partial_{\mu} + ieA_{\mu})\right) - m_f\right]\psi_{b,f} - \frac{1}{4}\mathrm{Tr}\left(F_{\mu\nu}F^{\mu\nu}\right),\quad F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$$

- electric charge vs color charge

$\psi \to e^{i\alpha}\psi$: $U(1)$ phase rotation vs $\begin{pmatrix}\psi_r\\ \psi_g\\ \psi_b\end{pmatrix} \to \left[e^{i\alpha^{c}T^{c}}\right]\begin{pmatrix}\psi_r\\ \psi_g\\ \psi_b\end{pmatrix}$: $SU(3)$ phase rotation

QCD

1. QCD is a renormalizable theory (D. Gross, F. Wilczek and D. Politzer)
2. Based on color $SU(3)$ Gauge symmetry
3. Chiral symmetry breaking
4. Fundamental constituents are colored states (quarks and gluons) but we see only hadronic states (baryons, mesons, tetra−quark states, penta−quark states etc)
5. But we don’t see colored states !!!!!!!

QCD in Euclidean spacetime

- Quantum ChromoDynamics Lagrangian: gauge theory of quark field and gluon field

$$\mathscr{L}_{QCD} = \bar{\psi}^i_{a,f}\left[i\gamma^\mu_{ab}\left(\delta_{ij}\partial_\mu + ig(A_\mu)_{ij}\right) - m_f\delta_{ij}\delta_{ab}\right]\psi^j_{b,f} - \frac{1}{4}\mathrm{Tr}\left(F_{\mu\nu}F^{\mu\nu}\right),\quad A_\mu = A_\mu{}^c T^c,\ F_{\mu\nu} = \partial_\mu A^c_\nu T^c - \partial_\nu A^c_\mu T^c + ig\left[A_\mu, A_\nu\right]^c T^c$$

$$\text{Path integral: } Z = \int dA_\mu \int d\bar{\psi} \int d\psi\, e^{iS_{\mathrm{QCD}}},\quad S_{\mathrm{QCD}} = \int d^3x\, dt\, \mathscr{L}_{\mathrm{QCD}}$$

- In Euclidean spacetime,

$$\mathscr{L}^E_{QCD} = \bar{\psi}^i_{a,f}\left[(\gamma_E)^\mu_{ab}\left(\delta_{ij}\partial_\mu + ig(A_\mu)_{ij}\right) + m_f\delta_{ij}\delta_{ab}\right]\psi^j_{b,f} + \frac{1}{4}\mathrm{Tr}\left(F_{\mu\nu}F^{\mu\nu}\right),\quad A_\mu = A_\mu{}^c T^c,\ F_{\mu\nu} = \partial_\mu A^c_\nu T^c - \partial_\nu A^c_\mu T^c + ig\left[A_\mu, A_\nu\right]^c T^c$$

$$\text{Path integral: } Z_E = \int dA_\mu \int d\bar{\psi} \int d\psi\, e^{-S^E_{\mathrm{QCD}}},\quad S^E_{\mathrm{QCD}} = \int d^3x\, d\tau\, \mathscr{L}^E_{\mathrm{QCD}}$$

Quark field, Grassmann number and effective action

1. Quark field is based on anti–commuting numbers (i.e. Grassmann number) which have no classical analogue

2. Formal integration over quark field and anti–quark field:

$$\int d\psi \int d\overline{\psi} \exp\left[-\overline{\psi} M \psi\right] \;\rightarrow\; \det(M)$$

3. Or can be mimicked by "pseudo fermion" (or boson field):

$$\int d\phi \int d\phi^\dagger \exp\left[-\phi^\dagger (M)^{-1} \phi\right] \;\rightarrow\; \det(M)$$

QCD in Euclidean spacetime

$$Z = \int dA_\mu \int d\psi \int d\overline{\psi}\, e^{-S^E_{\mathrm{QCD}}} = \int dA_\mu \int d\psi \int d\overline{\psi} \exp\left[-\int d^4x_E \mathscr{L}^E_{QCD}\right]$$

$$= \int dA_\mu \; \det(M)_1 \det(M)_2 \cdots \det(M)_f \; e^{-S_g} \,,$$

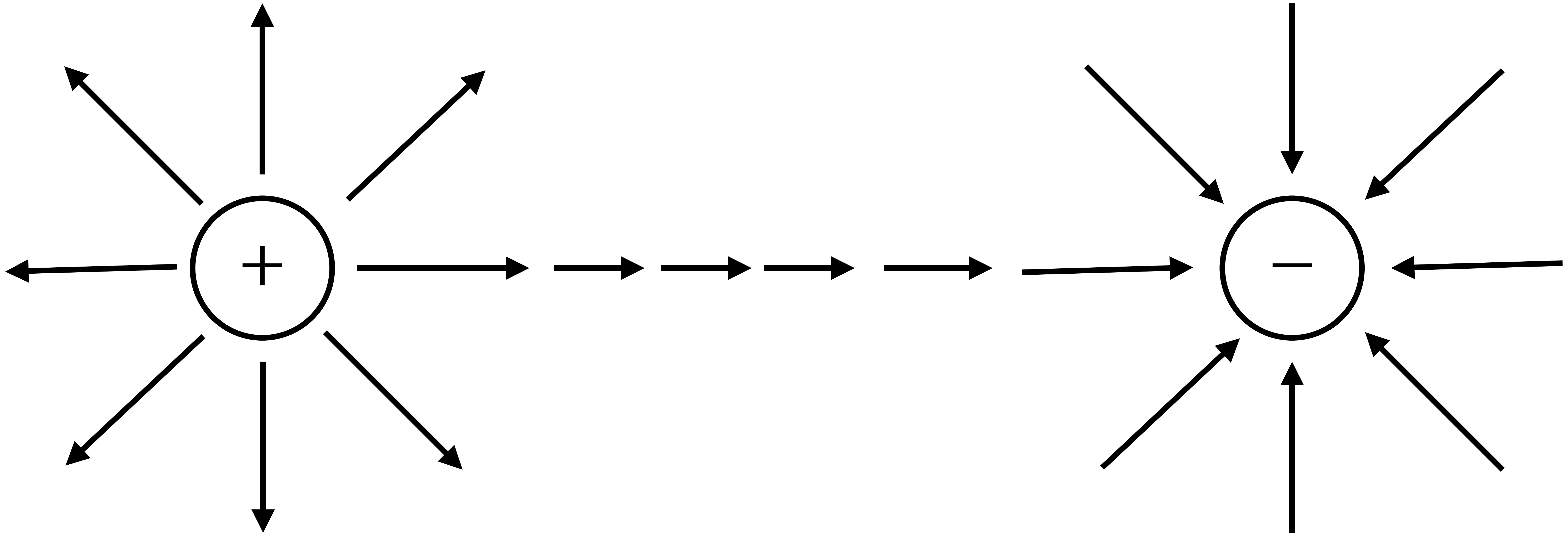
$$S_g = \frac{1}{4}\mathrm{Tr}F_{\mu\nu}F_{\mu\nu} \,, \quad M_1 = \gamma^\mu_E(\partial_\mu + igA_\mu) + m_1 \equiv \gamma^\mu_E D_\mu + m_1$$

Using $\det(M) = e^{\mathrm{Tr}\log(M)}$,

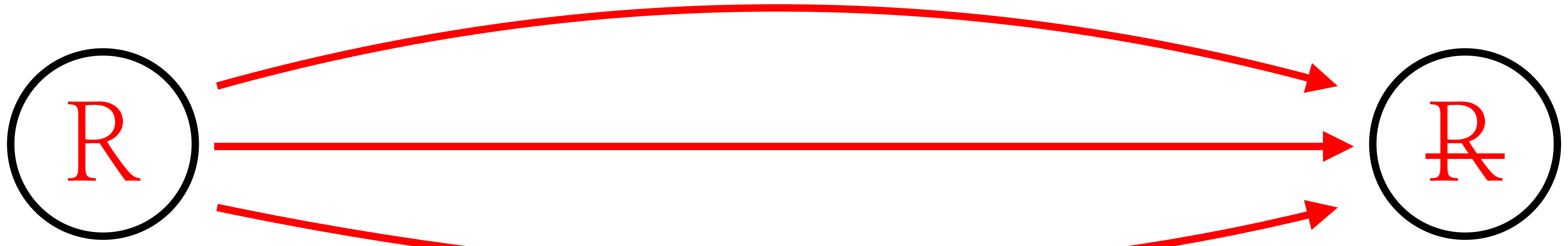
$$S_{\mathrm{eff}} = -\sum_f \mathrm{Tr}\log(M_f) \; + \; \frac{1}{4}\mathrm{Tr}F_{\mu\nu}F_{\mu\nu}$$

“Confinement of Quarks”,
K.G. Wilson, PRD10 (1974) 2445

1. “Coloumb’s law is not the only solution of Gauss’ law”
2. Flux tube of gauge field is also a solution of Gauss’ law
3. Energy cost of separating colored source can be proportional to the distance between the charges



$$\sim \frac{1}{r}$$



$$\sim r$$

"Confinement of Quarks", K.G. Wilson, PRD10 (1974) 2445

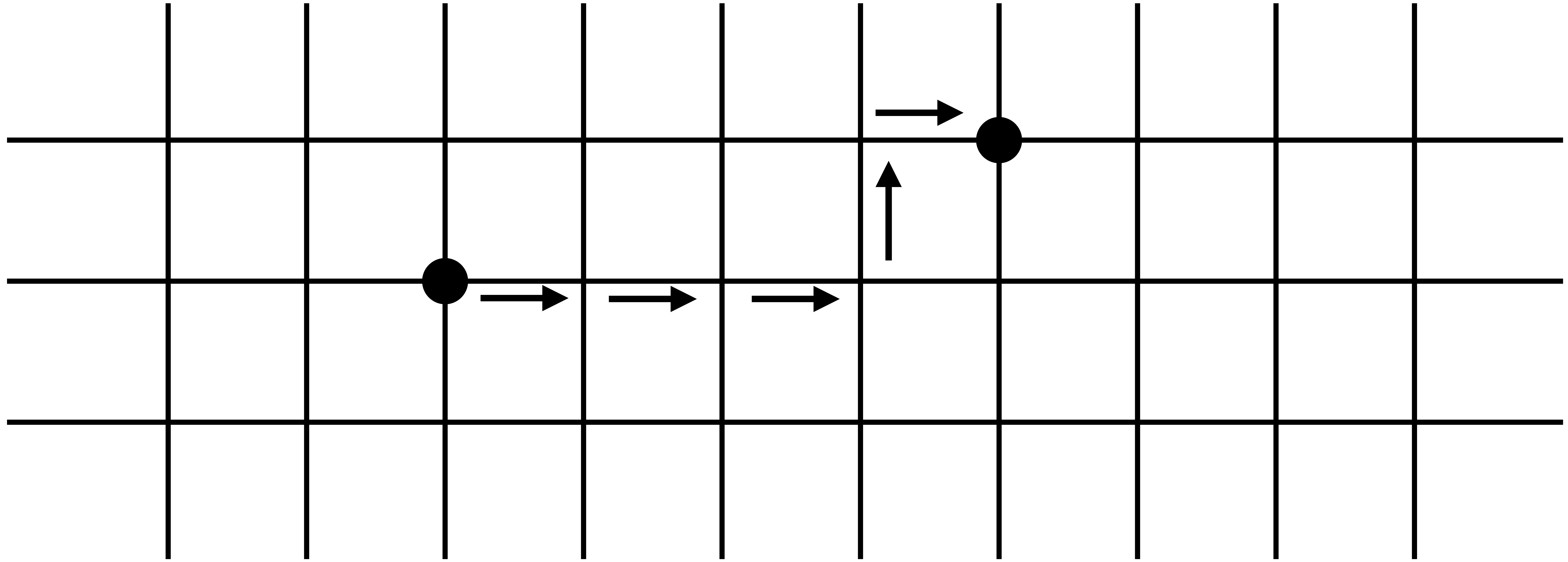
1. Lattice QCD is QCD on spacetime lattice
2. Lattice QCD has both IR−cutoff and UV−cutoff
3. Lattice QCD has a non−perturbative definition of QCD fully satisfying first principles of quantum field theory
4. Perturbative QCD vs Non−perturbative QCD
5. Keep gauge symmetry and give up continuous spacetime

QCD on Euclidean spacetime lattice

1. Needs to define quark field (fermonic field) and gluon field (gauge field)
2. Regulator, renormalization scheme and symmetry realized on a discrete Euclidean spacetime lattice

Quark field: $\psi(\mathbf{x}, \tau) \rightarrow \psi(\mathbf{x}_n, \tau_m)$

Gauge transform: $e^{i\alpha(\mathbf{x},\tau)\cdot T}\, \psi(\mathbf{x}, \tau) \rightarrow e^{i\alpha(\mathbf{x}_n,\tau_m)\cdot T}\psi(\mathbf{x}_n, \tau_m)$



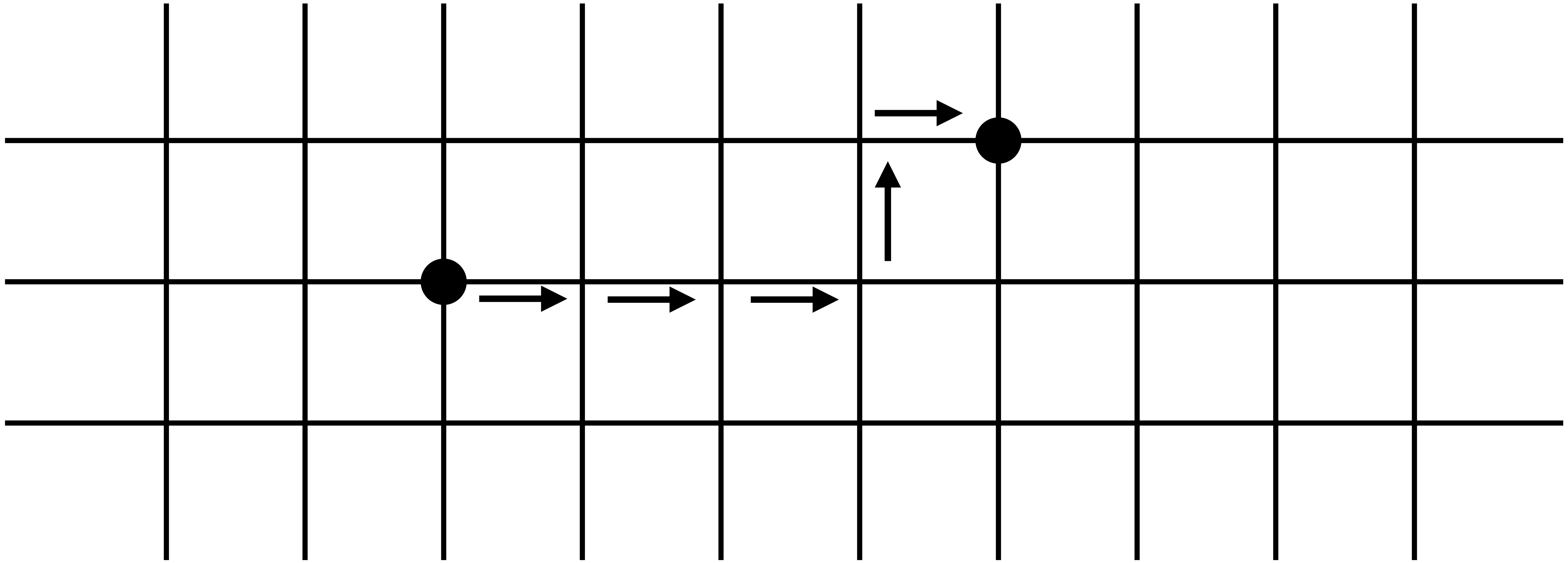
Lattice spacing: a

We have $\overline{\psi}(\mathbf{x}, \tau)\partial_\mu \psi(\mathbf{x}, \tau) \rightarrow \overline{\psi}(\mathbf{x}_{n'}, \tau_{m'})\psi(\mathbf{x}_n, \tau_m)$

$$\overline{\psi}(\mathbf{x}', \tau')\, e^{i\alpha(\mathbf{x}',\tau')\cdot T} e^{i\alpha(\mathbf{x},\tau)\cdot T}\, \psi(\mathbf{x}, \tau) \rightarrow \overline{\psi}(\mathbf{x}_{n'}, \tau_{m'})\, e^{i\alpha(\mathbf{x}_{n'},\tau_{m'})\cdot T} e^{i\alpha(\mathbf{x}_n,\tau_m)\cdot T}\psi(\mathbf{x}_n, \tau_m)$$

We also have $\bar{\psi}(\mathbf{x},\tau)\, A_\mu(\mathbf{x},\tau)\;\; \psi(\mathbf{x},\tau)$

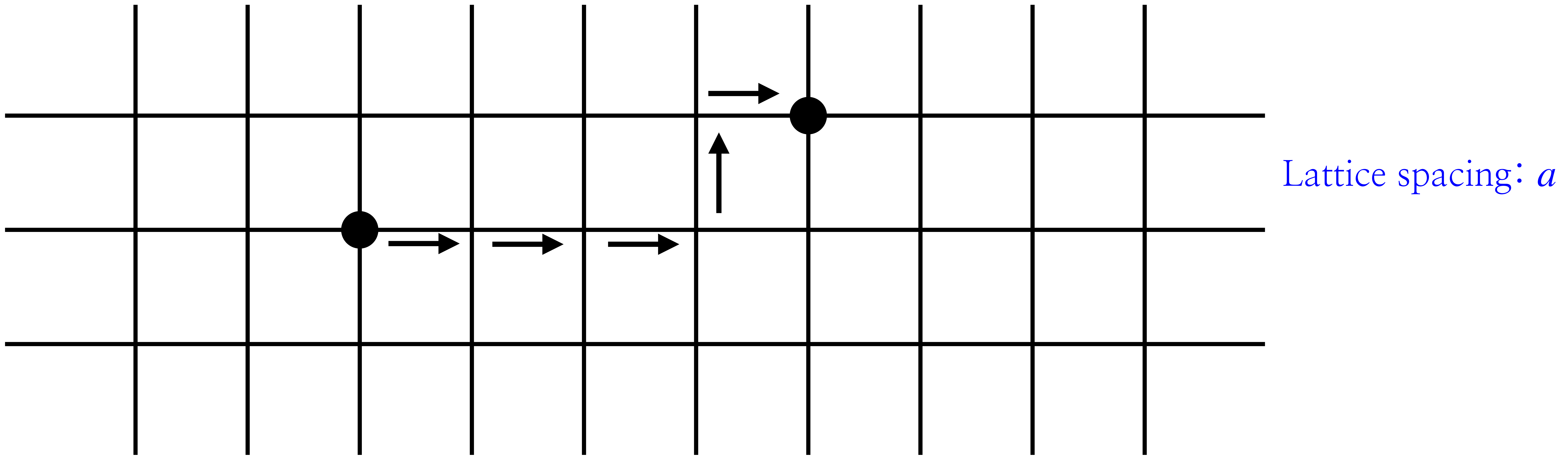
Gauge transform: $\bar{\psi}(\mathbf{x}_{n'},\tau_{m'})\; e^{i\alpha(\mathbf{x}_{n'},\tau_{m'})\cdot T}\Lambda(\mathbf{x}_{n'},\tau_{m'};\mathbf{x}_n,\tau_m)e^{i\alpha(\mathbf{x}_n,\tau_m)\cdot T}\psi(\mathbf{x}_n,\tau_m)$



Lattice spacing: a

Gluon field: $$A_\mu(\mathbf{x},\tau) \to \Lambda(\mathbf{x}',\tau';\mathbf{x},\tau) \equiv \exp\left[ig\int_{(\mathbf{x},\tau)}^{(\mathbf{x}',\tau')} dx_\nu\, A_\nu \cdot T\right]$$

$$\Lambda(\mathbf{x}_{n'},\tau_{m'};\mathbf{x}_n,\tau_m) \to U_\mu(x) \equiv e^{iaA_\mu(x)}$$



Quark field: defined on the lattice sites

Gluon field: defined between the lattice sites, called "links", $U_\mu(x) \equiv e^{iaA_\mu(x)}$
to respect gauge symmetry

Lattice QCD in Euclidean spacetime

$$\partial_\mu \psi(x) \simeq \frac{1}{2a}\left[\psi(x+\hat{\mu}a) - \psi(x-\hat{\mu}a)\right], \quad D_\mu \psi(x) \simeq \frac{1}{2a}\left[U_\mu(x)\psi(x+\hat{\mu}a) - U_\mu^\dagger(x-\hat{\mu}a)\psi(x-\hat{\mu}a)\right]$$

$$\overline{\psi}(x)\left[\gamma_E^\mu D_\mu \psi(x) + m\psi(x)\right] \;\rightarrow\; \overline{\psi}(x)\left[\frac{1}{2a}\gamma_E^\mu \left(U_\mu(x)\psi(x+\hat{\mu}a) - U_\mu^\dagger(x-\hat{\mu}a)\psi(x-\hat{\mu}a)\right) + m\psi(x)\right]$$

$$\overline{\psi}_a^i(x) M_{ab}^{ij}(x,y)\psi_b^j(y), \;\; M_{ab}^{ij}(x,y) = (\gamma_E^\mu)_{ab}\frac{1}{2a}\left[U_\mu(x)\delta_{x+\hat{\mu}a,y} - U_\mu^\dagger(y)\delta_{x-\hat{\mu}a,y}\right] + m\delta_{x,y}\delta_{ij}\delta_{ab}$$

$$F_{\mu\nu}(x)^c = \partial_\mu A_\nu^c - \partial_\nu A_\mu^c + ig\left[A_\mu, A_\nu\right]^c \rightarrow P_{\mu\nu} = U_\mu(x)U_\nu(x+\hat{\mu}a)U_\mu^\dagger(x+\hat{\nu}a)U_\nu^\dagger(x)$$

$$\frac{1}{4}\mathrm{Tr}F_{\mu\nu}F_{\mu\nu} \rightarrow \beta\left[1 - \frac{1}{2N_c}\mathrm{Tr}\left(P_{\mu\nu} + P_{\mu\nu}^\dagger\right)\right], \quad \beta = \frac{2N_c}{g^2}$$

Lattice QCD

$$Z = \int \mathscr{D}U_\mu \, e^{-S_{\text{eff}}} \,, \quad < \mathcal{O}[U] > = \frac{\int \mathscr{D}U_\mu \, \mathcal{O}[U] \; e^{-S_{\text{eff}}}}{\int \mathscr{D}U_\mu \, e^{-S_{\text{eff}}}}$$

$$S_{\text{eff}} = -\sum_f \text{Tr} \log \left[M_f \right] + \beta \left[1 - \frac{1}{2N_c} \text{Tr} \left(P_{\mu\nu} + P^\dagger_{\mu\nu} \right) \right], \quad \beta = \frac{2N_c}{g^2}$$

Remind you that $\int \mathscr{D}U_\mu = \int \int \cdots \int \prod_{x,\mu} dU_\mu(x)$

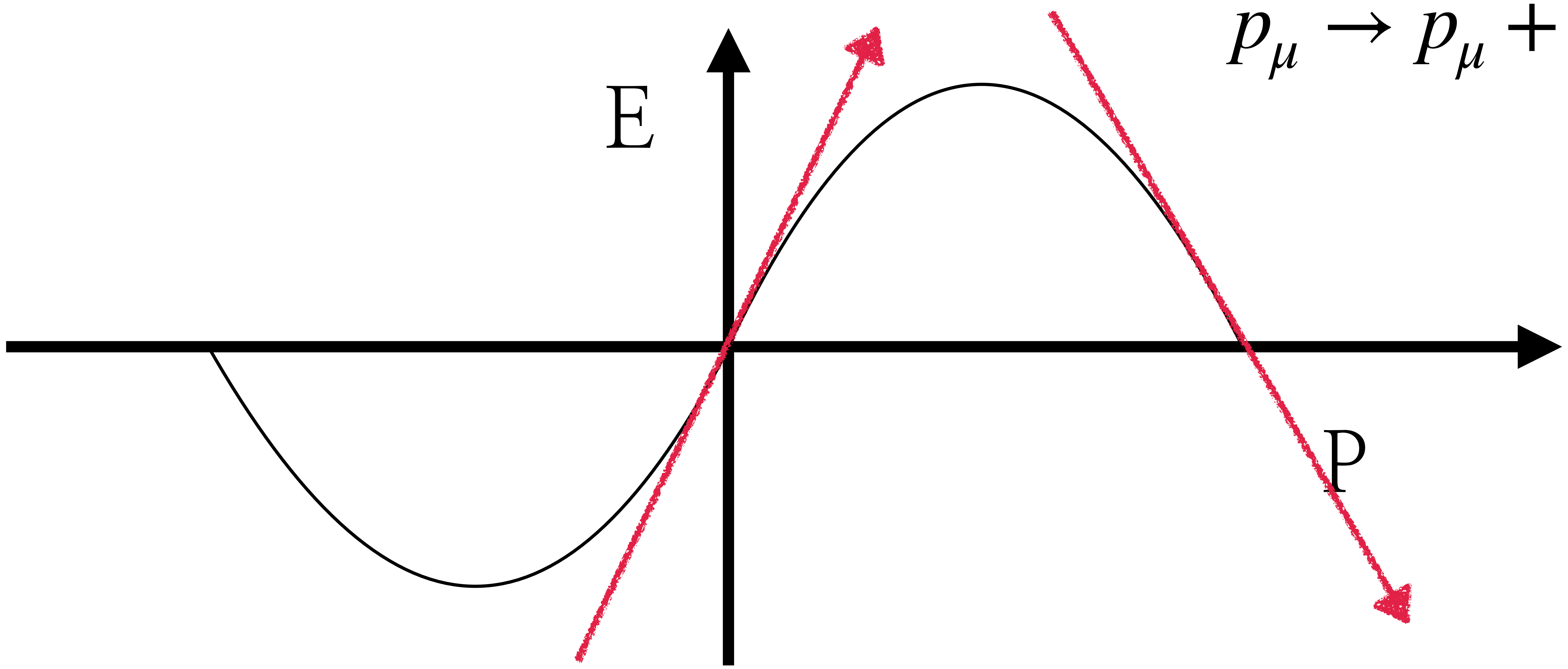
Anomaly and lattice regulator

1. Classical symmetry can be broken by quantum correction (e.g., Adler–Bell–Jackiw chiral anomaly of Quantum Electrodynamics)

2. Nielsen–Ninomya theorem: H.B. Nielsen and M. Ninomiya, "Absence of neutrinos on a lattice 1 & 2", Nucl. Phys. B185 (1981) 20 and Nucl. Phys. B193 (1981) 173

3. QCD is a "vector" gauge theory, not a chiral gauge theory

Fermion doubling problem



$$p_\mu \rightarrow p_\mu + \frac{\pi}{a}$$

In spacetime

$$\partial_\mu \psi \rightarrow \frac{\psi(x+\mu) - \psi(x-\mu)}{2a}$$

In momentum space

$$\frac{e^{ip\cdot(x+\mu)}\tilde{\psi}(p) - e^{ip\cdot(x-\mu)}\tilde{\psi}(p)}{2a} = i\frac{\sin(p_\mu a)}{a}\tilde{\psi}(p)$$

Fermion Doubling Problem

1. Unavoidable (Nielsen–Ninomya theorem)
2. Based on the first order derivative of Dirac equation
3. Topological property
4. Local chiral gauge theory is not possible

Solution to Fermion Doubling Problem

1. Wilson fermion
2. Staggered fermion
3. Domain wall fermion
4. Ginsparg–Wilson fermion
5. Random lattice

Euclidean Spacetime QFT and Statistical Mechanics

Path integral formulation of QFT means "summation of e^{-S_E} over all the possible field configurations"

$$Z = \int \mathscr{D}U_\mu \, e^{-S_{\text{eff}}}, \quad < \mathcal{O}[U] > = \frac{\int \mathscr{D}U_\mu \, \mathcal{O}[U] \; e^{-S_{\text{eff}}}}{\int \mathscr{D}U_\mu \, e^{-S_{\text{eff}}}}, \quad \int \mathscr{D}U_\mu = \int\int \cdots \int \prod_{x,\mu} dU_\mu(x)$$

Think about the partition function in statistical mechanics of 1−D Ising model,

$$Z = \text{Tr} \, \left(e^{-\frac{H}{k_B T}} \right), \quad < E > = \frac{\text{Tr}\left(H \, e^{-\frac{H}{k_B T}} \right)}{\text{Tr} \, \left(e^{-\frac{H}{k_B T}} \right)}, \quad H = -J \sum_i \sigma_i \sigma_{i+1} - h \sum_i \sigma_i$$

Here, "**Tr**" means sum over all the spin configurations, 2^N possibilities of $\sigma_1, \sigma_2, \cdots, \sigma_N$

Statistical Mechanics and Probability

Statistical mechanics of 1−D Ising model,

$$Z = \mathrm{Tr}\left(e^{-\frac{H}{k_B T}}\right), \quad < E > = \frac{\mathrm{Tr}\left(H\, e^{-\frac{H}{k_B T}}\right)}{\mathrm{Tr}\left(e^{-\frac{H}{k_B T}}\right)}, \quad H = -J\sum_i \sigma_i \sigma_{i+1} - h\sum_i \sigma_i$$

$$< E > = \mathrm{Tr}\left(H\,\frac{e^{-\frac{H}{k_B T}}}{Z}\right) = -\sum_{\sigma_1,\sigma_2,\cdots,\sigma_N=\pm 1}\left(J\sum_i \sigma_i\sigma_{i+1} + h\sum_i \sigma_i\right) P\left[\sigma_1, \sigma_2, \cdots, \sigma_N\right]$$

with a probability, $P\left[\sigma_1, \sigma_2, \cdots, \sigma_N\right] = \dfrac{e^{-\frac{H}{k_B T}}}{Z} = \dfrac{e^{-\frac{H}{k_B T}}}{\sum_{\sigma_1',\sigma_2',\cdots,\sigma_N'=\pm 1} e^{-\frac{H'}{k_B T}}}$

Statistical Mechanics and Probability

ex) for a 3−spin system,

$$P\left[\sigma_1, \sigma_2, \sigma_3\right] = \frac{\left[e^{J\left(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1\right)+h\left(\sigma_1 + \sigma_2 + \sigma_3\right)}\right]}{\left[e^{\frac{3J-3h}{k_BT}} + e^{-\frac{J+h}{k_BT}} + e^{-\frac{J+h}{k_BT}} + e^{-\frac{J+h}{k_BT}} + e^{\frac{-J+h}{k_BT}} + e^{\frac{-J+h}{k_BT}} + e^{\frac{-J+h}{k_BT}} + e^{\frac{3J+3h}{k_BT}}\right]}$$

Since $Z = \sum_{\sigma_1', \sigma_2', \cdots, \sigma_N' = \pm 1} e^{-\frac{H'}{k_BT}}$,

for $(\sigma_1', \sigma_2', \sigma_3') = (-,-,-)$, we have $e^{\frac{3J-3h}{k_BT}}$. for $(+,+,+)$, we have $e^{\frac{3J+3h}{k_BT}}$

$(-,-,+), (-,+,-), (+,-,-)$, we have $e^{-\frac{J+h}{k_BT}}$

$(-,+,+), (+,+,-), (+,-,+)$, we have $e^{\frac{-J+h}{k_BT}}$

Euclidean Spacetime QFT, Statistical Mechanics and Probability

Path integral formulation of QFT is "summation of e^{-S_E} over all the possible field configurations"

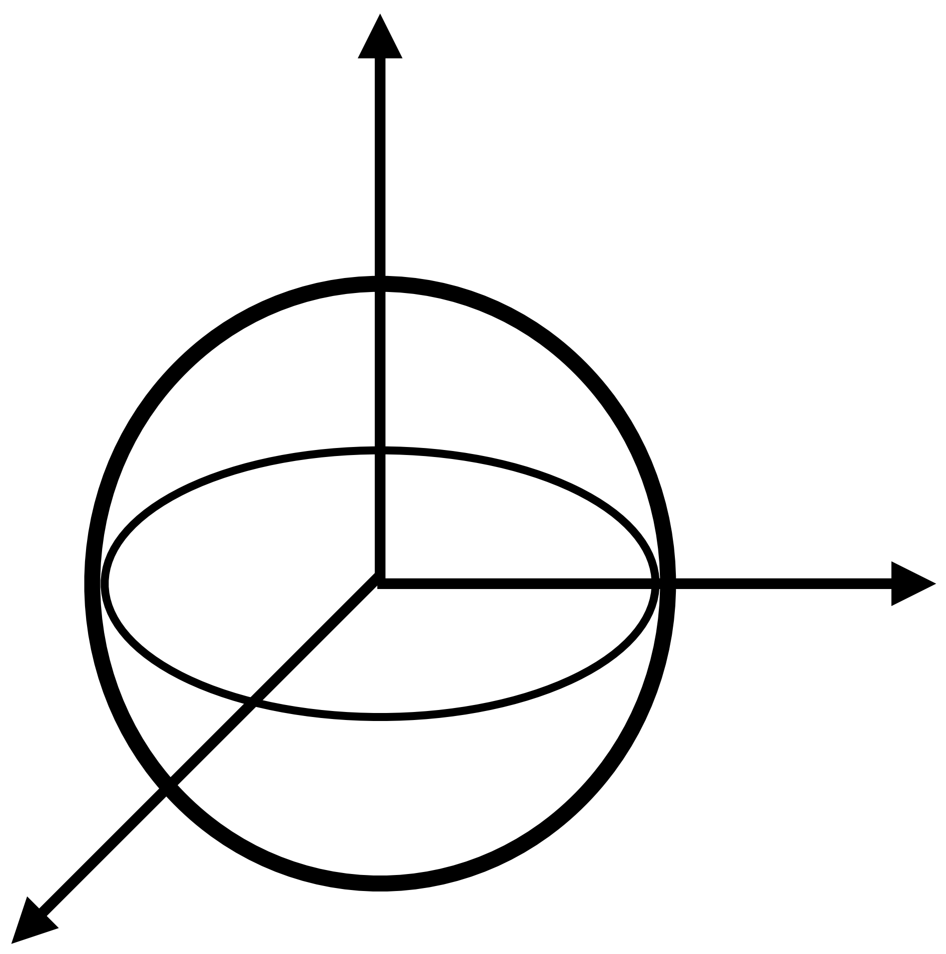
$$Z = \int \mathscr{D}U_\mu \, e^{-S_{\text{eff}}}, \ \ < \mathscr{O}[U] > = \frac{\int \mathscr{D}U_\mu \, \mathscr{O}[U] \ e^{-S_{\text{eff}}}}{\int \mathscr{D}U_\mu \, e^{-S_{\text{eff}}}}, \ \int \mathscr{D}U_\mu = \int\int \cdots \int \prod_{x,\mu} dU_\mu(x)$$

Expectation value of QCD in Euclidean spacetime can be interpreted as,

$$< \mathscr{O}[U] > = \int \mathscr{D}U_\mu \, \mathscr{O}[U] \, P[U], \ \ P[U] = \frac{e^{-S_{\text{eff}}}}{\int \mathscr{D}U_\mu \, e^{-S_{\text{eff}}}}$$

Monte Carlo Simulation/Integration

ex) calculate the volume of a sphere whose radius is R: $\frac{4}{3}\pi R^3$



Throw random numbers in $x_1 \in [-R, R], x_2 \in [-R, R], x_3 \in [-R, R]$,
and count $x_1^2 + x_2^2 + x_3^2 \leq R^3$

Monte Carlo Simulation/Integration

1. Here we mean Monte Carlo simulation as a sampling method
2. Path integral formulation of QFT means "summation of e^{-S_E} over all the possible field configurations"
3. Choose sample of field configurations, calculate e^{-S_E} for each elements in the sample, and sum over them
4. How many field configurations are there?

Importance Sampling

1. If we have too many degrees of freedom, we can't Monte Carlo sample all the possibilities. If we need N−dimensional variables and if we choose e.g., 10 values for each variable, we need $\mathbf{10}^N$
2. Prepare Monte Carlo ensemble according to their "importance" (i.e., which gives large e^{-S_E} for our case)

How: Algorithm

1. Detailed balance, $W(U' \to U)P[U'] = W(U \to U')P[U]$ is a sufficient condition
2. Ergodicity (algorithm ensures that all the possible states are visited, i.e, there is a finite probability to visit all the possible states) is a necessary condition

How Monte Carlo Algorithm works

Expectation value of QCD in Euclidean spacetime can be interpreted as,

$$< \mathcal{O}[U] > = \int \mathcal{D}U_\mu \, \mathcal{O}[U] \, P[U], \quad P[U] = \frac{e^{-S_{\text{eff}}}}{\int \mathcal{D}U_\mu \, e^{-S_{\text{eff}}}} \equiv P_{\text{eq}}[U]$$

Note that the condition for $P_{\text{eq}}[U]$ which we require is

$$P_{\text{eq}}[U] = \sum_{U'} P_{\text{eq}}[U'] W(U' \to U)$$

Let us define $P_N[U_N]$ which we obtain after N updates from some initial configurations

$$P_N[U_N] = \sum_{\{U_i\}} W(U_0 \to U_1) W(U_1 \to U_2) \cdots W(U_{N-1} \to U_N)$$

$$P_{N+1}[U_{N+1}] = \sum_{\{U_N\}} \sum_{\{U_i\}} W(U_0 \to U_1) W(U_1 \to U_2) \cdots W(U_{N-1} \to U_N) W(U_N \to U_{N+1}) = \sum_{\{U_N\}} P_N[U_N] W(U_N \to U_{N+1})$$

How Monte Carlo Algorithm works

Let us define $\epsilon_N = \sum_{U_N} |P_N[U_N] - P_{\text{eq}}[U_N]|$, the difference between the probability we obtain after N updates and the equilibrium probability. Then the next update gives

$$\epsilon_{N+1} = \sum_{U_{N+1}} |P_{N+1}[U_{N+1}] - P_{\text{eq}}[U_{N+1}]| = \sum_{U_{N+1}} |\sum_{U_N} P_N[U_N] W(U_N \to U_{N+1}) - P_{\text{eq}}[U]|$$

From the requirement for $P_{\text{eq}}[U]$, $P_{\text{eq}}[U] = \sum_{U'} P_{\text{eq}}[U'] W(U' \to U)$,

$$\epsilon_{N+1} = \sum_{U_{N+1}} |\sum_{U_N} P_N[U_N] W(U_N \to U_{N+1}) - \sum_{U_N} P_{\text{eq}}[U_N] W(U_N \to U_{N+1})|$$

$$= \sum_{U_{N+1}} |\sum_{U_N} \left(P_N[U_N] - P_{\text{eq}}[U_N]\right) W(U_N \to U_{N+1})| \leq \sum_{U_{N+1}} \sum_{U_N} |P_N[U_N] - P_{\text{eq}}[U_N]| W(U_N \to U_{N+1}) \leq \epsilon_N$$

Probability and Fokker–Planck equation

Time evolution of the probability function (in case of small time step algorithm) and Fokker–Planck equation: change of the probability for U at Monte Carlo time (fictitious time), t, is equal to (the transition from other states, U', to the desired state, U) minus (the transition from the desired state to other states, U')

$$P[U, t + \Delta t] - P[U, t] = \sum_{U'} \left[W(U' \to U) P[U', t] - W(U \to U') P[U, t] \right]$$

Metropolis Algorithm for 1−D Ising Model

1. Choose any initial spin configuration

2. Propose update on a spin σ_i with σ_i'

3. Calculate $E_{\text{old}} = H[\sigma_i], E_{\text{new}} = H[\sigma_i']$

4. If $E_{\text{new}} < E_{\text{old}}$, accept new spin σ_i'

5. If $E_{\text{new}} \geq E_{\text{old}}$, accept new spin σ_i' with the probability,

   $min\{1, e^{-\frac{\Delta E}{k_B T}}\}, \ \ \Delta E = E_{\text{new}} - E_{\text{old}}$

High Performance Computing

1. Large amount of computations: number of variables is $\sim L^4$
2. Statistical error associated with Monte Carlo sampling
3. “Grand Challenge problems in high performance computing

A lattice QCD project

Lattice field theory formulation

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Monte Carlo simulation of quark–gluon fields

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Calculation of observables

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Analysis/Lattice perturbation theory

Gauge field ensemble and physical observables

1. Ensemble of gauge fields has a distribution according to "the importance"
2. Expectation value of observables can be calculated using this ensemble just by averaging over the calculated observables: $< \mathcal{O} > = \frac{1}{N_{\text{sample}}} \sum_{i=1}^{N_{\text{sample}}} \mathcal{O}_i$

Continuum limit and field theory limit

1. Removal of regulator: lattice spacing, $a \to 0$

   it is equivalent to the continuum limit

2. Scale setting
3. Removal of finite volume effect
4. Quark mass