Algorithms for Lattice Quantum Chromodynamics

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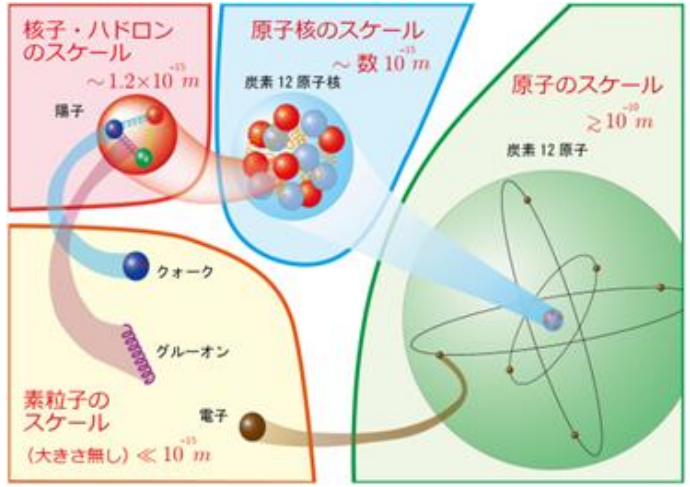
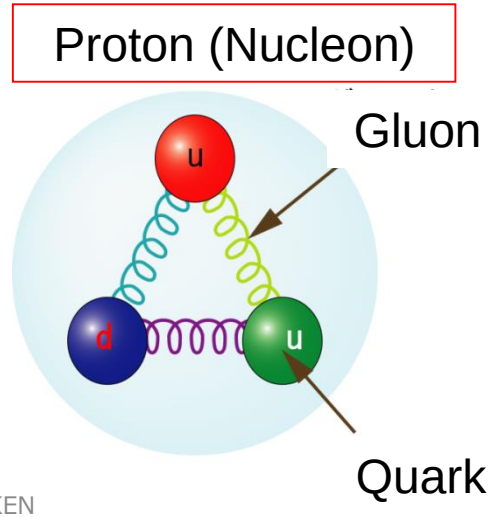
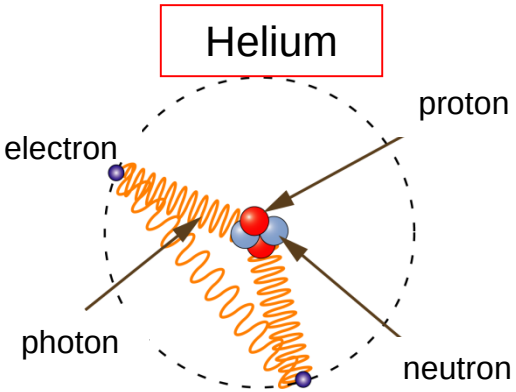
Contents

1. What is Lattice Quantum Chromodynamics?

- QCD (Quantum Chromodynamics)
  - Describes the properties of
    - Nucleons (Proton, Neutron)
    - (Mesons, Baryons =Hadrons)
    - Strong interaction (atomic nuclei)
  - from further fundamental particles;
    Quarks and Gluons
    - Dynamics by exchanging gluons. => Proton Mass, spin, … etc.
    - Quarks and gluons can not be isolated. Conefinment.
    - Quark has a kind of charge (not electric) :
      color charge(3types x +/- = 6 types).
  - e.g. QED (Quantum Electrodynamics)
    - Molecules/Atoms from nucleus/electrons and photons
    - Charge is + and − only.







- QCD (Quantum Chromodynamics)
  - We need Quantum Field Theory (QFT)
    to describe sub-atomic and high-energy phenomena.
  - E.x. QED := Quantized Maxwell and Dirac equations
    := Abelian(U(1)) Yang-Mills theory

$$\partial_\mu F^{\mu\nu} = j^\nu \qquad \left[i\gamma^\mu\partial_\mu - e\gamma^\mu A_\mu - m\right]\psi = 0$$

$$F^{\mu\nu} \equiv \partial^\mu A^\nu - \partial^\nu A^\mu$$

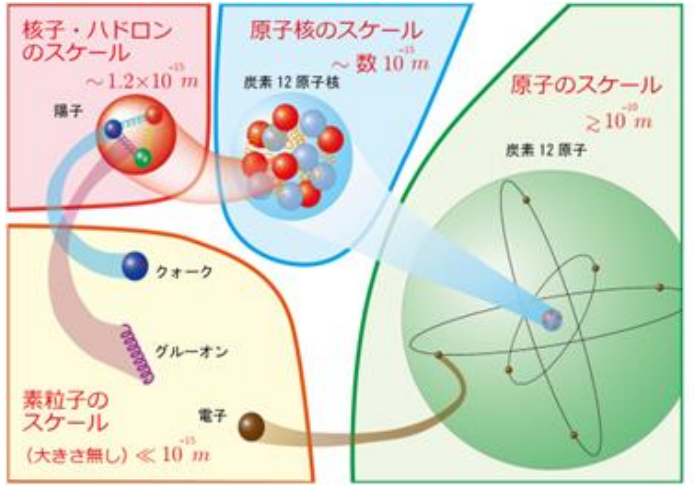
$$j^\mu \equiv e\bar{\psi}\gamma^\mu\psi$$ Electric current

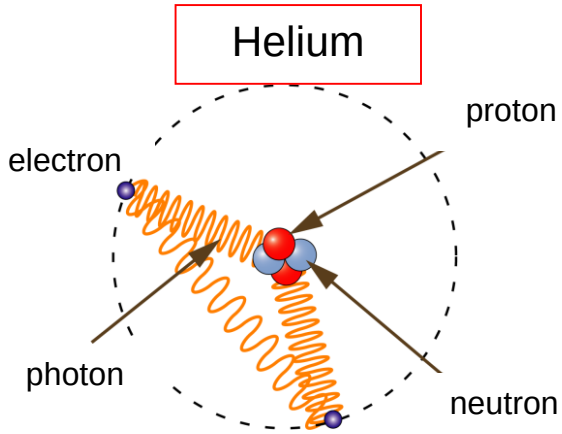
$$\nabla\cdot\vec{E} = \rho, \nabla\cdot\vec{B} = 0,$$

$$\nabla\times\vec{E} + \frac{\partial\vec{B}}{\partial t} = 0, \nabla\times\vec{B} - \frac{\partial\vec{E}}{\partial t} = \vec{j}$$

$A_\mu(x)$ Vector potential => Photon

$\psi_\alpha(x)$ Dirac Field =>Electrons/Atomic neuclei





- Quantize $A_\mu(x), \psi_\alpha(x)$ via Canonical/Path-integral quantization
- due to the electromagnetic interaction, the system cannot be solved exactly. But.

Thanks to the smallness of the electric charge *e*, the perturbative QED is the most successful theory we have.

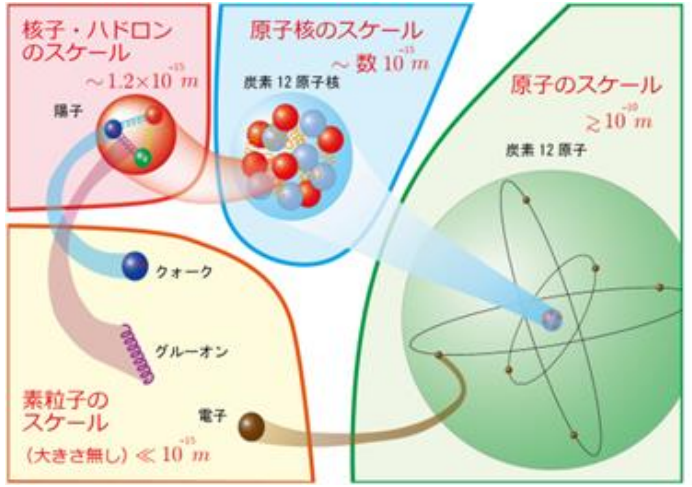
Fine Structure constant
$\alpha = e^2/(4\pi\varepsilon_0\hbar c)$ from Electron g-2

$$\alpha^{-1} = 137.035\ 999\ 084(51)$$

(4^{th} order perturbation), 10 digits accuracy!

1. What is Lattice Quantum Chromodynamics?

- QCD
- Quantum Field Theory (QFT) for Non-Abelian Yang-Mills theory.
  - Quark Field and Gluon Field. They have color charge (based on SU(3)).
    - Gluon: Very similar to Maxwell equation(photon). But the vector potential has color charge (8 types of charge).
    - Quark: Very similar to Dirac equation(Electron). But the field has color charge (3 types of charge).

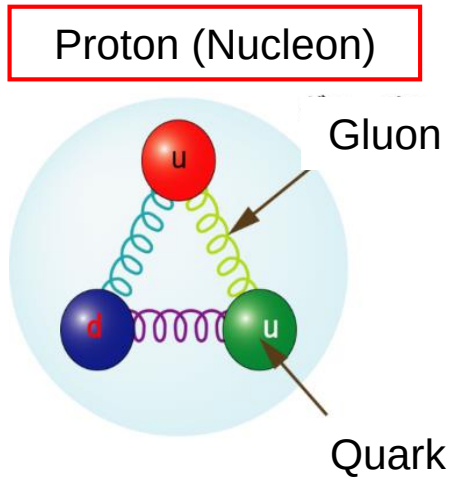


$$\left(\delta^{\bar{a}b}\partial_\mu - ig\overline{G_\mu^c f^{cab}}\right)G^{\bar{b}\mu\nu} = j^{\bar{a}\nu} \qquad \left[i\delta^{ab}\gamma^\mu\partial_\mu - e\gamma^\mu\overline{G_\mu^{ab}} - m_f\right]\psi_f^{\bar{b}} = 0$$

$$G^{a\mu\nu} \equiv \partial^\mu G^{a\nu} - \partial^\nu G^{a\mu} - igf^{abc}G^{b\mu}G^{c\nu}$$

$G_\mu^a(x)$ 8 charge types of Vector potential =>Gluon

$\psi_{f\beta}^a(x)$ 3 charge types of Dirac Field =>Quarks

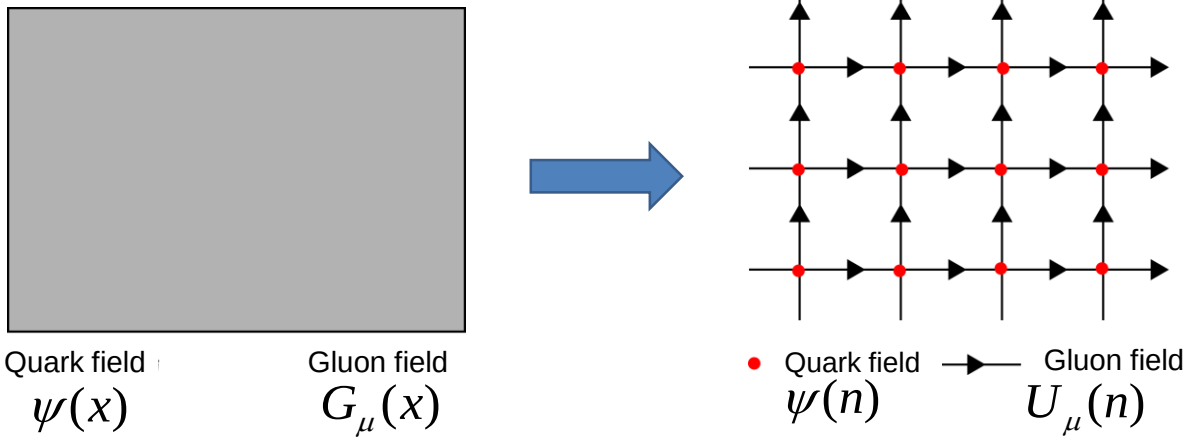


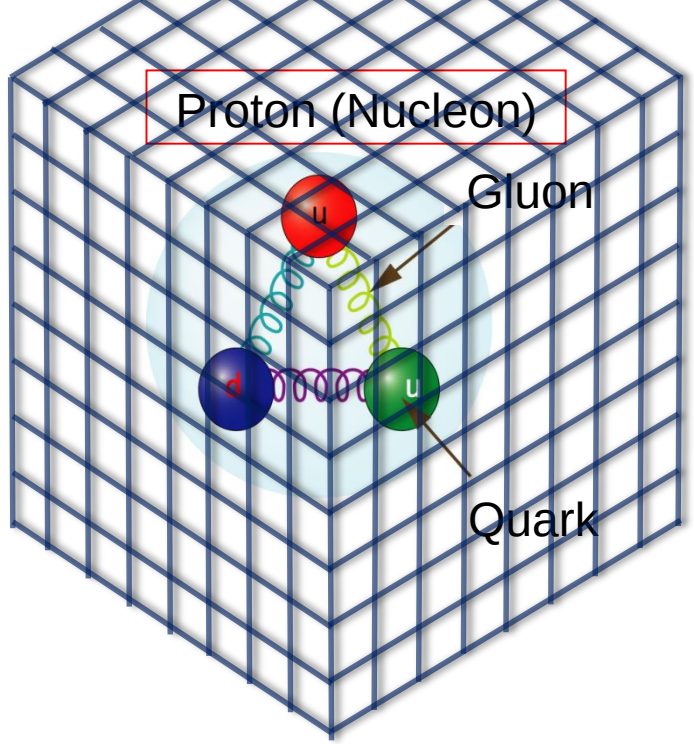
- Quantize $G_\mu^a(x), \psi_\alpha^a(x)$ via Canonical/Path-integral quantization
- Due to the colored property of Gluon, the equations are highly non-linear
- and the coupling g is known to be very large.

=> Perturbative treatment fails

1. What is Lattice Quantum Chromodynamics?

- Lattice QCD [K.G.Wilson (1974)]
  - 4 Dim Space-Time => Euclidean 4Dim Lattice Box
  - Fields on Discretized Space-Time





  - Quantize the Quark and Gluon fields on the 4-Dim grid lattice.
    - Discrete number of degree of freedom.
    - Numerical treatment is possible via Feynman's path integral formulation. Differential equations are discredited on the lattice.

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- Lattice QCD [K.G.Wilson (1974)]
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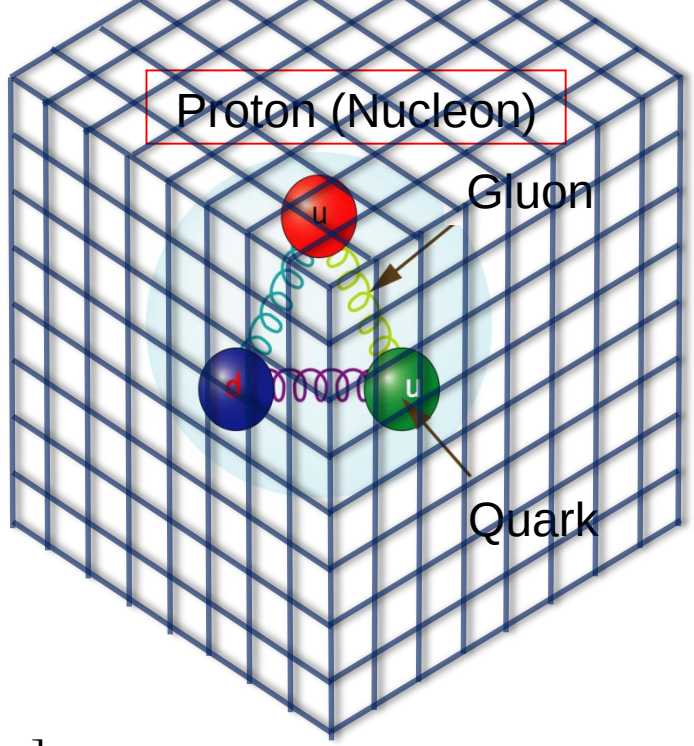
  - Fields on Discretized Space-Time
  - Quantize the Quark and Gluon fields on the 4-Dim grid lattice.
    - Discrete number of degree of freedom.
    - Numerical treatment is possible via Feynman's path integral formulation. Differential equations are discredited on the lattice.
    - The quantum expectation value of an observable $O[U,\bar{q},q]$ made of gluons and quarks is evaluated by



$$\langle O \rangle = \frac{1}{Z}\int DU \prod_{f=u,d,s} D\bar{q}_f Dq_f O[U,\bar{q},q]U, e^{-S[U,\bar{q},q]}$$

$$Z = \int DU \prod_{f=u,d,s} D\bar{q}_f Dq_f e^{-S[U,\bar{q},q]}$$

Lattice QCD Partition Function

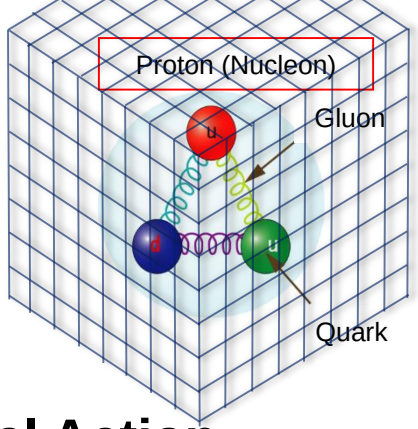
$$S = S_G[U] + \sum_{f=u,d,s} S_{Q_f}[\bar{q}_f, q_f, U]$$ ← **Total Action**

$$S_G[U] = \beta \sum_n \sum_{\mu,\nu} \left[1 - \frac{1}{6} Tr\left[P_{\mu\nu}(n) + P_{\mu\nu}(n)^\dagger\right]\right]$$ ← **Wilson Gauge Action**

$$S_{Q_f}[\bar{q}_f, q_f, U] = \sum_{n,m} \bar{q}_f(n) D_f[U](n,m) q_f(m)$$ ← **Wilson Fermion Action**

$$D_f[U](n,m) = (\hat{M}_f + 4)\delta_{n,m} - \frac{1}{2}\sum_{\mu=1,2,3,4}\left[(1-\gamma_\mu)U_\mu(n)\delta_{n+\hat{\mu},m} + (1+\gamma_\mu)U_\mu(m)^\dagger \delta_{n-\hat{\mu},m}\right]$$

1. What is Lattice Quantum Chromodynamics?



- Lattice QCD [K.G.Wilson (1974)]

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$$D_f[U](n,m) = \delta_{n,m} - \kappa_f \sum_{\mu=1,2,3,4} \left[(1-\gamma_\mu) U_\mu(n) \delta_{n+\hat{\mu},m} + (1+\gamma_\mu) U_\mu(m)^\dagger \delta_{n-\hat{\mu},m} \right]$$

$\beta = \frac{6}{g^2}$, $\kappa_f = \frac{1}{m_f + 4}$

g^2 : coupling constant (color charge unit)
m_f : quark mass (flavor f)

- Lattice QCD is a theory based on this path-integral (multi dimensional integration) form. We can extract properties of nucleon or hadrons or atomic nuclei without relying on the perturbation theory by evaluating this integral.
  - Strictly maintain SU(3) gauge symmetry.
  - Discard the full Poincare symmetry but maintain the subgroup on the lattice.
  - A lot of variants of actions with various discretization schemes.
  - The multi-dimensional integration is evaluated via a Monte Carlo Method.

2. Monte Carlo Integration Methods

- We fist integrate the quark fields out as they are described by Gassmann numbers (explaining Pauli's exclusion rule).

$$\langle O \rangle = \frac{1}{Z} \int DU \prod_{f=u,d,s} D\bar{q}_f Dq_f O[U,\bar{q},q] e^{-S[U,\bar{q},q]} \qquad Z = \int DU \prod_{f=u,d,s} D\bar{q}_f Dq_f e^{-S[U,\bar{q},q]}$$

$$\left\langle O[U,D[U]^{-1}] \right\rangle = \frac{1}{Z_{LQCD}} \int \prod_{n,\mu} dU_\mu(n) O[U,D[U]^{-1}] \prod_{f=u,d,s} \det[D_f[U]] \exp\left[-S_G[U]\right]$$

$$Z_{LQCD} = \int \prod_{n,\mu} dU_\mu(n) \prod_{f=u,d,s} \det[D_f[U]] \exp\left[-S_G[U]\right]$$

- Now the integral becomes the integration on the SU(3) valued matrices $U_\mu(n)$.
- Pairs of $q_f(n)\overline{q_f}(m)$ in $O[U,\bar{q},q]$ are replaced by D_f^{-1}, and the quark actions are by $\prod_{f=u,d,s} \det[D_f]$.
- Various methods to evaluate multi-dimensional integration.
- Naive method, trapezoidal quadrature rule, fails as its high-dimensionality (curse of dimensionality).
  - For a 16^4 lattice, the DoF is $16^4 \times (8 \times 4) = 2097152$ real variables.
- Monte Carlo Methods are inevitable.

2. Monte Carlo Integration Methods

- Hybrid Monte Carlo Algorithm (HMC algorithm) [Duane, Kennedy, Pendleton, Roweth (1987)]

  [called "Hamiltonian Monte Carlo" in other fields]

  - Stochastic estimate of

$$\langle O \rangle = \frac{1}{Z} \int \mathrm{d}\vec{x} O(\vec{x}) \mathrm{e}^{-S(\vec{x})}, Z = \int \mathrm{d}\vec{x} \mathrm{e}^{-S(\vec{x})}, S(\vec{x}) \in \mathbb{R}, S(\vec{x}) > 0$$

Stochastic variable X : $\vec{x}$, Probability density/distribution : $P_X(\vec{x})\mathrm{d}\vec{x} = \mathrm{d}\vec{x} \frac{1}{Z} \mathrm{e}^{-S(\vec{x})}$

  - If we could obtain the stochastic ensemble for $X = \{\vec{x}^{(1)}, \vec{x}^{(2)}, \vec{x}^{(3)}, \ldots, \vec{x}^{(N-1)}, \vec{x}^{(N)}\}$, then

$$\langle O \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{s=1}^{N} O\left(\vec{x}^{(s)}\right)$$ Statistical average $$\Delta\langle O \rangle = \frac{1}{\sqrt{N}} \sigma(O)$$ Statistical Error

Low of Large Numbers, No curse of dimension

  - How to generate the ensemble satisfying the desired probability distribution? => Markov Chain Monte Carlo (MCMC)

- HMC algorithm is a kind of MCMC.
- HMC algorithm is a composition of Molecular Dynamics Algorithm and Metropolis-Hasitings Algorithm.
- MCMC evolution of HMC satisfies the detailed balance to realize the desired probability distribution.

2. Monte Carlo Integration Methods

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Stochastic variable X : $\vec{x}$, Probability density/distribution : $P_X(\vec{x})\mathrm{d}\vec{x} = \mathrm{d}\vec{x} \frac{1}{Z} \mathrm{e}^{-S(\vec{x})}$

  - Idea: Introduce auxiliary stochastic variable P: $\vec{p}$ with Gaussian distribution $P_P(\vec{p})\mathrm{d}\vec{p} = \mathrm{C}\mathrm{e}^{-\frac{1}{2}|\vec{p}|^2} \mathrm{d}\vec{p}$, and rewrite the equations as

$$\langle O \rangle = \frac{1}{Z_{\mathrm{HMC}}} \int \mathrm{d}\vec{p}\mathrm{d}\vec{x} O(\vec{x}) \mathrm{e}^{-H(\vec{p},\vec{x})}, Z_{\mathrm{HMC}} = \int \mathrm{d}\vec{p}\mathrm{d}\vec{x} \mathrm{e}^{-H(\vec{p},\vec{x})},$$

$$H(\vec{p},\vec{x}) = \frac{1}{2}|\vec{p}|^2 + S(\vec{x}) \in \mathbb{R}, H(\vec{p},\vec{x}) > 0$$

Stochastic variable (P,X): $(\vec{p},\vec{x})$, Probability density/distribution : $P_{(P,X)}(\vec{p},\vec{x})\mathrm{d}\vec{p}\mathrm{d}\vec{x} = \mathrm{d}\vec{p}\mathrm{d}\vec{x} \frac{1}{Z_{HMC}} \mathrm{e}^{-H(\vec{p},\vec{x})}$

  - This resembles/equivalent to the thermal average with Canonical ensemble method in equilibrium with temperature 1 in statistical mechanics.
  - The thermal averaging can also be evaluated with Micro-Canonical ensemble method. This reduces the problem to the problem in Classical mechanics. H(p,x): Hamitonian, p is the canonical momentum of x.

2. Monte Carlo Integration Methods

- Hybrid Monte Carlo Algorithm (HMC algorithm) [Duane, Kennedy, Pendleton, Roweth (1987)]

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  - Translation to Micro-Canonical ensemble

$$\langle O \rangle = \frac{\int \mathrm{d}\vec{p}\mathrm{d}\vec{x} O(\vec{x}) \mathrm{e}^{-H(\vec{p},\vec{x})}}{\int \mathrm{d}\vec{p}\mathrm{d}\vec{x} \mathrm{e}^{-H(\vec{p},\vec{x})}} = \frac{\int_0^\infty \mathrm{d}E \int \mathrm{d}\vec{p}\mathrm{d}\vec{x} O(\vec{x}) \delta(E - H(\vec{p},\vec{x})) \mathrm{e}^{-E}}{\int_0^\infty \mathrm{d}E \int \mathrm{d}\vec{p}\mathrm{d}\vec{x} \delta(E - H(\vec{p},\vec{x})) \mathrm{e}^{-E}}$$

$$= \frac{\int_0^\infty \mathrm{d}E \langle O \rangle_{MiC}(E) Z_{MiC}(E) \mathrm{e}^{-E}}{\int_0^\infty \mathrm{d}E Z_{MiC}(E) \mathrm{e}^{-E}} = \frac{\int_0^\infty \mathrm{d}E \langle O \rangle_{MiC}(E) \mathrm{e}^{-E+s(E)}}{\int_0^\infty \mathrm{d}E \mathrm{e}^{-E+s(E)}}$$

$$\langle O \rangle_{MiC}(E) = \frac{1}{Z_{MiC}(E)} \int \mathrm{d}\vec{p}\mathrm{d}\vec{x} O(\vec{x}) \delta\big(E - H(\vec{p},\vec{x})\big), \qquad Z_{MiC}(E) = \int \mathrm{d}\vec{p}\mathrm{d}\vec{x} \delta(E - H(\vec{p},\vec{x}))$$

$$s(E) = \log Z_{MiC}(E) \quad : \text{Entropy} \qquad \frac{\partial\big(E - s(E)\big)}{\partial E} = 0 \to \left.\frac{\partial s(E)}{\partial E}\right|_{E=\bar{E}} = 1, \qquad \text{Peak of } \exp\big(-E + s(E)\big)$$

  - In the thermodynamic limit: $\langle O \rangle \simeq \langle O \rangle_{MiC}(\bar{E})$
  - Micro-Canonical ensemble can be evaluated/generated by solving the classical equation of motion

$$\langle O \rangle_{MiC}(\bar{E}) = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}\tau O\big(\vec{x}(\tau)\big), @E = \bar{E} \qquad \dot{\vec{x}} = \vec{p}, \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{x}}$$

2. Monte Carlo Integration Methods

- Hybrid Monte Carlo Algorithm (HMC algorithm) [Duane, Kennedy, Pendleton, Roweth (1987)]

  [called "Hamiltonian Monte Carlo" in other fields]

  - Hybrid Molecular Dynamics (HMD) algorithm
  - Micro-Canonical ensemble can be evaluated/generated by solving the classical equation of motion

$$\langle O \rangle = \langle O \rangle_{MiC}(\bar{E}) = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{d}\tau O\left(\vec{x}(\tau)\right), @E = \bar{E} \qquad \dot{\vec{x}} = \vec{p}, \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{x}}$$

  - $E = \bar{E}$ can be realized by the heating/cooling process during the time evolution by introducing energy conservation violation.
  - Solving the classical Hamiltonian equation of motion = Molecular Dynamics (MD) evolution
  - The time parameter τ is introduced and is called fictitious time (not real time but virtual).
  - In terms of MCMC context, the MD evolution corresponds to the MC step evolution.
  - The initial momentum should be distributed in Gaussian as we introduced.
  - HMD algorithm has been introduced before HMC [Duane (1985), Duane,Kogut (1986)]

- One MCMC step of the HMD algorithm goes as
  1. Give an initial $\vec{x}$
  2. Draw an initial $\vec{p}$ from Gaussian distribution $P(\vec{p}) \sim \exp\left(-\frac{|\vec{p}|^2}{2}\right)$
  3. Solve Hamiltonian EoM for a fixed fictitious time duration τ [MD evolution=>Numerical computation=> needs HPC]
  4. Store $\vec{x}$ for ensemble
  5. Goto (2)

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- Hybrid Monte Carlo Algorithm (HMC algorithm) [Duane, Kennedy, Pendleton, Roweth (1987)]

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- Hybrid Molecular Dynamics (HMD) algorithm

  - We can solve the EoM with MD schemes.
  - The fictitious time evolution is discretized.

  - To make the HMD algorithm correct in terms of MCMC context, we need

  - Area preservation
  - [Time reversal to satisfy detailed balance]
  - Symplectic scheme / integrator has been used. (Shadow-Hamitonian conserves)

- The time discretization introduces systematics. The distribution obtained will be distorted from the desired one exp(-H). Naively we need to take the limit $\Delta\tau \to 0$, using several ensemble sets with different step size $\Delta\tau$. This is to time consuming.
- To resolve this issue, HMC algorithm appears.
  - HMC adds one Metropolis test at the end of the MD evolution to fix the distorted distribution to the desired one.

2. Monte Carlo Integration Methods

- Hybrid Monte Carlo Algorithm (HMC algorithm) [Duane, Kennedy, Pendleton, Roweth (1987)]

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① Give an initial $\vec{x}_0$

② Draw an initial $\overrightarrow{p_0}$ from Gaussian distribution $P(\vec{p}) \sim \exp\left(-\frac{|\vec{p}|^2}{2}\right)$

③ Compute the initial Energy (Hamiltonian) $E_0 = H(\vec{p}_0, \vec{x}_0)$

④ Solve Hamiltonian EoM for a fixed fictitious time duration τ [MD evolution=>Numerical computation=> needs HPC]

⑤ [Negate momentum $\vec{p}_1 := -\vec{p}_1$and] Compute the last Energy $E_1 = H(\vec{p}_1, \vec{x}_1)$

⑥ Do Metropolis test : Prob = $\min\left(1, \exp\left(-(E_1 - E_0)\right)\right)$: on accept $\vec{x} = \overrightarrow{x_1}$, on rejecgt $\vec{x} = \overrightarrow{x_0}$

⑦ Store $\vec{x}$ for ensemble

⑧ Set $\vec{x}_0 = \vec{x}$, Goto (2)

- MCMC context: The MD evolution should be
  - Time reversal, area preserving. Symplectic scheme has been used.

- HMC algorithm for Lattice QCD $\vec{x} = (x_i) \Leftrightarrow U_\mu(n)^{ab}$: SU(3) matrices

$$H(\vec{p}, \vec{x}) = \frac{1}{2}|\vec{p}|^2 + S(\vec{x})$$

$$\dot{\vec{x}} = \vec{p}$$

$$\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{x}}$$

$$\left\langle O[U, D[U]^{-1}] \right\rangle = \frac{1}{Z_{LQCD}} \int \prod_{n,\mu} dU_\mu(n) O[U, D[U]^{-1}] \prod_{f=u,d,s} \det[D_f[U]] \exp\left[-S_G[U]\right]$$

How to introduce the canonical momentum for U?
How to treat the determinant $\prod \det D[U]$ part?

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How to introduce the canonical momentum for U?
How to treat the determinant $\prod \det D[U]$ part?

- Introduce an auxiliary variable for the determinant factor.
- Two flavors of fermions : case that up and down quarks have an identical mass.

$$\det[D_u]\det[D_d] = \det[D_u]\det[D_u] = \det[D_u]\det\left[D_u^\dagger\right] = |\det[D_u]|^2 = C \int \mathrm{d}\phi^\dagger \mathrm{d}\phi \, \mathrm{e}^{-\left(D_u^{-1}\phi\right)^\dagger \left(D_u^{-1}\phi\right)}$$

Lattice Dirac operator D_u satisfies $D_u^\dagger = \gamma_5 D_u \gamma_5, \gamma_5^2 = I$

$\phi_\alpha^a(n)$: complex number field with color and spin indices. Pseudo-fermion field

$$\langle O \rangle = \frac{1}{Z} \int \mathrm{d}\phi^\dagger \mathrm{d}\phi \, \mathrm{d}U O[U, D[U]^{-1}] \mathrm{e}^{-\left(S_G[U] - \left(D_u^{-1}\phi\right)^\dagger \left(D_u^{-1}\phi\right)\right)}, Z = \int \mathrm{d}\phi^\dagger \mathrm{d}\phi \, \mathrm{d}U \mathrm{e}^{-\left(S_G[U] - \left(D_u^{-1}\phi\right)^\dagger \left(D_u^{-1}\phi\right)\right)}$$

- Single flavor of fermion case (Skip): The (inverse) square or (inverse) quadruple root of $\gamma_5 D_u$ are required.

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$$\dot{\vec{x}} = \vec{p}$$
$$\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{x}}$$

$$\left\langle O[U, D[U]^{-1}] \right\rangle = \frac{1}{Z_{LQCD}} \int \prod_{n,\mu} dU_\mu(n) O[U, D[U]^{-1}] \prod_{f=u,d,s} \det[D_f[U]] \exp\left[-S_G[U]\right]$$

How to introduce the canonical momentum for U?
How to treat the determinant $\prod \det D[U]$ part?

$$\langle O \rangle = \frac{1}{Z} \int \mathrm{d}\phi^\dagger \mathrm{d}\phi \, \mathrm{d}U O[U, D[U]^{-1}] \mathrm{e}^{-(S_G[U] - (D_u^{-1}\phi)^\dagger (D_u^{-1}\phi))}, Z = \int \mathrm{d}\phi^\dagger \mathrm{d}\phi \, \mathrm{d}U \mathrm{e}^{-(S_G[U] - (D_u^{-1}\phi)^\dagger (D_u^{-1}\phi))}$$

$$\langle O \rangle = \frac{1}{Z_{HMC}} \int \mathrm{d}\phi^\dagger \mathrm{d}\phi \, \mathrm{d}P \mathrm{d}U O[U, D[U]^{-1}] \mathrm{e}^{-H[P,U,\phi]}, Z_{HMC} = \int \mathrm{d}\phi^\dagger \mathrm{d}\phi \, \mathrm{d}P \mathrm{d}U \mathrm{e}^{-H[P,U,\phi]}$$

$$H[P,U,\phi] = \frac{1}{2} \sum_{n,\mu} Tr[P_\mu(n) P_\mu(n)] + S_G[U] + |(D_u[U])^{-1}\phi|^2$$

EoM of LQCD used in MD

$$\dot{U}_\mu(n) = iP_\mu(n) U_\mu(n)$$
$$\dot{P}_\mu(n) = -\frac{\delta H[P,U,\phi]}{\delta U_\mu(n)}$$

$P_\mu(n)$: 3x3 Hermitian-trace less matrix (su(3) Lie algebra valued)

ϕ is treated as external field and kept fixed during the MD evolution
Randomly generated at the beginning of the MD evolution according to the distribution $\exp[-|(D_u[U])^{-1}\phi|^2]$. This is Gaussian.

2. Monte Carlo Integration Methods

- Hybrid Monte Carlo Algorithm (HMC algorithm) [Duane, Kennedy, Pendleton, Roweth (1987)]

[called "Hamiltonian Monte Carlo" in other fields]

- HMC algorithm for Lattice QCD

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ϕ is treated as external field and kept fixed during the MD evolution
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$$F_\mu(n) = i\left[\left(V_\mu(n) - V_\mu(n)^\dagger\right) - \frac{1}{3}Tr\left[\left(V_\mu(n) - V_\mu(n)^\dagger\right)\right]\right] \qquad V_\mu(n) = V_\mu^G(n) + V_\mu^Q(n)$$

$$V_\mu^G(n) = \frac{\beta}{6}\sum_{\nu\neq\mu}\left[U_\mu(n)\left\{U_\nu(n+\hat{\mu})U_\mu(n+\hat{\nu})^\dagger U_\nu(n)^\dagger + U_\nu(n+\hat{\mu}-\hat{\nu})^\dagger U_\mu(n-\hat{\nu})^\dagger U_\nu(n-\hat{\nu})\right\}\right]$$

Contribution from Gluon action

$$V_\mu^Q(n) = -\kappa\left[U_\mu(n)\left\{\mathrm{tr}\left((1-\gamma_\mu)X(n+\hat{\mu})Y(n)^\dagger\right) + \mathrm{tr}\left((1+\gamma_\mu)Y(n+\hat{\mu})X(n)^\dagger\right)\right\}\right]$$

Contribution from Quark action

$$X(n) = ((D_u[U])^{-1}\phi)(n), Y(n) = (\gamma_5(D_u[U])^{-1}\gamma_5(D_u[U])^{-1}\phi)(n)$$

MD force contains two inversions of quark matrix $D_u[U]$ => solve Dirac equation twice in each MD step

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MD force contains two inversions of quark matrix $D_u[U]$ => solve Dirac equation twice in each MD step

- The quark part is the most time consuming part of the HMC in LQCD.
  - explicit form of D[U]

$$D_f[U]^{ab}_{\alpha\beta}(n,m) = \delta^{ab}\delta_{\alpha\beta}\delta(n,m) - \kappa_f\sum_{\mu=1}^{4}\left[\left(1-\gamma_\mu\right)_{\alpha\beta}U_\mu^{ab}(n)\delta(n+\hat{\mu},m) + \left(1+\gamma_\mu\right)_{\alpha\beta}\left\{U_\mu^{ba}(m)\right\}^*\delta(n-\hat{\mu},m)\right]$$

$a,b = 1,2,3$:color index, $\alpha,\beta = 1,2,3,4$: spin index, n,m : 4dim site index

  - matrix dimension (complex number) for $L^4 = 64^4$ lattice: $(3\times4\times L^4) = 201\,326\,592 \sim 2\times10^8$

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- MD evolution method/scheme : Typically Leapfrog method and its variants have been used.
  - Higher order scheme is not efficient in HMC.
  - Although a higher order scheme yields a better energy conservation and a high Metropolis acceptance rate, the acceptance would saturate at 100% and increasing computational cost does not pay [Creutz,Gockch (1989) Takaishi (2000)].

$$\text{Efficiency} = \frac{P_{acc}}{\text{Cost}}$$

Cost: computational cost for unit τ evolution, P_{acc} : HMC acceptance rate

  - However there are lots of efforts to improve P_{acc} with a lower computational cost.
    - Multiple time step scheme combined with transformations of the quark determinant part [Sexton, Weingarten (1992), ...]
    - minimizing error terms of the shadow-Hamiltonian [Omelyan,Mryglod,Folk (2002), Takaishi (2006), ...]
    - etc.
    - I will skip this topic.

• HMC algorithm for Lattice QCD

• Typical setup

- Lattice size : 64^4 – 128^4 for Wilson type fermions
- Simulation (physics) parameters :
  - β (coupling constant): 3 – 5 combinations, determine the lattice spacing and extrapolate to zero lattice spacing.
  - κ (quark mass) : 3 – 5 combinations, extrapolate/interpolate to the physical mass.
  - Lattice size : 2—3 combinations, physical volume has to be kept fixed and extrapolated to infinite volume.
- Total number of combinations (Ideal case) : (3 – 5)(3 – 5)(2 – 3)=18 – 75
- For each parameter set, we have to accumulate ~ 1000 independent Monte Carlo samples for statistical errors smaller than 10% (these numbers depend on physics target and observable).
- The samples generated with the HMC algorithm have autocorrelation. Typically we store samples every ~ 10 HMC steps with $\tau = 1$ at 70—90% acceptance rate to eliminate/reduce the correlation between the samples.
- The number of MD step is N_{MD} ~100—1000 to keep the above acceptance rate (N_{MD} strongly depends on the physics parameters).

Total number of inversion of quark matrix $D_u[U]$ to accomplish the above requirements is

$$(18 - 75) \times (1000) \times (10) \times (100 — 1000) \times 2 = (36 — 1500) \times 10^6 \sim 10^7 — 10^9$$

When the computational time for one inversion is 60[sec], the total time is $\sim 19 - 1902$ [years]

Parameter set parallelism can be used.
A single Markov-Chain cannot be parallelized.

3. Quark solvers

- Total performance of LQCD simulations strongly rely on the performance of computing the inversion of $D[U]$.

$$D_f[U]^{ab}_{\alpha\beta}(n,m) = \delta^{ab}\delta_{\alpha\beta}\delta(n,m) - \kappa_f \sum_{\mu=1}^{4}\left[(1-\gamma_\mu)_{\alpha\beta}U^{ab}_\mu(n)\delta(n+\hat{\mu},m) + (1+\gamma_\mu)_{\alpha\beta}\{U^{ba}_\mu(m)\}^*\delta(n-\hat{\mu},m)\right]$$

$a,b = 1,2,3$:color index, $\alpha,\beta = 1,2,3,4$: spin index, n,m : 4dim site index

- The matrix size is huge, the direct solve is impossible. => iterative methods have been employed.

$$\sum_{b,\beta,m} D[U]^{ab}_{\alpha\beta}(n,m)X^b_\beta(m) = \phi^a_\alpha(n) \qquad DX = \phi \quad \text{Linear equation for X}$$

$$X = D^{-1}\phi \quad \text{Solution X, used in MD of HMC}$$

- The performance of the linear solver is important in LQCD. Various algorithms are available in applied math field.
  - Conjugate Gradient (CG) algorithm, Bi-Conjugate Gradient Stabilized (BiCGStab) algorithm, Generalized Minimal Residual (GMRES) algorithm, ... etc.
  - and many improved versions...

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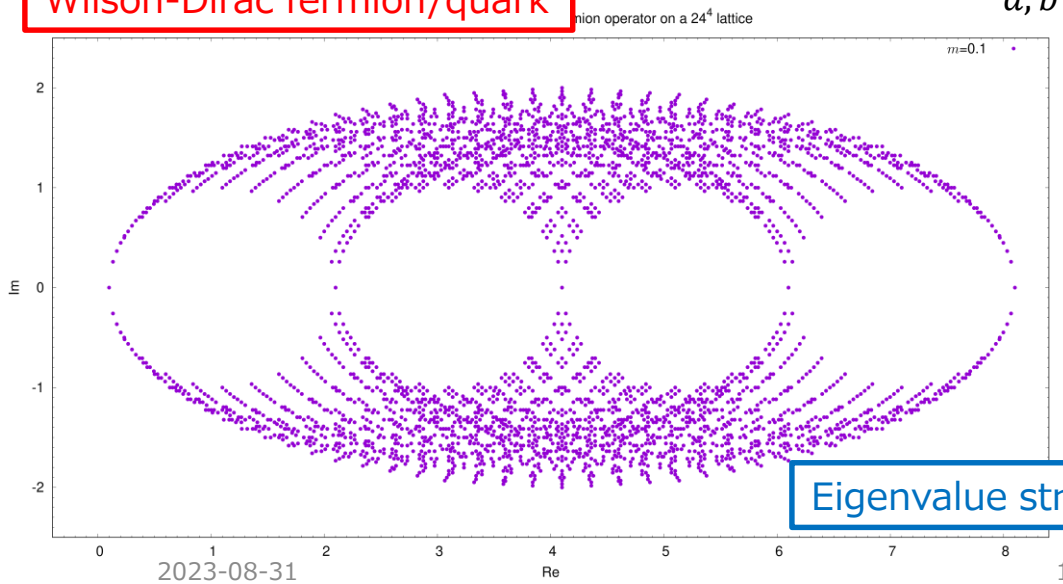
  - and many improved versions...
- Choice of solver algorithm depends on the property of the coefficient matrix.

$DX = \phi$ Linear equation for X $X = D^{-1}\phi$ Solution X, used in MD of HMC

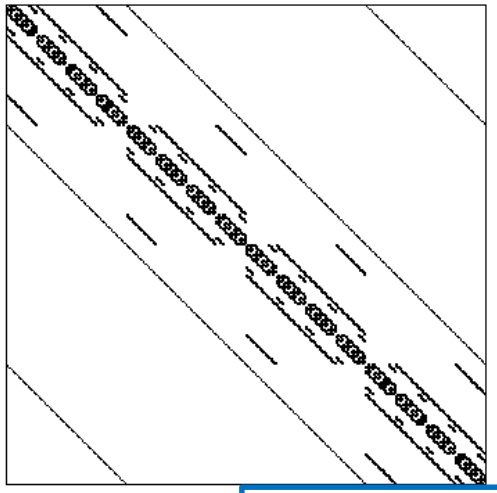
$$D_f[U]^{ab}_{\alpha\beta}(n,m) = \delta^{ab}\delta_{\alpha\beta}\delta(n,m) - \kappa_f \sum_{\mu=1}^{4}\left[(1-\gamma_\mu)_{\alpha\beta}U^{ab}_{\mu}(n)\delta(n+\hat{\mu},m) + (1+\gamma_\mu)_{\alpha\beta}\left\{U^{ba}_{\mu}(m)\right\}^{*}\delta(n-\hat{\mu},m)\right]$$

Wilson-Dirac fermion/quark

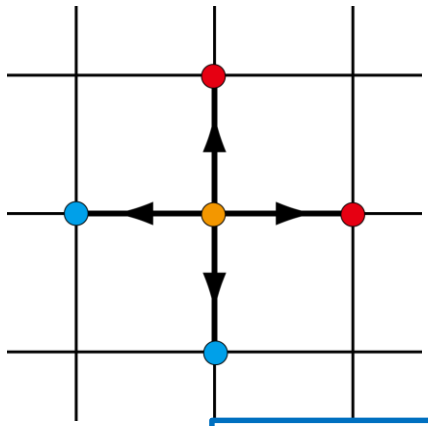
$a, b = 1,2,3$:color index, $\alpha, \beta = 1,2,3,4$: spin index, n, m : 4dim site index



Eigenvalue structure



Sparse matrix structure



Stencil structure

3. Quark solvers

- Choice of solver algorithm depends on the property of the coefficient matrix.

$DX = \phi$ Linear equation for X $X = D^{-1}\phi$ Solution X, used in MD of HMC

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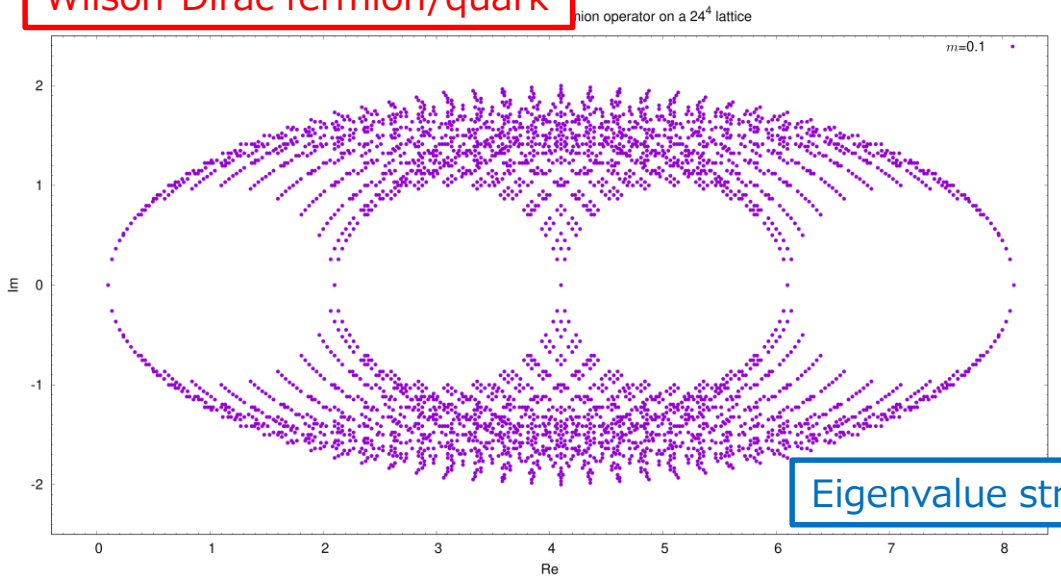
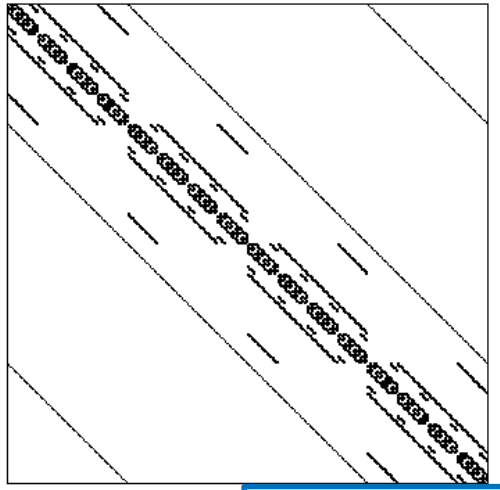
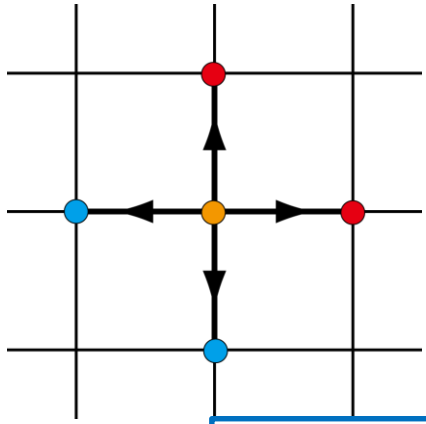


Eigenvalue structure



Sparse matrix structure



Stencil structure

- The coefficient matrix is not Hermite, but has γ_5-Hermiticity $\gamma_5 D \gamma_5 = D^\dagger$ => CGLS can be used.
- Wilson quark case: The complex eigenvalue Re(λ)>0 for a positive mass. => BiCGStab is more effective.
- For other fermion actions (overlap, domainwall, staggered fermion actions), other choices will be applied.

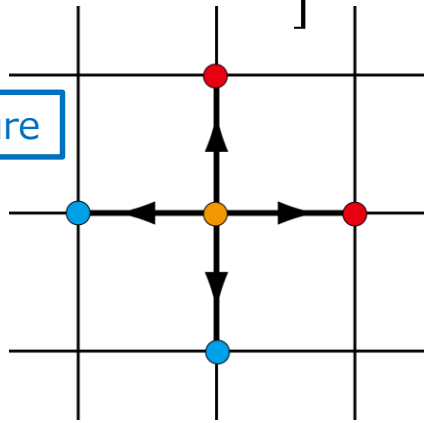
3. Quark solvers

- HPC-Phys context: Sparse matrix-vector multiplication $\chi = D\eta$

$$\chi^a_\alpha(n) = \eta^a_\alpha(n) - \kappa_f \sum_{\mu=1}^{4} \left[\sum_{b=1,2,3;\beta=1,2,3,4} (1-\gamma_\mu)_{\alpha\beta} U^{ab}_\mu(n) \eta^b_\beta(n+\hat{\mu}) + \sum_{b=1,2,3;\beta=1,2,3,4} (1+\gamma_\mu)_{\alpha\beta} \{U^{ba}_\mu(n-\hat{\mu})\}^* \eta^b_\beta(n-\hat{\mu}) \right]$$

  - The structure of coefficient matrix is rather simple.
  - No room for optimization at the local level (site level).
  - Compute complexity/ input-output data movement at a site : (Flop/Byte)/site

Stencil structure

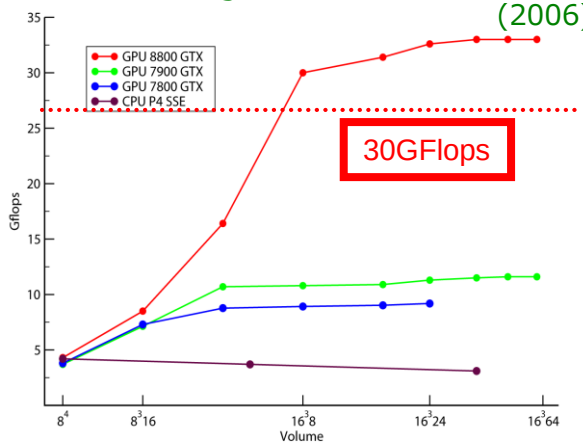


Action type	Double precision Flop/Byte	Single precision Flop/Byte
Wilson-Dirac (1296Flop/site, 168 complx/site)	0.9643	0.4821
O(a)-improved Wilson-Dirac(1896Flop/site,210 cmplx/site)	1.129	0.5643

Numbers in the Flop/Byte table could be incorrect by a factor two. Anyway, the memory bandwidth is the bottleneck of this computation.

  - Mixed-precision/single precision acceleration has become popular.
  - GPU acceleration is applicable and is popular now.
  - Short vector (SIMD) for color/spin/complex indices
  - Long vector (vector machine/GPU) for site indices
  - Domain decomposed parallelism is inevitable.
    - MPI + OpenMP or GPU mutithread

"**Lattice QCD as a video game**", G.I.Egri, Z.Fodor, S.D.Katz, D.Nogradi, K.K.Szabo, (2006) hep-lat/0611022.



- (Skip) Applied math context :
  - Preconditioner, low-mode recycling, algebraic-Multi-Grid etc.

4. Summary

- I have explained the Lattice QCD.
- Monte Carlo sampling is used for quantum expectation values.
- HMC algorithm is explained.
- Quark contribution in the MD evolution is the most heavy part of the algorithm.
- The contribution is inversion of the quark matrix, and it needs linear equation solvers.
- The structure of Wilson-Dirac quark matrix is explained, and it is rather simple.
- The performance of computer could directly reflect the performance of quark solver, or vice-versa.