Numerical Time Integration in Hybrid Monte Carlo Schemes for Lattice Quantum Chromo Dynamics

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Contents

Physical background

Quantum Chromo Dynamics (QCD)

- QCD is the theory of the strong interaction (=color force) between quarks and gluons inside subatomic particles.
- Quark = elementary particle, fundamental constituent of matter, e.g., protons and neutrons.
- Gluons = exchange particles for the strong force between quarks.

Lattice QCD

- approach to solve the theory of QCD
- investigation of elementary particles using computer simulations
- formulated on a lattice of points in space and time
- links $U_\mu(x) \in SU(3)$ between points x and $x + a\hat{\mu}$

Task of Lattice QCD

Compuation of observables (particle mass, e.g.)

observables given as expectation of certain operators O:

$$\langle O \rangle = \int_\Omega O(U)\Pi(U)\mathrm{d}U \quad \text{with}$$

- probability space $(\Omega, \sigma(\Omega), F_\Pi)$
- $\Omega = (SU(3))^N$, $N =$ lattice size
- probability density $\Pi(U) = \exp(-S(U))/Z$ with $Z = \int_\Omega \exp(-S(U))\mathrm{d}U$,
- action S acting on $U \in \Omega$.

Problem: integral has very high dimension

$N = 64 \cdot 32^3$, for example

Importance sampling

Approximate integral by

$$\langle O \rangle \approx \frac{1}{n} \sum_{i=1}^{n} O(U_i)$$

- choose configurations U_i according to the probability density $\exp(-S(U))/Z$
- prefer configurations that occur with a higher probability
- sequence
  - is generated by a Markov chain
  - is ergodic
  - satisfies the detailed balance condition

$\Longrightarrow$ convergence to the unique fixed point distribution given by the density $\Pi(U)$

Hybrid Monte Carlo

Method of choice in Lattice QCD

- uses augmented Markov chain
- constructs samples of pairs of links $U \in \Omega$ and momenta $P \in \hat{\Omega} = (\mathfrak{su}(3))^N$
- samples generated according to the probability density $\nu(U,P)$ given by

$$\begin{aligned}\nu(U,P) &= \underbrace{\frac{(2\pi)^{N/2}}{Z_H}\exp(-S(U))}_{:=\Pi(U)} \cdot \underbrace{\frac{1}{(2\pi)^{N/2}}\exp(-\langle P,P\rangle/2)}_{:=\varphi(P)} \\ &= \frac{1}{Z_H}\exp(-H(U,P)) \qquad \text{with}\end{aligned}$$

$$Z_H = \int_{\Omega\times\hat{\Omega}} \nu(U,P)\mathrm{d}(U,P), \qquad H(U,P) = \langle P,P\rangle/2 + S(U)$$

Transition $(U_0, P_0) \to (U^\star, P^\star)$

Proposal step

$$(U_0, P_0) \to g(U_0, P_0)$$

for the moment: arbitrary mapping $g : \Omega \times \hat{\Omega} \to \Omega \times \hat{\Omega}$

Acceptance step

- $(U^*, P^*) := g(U_0, P_0)$
  $g(U_0, P_0)$ is accepted with probability

$$\begin{aligned} \alpha((U_0, P_0) g(U_0, P_0)) &= \min\left(1, \frac{\nu(g(U_0, P_0))}{\nu(U_0, P_0)}\right) \\ &= \min\left(1, e^{-(H(g(U_0,P_0)) - H(U_0,P_0))}\right) \end{aligned}$$

- otherwise the old configuration is kept:
  $(U^*, P^*) := (U_0, P_0)$

Demand on g

Detailed balance condition holds if

- g is time-reversible:

$$S \cdot g(S \cdot g(U_0, P_0)^\top) = (U_0, P_0)^\top$$

with $S = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ flipping the momenta

- g is volume-preserving:

$$\left| \det \left(\frac{\partial g(U_0, P_0)}{\partial (U_0, P_0)} \right) \right| = 1.$$

Choice of g?

Detailed Balance condition I

Transition kernel in HMC

$$\begin{aligned} K((U_0,P_0),(\Omega'\times\hat{\Omega}')) &= P((U^*,P^*)\in(\Omega'\times\hat{\Omega}')|(U_0,P_0)) \\ &= \alpha((U_0,P_0),g(U_0,P_0))\delta_{g(U_0,P_0)}(\Omega'\times\hat{\Omega}') + \\ &\quad (1-\alpha((U_0,P_0),g(U_0,P_0)))\delta_{(U_0,P_0)}(\Omega'\times\hat{\Omega}'). \end{aligned}$$

Restricted Transition kernel

$$K_L(U_0,\Omega') = P(U_0\in\Omega'|U_0) = \int_{\hat{\Omega}} K((U_0,P),(\Omega'\times\hat{\Omega}))\varphi(P)\mathrm{d}P$$

Detailed Balance condition for all $A,B\in\sigma(\Omega)$

$$\int_A K_L(U,B)\Pi(U)\mathrm{d}U = \int_B K_L(U,A)\Pi(U)\mathrm{d}U$$

Detailed Balance condition II

Detailed Balance condition for all $A, B \in \sigma(\Omega)$

$$\int_A K_L(U, B)\Pi(U)\mathrm{d}U = \int_B K_L(U, A)\Pi(U)\mathrm{d}U$$

Left-hand side

$$\int_A \int_{\hat{\Omega}} \min\left(1, \frac{\nu(g(U,P))}{\nu(U,P)}\right) \delta_{g(U,P)}(B \times \hat{\Omega})\varphi(P)\Pi(U)\mathrm{d}P\mathrm{d}U +$$
$$\int_{A\cap B} \int_{\hat{\Omega}} \left(1 - \min\left(1, \frac{\nu(g(U,P))}{\nu(U,P)}\right)\right) \varphi(P)\Pi(U)\mathrm{d}P\mathrm{d}U.$$

Right-hand side

$$\int_B \int_{\hat{\Omega}} \min\left(1, \frac{\nu(g(U,P))}{\nu(U,P)}\right) \delta_{g(U,P)}(A \times \hat{\Omega})\varphi(P)\Pi(U)\mathrm{d}P\mathrm{d}U +$$
$$\int_{B\cap A} \int_{\hat{\Omega}} \left(1 - \min\left(1, \frac{\nu(g(U,P))}{\nu(U,P)}\right)\right) \varphi(P)\Pi(U)\mathrm{d}P\mathrm{d}U.$$

Detailed Balance condition III

To be shown

$$\int_A \int_{\hat{\Omega}} \min\left(\nu(U,P), \nu(g(U,P))\right) \delta_{g(U,P)}(B \times \hat{\Omega}) \mathrm{d}(P,U) =$$
$$\int_B \int_{\hat{\Omega}} \min\left(\nu(U,P), \nu(g(U,P))\right) \delta_{g(U,P)}(A \times \hat{\Omega}) \mathrm{d}(P,U) \,.$$

With $\delta_{g(U,P)}(B \times \hat{\Omega}) = \delta_{(U,P)}(g^{-1})(B \times \hat{\Omega}))$

$$\underbrace{\int_{(A\times\hat{\Omega})\cap g^{-1}(B\times\hat{\Omega})} \min\left(\nu(U,P), \nu(g(U,P))\right) \mathrm{d}(P,U)}_{F_1 =} =$$

$$\underbrace{\int_{(B\times\hat{\Omega})\cap g^{-1}(A\times\hat{\Omega})} \min\left(\nu(U,P), \nu(g(U,P))\right) \mathrm{d}(P,U)}_{F_2 =}$$

Detailed Balance condition IV

$\varphi(P) = \varphi(-P)$, $\nu(U,P) = \nu(U,-P)$ & g time reversible

$$\nu(g(U,P)) = \nu(g^{-1}(U,-P)) \quad \& \quad g(U,-P) = g^{-1}(U,P)$$

Rewrite F_1 as

$$F_1 = \int_{g^{-1}(B\times\hat{\Omega})} \min\left(\nu(U,P), \nu(g(U,P))\right) \delta_{(U,P)}(A\times\hat{\Omega}) d(P,U) =$$

$$\int_{B\times\hat{\Omega}} \min\left(\nu(g^{-1}(U,P)), \nu(U,P)\right) \delta_{g^{-1}(U,P)}(A\times\hat{\Omega}) \cdot \left|\det \frac{dg^{-1}(U,P)}{d(U,P)}\right| d(P,U) =$$

$$\int_{B\times\hat{\Omega}} \min\left(\nu(g(U,-P)), \nu(U,-P)\right) \delta_{g^{-1}(U,P)}(A\times\hat{\Omega}) \cdot \left|\det \frac{dg^{-1}(U,P)}{d(U,P)}\right| d(P,U) =$$

$$\int_{B\times\hat{\Omega}} \min\left(\nu(g(U,-P)), \nu(U,-P)\right) \delta_{g(U,-P)}(A\times\hat{\Omega}) \cdot \left|\det \frac{dg^{-1}(U,P)}{d(U,P)}\right| d(P,U) =$$

$$\int_{(B\times\hat{\Omega})\cap g^{-1}(A\times\hat{\Omega})} \min\left(\nu(g(U,P)), \nu(U,P)\right) \underbrace{\left|\det \frac{dg^{-1}(U,P)}{d(U,P)}\right|}_{=1} d(P,U) = F_2$$

Choice of g

Demand on g: time-reversible and volume-preserving mapping

- Natural choice: use Hamiltonian flow $H(U,P) = \langle P, P\rangle/2 + S(U)$
- Problem: analytical flow not available
- Way-out: use numerical approximation using geometric integration
- accuracy of less importance (only to get high acceptance rate)

Demand on numerical approximation of g

- time-reversible & volume preserving numerical flow
- compatible with non-Abelian structure of $U \in (SU(3))^N$ and $P \in (\mathfrak{su}(3))^N$

Derivation of Equation of Motion

Time Derivative of Links $U_\mu(x) \in SU(3)$

derived via an infinitesimal rotation on the group manifold

$$\dot{U}_\mu(x) = P_\mu(x) U_\mu(x)$$

Time Derivative of Momenta $P_\mu(x) \in \mathfrak{su}(3)$

- usually: solve $\dot{H}(U,P) = 0$ for $\dot{P}_\mu(x)$
- via the link differential operator

$$\dot{P}_\mu(x) = -\partial_{x,\mu} H(U,P) = -\partial_{x,\mu} S(U)$$

$$\partial_{x,\mu} f(U) = T^i \partial^i_{x,\mu} f(U) \quad \text{with} \quad \partial^i_{x,\mu} f(U) = \left. \frac{\mathrm{d} f(U_s)}{\mathrm{d}s} \right|_{s=0}$$

$$(U_s)_\nu(y) = \begin{cases} \mathrm{e}^{sT^i} U_\mu(x) & \text{if } (y,\nu) = (x,\mu) \\ U_\nu(y) & \text{otherwise} \end{cases} .$$

Example: Wilson action

$S_g(U) = -\frac{\beta}{N}\mathrm{Re}\,\mathrm{tr}(U_\mu(x)\Sigma_\mu^\dagger(x)) + \text{terms indep. of } U_\mu(x)$

Staples $\Sigma_\mu(x)$ defined by

$$\sum_{\nu\neq\mu}\left[U_\nu(x)U_\mu(x+a\hat{\nu})U_\nu(x+a\hat{\mu})^{-1} + U_\nu(x-a\hat{\nu})^{-1}U_\mu(x-a\hat{\nu})U_\nu(x-a\hat{\nu}+a\hat{\mu})\right]$$

$$\begin{aligned}
\Rightarrow \partial^i_{x,\mu} S_g(U) &= -\frac{\beta}{N}\mathrm{Re}\,\mathrm{tr}\Big\{T^i U_\mu(x)\Sigma_\mu^\dagger(x)\Big\} \\
\Rightarrow \partial_{x,\mu} S_g(U) &= -\frac{\beta}{N}T^i\mathrm{Re}\,\mathrm{tr}\Big\{T^i U_\mu(x)\Sigma_\mu^\dagger(x)\Big\} \\
&= \frac{\beta}{2N}\{U_\mu(x)\Sigma_\mu^\dagger(x)\}_{TA}
\end{aligned}$$

Time Derivative of Momenta $P_\mu(x) \in \mathfrak{su}(3)$

$$\dot{P}_\mu(x) = -\partial_{x,\mu} S_g(U) = -\frac{\beta}{2N}\{U_\mu(x)\Sigma_\mu^\dagger(x)\}_{TA}$$

Numerical integration on Lie groups

Structure of ODE-IVP

$$\begin{aligned} \dot{U} &= \operatorname{diag}(P_\mu(x)U_\mu(x)), & U(t_0) &= U_0 \\ \dot{P} &= -\partial_{x,\mu}S(U), & P(t_0) &= P_0 \end{aligned}$$

with $U \in (SU(3))^N$, $P \in (\mathfrak{su}(3))^N$.

Problem for Numerical integration schemes

- multiplicative structure of Lie group does not fit the additive structure of integrations schemes (RK and others)
- way-out: bypass via the Lie algebra with its additive structure (Magnus, 1954)

Bypass via Lie algebra

Lie algebra parameterization of U

$$U(t) = \Psi(\Omega(t))U_0 \quad \text{with } \Psi(t_0) = 0$$

Transformation of ODE

$$\begin{aligned}
\dot{U} &= \left(\frac{\mathrm{d}}{\mathrm{d}\Omega}\Psi(\Omega(t))\right)\dot{\Omega}(t)U_0 \\
&= \left(\mathrm{d}\Psi_{\Omega(t)}\left(\dot{\Omega}(t)\right)\right)\Psi(\Omega(t))U_0 \\
&= \underbrace{\left(\mathrm{d}\Psi_{\Omega(t)}\left(\dot{\Omega}(t)\right)\right)}_{=P(t)!}U(t) \\
\Rightarrow P(t) &= \mathrm{d}\Psi_{\Omega(t)}\left(\dot{\Omega}(t)\right) \\
\Rightarrow \dot{\Omega}(t) &= \mathrm{d}\Psi^{-1}_{\Omega(t)}\left(P(t)\right).
\end{aligned}$$

Transformed ODE system

Solve ODE-IVP on Lie-algebra

$$\begin{aligned} \dot{\Omega}_\mu(x) &= \mathrm{d}\Psi^{-1}_{\Omega_\mu(x)}\left(P_\mu(x)\right), & \Omega_\mu(x)(t_0) &= 0, \\ \dot{P} &= -\partial_{x,\mu} S(\Psi(\Omega)U_0), & P(t_0) &= P_0 \end{aligned}$$

$\Rightarrow$ links can be obtained via the transformation

$$U_\mu(x)(t) = \Psi(\Omega_\mu(x)(t))U_0$$

Possible choice of parameterization

- Exponential map: $\Psi(\Omega) = \exp(\Omega) = \sum_{k=0}^{\infty} \frac{1}{k!}\Omega^k$
- Cayley map: $\Psi(\Omega) = \mathrm{cay}(\Omega) = (I - \Omega)^{-1}(I + \Omega)$

Exponential map

$\psi(\Omega) = \exp(\Omega) = \sum_{k=0}^{\infty} \frac{1}{k!}\Omega^k$

$$\begin{aligned}
\dot{\Omega}(t) &= \mathrm{d}\exp_{\Omega}^{-1}(P(t)) \\
&= \sum_{k\geq 0} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k}(P(t)) \\
&= P(t) - \frac{1}{2}\left[\Omega(t), P(t)\right] + \frac{1}{12}\left[\Omega(t), \left[\Omega(t), P(t)\right]\right] + \ldots
\end{aligned}$$

- Problem: for numerical integration schemes, infinite sum has to be truncated: $\sum_{k\geq 0} \rightsquigarrow \sum_{k=0}^{q}$
- Compatability with numerical integration schemes: Order p if a) RK scheme has order p and b) $q + 2 \geq p$ holds (Munthe-Kaas).

Cayley map

$$\psi(\Omega) = \mathrm{cay}(\Omega) = (I - \Omega)^{-1}(I + \Omega)$$

$$\begin{aligned} \dot{\Omega}(t) &= \mathrm{d}cay_{\Omega}^{-1}(P(t)) \\ &= \frac{1}{2}(I - \Omega(t))P(t)(I + \Omega(t)) \end{aligned}$$

- No infinite series, no trunaction needed
- No compatability condition
- cheap evaluations!

The basis scheme: leap frog

Exponential map: Update $(U_n, P_n) \rightsquigarrow (U_{n+1}, P_{n+1})$

$$
\begin{aligned}
P_{n+\frac{1}{2}} &= P_n - \frac{h}{2}\partial_{x,\mu} S(U_n), \\
\Omega_{n+1} &= \Omega_n + h \cdot d\exp_\Omega^{-1}(P_{n+\frac{1}{2}}) \approx \Omega_n + h \cdot P_{n+\frac{1}{2}}, \\
U_{n+1} &= \exp(\Omega_{n+1}) U_n, \\
P_{n+1} &= P_{n+\frac{1}{2}} - \frac{h}{2}\partial_{x,\mu} S(U_{n+1}).
\end{aligned}
$$

Elimination of the auxiliary Ω variable

$$
\begin{aligned}
U_{n+1} &= \exp(h \cdot (P_n - \frac{h}{2}\partial_{x,\mu} S(U_n))) U_n, \\
P_{n+1} &= P_n - \frac{h}{2}\partial_{x,\mu} S(U_n) - \frac{h}{2}\partial_{x,\mu} S(\exp(h \cdot (P_n - \frac{h}{2}\partial_{x,\mu} S(U_n))))
\end{aligned}
$$

The basis scheme: leap frog

Cayley map: Update $(U_n, P_n) \rightsquigarrow (U_{n+1}, P_{n+1})$

$$
\begin{aligned}
P_{n+\frac{1}{2}} &= P_n - \frac{h}{2}\partial_{x,\mu} S(U_n), \\
\Omega_{n+1} &= \Omega_n + h \cdot d\mathrm{cay}_\Omega^{-1}(P_{n+\frac{1}{2}}) \\
&= \Omega_n + \frac{h}{2}(I - \Omega_n) P_{n+\frac{1}{2}} (I + \Omega_n), \\
U_{n+1} &= \mathrm{cay}(\Omega_{n+1}) U_n = (I - \Omega_{n+1})^{-1}(I + \Omega_{n+1}) U_n, \\
P_{n+1} &= P_{n+\frac{1}{2}} - \frac{h}{2}\partial_{x,\mu} S(U_{n+1}).
\end{aligned}
$$

Elimination of the auxiliary Ω variable

$$
\begin{aligned}
U_{n+1} &= \mathrm{cay}(h \cdot d\mathrm{cay}_\Omega^{-1}(P_n - \frac{h}{2}\partial_{x,\mu} S(U_n))) U_n, \\
P_{n+1} &= P_n - \frac{h}{2}\partial_{x,\mu} S(U_n) - \frac{h}{2}\partial_{x,\mu} S(\mathrm{cay}(h \cdot d\mathrm{cay}_\Omega^{-1}(P_n - \frac{h}{2}\partial_{x,\mu} S(U_n))))
\end{aligned}
$$

Higher-order schemes — Composition

Starting point: basis scheme φ_t^h order p, time-reversible & volume-preserving

$$\begin{pmatrix} U_{n+1} \\ P_{n+1} \end{pmatrix} = \varphi_{t_n}^h \begin{pmatrix} U_n \\ P_n \end{pmatrix}$$

Composition of m basic schemes

$$\tilde{\varphi}_{t_n}^h = \varphi_{t_n}^{\gamma_1 h} \circ \varphi_{t_n}^{\gamma_2 h} \circ \cdots \circ \varphi_{t_n}^{\gamma_m h}$$

- Volume-preservation $\surd$
- Condition for time-reversibility:

$$\gamma_{m+1-k} = \gamma_k, \quad k = 1, \ldots, m-1$$

- Order $p+1$, if the underlying scheme has order p:

$$\sum_{j=1}^{m} \gamma_j = 1, \qquad \sum_{j=1}^{m} \gamma_j^p = 0$$

- For leap-frog to get $p = 4$: $m = 3$, $\gamma_1 = \gamma_3 = (2 - \sqrt[3]{2})^{-1/3}$, $\gamma_2 = 1 - 2\gamma_1$.

Higher-order schemes — Splitting

Starting point: sequence of link and momenta updates

Momenta Update

$$\begin{aligned} \dot{U}_\mu(x) &= 0 \\ \dot{P}_\mu(x) &= -\partial_{x,\mu} S(U) \end{aligned}$$

Link Updata

$$\begin{aligned} \dot{U}_\mu(x) &= P_{\mu,x} \cdot U_{\mu,x} \\ \dot{P}_\mu(x) &= 0 \end{aligned}$$

- in general: order 1
- at least order 2, if splitting symmetric
- important classes: Omelyan and force-gradient schemes

Higher-order schemes — Examples

Symmetric five-stage Omelyan scheme

$$P_{\lambda h} \circ U_{h/2} \circ P_{(1-2\lambda)h} \circ U_{h/2} \circ P_{\lambda h} \quad \text{with}$$

$$\lambda = \frac{1}{2} - \frac{(2\sqrt{326}+36)^{1/3}}{12} + \frac{1}{6(2\sqrt{326}-36)^{1/3}}$$

Still order 2, but minimal leading error coefficient

Five stage force-gradient scheme of order 4

$$\tilde{P}_{\lambda h,\xi h^3} \circ U_{h/2} \circ \tilde{P}_{(1-2\lambda)h,\chi h^3} \circ U_{h/2} \circ \tilde{P}_{\lambda h,\xi h^3} \quad \text{with}$$

$$\lambda = \frac{1}{6}, \quad \xi = 0, \quad \chi = \frac{1}{72}$$

Higher-order schemes — Discussion

Exponential mapping

- leap-frog scheme used as basic scheme
- time-reversibility & volume preservation $\surd$
- but: truncation order $q = 0$
- Problem: $-(H(g(U_0, P_0) - H(U_0, P_0)) = \mathcal{O}((\Delta t)^2)$ only
- high order only with respect to modified equation of motion

$$\begin{aligned} \dot{\Omega}_\mu(x) &= P_\mu(x), \\ U_{\mu,x}(t) &= \exp\left(\Omega_\mu(x)(t)\right) U_\mu(x)(0) \\ \dot{P}_\mu(x) &= -\partial_{x,\mu} S(U) \end{aligned}$$

- possible way out: if modified equation of motion based on modified Hamiltonian $\tilde{H}(U, P)$, use $g(U, P) := \tilde{H}(U, P)$ instead of $H(U, P)$

Fermionic fields

Additional action: pseudofermionic field

Partition function now given by

$$
\begin{aligned}
Z &= \int \exp\left(-S_g(U)\right)\det(DD^\dagger)\mathrm{d}U \quad \text{with} \\
\det(DD^\dagger) &= \int \exp\left(-S_{pf}(U,\phi)\right)\mathrm{d}\phi, \\
S_{pf}(U,\phi) &= \langle \phi, (DD^\dagger)^{-1}\phi \rangle
\end{aligned}
$$

$$
\Rightarrow H(U,P) = \frac{1}{2}\langle P, P\rangle + S_g(U) + S_{pf}(U,\phi)
$$

Computation of pseudofermionic force

Additional action: pseudofermionic field

$$
\begin{aligned}
\partial_{x,\mu} S_{pf(U,\phi)} &= -2\mathrm{Re} T^i \langle (DD^\dagger)^{-1}\phi, \delta^i_{x,\mu}\phi \rangle \\
(\delta^i_{x,\mu}\phi)(y) &= -\delta_{y,x}\frac{1}{2}(1-\gamma_\mu)T^i U_\mu(x) D^{-1}\phi(x+\hat{\mu}) \\
&\quad +\delta_{y,x+\hat{\mu}}\frac{1}{2}(1+\gamma_\mu)U_\mu^{-1}(x)T_i D^{-1}\phi(x)
\end{aligned}
$$

Note: Computation requires two expensive inversions of the Wilson-Dirac operator

Nested integration - multirate schemes

Idea: use different activity levels

- gauge field S_g: fast dynamics, cheap evaluations
- pseudofermionic field S_{pf}: slow dynamics, expensive evaluations
- exploit different dynamics by multirate schemes: higher/lower sample rate for fast/slow part
- introduce additional activity splitting of pseudofermionic field: even-odd preconditioning, domain decomposition and determinant splitting

$$S_{pf}(U,\phi\ \ ) = \sum_{m=1}^{M} S_k[U,\phi],$$

$$\Rightarrow H(U,P) \quad = \quad \langle P,P\rangle/2 + S_g(U) + \sum_{m=1}^{M} S_k[U,\phi].$$

Sexton and Weingarten

First step

- macro step size h_0
- micro step size $h_1 = h_0/m_1$

Leap-frog step

$$V_H(h_0) = V_{H_2}(h_0/2)\left(V_{H_1}(h_1)\right)^{m_1} V_{H_2}(h_0/2) \quad \text{with}$$

$$H_1(U,P) = \langle P,P\rangle/2 + S_g[U] + \sum_{m=1}^{M-1} S_k[U,\phi], \quad H_2(U,P) = S_M[U,\phi]$$

Nesting

- next finer step size $h_2 = h_1/m_2$
- further splitting H_1 into

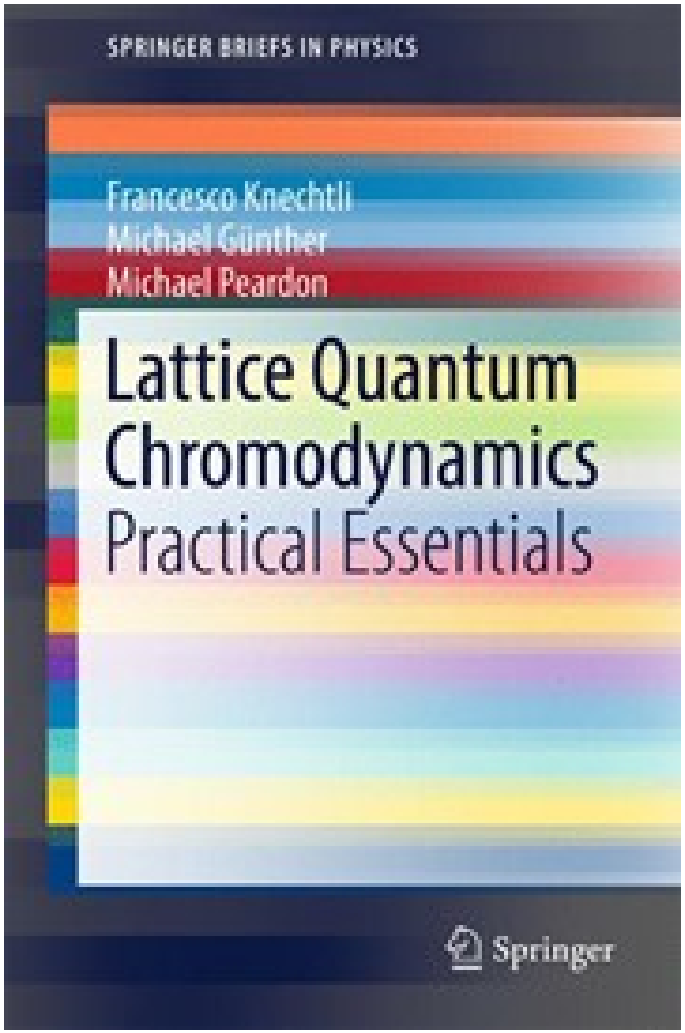
$$H_1(U,P) = H_{11}(U,P) + H_{12}(U,P) \quad \text{with}$$

$$H_{11}(U,P) = \langle P,P\rangle/2 + S_g[U] + \sum_{m=1}^{M-2} S_k[U,\phi], \quad H_{12}(U,P) = S_{M-1}[U,\phi]$$

- replace $V_{H_1}(h_1)$ above by

$$V_{H_1}(h_1) = V_{H_{12}}(h_1/2)\left(V_{H_{11}}(h_2)\right)^{m_2} V_{H_{12}}(h_1/2).$$

More to read ...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