

# Object of the Talk



Discuss the rôle of <u>symmetric symplectic integrators</u> in the HMC algorithm Show that there is a <u>shadow Hamiltonian</u> that is exactly conserved by each such integrator, and that we may express it using a BCH expansion in terms of Poisson brackets Explain how we may tune the choice of integrator by measuring these Poisson brackets Explain how we construct symplectic integrators on Lie groups, and what the corresponding Poisson brackets are

#### Caveat



A recent (published) paper had near the beginning the passage

"The object of this paper is to prove (something very important)."

It transpired with great difficulty, and not till near the end, that the "object" was an unachieved one.

Littlewood, "A Mathematician's Miscellany"

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# HMC



 The HMC Markov chain repeats three Markov steps
 Molecular Dynamics Monte Carlo (MDMC)

- Momentum heatbath
- Pseudofermion heatbath
- All have the desired fixed point
- Together they are ergodic (we hope!)

# MDMC

- If we could integrate Hamilton's equations exactly we could follow a trajectory of constant fictitious energy
  - This corresponds to a set of equiprobable fictitious phase space configurations
  - Liouville's theorem tells us that this also preserves the functional integral measure dp dq as required
- Any approximate integration scheme which is reversible and area preserving may be used to suggest configurations to a Metropolis accept/reject test
  - With acceptance probability min[1,exp( $-\delta H$ )]













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Baker-Campbell-Hausdorff (BCH) formula

If *A* and *B* belong to any (non-commutative) algebra then  $e^A e^B = e^{A+B+\delta}$ , where  $\delta$  constructed from commutators of *A* and *B* (i.e., is in the Free Lie Algebra generated by  $\{A, B\}$ )

• More precisely,  $\ln(e^A e^B) = \sum_{n>1} c_n$  where  $c_1 = A + B$  and

 $C_{n+1} = \frac{1}{n+1} \left\{ -\frac{1}{2} \left[ C_n, A - B \right] + \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{B_{2m}}{(2m)!} \sum_{k_1, \dots, k_{2m} \ge 1} \left[ C_{k_1}, \left[ \dots, \left[ C_{k_{2m}}, A + B \right] \dots \right] \right] \right\}$ 



 $+ \frac{1}{5760} \begin{cases} 7 \Big[ A, \Big[ A, \Big[ A, [A, B \Big] \Big] \Big] + 28 \Big[ B, \Big[ A, \Big[ A, [A, B \Big] \Big] \Big] \\ + 12 \Big[ [A, B], \Big[ A, [A, B \Big] \Big] + 32 \Big[ B, \Big[ B, \Big[ A, [A, B \Big] \Big] \Big] \\ - 16 \Big[ [A, B], \Big[ B, [A, B \Big] \Big] + 8 \Big[ B, \Big[ B, [B, [A, B \Big] \Big] \Big] \end{cases} + \cdots$ 



- We are interested in finding the classical trajectory in phase space of a system described by the Hamiltonian  $H(q, p) = T(p) + S(q) = \frac{1}{2}p^2 + S(q)$ 
  - The basic idea of such a <u>symplectic integrator</u> is to write the time evolution operator as

$$\exp\left(\tau \frac{d}{dt}\right) \equiv \exp\left(\tau \left\{\frac{dp}{dt} \frac{\partial}{\partial p} + \frac{dq}{dt} \frac{\partial}{\partial q}\right\}\right)$$
$$= \exp\left(\tau \left\{-\frac{\partial H}{\partial q} \frac{\partial}{\partial p} + \frac{\partial H}{\partial p} \frac{\partial}{\partial q}\right\}\right) \equiv e^{\tau}$$
$$= \exp\left(\tau \left\{-S'(q) \frac{\partial}{\partial p} + T'(p) \frac{\partial}{\partial q}\right\}\right)$$

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Define 
$$\hat{Q} \equiv T'(p) \frac{\partial}{\partial q}$$
 and  $\hat{P} \equiv -S'(q) \frac{\partial}{\partial p}$  so that  $\hat{H} = \hat{P} + \hat{Q}$ 

Since the kinetic energy *T* is a function only of *p* and the potential energy *S* is a function only of *q*, it follows that the action of  $e^{\tau \hat{p}}$  and  $e^{\tau \hat{q}}$  may be evaluated trivially

 $e^{\tau \hat{Q}}: f(q,p) \mapsto f(q+\tau T'(p),p)$  $e^{\tau \hat{P}}: f(q,p) \mapsto f(q,p-\tau S'(q))$ 

This is just Taylor's theorem

 $U_0(\delta\tau)^{\tau/\delta\tau} = \left(e^{\frac{1}{2}\delta\tau\hat{P}}e^{\delta\tau\hat{Q}}e^{\frac{1}{2}\delta\tau\hat{P}}\right)^{\tau/\delta\tau}$ 

From the BCH formula we find that the <u>PQP</u> symmetric symplectic integrator is given by

 $= \left( \exp\left[ \left( \hat{P} + \hat{Q} \right) \delta \tau - \frac{1}{24} \left( \left[ \hat{P}, \left[ \hat{P}, \hat{Q} \right] \right] + 2 \left[ \hat{Q}, \left[ \hat{P}, \hat{Q} \right] \right] \right) \delta \tau^{3} + O\left( \delta \tau^{5} \right) \right] \right)^{\tau/\delta \tau}$  $= \exp\left[ \tau \left( \left( \hat{P} + \hat{Q} \right) - \frac{1}{24} \left( \left[ \hat{P}, \left[ \hat{P}, \hat{Q} \right] \right] + 2 \left[ \hat{Q}, \left[ \hat{P}, \hat{Q} \right] \right] \right) \delta \tau^{2} + O\left( \delta \tau^{4} \right) \right) \right]$  $= e^{\tau \hat{H}'} = e^{\tau \left( \hat{P} + \hat{Q} \right)} + O\left( \delta \tau^{2} \right)$ 

In addition to conserving energy to  $O(\delta \tau^2)$  such symmetric symplectic integrators are manifestly area preserving and reversible



# **Digression on Differential Forms**

The natural language for Hamiltonian dynamics is that of differential forms  $\alpha = \frac{\mathbf{L}}{\mathbf{k}} \alpha_{\mu_1 \cdots \mu_k} \mathbf{e}^{\mu_1} \wedge \cdots \wedge \mathbf{e}^{\mu_k}$ The 1-forms lie in the dual space to vector fields (linear differential operators)  $e^{\mu}(e_{\nu}) = \delta^{\mu}_{\nu}$ There is an antisymmetric wedge product  $\alpha \wedge \beta = (-1)^{\deg \alpha \deg \beta} \beta \wedge \alpha$ 

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# **Digression on Differential Forms**

and a natural antiderivation df(v) = vf  $d(\alpha + \beta) = d\alpha + d\beta$  $d(\alpha \wedge \beta) = (d\alpha) \wedge \beta + (-1)^{\deg \alpha} \alpha \wedge d\beta$ • which therefore satisfies  $d^2 = 0$  and  $d\theta(a,b) = a\theta(b) - b\theta(a) - \theta(\lceil a,b \rceil)$  $d\omega(a,b,c) = a\omega(b,c) + b\omega(c,a) + c\omega(a,b)$  $-\omega(\lceil a,b \rceil,c) - \omega(\lceil b,c \rceil,a) - \omega(\lceil c,a \rceil,b)$ 

Note the commutator of two vector fields is a vector field

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# Hamiltonian Mechanics



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#### Lemma



Consider a Hamiltonian vector field acting on a 0-form

 $\hat{HF} = dF(\hat{H}) \quad \text{definition of } dF$   $= i_{\hat{F}}\omega(\hat{H}) \quad \hat{F} \text{ is a Hamiltonian vector field}$   $= \omega(\hat{F}, \hat{H}) \quad \text{definition of } i_{\hat{F}}$   $= \{H, F\} \quad \text{definition of Poisson bracket}$ 

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# Corollary



The fundamental 2-form is closed, so for any Hamiltonian vector fields  $d\omega(\hat{A},\hat{B},\hat{C}) = \hat{A}\omega(\hat{B},\hat{C}) + \hat{B}\omega(\hat{C},\hat{A}) + \hat{C}\omega(\hat{A},\hat{B})$  $-\omega\left(\left\lceil \hat{A}, \hat{B} \rceil, \hat{C}\right) - \omega\left(\left\lceil \hat{B}, \hat{C} \rceil, \hat{A} \right) - \omega\left(\left\lceil \hat{C}, \hat{A} \rceil, \hat{B} \right) = 0\right)$ but by the lemma  $\hat{A}\omega(\hat{B},\hat{C}) = -\hat{A}\{B,C\} = -\{A,\{B,C\}\}$ and  $-\omega\left(\left\lceil \hat{A}, \hat{B} \right\rceil, \hat{C}\right) = \omega\left(\hat{C}, \left\lceil \hat{A}, \hat{B} \right\rceil\right) = i_{\hat{C}}\omega\left(\left\lceil \hat{A}, \hat{B} \right\rceil\right) = dC\left(\left\lceil \hat{A}, \hat{B} \right\rceil\right)$  $= \begin{bmatrix} \hat{A}, \hat{B} \end{bmatrix} C = \hat{A}\hat{B}C - \hat{B}\hat{A}C = \{A, \{B, C\}\} - \{B, \{A, C\}\}$ hence  $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$ 

# Poisson Lie Algebra



Poisson brackets therefore satisfy all of the axioms of a Lie algebra Antisymmetry  $\{A,B\} = -\{B,A\}$  $\omega(\hat{A},\hat{B}) = -\omega(\hat{B},\hat{A})$ Jacobi identity  $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$  $\omega(\widehat{\omega}(\hat{A},\hat{B}),\hat{C}) + \omega(\widehat{\omega}(\hat{B},\hat{C}),\hat{A}) + \omega(\widehat{\omega}(\hat{C},\hat{A}),\hat{B}) = 0$ 

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# **Shadow Hamiltonians**



• **Theorem:** The commutator of two Hamiltonian vector fields is a Hamiltonian vector field  $[\hat{A}, \hat{B}]F = \hat{A}\hat{B}F - \hat{B}\hat{A}F = \hat{A}\{B, F\} - \hat{B}\{A, F\}$  $= \{A, \{B, F\}\} - \{B, \{A, F\}\}$  $= -\{F, \{A, B\}\} \quad \text{Jacobi identity}$ thus  $[\hat{A}, \hat{B}]F = \{\{A, B\}, F\} \Rightarrow [\hat{A}, \hat{B}] = \{A, B\}$ 

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# **Shadow Hamiltonians**



For each symplectic integrator there exists a Hamiltonian *H'* which is *exactly conserved*This may be obtained by replacing the commutators [*s*,*t*] in the BCH expansion of ln(*e* <sup>s</sup>*e* <sup>t</sup>) with the <u>Poisson bracket</u> {*S*,*T*}

# **Conserved Hamiltonian**



• For the PQP integrator we have  $H' = T + S + \frac{1}{24} \Big[ \{S, \{S, T\}\} - 2\{T, \{S, T\}\} \Big] \\
+ \frac{1}{5760} \begin{bmatrix} 7\{S, \{S, \{S, \{S, T\}\}\} - 2\{T, \{S, \{S, \{S, T\}\}\} \} \\ + 12\{\{S, T\}\{S, \{S, T\}\}\} + 28\{T, \{S, \{S, \{S, T\}\}\} \} \\ + 12\{\{S, T\}\{S, \{S, T\}\} + 32\{T, \{T, \{S, \{S, T\}\}\} \} \end{bmatrix} + \cdots \\
- 16\{\{S, T\}\}\{T, \{S, T\}\} + 8\{T, \{T, \{T, \{S, T\}\}\} \} \Big]$ 

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#### How Many Poisson Brackets Are There?

Witt's formula for the number of independent elements  $a_N$  of degree N of a Free Lie Algebra on q generators is  $a_N = \sum \mu(d)q^{\frac{N}{d}}$ , where  $\mu$ is the Möbius function  $d|\Lambda$ The first two terms in our case are  $a_3 = \frac{(q-1)q(q+1)}{3}; \quad a_5 = \frac{(q-1)q(q+1)(q^2+1)}{5}$ but some of these vanish (e.g.,  $[S_1, S_2]$ )

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# **Results for Scalar Theory**



 Evaluating the Poisson brackets gives
 H' = H + 1/24 { 2p<sup>2</sup>S" - S'<sup>2</sup> } δτ<sup>2</sup> + 1/720 { -p<sup>4</sup>S<sup>(4)</sup> + 6p<sup>2</sup> (S'S"" + 2S"<sup>2</sup>) - 3S'<sup>2</sup>S" } δτ<sup>4</sup> + O(δτ<sup>6</sup>)
 Note that H' cannot be written as the sum of a *p*-dependent kinetic term and a *q*-dependent potential term
 So, sadly, it is not possible to construct an integrator that

conserves the Hamiltonian we started with

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# Tuning HMC



For any (symmetric) symplectic integrator the conserved Hamiltonian is constructed from the same Poisson brackets

#### The proposed procedure is therefore

- Measure the Poisson brackets during an HMC run
- Optimize the integrator (number of pseudofermions, stepsizes, order of integration scheme, etc.) offline using these measured values
- This can be done because the acceptance rate (and instabilities) are completely determined by  $\delta H = H' H$

# Simple Example (Omelyan)



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# Another Caveat (Creutz)



 $\langle 1 \rangle = \frac{1}{Z} \int dq \, dp \, e^{-H(q,p)} = \frac{1}{Z} \int dq' \, dp' \, e^{-H(q',p')}$   $= \frac{1}{Z} \int dq \, dp \, e^{-[H(q,p)+\delta H]} = \left\langle e^{-\delta H} \right\rangle$   $1 = 1 - \left\langle \delta H \right\rangle + \frac{1}{2} \left\langle \delta H^2 \right\rangle + \cdots$   $\left\langle \delta H \right\rangle = \frac{1}{2} \left\langle \delta H^2 \right\rangle + \cdots = O\left(\delta \tau^4\right)$ 

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# **Beyond Scalar Field Theory**

We need to extend the formalism beyond a scalar field theory "In theory, theory and practice are the same; in practice they aren't" – Yogi Berra Fermions are easy  $S_{F}(U) = \phi^{\dagger} M^{-1}(U) \phi = \operatorname{Tr} \left[ M^{-1}(U) \phi \otimes \phi^{\dagger} \right]$  $\frac{\partial M^{-1}}{\partial U} = -M^{-1} \frac{\partial M}{\partial U} M^{-1}$ How do we extend all this fancy differential geometry formalism to gauge fields?

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# **Digression on Lie Groups**

- Gauge fields take their values in some Lie group, so we need to define classical mechanics on a group manifold which preserves the group-invariant Haar measure
  - A Lie group G is a smooth manifold on which there is a natural mapping  $L: G \times G \rightarrow G$  defined by the group action
  - This induces a map called the *pull-back* of *L* on the cotangent bundle defined by
    - $L^{*}: G \times \Lambda^{0} \to \Lambda^{0} \qquad L^{*}_{g}f = f \circ L_{g} \qquad \text{covariant}$   $L_{*}: G \times TG \to TG \qquad (L_{g*}v)(f) = v(L^{*}_{g}f) \qquad \text{contravariant}$   $L^{*}: G \times T^{*}G \to T^{*}G \qquad (L^{*}_{g}\theta)(v) = \theta(L_{g*}v) \qquad \text{covariant}$

<sup> $\bigcirc$ </sup>  $A^{0}$  is the space of 0 *forms*, which are smooth mappings from *G* to the real numbers  $\Lambda^{0}$  : *G* →  $\Re$ 

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## Left Invariant 1-forms



- A form is *left invariant* if  $L^* \theta = \theta$
- The tangent space to a Lie group at the origin is called the *Lie algebra*, and we may choose a set of basis vectors  $\{e_i(0)\}$  that satisfy the commutation relations  $[e_i, e_j] = \sum_{ij} c_{ij}^k e_k$  where  $c_{ij}^k$  are the *structure constants* of the algebra
- We may define a set of left invariant vector fields on TG by  $e_i(g) \equiv L_{g^*}e_i(0)$

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# **Maurer-Cartan Equations**



The corresponding left invariant dual forms  $\{\theta_i\}$  satisfy the *Maurer-Cartan* equations

 $d\theta^{i}(e_{j},e_{k}) = e_{j}d\theta^{i}(e_{k}) - e_{k}d\theta^{i}(e_{j}) - \theta^{i}([e_{j},e_{k}])$  $= -\theta^{i}(C_{jk}^{\ell}e_{\ell}) = -C_{jk}^{i}$ 

$$\boldsymbol{d}\theta^{i} = -\frac{1}{2}\sum_{jk}\boldsymbol{C}_{jk}^{i}\,\theta^{j}\wedge\theta^{k}$$

## **Fundamental 2-form**



We can invent any Classical Mechanics we want...
 So we may therefore define a closed *symplectic 2-form* which globally defines an invariant Poisson bracket by

$$\omega \equiv -d\sum_{i} \theta^{i} p^{i}$$
$$= \sum_{i} \left( \theta^{i} \wedge dp^{i} - p^{i} d\theta^{i} \right)$$

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 $=\sum_{i}\left(\theta^{i}\wedge dp^{i}+\frac{1}{2}p^{i}C_{jk}^{i}\theta^{j}\wedge\theta^{k}\right)$ 

# Hamiltonian Vector Field



- We may now follow the usual procedure to find the equations of motion:
- Introduce a Hamiltonian function (0-form) *H* on the cotangent bundle (phase space) over the group manifold
- Define a vector field  $h \equiv \hat{H}$  such that  $dH = i_h \omega$  $h = \sum_i \left( \frac{\partial H}{\partial p^i} e_i + \left[ \sum_{jk} c_{ji}^k \hat{p}^k \frac{\partial H}{\partial p^j} - e_i (H) \right] \frac{\partial}{\partial p^i} \right)$

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# **Integral Curves**



• The classical trajectories  $\sigma_t = (Q_t, P_t)$  are then the *integral curves* of *h*:  $\dot{\sigma}_t = h(\sigma_t)$ 



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# **Equations of Motion**



The equations of motion in the local coordinates  $e_j = \sum_i e_j^i \frac{\partial}{\partial q^j}$  are therefore  $\dot{Q}_{t}^{j} = \sum_{i} \frac{\partial H}{\partial p^{i}} e_{i}^{j}, \ \dot{P}_{t}^{j} = \sum_{k} \left( \sum_{i} c_{kj}^{i} P_{t}^{i} \frac{\partial H}{\partial p^{k}} - e_{j}^{k} \frac{\partial H}{\partial q^{k}} \right)$ Which for a Hamiltonian of the form  $H = f(p^2) + S(q)$  reduces to  $\dot{Q}_{t}^{j} = \sum_{i} \frac{\partial H}{\partial n^{i}} e_{i}^{j}, \dot{P}_{t}^{j} = -\sum_{k} e_{j}^{k} \frac{\partial H}{\partial n^{k}}$ 

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#### **Constrained Variables**



The representation of the generators is  $U(q) = e^{\sum_{i} q^{i} \tau_{i}}$  $T_{i} = \frac{\partial U(g)}{\partial g^{i}} \bigg|_{g=0} = e_{i}(g)U(g) \bigg|_{g=0}$ • from which it follows that  $e_i(U) = UT_i$ • and for the Hamiltonian  $H = \frac{1}{2}\sum_{i=1}^{\infty} (p^{i})^{2} + S(U)$  leads to the equations of motion  $\dot{U} = PU$  $\dot{P} = \sum_{iab} T_i \left[ \frac{\partial S}{\partial U_{ab}} (UT_i)_{ab} - \frac{\partial S}{\partial U_{ab}^{\dagger}} (T_i U^{\dagger})_{ab} \right] = -T \left[ S'(U) U \right]$ 

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# **Discrete Equations of Motion**

We can now easily construct a discrete PQP symmetric integrator (for example) from these equations

 $P\left(\frac{1}{2}\delta\tau\right) = P\left(0\right) - T\left[S'\left(U\left(0\right)\right)U\left(0\right)\right]\frac{1}{2}\delta\tau$  $U\left(\delta\tau\right) = \exp\left[P\left(\frac{1}{2}\delta\tau\right)\delta\tau\right]U\left(0\right)$  $P\left(\delta\tau\right) = P\left(\frac{1}{2}\delta\tau\right) - T\left[S'\left(U\left(\delta\tau\right)\right)U\left(\delta\tau\right)\right]\frac{1}{2}\delta\tau$ 

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## Matrix Exponential



The exponential map from the Lie algebra to the Lie group may be evaluated exactly using the Cayley-Hamilton theorem

- All functions of an n × n matrix M may be written as a polynomial of degree n - 1 in M
- The coefficients of this polynomial can be expressed in terms of the invariants (traces of powers) of *M*

## **Poisson Brackets**



Recall our Hamiltonian vector field  $\hat{H} = \sum_{i} \left( \frac{\partial H}{\partial p^{i}} e_{i} + \left| \sum_{ik} c_{ji}^{k} p^{k} \frac{\partial H}{\partial p^{j}} - e_{i} (H) \right| \frac{\partial}{\partial p^{i}} \right)$ For H(q,p) = T(p) + S(q) we have vector fields  $\hat{S} = -\sum_{i} e_{i}(S) \frac{\partial}{\partial p^{i}} \quad \hat{T} = \sum_{i} \left( \frac{\partial T}{\partial p^{i}} e_{i} + \left[ \sum_{jk} c_{ji}^{k} p^{k} \frac{\partial T}{\partial p^{j}} \right] \frac{\partial}{\partial p^{i}} \right)$  $= \sum_{i} \left( p^{i} e_{i} + \sum_{jk} c_{ji}^{k} p^{k} p^{j} \frac{\partial}{\partial p^{i}} \right) \text{ if } T(p) = \frac{p^{2}}{2}$ 

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### **More Poisson Brackets**



• We thus compute the lowest-order Poisson bracket  $\{S,T\} = -\omega(\hat{S},\hat{T}) = -(\theta^i \wedge dp^i + \frac{1}{2}p^i c^i_{jk}\theta^j \wedge \theta^k)(\hat{S},\hat{T})$  $= -p^i e_i(S) = -\operatorname{tr}\left(\frac{\partial S}{\partial U}PU\right)$ 

and the Hamiltonian vector corresponding to it

 $\{S,T\} = \sum_{i} \left( \frac{\partial \{S,T\}}{\partial p^{i}} e_{i} + \left[ \sum_{jk} c_{ji}^{k} p^{k} \frac{\partial \{S,T\}}{\partial p^{j}} - e_{i} \left( \{S,T\} \right) \right] \frac{\partial}{\partial p^{i}} \right)$  $= -e_{i} \left( S \right) e_{i} + \left[ -c_{ji}^{k} p^{k} e_{j} \left( S \right) + p^{j} e_{i} e_{j} \left( S \right) \right] \frac{\partial}{\partial p^{i}}$ 

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# Yet More Poisson Brackets

- Continuing in the same manner we may compute all the higher-order Poisson brackets we like
- In terms of the variables  $U \in SU(n)$  and  $P \in su(n) = T^* SU(n)$  the lowest-order Poisson brackets are

$$\{S, \{S, T\}\} = \operatorname{tr}\left(\frac{\partial S}{\partial U}U\frac{\partial S}{\partial U}U\right) - \frac{1}{3}\left[\operatorname{tr}\left(\frac{\partial S}{\partial U}U\right)\right]$$
$$\{T, \{S, T\}\} = -\operatorname{tr}\left(\frac{\partial^2 S}{\partial U^2}PUPU + \frac{\partial S}{\partial U}P^2U\right)$$

Remember that S(U) includes not only the pure gauge part but also the pseudofermion part

# Questions?



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