Structure Preserving Discretisation of Kinetic and Gyrokinetic Equations

Discrete Geometric Field Theory in Plasma Physics

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Structure Preserving Integration Schemes

- Courant, Friedrichs, Lewy (1928): preserving first integrals of an equation during discretisation is advantageous for the stability of the resulting scheme
- preserving as much structure of an equation as possible when performing a discretisation produces not only more stable schemes but more realistic and more accurate representations of the physical system at hand
- geometric structures: momentum maps / Casimirs (e.g. momentum, energy, enstrophy), symplecticity, phasespace volume, symmetries (e.g. particle relabeling, gauge), ...
- while structure preserving integration schemes for ODEs have been known for several decades, the development of general methods for PDEs is a rather young and lively field of research

Structure Preserving Integration Schemes

- Can we preserve all these structures at once? Unfortunately not...

→ classes of schemes, that preserve

  - symplecticity and Noether's theorem (and thus momentum maps)
    - → variational integrators (discrete action principle)
    - → multi-symplectic integrators for Hamiltonian PDEs
  - local and/or global energy
    - → variational integrators with local or global time step adaption
  - first integrals
    - → discrete variational derivative
    - → discrete gradients
  - phasespace volume
    - → discretisation of the group of volume-preserving diffeomorphisms
  - constraints ($\nabla \cdot \vec{E} = \rho$, $\nabla \cdot \vec{B} = 0$)
    - → discrete differential forms

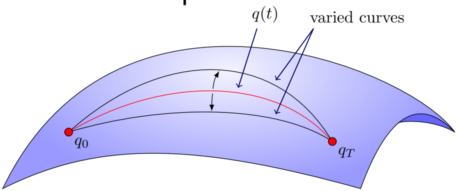
- Arakawa (bracket antisymmetry, kinetic energy, L1 and L2 norm)
- Morinishi (mass, momentum, kinetic energy, L1 and L2 norm)

Variational Integrators (VIs)

- common practice: discretisation of the Euler-Lagrange equations derived from a continuous Lagrangian via a variational principle
- VIs: discretise the Lagrangian and the accompanying Hamiltonian action principle to obtain discrete Euler-Lagrange equations
  - → automatically preserve symplecticity and discrete momenta associated to symmetries of the Lagrangian through a discrete version of Noether's theorem
  - → good long-time energy behaviour, no artificial numerical damping
  - → simultaneous discretisation in (phase)space and time
  - → easily applicable to different meshes
- the discrete theory mimics the continuous theory as closely as possible
- idea: instead of solving the exact system approximately, we solve an approximate system exactly

Continuous Variational Principle

- action



$$\mathcal{A} = \int_0^T L\big(q(t), \dot{q}(t)\big)\, dt$$

- variation and partial integration (endpoints fixed: $\delta q(0) = \delta q(T) = 0$)

$$\delta \mathcal{A} = \int_0^T \left[\frac{\partial L}{\partial q} \cdot \delta q + \frac{\partial L}{\partial \dot{q}} \cdot \delta \dot{q} \right] dt = \int_0^T \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) \right] \cdot \delta q \, dt$$

- the variation of the action has to vanish for all δq, thus the integrand has to vanish, and we get the Euler-Lagrange equations

$$\frac{\partial L}{\partial q}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \right) = 0$$

Discrete Variational Principle

- approximate q as the average of two neighbouring points

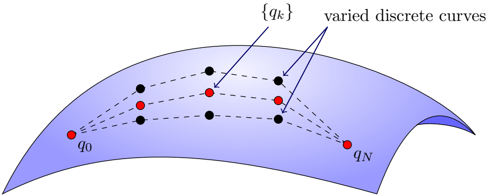
$$q \rightarrow \frac{q_k + q_{k+1}}{2}$$

and $\dot{q}$ with finite differences (timestep h)

$$\dot{q} \rightarrow \frac{q_{k+1} - q_k}{h}$$

- discrete action

$$\mathcal{A}_d = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}, h)$$



- discrete variational principle

$$\delta \mathcal{A}_d = \sum_{k=0}^{N-1} \left[D_1 L_d(q_k, q_{k+1}, h) \cdot \delta q_k + D_2 L_d(q_k, q_{k+1}, h) \cdot \delta q_{k+1} \right]$$

Discrete Variational Principle

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- discrete partial integration (use $\delta q_0 = \delta q_N = 0$)

$$\begin{aligned} \delta \mathcal{A}_d &= D_1 L_d(q_0, q_1, h) \cdot \delta q_0 + \sum_{k=1}^{N-1} D_1 L_d(q_k, q_{k+1}, h) \cdot \delta q_k \\ &+ \sum_{k=1}^{N-1} D_2 L_d(q_{k-1}, q_k, h) \cdot \delta q_k + D_2 L_d(q_{N-1}, q_N, h) \cdot \delta q_N \\ &= \sum_{k=1}^{N-1} \big[D_1 L_d(q_k, q_{k+1}, h) + D_2 L_d(q_{k-1}, q_k, h) \big] \cdot \delta q_k \end{aligned}$$

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- the variation $\delta \mathcal{A}_d$ has to vanish for all δq_k, thus for all k we get the

Discrete Euler-Lagrange Equations

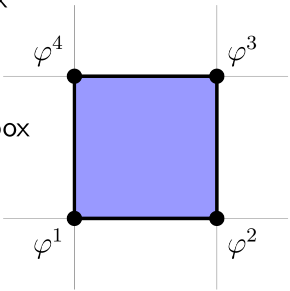
$$D_2 L_d(q_{k-1}, q_k, h) + D_1 L_d(q_k, q_{k+1}, h) = 0$$

- in general: fully nonlinear algebraic equation
- often recovering well-known schemes

VIs for Field Dynamics (Discrete Field Theory)

- average the fields over all vertices of a grid box

$$\varphi \to \bar{\varphi} = \frac{1}{4} \left(\varphi^1 + \varphi^2 + \varphi^3 + \varphi^4 \right)$$



- define derivatives along the edges of the grid box

$$\frac{\partial \varphi}{\partial x} \to \frac{1}{2} \left(\frac{\varphi^2 - \varphi^1}{h_x} + \frac{\varphi^3 - \varphi^4}{h_x} \right)$$

$$\frac{\partial \varphi}{\partial y} \to \frac{1}{2} \left(\frac{\varphi^4 - \varphi^1}{h_y} + \frac{\varphi^3 - \varphi^2}{h_y} \right)$$

- replace the continuous Lagrangian density with its discrete counterpart

$$L(\varphi, \varphi_x, \varphi_y) \to L_d(\varphi^1, \varphi^2, \varphi^3, \varphi^4)$$

$$\mathcal{A} = \int L(\varphi, \varphi_x, \varphi_y) \, dx \, dy \to \mathcal{A}_d = \sum_{\text{grid boxes}} L_d(\varphi^1, \varphi^2, \varphi^3, \varphi^4)$$

VIs for Field Dynamics (Discrete Field Theory)

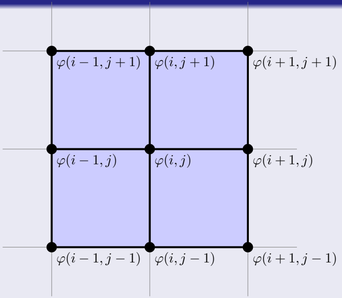
- apply discrete variational principle

$$\delta \mathcal{A}_d = \sum_{\text{grid boxes}} \frac{\partial L_d}{\partial \varphi^i}(\varphi^1, \varphi^2, \varphi^3, \varphi^4) \cdot \delta\varphi^i \qquad (1 \leq i \leq 4)$$

to obtain

Discrete Euler-Lagrange Field Equations

$$\begin{aligned} 0 = &\frac{\partial L_d}{\partial \varphi^1}\left(\varphi_{i,j}, \varphi_{i+1,j}, \varphi_{i+1,j+1}, \varphi_{i,j+1}\right) \\ &+ \frac{\partial L_d}{\partial \varphi^2}\left(\varphi_{i-1,j}, \varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i-1,j+1}\right) \\ &+ \frac{\partial L_d}{\partial \varphi^3}\left(\varphi_{i-1,j-1}, \varphi_{i,j-1}, \varphi_{i,j}, \varphi_{i-1,j}\right) \\ &+ \frac{\partial L_d}{\partial \varphi^4}\left(\varphi_{i,j-1}, \varphi_{i+1,j-1}, \varphi_{i+1,j}, \varphi_{i,j}\right) \end{aligned}$$



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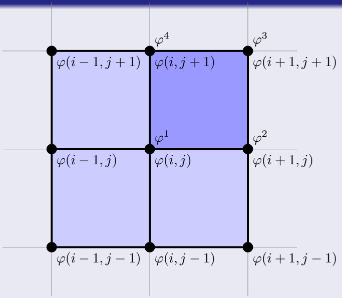

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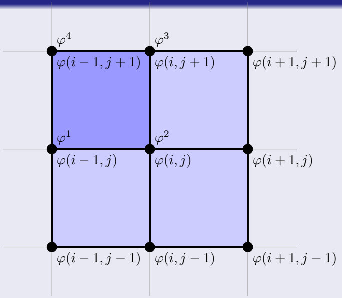

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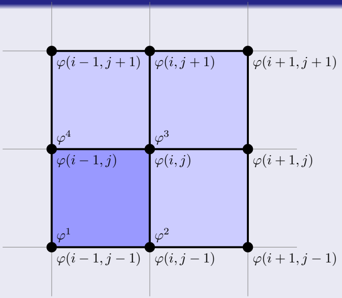

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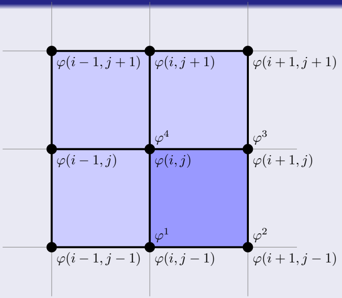

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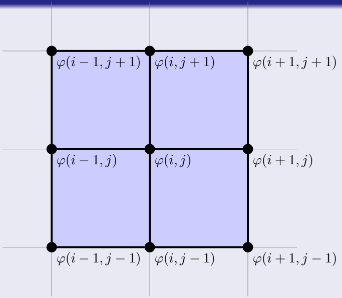

Kinetic and Gyrokinetic Theory

- Lagrangian formulations of gyrokinetics allow for rigorous proofs of energy and momentum conservation through Noether's theorem
- other conserved quantities: L1 and L2 norm of f, entropy

$$\int f \, d^3x \, d^3p, \qquad \int f^2 \, d^3x \, d^3p, \qquad \int f \, \log f \, d^3x \, d^3p$$

- test bed: Vlasov-Poisson in 1D, determining the evolution of the distribution function f and the electrostatic potential ϕ selfconsistently

$$\frac{\partial f}{\partial t} + \frac{p}{m} \frac{\partial f}{\partial x} - e \frac{\partial \phi}{\partial x} \frac{\partial f}{\partial p} = 0, \qquad \nabla^2 \phi = -e \int f \, dp$$

- two possibilities for variational principles for Vlasov-Poisson:
  - a) the Poisson equation enters only as a constraint in the action for the Vlasov equation (ϕ is a functional of f)
  - b) the Poisson equation is also obtained from the variational principle (ϕ is a dynamical variable)

Kinetic and Gyrokinetic Theory

- the natural basis for a full-f Vlasov (Eulerian) code is a purely Eulerian field theoretic description

→ Eulerian action principles for the Vlasov-Poisson/Maxwell system?

$$\mathcal{A} = \mathcal{A}_f + \frac{1}{2} \int |\nabla \phi|^2 \, dt \, dx$$

1. canonical Hamiltonian action principle

$$\mathcal{A}_f(f, g) = \int \left(\dot{f} g - \mathcal{H} \right) dt \, dx \, dp$$

→ no canonical conjugate field variable g, only f

2. Clebsch parametrisation of f

$$f = [\alpha, \beta] \quad \rightarrow \quad \mathcal{A}_f(\alpha, \beta) = \int \left(\alpha \dot{\beta} - \mathcal{H} \right) dt \, dx \, dp$$

→ α and β are canonical conjugate variables, but not well-behaved

Kinetic and Gyrokinetic Theory

→ Eulerian action principles for the Vlasov-Poisson/Maxwell system?

3. weak formulation

3a. just the Vlasov equation

$$\mathcal{A}(f,g) = \int g \left(\frac{\partial f}{\partial t} + \frac{p}{m} \frac{\partial f}{\partial x} - e \frac{\partial \phi}{\partial x} \frac{\partial f}{\partial p} \right) dt\, dx\, dp$$

→ in theory applicable to any differential operator that equals zero

3b. with two auxiliary fields g and ψ [Ibragimov '06, '10]

$$\mathcal{A}(f,g,\phi,\psi) = \int g \left(\frac{\partial f}{\partial t} + \frac{p}{m} \frac{\partial f}{\partial x} - e \frac{\partial \phi}{\partial x} \frac{\partial f}{\partial p} \right) dt\, dx\, dp + \int \psi \left(\Delta \phi - e \int f\, dv \right) dt\, dx$$

→ rigorous theory with Noether theorem recovering the conserved quantities of the original system

→ Eulerian action principles for the Vlasov-Poisson/Maxwell system?

4. constrained variations

4a. Brizards action principle in extended 8D phasespace $(t, \epsilon; x, p)$

$$\mathcal{A}_f(f) = \int (h - \epsilon)\, f\, \delta(h - \epsilon)\, dt\, d\epsilon\, dx\, dp \qquad \text{with} \qquad \delta f = [\delta S, f]_{\text{cov}}$$

4b. Cendra's reduced Euler-Poincaré action principle using Lin constraints

$$\mathcal{A}_f(\vec{u}, f) = \int f \left(\frac{m}{2} \vec{u}_s^2 + \frac{m}{2} (\vec{u}_s - \vec{v})^2 - q\phi \right) dt\, dx\, dv$$

$$\delta \vec{u} = \frac{\partial \vec{w}}{\partial t} + [\vec{u}, \vec{w}] \qquad \text{and} \qquad \delta f = -\nabla_{\vec{z}} \cdot (f \vec{w})$$

→ starts from Low's Lagrangian, just as Sugama's gyrokinetic field action

→ analogous to incompressible fluid theory ($\vec{u}$: phasespace velocity field)

→ discretisation of the volume preserving diffeomorphism group

→ exact conservation of energy and phasespace volume, time-reversibility

Kinetic and Gyrokinetic Theory

→ Eulerian action principles for the Vlasov-Poisson/Maxwell system?

5. semi-discretisation of the phasespace part (Poisson bracket)

5a. keep f_t continuous, discretise only the derivatives of the Poisson bracket:

$$\mathcal{A} = \int g \left(\bar{f}_t + [f, h] \right) dx \, dp$$

→ retains certain properties of the variational integrator [Leon '08]

→ still implicit (due to the averaging of f in the time-derivative)

5b. use the variational integrator formalism to discretise the functional derivative:

$$\mathcal{A} = \int S \, [f, h] \, dx \, dp$$

→ weak formulation with (arbitrary) generating function S

→ Poisson bracket is retained via functional derivative

$$\frac{\delta \mathcal{A}}{\delta S} = [f, h] \qquad \rightarrow \qquad \frac{\partial f}{\partial t} = - \frac{\delta \mathcal{A}}{\delta S}$$

Semidiscretisation

- idea: discrete functional derivative $\leftrightarrow$ discrete variational derivative

$$\mathcal{A} = \int S\,[f, h]\, dx\, dp \quad \rightarrow \quad \frac{\delta \mathcal{A}}{\delta S} = [f, h] = -\frac{\partial f}{\partial t}$$

- to retain the antisymmetry properties of the bracket, one has to realise the equality of permutations in the integrand (by partial integration)

$$\int S\,[f, h]\, dx\, dp = \int f\,[h, S]\, dx\, dp = \int h\,[S, f]\, dx\, dp$$

- thus the "action" can be written as $(\alpha + \beta + \gamma = 1)$

$$\mathcal{A} = \int \Big(\alpha\, S\,[f, h] + \beta\, f\,[h, S] + \gamma\, h\,[S, f] \Big)\, dx\, dp$$

- applying the variational integrator scheme to this functional with $\alpha = \beta = \gamma = 1/3$, one obtains the well-known Arakawa scheme
- discretising the derivatives on a triangular grid, the very same formalism produces Sadourney's scheme ("Arakawa on triangles")

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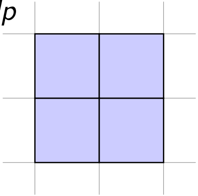

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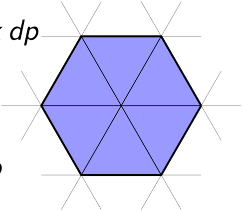

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Semidiscretisation

- generalise to a Nambu three bracket ($(a, b, c) \in \{x, y, z\}$)

$$[f, g, h] \equiv \mathcal{E}^{abc} \, f_{,a} \, g_{,b} \, h_{,c} = \frac{\partial f}{\partial x} \, [g, h]_{yz} + \frac{\partial f}{\partial y} \, [g, h]_{zx} + \frac{\partial f}{\partial z} \, [g, h]_{xy}$$

- the action functional is completely analogous to the previous one

$$\mathcal{A} = \int S \, [f, g, h] \, dx \, dy \, dz$$
$$= \frac{1}{4} \int \Big(S \, [f, g, h] + f \, [S, h, g] + g \, [S, f, h] + h \, [S, g, f] \Big) \, dx \, dy \, dz$$

- results in quite large integrators
  - → use scripts for the derivation
  - → easily adaptable to different meshes, discretisation schemes, and actions
  - → produces ready-to-use Fortran code

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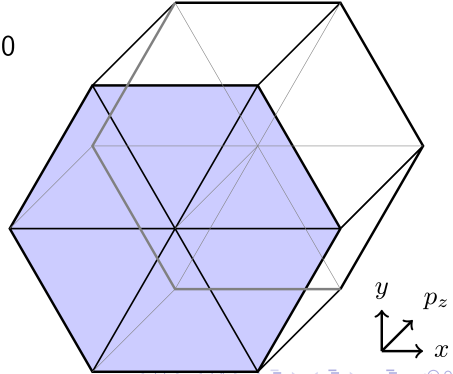
- application: gyrokinetic Vlasov equation on extruded triangular mesh

$$\frac{\partial f}{\partial t} + \frac{1}{\sqrt{g} \, B_{\parallel}^{*}} \left[h, f, A_{\varphi}^{*} \right]_{xyp_z} = 0$$



x, y	coordinates of the poloidal plane
p_z	parallel momentum
g	metric
f	distribution function
h	particle Hamiltonian
$\vec{A}^{*}$	$= \vec{A} + \frac{c}{e} p_z \vec{b}$
$B_{\parallel}^{*}$	$= \vec{b} \cdot (\nabla \times \vec{A}^{*})$

Noncanonical Hamiltonian Field Theory

- the dynamics of Hamiltonian systems is usually expressed with the help of conjugate variables (q, p) and Hamilton's equations

$$\dot{q} = \frac{\partial H}{\partial p} \quad \text{and} \quad \dot{p} = -\frac{\partial H}{\partial q} \qquad \text{or} \qquad \dot{F}(q,p) = [F, H]$$

- a lot of (esp. infinite-dimensional) Hamiltonian systems do not fit into this form (Vlasov-Poisson, reduced and ideal MHD, incompressible Fluid dynamics, ...)
- noncanonical Hamiltonian formulation for functionals of a vector of state variables $\vec{\xi}(\vec{x}, t)$ (distribution function, vorticity, temperature, ...)

$$\dot{F}(\xi^{\mu}) = \{F, H\}$$

$H(\xi^{\mu})$: Hamiltonian functional
$\{\cdot,\cdot\}$: generalised Poisson bracket (antisymmetry, Jacobi identity)

- Lie-Poisson bracket formulation of the Vlasov equation

$$\dot{F} = \{F, H\} \equiv \int f \left[\frac{\delta F}{\delta f}, \frac{\delta H}{\delta f} \right] dx\, dp$$

where F is any functional of f and H is the total energy functional

$$H = \int \frac{|\vec{p}|^2}{2m} f(\vec{x}, \vec{p})\, dx\, dp + \frac{1}{2} \int |\nabla \phi(\vec{x})|^2\, dx$$

- with the L2 norm

$$Z = \frac{1}{2} \int f^2\, dx\, dp$$

the Lie-Poisson bracket can be expressed as a Nambu three bracket

$$\dot{F} = \{F, H, Z\} \equiv \int \frac{\delta Z}{\delta f} \left[\frac{\delta F}{\delta f}, \frac{\delta H}{\delta f} \right] dx\, dp$$

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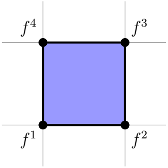

- discretise the functionals Z and H in the Nambu bracket as

$$Z = \frac{1}{2} \sum_{ij} f_{ij}^2 , \qquad H = \sum_{ij} f_{ij} \, h_{ij} = \sum_{ij} f_{ij} \left(p_j^2 / m + q \phi_{ij} \right)$$

- to get the Arakawa scheme, approximate $\delta Z / \delta f$

$$\{F, H, Z\}_D = \sum_{\text{grid boxes}} \frac{1}{4} \left(\frac{\partial Z}{\partial f^1} + \frac{\partial Z}{\partial f^2} + \frac{\partial Z}{\partial f^3} + \frac{\partial Z}{\partial f^4} \right) \left[\frac{\delta F}{\delta f} , \frac{\delta H}{\delta f} \right]_D$$

and the discrete Poisson bracket as

$$\left[\frac{\delta F}{\delta f} , \frac{\delta H}{\delta f} \right]_D = \frac{1}{4 \, h_x \, h_p} \Bigg[\left(\frac{\partial F}{\partial f^2} - \frac{\partial F}{\partial f^1} + \frac{\partial F}{\partial f^3} - \frac{\partial F}{\partial f^4} \right) \left(\frac{\partial H}{\partial f^4} - \frac{\partial H}{\partial f^1} + \frac{\partial H}{\partial f^3} - \frac{\partial H}{\partial f^2} \right)$$
$$- \left(\frac{\partial F}{\partial f^4} - \frac{\partial F}{\partial f^1} + \frac{\partial F}{\partial f^3} - \frac{\partial F}{\partial f^2} \right) \left(\frac{\partial H}{\partial f^2} - \frac{\partial H}{\partial f^1} + \frac{\partial H}{\partial f^3} - \frac{\partial H}{\partial f^4} \right) \Bigg]$$

→ discrete analogue of the Vlasov-Poisson equation

$$\frac{\partial f_{ij}}{\partial t} = \{ f_{ij}, H, Z \}_D$$

Summary and Outlook

Achievements:

- variational derivation of Arakawa's scheme: easily generalisable to higher dimensions, different meshes, and/or higher order
- antisymmetry-preserving discretisation of the three-bracket on an extruded triangular grid
- Nambu field bracket formulation of the noncanonical Hamiltonian description of the Vlasov equation and application of antisymmetry-preserving semi-discretisation schemes

Next Steps:

- discretisation of Cendra's constrained variational principle via discretisation of the volume preserving diffeomorphism group
- reduction of Sugama's gyrokinetic field action to Euler-Poincaré form
- discretisation of electromagnetic field action with discrete diff. forms
- numerical validation of the three-bracket discretisation
- further generalisation and exploration of the Nambu field bracket