The geometric exegesis of the Dirac algorithm

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Extend the use of Hamiltonian methods to **field theories in bounded regions**. No obstructions in principle but problematic in practice.

The computation of Poisson brackets when boundaries are present is not trivial. At some point functional-analytic issues become relevant.

Can we somehow avoid these problems? Yes, but to this end the standard approach must be suitably (subtly?) modified.

**A geometric reinterpretation of the usual method helps**

**exegesis: critical interpretation of a text, particularly a sacred text**
Lectures on Quantum Mechanics

Paul A. M. Dirac
<table>
<thead>
<tr>
<th>The Dirac algorithm in words</th>
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<tbody>
<tr>
<td><strong>Write the canonical momenta</strong> ( p ) in terms of ( q ) and ( \dot{q} ).</td>
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<tr>
<td><strong>Find the primary constraints</strong>, i.e. relations ( \phi_m(q, p) = 0 ) between ( q ) and ( p ) originating in the “impossibility to solve for all the velocities” in terms of positions and momenta.</td>
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<tr>
<td><strong>Find a Hamiltonian</strong> ( H ) and build the <strong>total Hamiltonian</strong> ( H_T = H + \sum u_m \phi_m ) in which the <strong>primary constraints</strong> are introduced together with some multipliers ( u_m(t) ).</td>
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<tr>
<td><strong>The</strong> ( u_m ) <strong>must be fixed by enforcing the consistency of the time evolution of the system.</strong> This consistency requires, for instance, that the primary constraints be <strong>preserved in time</strong>:</td>
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| \[
\{\phi_m, H\} + u_n \{\phi_m, \phi_n\} \approx 0
\] |
| The weak equality symbol \( \approx \) means that the previous identity must hold when the primary constraints are enforced. |
The Dirac algorithm in words (continued)

Several possibilities:

1. The consistency conditions may be impossible to fulfill. This means that our starting point (the Lagrangian) makes no sense.
2. The consistency conditions may be trivial, i.e. identically satisfied once the primary constraints are enforced.
3. The $u_m$ may not appear in the consistency conditions. In this case we have secondary constraints.
4. The consistency conditions can be solved for the $u_m$.

If we find secondary constraints their “stability under time evolution” must be enforced, exactly as we did for the primary constraints. However we do not have to modify the total Hamiltonian (i.e. we do not have to include them in a new, “more total” Hamiltonian).
The Dirac algorithm in words (continued)

- Let us look with some care at the equations
  \[
  \{\phi_j, H\} + u_n\{\phi_j, \phi_n\} \approx 0
  \]
  These are **linear, inhomogeneous** equations for the unknowns $u_n$. As such, the inhomogeneous term will be subject, generically, to conditions necessary to guarantee solvability.

- **These are the secondary constraints.** Their number is determined by the **rank of the matrix** $\{\phi_j, \phi_n\}$ (beware of *bifurcation*!).

- Once solvability is guaranteed we can find the $u_n$ (as functions of the generalized coordinates and momenta) and, maybe, arbitrary parameters.

  \[
  u_m = U_m(q, p) + \nu_a(t)V_{am}(q, p),
  \]

  where $V_{an}\{\phi_j, \phi_n\} = 0$ and the $\nu_a(t)$ are arbitrary functions of time.
The Hamiltonian \[ \hat{H} = H + (U_m(q, p) + v_a(t)V_{am}(q, p))\phi_m \] defines consistent dynamics equivalent to the one given by the singular Lagrangian used to define our system for initial data for \((q, p)\) satisfying all the constraints (primary and secondary).

Comments on the Dirac algorithm

- Its logic is difficult to follow at times. For instance, sentences such as
  
  *The Poisson bracket \([g, u_m]\) is not defined, but it is multiplied by something that vanishes, \(\phi_m\). So the first term of (1-18) vanishes.*
  
  (P.A.M. Dirac, LQM)
  
  sound strange.

- It is not so straightforward to extended it to field theories.

- This notwithstanding, **the algorithm works well if followed to the letter**! (and if the results are correctly interpreted).
Scalar field with Dirichlet boundary conditions

\[ S[\varphi, \psi_0, \psi_1] = \int_{t_1}^{t_2} dt \left[ \frac{1}{2} \int_0^1 dx (\dot{\varphi}^2 - \varphi'^2) - \psi_0 (\varphi(0) - \varphi_0) + \psi_1 (\varphi(1) - \varphi_1) \right] \]

- The configuration variables are \( \varphi(x) \), \( \psi_0 \) and \( \psi_1 \).
- \( \psi_0 \) and \( \psi_1 \) are Lagrange multipliers introduced to enforce the boundary conditions \( \varphi(0) = \varphi_0 \) and \( \varphi(1) = \varphi_1 \).
- \( \varphi_0, \varphi_1 \in \mathbb{R} \), (boundary values of \( \varphi \)).
- \( \varphi \in C^2(0, 1) \cap C^1[0, 1] \) (smooth enough).

Do we get the right field equations?

We should better check...
Scalar field with Dirichlet boundary conditions

Field equations: variations of the action

\[
\delta S = \int_{t_1}^{t_2} dt \left( \int_0^1 dx (-\ddot{\varphi}(x) + \varphi''(x)) \delta \varphi(x) - \varphi'(x) \delta \varphi(x) \bigg|_0^1 \right) \\
- \int_{t_1}^{t_2} dt (\varphi(0) - \varphi_0) \delta \psi_0 + \int_{t_1}^{t_2} dt (\varphi(1) - \varphi_1) \delta \psi_1 \\
- \int_{t_1}^{t_2} dt \psi_0 \delta \varphi(0) + \int_{t_1}^{t_2} dt \psi_1 \delta \varphi(1)
\]

\[\ddot{\varphi}(x) - \varphi''(x) = 0, \quad x \in (0, 1)\]
\[\varphi(0) = \varphi_0\]
\[\varphi(1) = \varphi_1\]
\[\psi_1 - \varphi'(1) = 0\]
\[\psi_0 - \varphi'(0) = 0\]
Scalar field with Dirichlet boundary conditions

- **Canonical momenta:**
  \[ \pi(x) := \frac{\delta L}{\delta \dot{\phi}(x)} = \dot{\phi}(x), \quad p_0 := \frac{\partial L}{\partial \dot{\psi}_0} = 0, \quad p_1 := \frac{\partial L}{\partial \dot{\psi}_1} = 0 \]

- **Primary constraints** \( p_0 = 0 \) and \( p_1 = 0 \).
- **Non-zero Poisson brackets**
  \[ \{\phi(x), \pi(y)\} = \delta(x, y), \quad \{\psi_0, p_0\} = 1, \quad \{\psi_1, p_1\} = 1 \]

- **Total hamiltonian**
  \[ H_T = \psi_0(\phi(0) - \phi_0) - \psi_1(\phi(1) - \phi_1) + u_0 p_0 + u_1 p_1 + \frac{1}{2} \int_0^1 dx (\pi^2 + \phi'^2) \cdot \]

- Here \( u_0 \) and \( u_1 \) are the Lagrange multipliers that enforce the primary constraints in the Dirac algorithm.

**Before going further just a short question...**
What is the value of \( \{\varphi(0), \pi(0)\}\) ?, Is it 1 ?, Is it \( \delta(0, 0)\) ?

This is not an academic question

**Secondary constraints** (at \( x = 0 \), analogously at \( x = 1 \))

\[
\{H_T, p_0\} = \varphi(0) - \varphi_0 = 0 \quad \text{(OK)}
\]

\[
\{H_T, \varphi(0) - \varphi_0\} = \int_0^1 dx \pi(x) \{\pi(x), \varphi(0)\} = -\pi(0) = 0 \quad \text{(uhm...)}
\]

\[
\{H_T, \pi(0)\} = \{\varphi(0), \pi(0)\} \psi_0 + \int_0^1 dx \varphi'(x) \{\varphi'(x), \pi(0)\}
\]

\[
= \{\varphi(0), \pi(0)\} \psi_0 + \varphi'(x) \{\varphi(x), \pi(0)\} \bigg|_0^1
\]

\[
- \int_0^1 dx \varphi''(x) \{\varphi(x), \pi(0)\} \quad (???)
\]

The algorithm **crashes**. One has to be careful...
Geometric interpretation of the Dirac algorithm
The geometric exegesis of the Dirac algorithm, preliminaries.

- The goal is to find a Hamiltonian $H$ defined on the whole phase space such that the integral curves of the Hamiltonian vector field $X_H$ describe the dynamics of the system for allowed initial data. This is important to implement the quantization programme à la Dirac.

- The dynamics must take place on the primary constraint submanifold of the phase space given by $FL(TQ)$ (the image of the fiber derivative defining the momenta).

- The Hamiltonian vector field, when restricted to the submanifold where the dynamics takes place, must be tangent to it (otherwise the integral curves would fail to remain there!)

The gist of Dirac’s algorithm is this tangency condition.
The geometric exegesis of the Dirac algorithm (continued).

The starting point is the identification of the **primary constraints** $\phi_n$. These are found by computing the **fiber derivative** (definition of momenta)

$$FL : TQ \to T^*Q$$

From the energy $E$ we get the **Hamiltonian** from $H \circ FL = E$ (a real function in $T^*Q$ which is uniquely defined only on the **primary constraint submanifold** $M_0 := FL(TQ)$, given by constraints $\phi_n = 0$).

Find the vector fields $X$ satisfying

$$\iota_X \Omega - dH - u_n d\phi_n = 0$$

and require also

$$\phi_n(q, p) = 0.$$
In order to have consistent dynamics we must require $X$ to be tangent to the primary constraint submanifold $\mathcal{M}_0$.

$\mathcal{I}_X d\phi_i|_{\mathcal{M}_0} = 0$

$\mathcal{I}_X d\phi_n$ just gives, at each point, the directional derivative of $\phi_i$ along $X$. Notice that it can be computed without using the symplectic form.

Three things may happen at this point:

1. The tangency condition is **identically satisfied**.
2. The tangency condition is only satisfied **on a proper submanifold** of the primary constraint submanifold.
3. The tangency condition **fixes some** of the arbitrary $u_n$. 
The geometric exegesis of the Dirac algorithm, (continued).

- In the **first case** we are done.
- In the **second case** the conditions defining the submanifold are **secondary constraints**. The Hamiltonian vector field $X$ will be tangent to the primary constraint manifold but may fail to be tangent to the new submanifold. If this is the case we must persevere with tangency.
- In the **third case** the specific values of $u_n$, when introduced in $X$ will give us a Hamiltonian vector field defining the right evolution.

The dynamics that we obtain by projecting the integral curves of the Hamiltonian vector fields onto $Q$ is the same as the Lagrangian dynamics. We also obtain the additional conditions that the initial data (on the generalized positions and momenta) must satisfy.
Scalar field with Dirichlet boundary conditions

(Homogeneous conditions $\varphi(0) = \varphi(1) = 0$)

Lagrangian

$$L(v) = \frac{1}{2} \int_0^1 \left( v_\varphi^2 - \varphi'^2 + 2 (\psi \varphi)' \right)$$

Fiber derivative

$$\langle FL(v) | w \rangle = \int_0^1 v_\varphi w_\varphi, \quad \rightarrow \quad p_\varphi(\cdot) := \int_0^1 v_\varphi \cdot ,$$

$$p_\psi(\cdot) := 0.$$ 

Hamiltonian (extension to the full phase space)

$$H = \frac{1}{2} \int_0^1 \left( p_\varphi^2 + \varphi'^2 - 2 (\psi \varphi)' \right),$$
Scalar field with Dirichlet boundary conditions

Vector fields

\[ Y \in T(\varphi, \psi; p_\varphi, p_\psi) \quad T^* Q \to Y = ( (\varphi, \psi; p_\varphi, p_\psi), (Y_\varphi, Y_\psi, Y_{p_\varphi}(\cdot), Y_{p_\psi}(\cdot)) ). \]

\( Y_{p_\varphi}(\cdot), Y_{p_\psi}(\cdot) \) can be represented by real functions \( Y_{p_\varphi}, Y_{p_\psi} \) such that over functions \( f, g \in Q \)

\[ Y_{p_\varphi}(f) := \int_0^1 Y_{p_\varphi} f, \quad Y_{p_\psi}(g) := \int_0^1 Y_{p_\psi} g. \]

Differential of \( H \) acting on a vector field \( Y \)

\[ dH(Y) = \int_0^1 (Y_{p_\varphi} p_\varphi - \varphi'' Y_\varphi) - [(\psi - \varphi') Y_\varphi + \varphi Y_\psi](1) + [(\psi - \varphi') Y_\varphi + \varphi Y_\psi](0). \]

Canonical symplectic form in \( T^* Q \), acting on a pair of vector fields \( X, Y \)

\[ \Omega(X, Y) = \int_0^1 (Y_{p_\varphi} X_\varphi - X_{p_\varphi} Y_\varphi + Y_{p_\psi} X_\psi - X_{p_\psi} Y_\psi). \]
We solve for $X$ in the equation (for all $Y$)

$$
\Omega(X, Y) = dH(Y) + \langle u|dp_\psi \rangle(Y) = dH(Y) + \int_0^1 uY_{p_\psi}
$$

By considering first fields $Y$ vanishing at 0 and 1 we get the Hamiltonian vector field $X$ in the interval $[0, 1]$

$$
X_\varphi = p_\varphi, \quad X_\psi = u, \quad X_{p_\varphi} = \varphi'', \quad X_{p_\psi} = 0.
$$

Once we know $X$, we can allow $Y$ to be arbitrary on the boundary. This gives us, then, the following secondary constraints

$$
\varphi(0) = 0, \quad \varphi(1) = 0, \quad (1)
$$

$$
\psi(0) - \varphi'(0) = 0, \quad \psi(1) - \varphi'(1) = 0, \quad (2)
$$

which include both the Dirichlet boundary conditions and the values of $\psi$ at the boundary. This is the result given by the Euler-Lagrange equations.
We must check now the tangency of the Hamiltonian field, to the submanifold in $T^*Q$ defined by the constraints $p_\psi = 0$ and the boundary conditions

\[
0 = \iota_X dp_\psi = X_{p_\psi},
\]
\[
0 = \iota_X d(\varphi(j)) = X_{\varphi}(j) = p_\varphi(j), \quad j \in \{0, 1\}
\]
\[
0 = \iota_X d(\psi(j) - \varphi'(j)) = X_\psi(j) - X_{\varphi}'(j) = u(j) - p_{\varphi}'(j) \quad j \in \{0, 1\}.
\]

- The first gives nothing new.
- The next pair of conditions are new secondary constraints at 0 and 1.
- The last pair fixes the Dirac multiplier at the boundary $u(0) = p_{\varphi}'(0)$, $u(1) = p_{\varphi}'(1)$. 

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**Tangency of the Hamiltonian vector field**

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<th>Expression</th>
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<td>$u(j) - p_{\varphi}'(j) \quad j \in {0, 1}$.</td>
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Scalar field with Dirichlet boundary conditions

We must demand now that the vector field \( X \) be tangent to the new submanifold defined by the secondary constraints just obtained. These new tangency conditions give

\[
0 = \iota_X d(p\varphi(j)) = X_{p\varphi}(j) = D^2\varphi(j), \quad j \in \{0, 1\}
\]

where \( D^n \) denotes the \( n \)-th order spatial derivative.

As we see, there are more secondary constraints and additional tangency requirements. Iterating this process, we find an infinite number of boundary constraints of the form \( (n \in \mathbb{N}) \)

\[
D^{2n}\varphi(0) = 0, \quad D^{2n}p\varphi(0) = 0, \\
D^{2n}\varphi(1) = 0, \quad D^{2n}p\varphi(1) = 0.
\]
## Scalar field (final result)

### Hamiltonian vector field

- $X_\varphi = p_\varphi$
- $X_\psi = u$
- $X_{p_\varphi} = \varphi''$
- $X_{p_\psi} = 0$

### Primary constraints

- $p_\psi(\cdot) := 0$

### Secondary constraints

- $\varphi(0) = 0$, $\varphi(1) = 0$
- $\psi(0) - \varphi'(0) = 0$, $\psi(1) - \varphi'(1) = 0$
- $p_\varphi(0) = 0$, $p_\varphi(1) = 0$
- $D^{2n}\varphi(0) = 0$, $D^{2n}\varphi(1) = 0$, $n \in \mathbb{N}$
- $D^{2n}p_\varphi(0) = 0$, $D^{2n}p_\varphi(1) = 0$, $n \in \mathbb{N}$

The Lagrange multiplier $u$ is **arbitrary** in $(0, 1)$ but $u(0) = u(1) = 0$
Meaning of the boundary constraints $D^{2n}\varphi(j) = 0, D^{2n}p\varphi(j) = 0, j = 0, 1$
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The geometric approach to the Dirac algorithm

- The steps of the Dirac algorithm can be conveniently interpreted in geometric terms.
- The stability of the constraints is the tangency condition of the constraint submanifold to the Hamiltonian vector field.
- Actual computations can be performed in a way that avoids the use of formal Poisson brackets. This is sometimes useful, for instance, for field theories in bounded regions.
- In practice the computations are rather clean and quick.
- A similar approach—the so called Gotay-Nester-Hinds (GNH) method—does a similar thing on the primary constraint submanifold.
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Happy birthday, Jurek!!