The geometric exegesis of the Dirac algorithm

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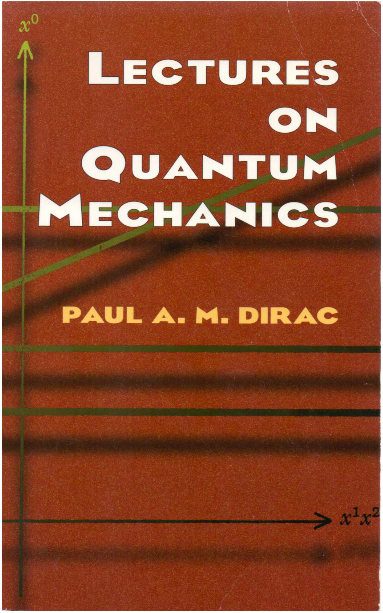
Motivation

back

- 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


x^0
LECTURES
ON
QUANTUM
MECHANICS
PAUL A. M. DIRAC
$x^1 x^2$

The Dirac algorithm in words

- Write the canonical momenta p in terms of q and $\dot{q}$.
- Find the **primary constraints**, 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.
- Find a Hamiltonian H and build the **total Hamiltonian** $H_T = H + \sum u_m \phi_m$ in which the **primary constraints** are introduced together with some multipliers $u_m(t)$.
- The u_m must be fixed by enforcing the **consistency of the time evolution of the system.** This consistency requires, for instance, that the primary constraints be **preserved in time**:

$$\boxed{\{\phi_m, H\} + u_n\{\phi_m, \phi_n\} \approx 0}$$

  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

$$\boxed{\{\phi_j, H\} + u_n\{\phi_j, \phi_n\} \approx 0}$$

- 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.

$$\boxed{u_m = U_m(q,p) + v_a(t)V_{am}(q,p)},$$

where $V_{an}\{\phi_j, \phi_n\} = 0$ and the $v_a(t)$ are arbitrary functions of time.

The Hamiltonian $\hat{\mathrm{H}} = \mathrm{H} + (U_m(q,p) + v_a(t)V_{am}(q,p))\phi_m$ 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,* ϕ_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 back

$$S[\varphi,\psi_0,\psi_1]=\int_{t_1}^{t_2}\mathrm{d}t\left[\frac{1}{2}\int_0^1\mathrm{d}x(\dot{\varphi}^2-\varphi'^2)-\psi_0\big(\varphi(0)-\varphi_0\big)+\psi_1\big(\varphi(1)-\varphi_1\big)\right]$$

- The configuration variables are $\varphi(x)$, ψ_0 and ψ_1.
- ψ_0 and ψ_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 φ).
- $\varphi\in C^2(0,1)\cap C^1[0,1]$ (smooth enough).

Do we get the right field equations?

We should better check...

Scalar field with Dirichlet boundary conditions back

Field equations: variations of the action

$$
\begin{aligned}
\delta S \ = \ & \int_{t_1}^{t_2} \mathrm{d}t \left(\int_0^1 \mathrm{d}x(-\ddot{\varphi}(x) + \varphi''(x))\delta\varphi(x) - \varphi'(x)\delta\varphi(x)\Big|_0^1 \right) \\
- \ & \int_{t_1}^{t_2} \mathrm{d}t(\varphi(0) - \varphi_0)\delta\psi_0 + \int_{t_1}^{t_2} \mathrm{d}t(\varphi(1) - \varphi_1)\delta\psi_1 \\
- \ & \int_{t_1}^{t_2} \mathrm{d}t\psi_0\delta\varphi(0) + \int_{t_1}^{t_2} \mathrm{d}t\psi_1\delta\varphi(1)
\end{aligned}
$$

$$
\begin{aligned}
& \ddot{\varphi}(x) - \varphi''(x) = 0\,, \quad x \in (0,1) \\
& \varphi(0) = \varphi_0 \\
& \varphi(1) = \varphi_1 \qquad \checkmark \\
& \psi_1 - \varphi'(1) = 0 \\
& \psi_0 - \varphi'(0) = 0
\end{aligned}
$$

Scalar field with Dirichlet boundary conditions back

- **Canonical momenta**:

$$\pi(x) := \frac{\delta \mathcal{L}}{\delta \dot{\varphi}(x)} = \dot{\varphi}(x)\,,\, p_0 := \frac{\partial \mathcal{L}}{\partial \dot{\psi}_0} = 0\,,\, p_1 := \frac{\partial \mathcal{L}}{\partial \dot{\psi}_1} = 0$$

- **Primary constraints** $p_0 = 0$ and $p_1 = 0$.
- Non-zero **Poisson brackets**

$$\{\varphi(x), \pi(y)\} = \delta(x, y)\,, \{\psi_0, p_0\} = 1\,, \{\psi_1, p_1\} = 1$$

- **Total hamiltonian**

$$H_T = \psi_0\big(\varphi(0) - \varphi_0\big) - \psi_1\big(\varphi(1) - \varphi_1\big) + u_0 p_0 + u_1 p_1 + \frac{1}{2}\int_0^1 \mathrm{d}x\big(\pi^2 + \varphi'^2\big)\,.$$

- 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...

Scalar field with Dirichlet boundary conditions back

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 $x=1$)

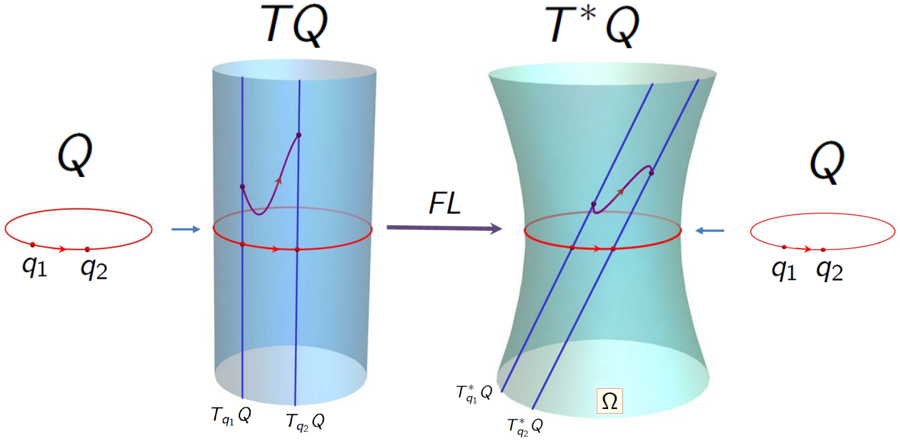
$$\{H_T,p_0\}=\varphi(0)-\varphi_0=0 \quad \text{(OK)}$$

$$\{H_T,\varphi(0)-\varphi_0\}=\int_0^1 \mathrm{d}x\pi(x)\underbrace{\{\pi(x),\varphi(0)\}}_{-\delta(x,0)}=-\pi(0)=0 \quad \text{(uhm...)}$$

$$\begin{aligned}\{H_T,\pi(0)\} &= \{\varphi(0),\pi(0)\}\psi_0+\int_0^1 \mathrm{d}x\varphi'(x)\{\varphi'(x),\pi(0)\}\\ &= \{\varphi(0),\pi(0)\}\psi_0+\varphi'(x)\{\varphi(x),\pi(0)\}\Big|_0^1\\ &\quad -\int_0^1 \mathrm{d}x\varphi''(x)\{\varphi(x),\pi(0)\} \quad \text{(???)}\end{aligned}$$

The algorithm **crashes**. One has to be careful...

Geometric interpretation of the Dirac algorithm back



Singular Hamiltonian systems: the Dirac algorithm back

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** ϕ_n. These are found by computing the **fiber derivative** (definition of momenta)
$$\boxed{FL : TQ \to T^*Q}$$
- 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** $\mathcal{M}_0 := FL(TQ)$, given by **constraints** $\phi_n = 0$).
- Find the vector fields X satisfying
$$\boxed{\imath_X \Omega - \mathrm{d}H - u_n \mathrm{d}\phi_n = 0}$$
and require also
$$\boxed{\phi_n(q,p) = 0}\,.$$

The geometric exegesis of the Dirac algorithm, (continued).

- In order to have consistent dynamics we must require X to be **tangent** to the primary constraint submanifold $\mathcal{M}_0$.

$$\boxed{\imath_X \mathrm{d}\phi_i \big| \mathcal{M}_0 = 0}$$

  $\imath_X \mathrm{d}\phi_n$ just gives, at each point, the **directional derivative** of ϕ_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.

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

Lagrangian

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

Fiber derivative

$$\langle FL(\mathrm{v})|\mathrm{w}\rangle \;=\; \int_0^1 v_\varphi w_\varphi, \quad\longrightarrow\quad \begin{array}{l} \mathbf{p}_\varphi(\cdot):=\displaystyle\int_0^1 v_\varphi\,\cdot\,, \\[2ex] \mathbf{p}_\psi(\cdot):=0\,. \end{array}$$

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 back

Vector fields

$$Y \in T_{(\varphi,\psi;p_\varphi,p_\psi)} T^*\mathcal{Q} \to Y = \big((\varphi,\psi;p_\varphi,p_\psi)\,,(Y_\varphi, Y_\psi, \boldsymbol{Y}_{\mathbf{p}_\varphi}(\cdot), \boldsymbol{Y}_{\mathbf{p}_\psi}(\cdot))\big)\ .$$

$\boldsymbol{Y}_{\mathbf{p}_\varphi}(\cdot)$, $\boldsymbol{Y}_{\mathbf{p}_\psi}(\cdot)$ can be represented by real functions $Y_{\mathbf{p}_\varphi}, Y_{\mathbf{p}_\psi}$ such that over functions $f, g \in \mathcal{Q}$

$$\boldsymbol{Y}_{\mathbf{p}_\varphi}(f) := \int_0^1 Y_{\mathbf{p}_\varphi} f\,, \quad \boldsymbol{Y}_{\mathbf{p}_\psi}(g) := \int_0^1 Y_{\mathbf{p}_\psi} g\,.$$

Differential of H acting on a vector field Y

$$\mathrm{d}H(Y) = \int_0^1 \left(Y_{p_\varphi} p_\varphi - \varphi'' Y_\varphi\right) - \left[\left(\psi - \varphi'\right) Y_\varphi + \varphi Y_\psi\right](1) + \left[\left(\psi - \varphi'\right) Y_\varphi + \varphi Y_\psi\right](0)\,.$$

Canonical symplectic form in $T^*\mathcal{Q}$, acting on a pair of vector fields X, Y

$$\Omega(X,Y) = \int_0^1 \left(Y_{p_\varphi} X_\varphi - X_{p_\varphi} Y_\varphi + Y_{p_\psi} X_\psi - X_{p_\psi} Y_\psi\right)\ .$$

Scalar field with Dirichlet boundary conditions back

We solve for X in the equation (for all Y)

$$\Omega(X,Y) = \mathbf{d}H(Y) + \langle \mathbf{u} | \mathbf{d}p_\psi \rangle(Y) = \mathbf{d}H(Y) + \int_0^1 u Y_{p_\psi}$$

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

$$\begin{aligned} X_\varphi &= p_\varphi\,, & X_\psi &= u\,, \\ X_{p_\varphi} &= \varphi''\,, & X_{p_\psi} &= 0\,. \end{aligned}$$

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

$$\varphi(0) = 0 \qquad \varphi(1) = 0\,, \tag{1}$$

$$\psi(0) - \varphi'(0) = 0 \qquad \psi(1) - \varphi'(1) = 0\,, \tag{2}$$

which include both the **Dirichlet boundary conditions** and the **values of ψ at the boundary**. This is the result given by the Euler-Lagrange equations.

Scalar field with Dirichlet boundary conditions back

We must check now the tangency of the Hamiltonian field, to the submanifold in $T^*\mathcal{Q}$ defined by the constraints $p_\psi = 0$ and the boundary conditions

Tangency of the Hamiltonian vector field

$$0 = \imath_X \mathbf{d} p_\psi = X_{p_\psi} \,,$$
$$0 = \imath_X \mathbf{d}\left(\varphi(j)\right) = X_\varphi(j) = p_\varphi(j) \,, \quad j \in \{0,1\}$$
$$0 = \imath_X \mathbf{d}\left(\psi(j) - \varphi'(j)\right) = X_\psi(j) - X'_\varphi(j) = u(j) - p'_\varphi(j) \quad j \in \{0,1\} \,.$$

- 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 $u(0) = p'_\varphi(0)$, $u(1) = p'_\varphi(1)$.

Scalar field with Dirichlet boundary conditions back

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

$$0 = \imath_X \mathbf{d}\left(p_\varphi(j)\right) = X_{p_\varphi}(j) = D^2\varphi(j)\,, \quad j \in \{0,1\}$$

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 ($n \in \mathbb{N}$)

$$\begin{aligned} D^{2n}\varphi(0) &= 0\,, & \qquad D^{2n}p_\varphi(0) &= 0\,,\\ D^{2n}\varphi(1) &= 0\,, & \qquad D^{2n}p_\varphi(1) &= 0\,. \end{aligned}$$

Scalar field (final result)

back

Hamiltonian vector field

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

Primary constraints

$$\boxed{\mathbf{p}_\psi(\cdot) := 0}$$

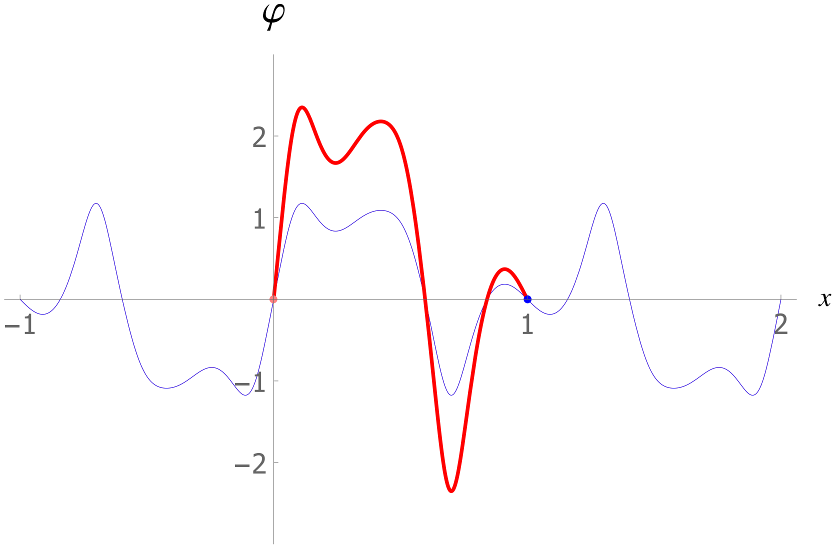
Secondary constraints

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

The Lagrange multiplier u is **arbitrary** in $(0,1)$ but $u(0) = u(1) = 0$

Scalar field with Dirichlet boundary conditions back

Meaning of the boundary constraints $D^{2n}\varphi(j) = 0\,, D^{2n}p_\varphi(j) = 0\,, j = 0\,,1$



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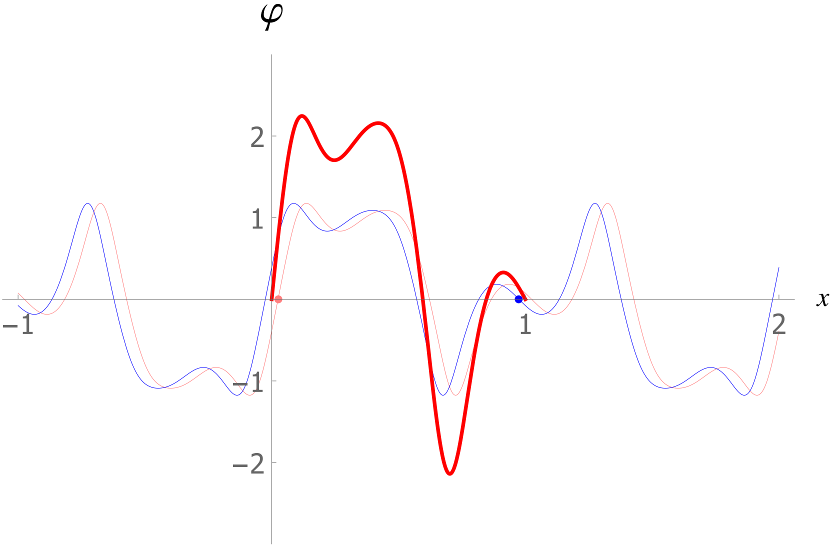

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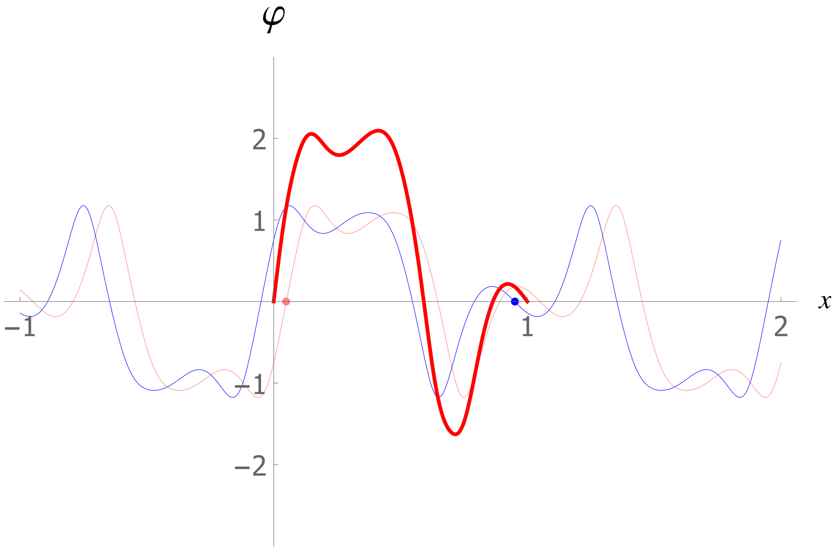

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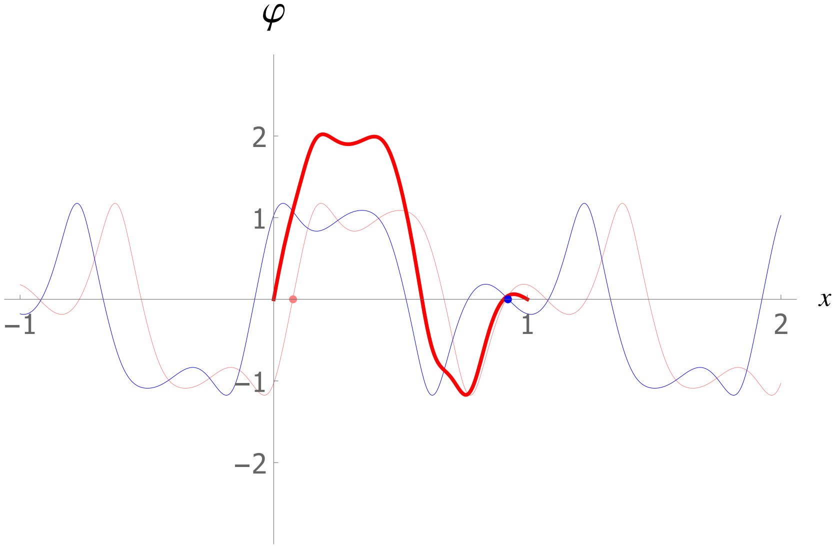

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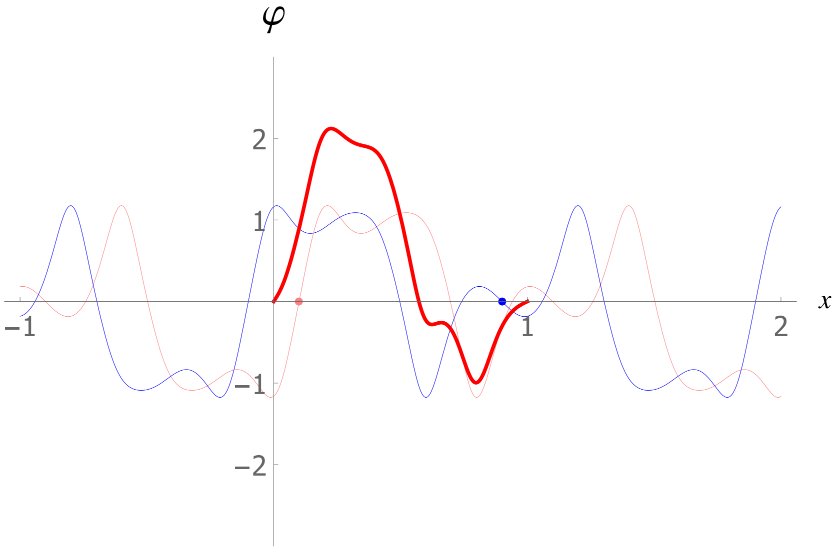

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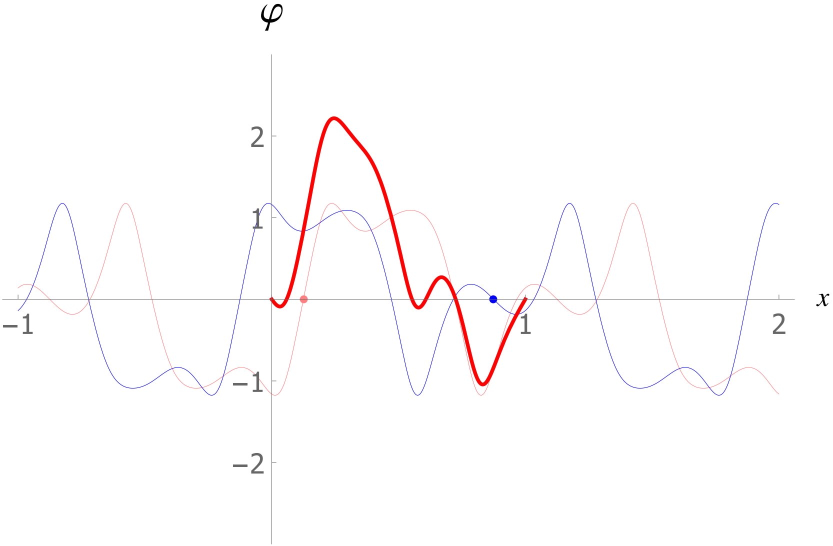

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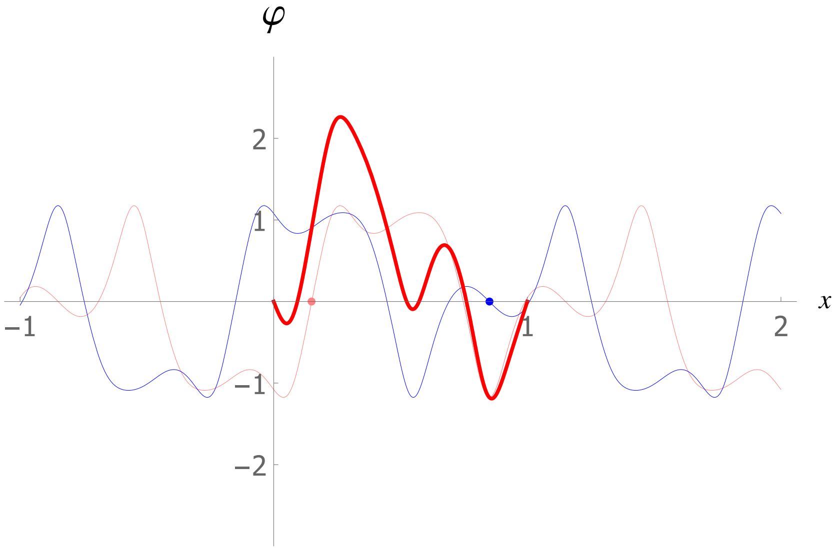

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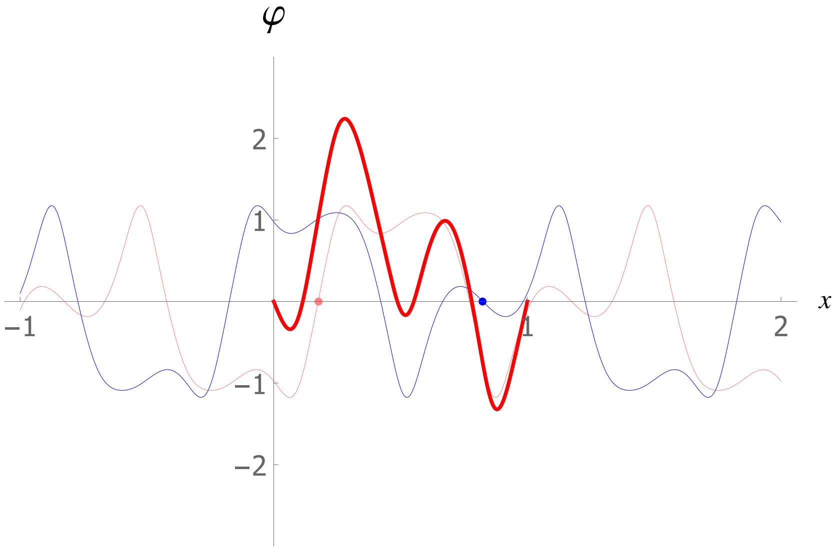

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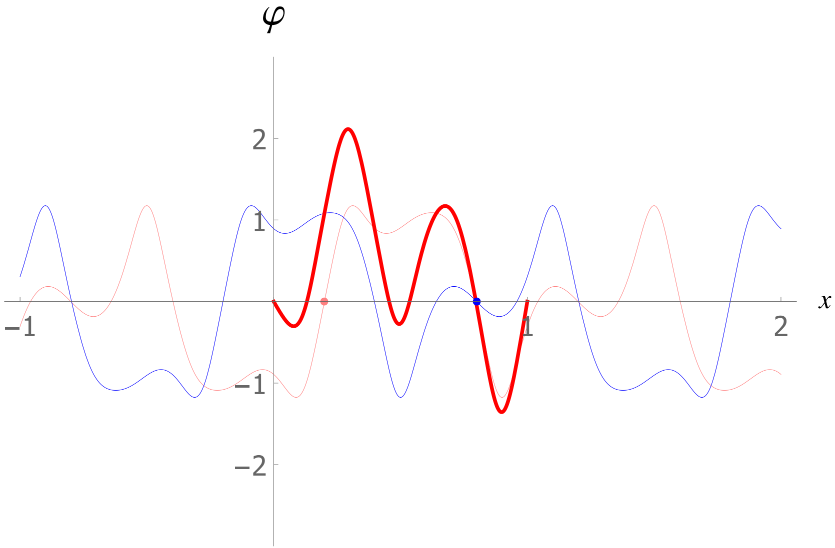

Conclusions

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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.

Conclusions

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Happy birthday, Jurek!!