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Boundary conditions as Dirac constraints

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Abstract. In this article we show that boundary conditions can be treated as Lagrangian and Hamiltonian constraints. Using the Dirac method, we find that boundary conditions are equivalent to an infinite chain of second class constraints, which is a new feature in the context of constrained systems. Constructing the Dirac brackets and the reduced phase space structure for different boundary conditions, we show why mode expanding and then quantizing a field theory with boundary conditions is the proper way. We also show that in a quantized field theory subjected to the mixed boundary conditions, the field components are non-commutative.

1 Introduction

It is well known that to formulate a general classical field theory defined in a box, besides the equations of motion one should know the behavior of the fields on the boundaries: the boundary conditions. Boundary conditions are usually relations between the fields and their various derivatives, including the time derivative, on the boundaries, which are expected to hold at all times. In Hamiltonian language the boundary conditions are in general functions of the fields and their conjugate momenta; hence the field theories subjected to the boundary conditions might be understood by the prescription for handling the constrained systems proposed by Dirac [1].

In the usual field theory arguments, since boundary conditions are usually linear combinations of fields and their momenta, one can easily impose them on the solutions of the equations of motion, and find the final result. But imposing the boundary conditions may in some special cases leads to inconsistencies with the canonical commutation relations [2–7].

In this article, considering the boundary conditions as constraints, we apply the Dirac procedure to this constrained system. Although this idea has been used in [5,6], the problem has new and special features in the context of constrained systems on which we mostly concentrate.

In the second section, we review the Lagrangian and Hamiltonian constrained systems. In Sect. 3, to visualize the seat of boundary conditions we take a toy model and by discretizing this model we show that boundary conditions are in fact the equations of motion for the points at the boundaries so that when we go to the continuum limit, i.e. the original theory, the acceleration term disappears. In other words, boundary conditions are Lagrangian constraints which are not consequences of a singular Lagrangian. In Sect. 4, going to the Hamiltonian picture we study the constraint structure resulting from the boundary conditions, and apply it explicitly to some field theories. Implying constraint consistency we show that although the Lagrange multiplier is determined, the constraint chain is not terminated. This is a new feature in the constrained systems analysis. Exhausting all the consistency checks we end up with an infinite constraint chain which all are of second class. This is another new feature of this constraint structure, which recently has also been addressed in [6]. Moreover, we construct the fundamental Dirac brackets, the Dirac brackets of fields and their conjugate momenta. In Sect. 5, by a canonical transformation we go to the Fourier modes, in terms of which the constraint chain obtained in the previous section can easily be solved. In this way we prove that using the proper mode expansions is equivalent to working in the *reduced phase space*. In Sect. 6, we apply the machinery developed in the previous sections to the case of mixed boundary conditions, i.e. we find the constraints chain, the Dirac bracket and the reduced phase space. The new and interesting result of this case is that the Dirac bracket of two field components is obtained to be non-zero, and hence in the quantum theory these field components are non-commuting. The last section is devoted to the concluding remarks.

2 Review of Dirac procedure

Given the Lagrangian $L(q,\dot q)$ (or $L(\phi,\partial\phi)$ in a field theory), the Lagrangian equations of motion are

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$$\boldsymbol{L}_i = W_{ij}\ddot{q}_j + \alpha_i = 0, \tag{2.1}$$

where $\boldsymbol{L}_i$ are Eulerian derivatives, $W_{ij}(q,\dot{q}) \equiv \partial^2 L/\partial\dot{q}^i\partial\dot{q}^j$ is called the Hessian matrix, and $\alpha_i \equiv \partial L/\partial q^i - \dot{q}_j\left(\partial^2 L/\partial\dot{q}^i\partial q^j\right)$. If $|W_{ij}| = 0$, the Lagrangian is called *singular*, and in this case the number of equations containing accelerations is less than the number of degrees of freedom. Hence a number of Lagrangian constraints, $\gamma^a(q,\dot{q}) = 0$, emerges. To obtain these constraints we should simply multiply both sides of (2.1) by the null eigenvector λ_i^a of W, so $\gamma^a(q,\dot{q}) = \lambda_i^a\alpha_i$ [8]. Then we should add the time derivatives of the constraints, $\dot{\gamma}^a(q,\dot{q})$, to the set of equations of motion to get new relations containing the accelerations. As a result two cases may occur.

(1) The rank of equations with respect to acceleration is equal to the number of degrees of freedom.
(2) New constraints, acceleration-free relations, may emerge.

In the first case the equations of motion can be solved completely; however, the solutions should obey the acceleration-free equations, the constraints. In the second one, the derivatives of new constraints and derivatives of previous constraints should be added to the equations of motion, and the scenario should be repeated.

In the end, there may remain a number of undetermined accelerations; it has been shown that these correspond to the gauge degrees of freedom and are related to the first class Hamiltonian constraints. Moreover, roughly speaking, there may exist some degrees of freedom which have no dynamics and are completely determined via the constraints. These are related to the second class Hamiltonian constraints [9].

Let us study the Hamiltonian formulation. Singularity of the Hessian matrix, $p_i/\partial\dot{q}^j$, implies the Legendre transformation, $(q,\dot{q}) \to (q,p)$, to have a zero Jacobian and hence, the set of momenta, p_i,

$$p_i = \frac{\partial L}{\partial \dot{q}^i}, \tag{2.2}$$

are not independent functions of q and $\dot{q}$. So a number of Hamiltonian primary constraints turns up:

$$\Phi_a^{(0)}(q,p) = 0. \tag{2.3}$$

It can be shown that [1] the dynamics of any function in phase space is obtained by

$$\dot{g} \approx \{g, H_T\}_{\text{P.B.}}, \tag{2.4}$$

where the weak equality, $\approx$, is the equality on the constraint surface, and

$$H_T = H + \lambda_a\Phi_a \tag{2.5}$$

is the total Hamiltonian, λ_a being the Lagrange multipliers.

Like the Lagrangian case the consistency conditions of the primary constraints should be investigated, i.e. the constraints should be valid under the time evolution:

$$\dot{\Phi}_a^{(0)} \approx \{\Phi_a^{(0)}, H_T\}_{\text{P.B.}} \approx \{\Phi_a^{(0)}, H\} + \lambda_b\{\Phi_a^{(0)}, \Phi_b^{(0)}\} \approx 0. \tag{2.6}$$

If the above relation does not hold identically, then two possibilities remain:

(i) (i) the $\{\Phi_a^{(0)}, \Phi_b^{(0)}\}$'s weakly vanish. In this case new Hamiltonian constraints,

$$\Phi^{(1)} = \{\Phi_a^{(0)}, H\}, \tag{2.7}$$

turn up;

(ii) the $\{\Phi_a^{(0)}, \Phi_b^{(0)}\}$ do not vanish, yielding equations for determining λ_a.

In general, depending on the rank of the matrix $\{\Phi_a^{(0)}, \Phi_b^{(0)}\}$, we may have a mixture of two possibilities. That is, some of the Lagrange multipliers are determined and a number of new constraints emerge. Here we do not bother the reader with the details. A complete and detailed discussion can be found in [9].

Now the consistency conditions of $\Phi_a^{(1)}$ should be verified which may result in some new constraints $\Phi_a^{(2)}$. The procedure goes on, and finally we end up with some *constraint chains*. Roughly speaking, each chain terminates if a Lagrange multiplier is determined or if we get an identically satisfied relation. The latter case occurs when the last constraint has a weakly vanishing Poisson bracket with the primary constraints and the Hamiltonian.

We denote the set of constraints $\Phi^{(1)}, \Phi^{(2)}, \ldots$ as *secondary constraints*. These are really consequences of primary constraints while the primary constraints, by themselves have their origin in the singularity of the Lagrangian (singularity of the Hessian matrix). In a pure Hamiltonian point of view, however, the origin of primary constraints is not essential. In any way given some primary constraints, we should build the total Hamiltonian, (2.5), and check consistency.

There is another important classification of constraints. If the Poisson bracket of some constraint with all the constraints in the chain vanishes, it is called *first class*. If the matrix of mutual Poisson brackets of a subset of constraints, C^{MN},

$$C^{MN} = \{\Phi^M, \Phi^N\}, \tag{2.8}$$

has the maximal rank, it is invertible; then we deal with *second class constraints*. It is shown that a constraint chain terminating with an identity is of the first class and when we end with determining Lagrange multipliers they are of the second class [9]. To find the dynamics of a system with second class constraints, one may use the Dirac bracket,

$$\{A,B\}_{\text{D.B.}} = \{A,B\}_{\text{P.B.}} - \{A,\Phi_M\}_{\text{P.B.}} (C^{-1})^{MN}\{\Phi_N, B\}_{\text{P.B.}}. \tag{2.9}$$

The important property of the Dirac bracket is that for an arbitrary function A and for all second class constraints Φ_M,

$$\{\Phi_M, A\}_{\rm D.B.} = 0. \qquad (2.10)$$

It can be shown that using the Dirac brackets instead of Poisson brackets is equivalent to a priori putting the second class constraints *strongly* equal to zero.

For second class constraints we can always find a *canonical transformation* such that the constraints, Φ_M, lie on the first $2n$ coordinates $(q_1, ..., q_n; p_1, ..., p_n)$ of the phase space and the remaining degrees of freedom, $(Q_1, ..., Q_{N-n}; P_1, ..., P_{N-n})$ are unconstrained. The Dirac bracket in the original phase space is equal to the Poisson bracket in the space $(Q_1, ..., Q_{N-n}; P_1, ..., P_{N-n})$, the *reduced phase space* [1,10,11]. Although finding the above canonical transformation is not an easy task, for the case we study in this paper, boundary conditions as constraints, we show that using the suitable mode expansions, is in fact equivalent to going to reduced phase space.

3 Boundary conditions as constraints

Boundary conditions are acceleration-free equations which in general are not related to a singular Lagrangian. To visualize this point, let us take a simple (1+1) field theory as a toy model:

$$S = \frac{1}{2}\int_0^l \mathrm{d}x \int_{t_1}^{t_2} \mathrm{d}t[(\partial_t\phi)^2 - (\partial_x\phi)^2]. \qquad (3.1)$$

Variation of the action with respect to ϕ gives

$$\delta S = \int_0^l \mathrm{d}x \int_{t_1}^{t_2} \mathrm{d}t\boldsymbol{L}(\phi)\delta\phi + \int_{t_1}^{t_2} \mathrm{d}t(\partial_x\phi)\delta\phi|_0^l + \int_0^l \mathrm{d}t(\partial_t\phi)\delta\phi|_{t_1}^{t_2}, \qquad (3.2)$$

where $\boldsymbol{L}(\phi) = \partial_t^2\phi - \partial_x^2\phi$ is the Eulerian derivative. For an arbitrary $\delta\phi$, the variation of the action vanishes if the three terms in the above equation vanish independently. The first term in (3.2) leads to equations of motion and the last term to the initial conditions. The second term, which is called the surface term, results in the boundary conditions. For this term to vanish, there are two choices: $\delta\phi|_{\rm boundary} = 0$, the Dirichlet boundary conditions, or $\partial_x\phi|_{\rm boundary} = 0$, the Neumann boundary conditions. The boundary conditions, unlike the equations of motion, are acceleration-free equations and should hold at all times. In other words, they can be treated as Lagrangian constraints. To clarify this point we repeat the above argument in the discrete version:

$$S = \frac{1}{2}\int_{t_1}^{t_2} \mathrm{d}t \sum_{i=0}^{N} \epsilon(\partial_t\phi_i)^2 - \sum_{i=0}^{N-1} \frac{1}{\epsilon}(\phi_i - \phi_{i+1})^2, \qquad (3.3)$$

$$\phi_i(t) = \phi(x,t)|_{x=x_i}; \quad x_n = n\epsilon, \qquad (3.4)$$

and $\epsilon = l/N$ so that $\epsilon \to 0$ ($N \to \infty$) reproduces the continuum theory.

Demanding the variation of (3.3) to vanish leads to[1]

$$\epsilon\partial_t^2\phi_0 = \frac{1}{\epsilon}(\phi_1 - \phi_0), \qquad (3.5)$$

$$\epsilon\partial_t^2\phi_i = \frac{1}{\epsilon}(\phi_{i+1} - 2\phi_i + \phi_{i-1}), \quad i \neq 0, N, \qquad (3.6)$$

$$\epsilon\partial_t^2\phi_N = \frac{1}{\epsilon}(\phi_N - \phi_{N-1}). \qquad (3.7)$$

Taking the continuum limit and assuming that accelerations of the end points are finite, the equations for $0, N$ give

$$\lim \frac{1}{\epsilon}(\phi_1 - \phi_0) = 0 \quad \text{and} \quad \lim \frac{1}{\epsilon}(\phi_N - \phi_{N-1}) = 0. \qquad (3.8)$$

Hence in the continuum limit *equations of motion* for the end points give acceleration-free equations, the Lagrangian constraints, whereas (3.6) leads to $\boldsymbol{L}(\phi) = 0$, which actually contains the acceleration term.

A new feature appearing here is that, unlike the usual Lagrangian constraints, boundary conditions are the constraints which are not consequences of the singularity of the Lagrangian, but a result of taking the continuum limit.

4 The Hamiltonian setup

In this section, by going to the Hamiltonian formulation, we apply the Dirac procedure to a field theory with given boundary conditions. Again, we take our simple toy model and treat the boundary conditions as Hamiltonian primary constraints:

$$\Phi^{(0)} = \partial_x\phi|_{x=0}. \qquad (4.1)$$

Here we explicitly work out the Neumann boundary condition at one end, the Neumann boundary condition at the other end, and the Dirichlet cases can be worked out similarly. The total Hamiltonian is built by adding the constraint to the Hamiltonian by an arbitrary Lagrange multiplier:

$$H_T = H + \lambda\Phi^{(0)}, \qquad (4.2)$$

with

$$H = \frac{1}{2}\int_0^l \mathrm{d}x\Pi^2 + (\partial_x\phi)^2, \qquad (4.3)$$

$$\Pi = \partial_t\phi. \qquad (4.4)$$

We should recall that as discussed in Sect. 2, the appearance of the constraints (4.1) is not a consequence of the definition of the momenta for an ordinary singular Lagrangian and hence, the transformation (4.4) between

[1] It is worth noting that we still have the options $\delta\phi_0$ or $\delta\phi_N = 0$, which in the continuum limit translate into the Dirichlet boundary conditions

the velocities and momenta is well defined and invertible throughout all the points, even at the boundaries.

Now we should check the consistency condition

$$\dot{\Phi}^{(0)} = \{\Phi^{(0)}, H_T\}_{\text{P.B.}} = \partial_x \Pi|_0 \equiv \Phi^{(1)}, \tag{4.5}$$

which leads to the secondary constraint, $\Phi^{(1)}$. It should be noted that to obtain (4.5), although the conditions are imposed at the boundaries, the fields can safely be extended into the neighborhood of the boundaries and we can use $\Phi^{(0)} = \int \delta(x)\partial_x\phi \mathrm{d}x$.

We should go further:

$$\dot{\Phi}^{(1)} = \{\Phi^{(1)}, H_T\} = \{\Phi^{(1)}, H\} + \lambda\{\Phi^{(1)}, \Phi^{(0)}\} = 0. \tag{4.6}$$

The second term on the right hand side,

$$\lambda\{\Phi^{(1)}, \Phi^{(0)}\} = \int \delta(x)\delta(x')\{\partial_x \Pi, \partial_{x'}\phi\}\mathrm{d}x\mathrm{d}x' = -\int \delta(x)\delta(x')\partial_x\partial_{x'}\delta(x-x')\mathrm{d}x\mathrm{d}x', \tag{4.7}$$

is not well defined, and formally can be written as $\partial_x^2\delta(x-x')|_{x=x'=0}$. This term compared to the first term is infinitely large. The only way to impose the consistency condition on the constraints is by

$$\lambda = 0 \tag{4.8}$$

and

$$\{\Phi^{(1)}, H\} = 0. \tag{4.9}$$

There is a new feature appearing which is not one of the cases (i) and (ii) discussed in Sect. 2. The consistency condition, (4.6), reduces to two equations, (4.8) and (4.9), and *although the Lagrange multiplier is determined the constraint chain is not terminated.*

The above discussion can be better understood if the calculation is regularized by considering the discrete case. Using the discrete version of (4.6), λ turns out to be of the order of ϵ; going to the continuum limit it vanishes, and the other term, $\{\Phi^{(1)}, H\}$, should vanish separately.

Defining $\{\Phi^{(1)}, H\}$ as $\Phi^{(2)}$, the other secondary constraint, we find

$$\Phi^{(2)} = \partial_x^3\phi|_0. \tag{4.10}$$

Furthermore,

$$\Phi^{(3)} \equiv \dot{\Phi}^{(2)} = \{\Phi^{(2)}, H_T\} = \{\Phi^{(2)}, H\} = \partial_x^3 \Pi|_0. \tag{4.11}$$

This process should be continued and finally we are left with an infinite number of constraints:

$$\Phi^{(n)} = \begin{cases} \partial_x^{(n+1)}\phi|_0, & n = 0, 2, 4, ..., \\ \partial_x^{(n)}\Pi|_0, & n = 1, 3, 5, ... \end{cases} \tag{4.12}$$

Having exhausted the constraint consistency conditions, we show that the Poisson bracket of the constraints,

$$C_{mn} \equiv \{\Phi^{(m)}, \Phi^{(n)}\}, \tag{4.13}$$

is non-singular and hence, the set of constraints (4.12) are all of second class. To show this, first we calculate

$$C_{mn} = \begin{cases} 0, & m, n = 0, 2, 4, ... \\ 0, & m, n = 1, 3, 5, ... \\ \int \delta(x)\delta(x')\partial_x^{m+1}\partial_{x'}^{n}\delta(x-x')\mathrm{d}x\mathrm{d}x', \\ \qquad m = 0, 2, 4, ..., n = 1, 3, 5, ... \end{cases} \tag{4.14}$$

In order to find $\det C$, the non-zero elements should be regularized. This regularization can be done by two methods, discretization or using a limit of a regular function, e.g. the Gaussian function, to represent $\delta(x)$. Here we choose the second one, but one can easily show that the other method gives the same results. Inserting

$$\delta(x-x') = \lim_{\epsilon\to 0} \frac{1}{\epsilon\sqrt{\pi}} \mathrm{e}^{-(x-x')^2/\epsilon^2} \tag{4.15}$$

into (4.14), using the properties of the Hermite polynomials [12] and performing the integration over x, x' by means of the corresponding delta functions, $\delta(x)$, $\delta(x')$, we find

$$\begin{aligned} &\int \delta(x)\delta(x')\partial_x^{m+1}\partial_{x'}^{n}\delta(x-x')\mathrm{d}x\mathrm{d}x' \\ &= \frac{-1}{\sqrt{\pi}}\epsilon^{-(m+n+2)}H_{m+n+1}(0) \\ &= \frac{-1}{\sqrt{\pi}}(-2)^{(n+m+1)/2}\epsilon^{-(m+n+2)}(m+n)!!, \\ &\qquad m = 0, 2, 4, ..., n = 1, 3, 5, ... \end{aligned} \tag{4.16}$$

$H_n(0)$ denotes the Hermite polynomials at $x = 0$ [12]. Putting these together, C is finally found to be

$$C = A \otimes B, \tag{4.17}$$

where

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

and B is an infinite dimensional matrix with

$$B_{mn} = \frac{-1}{\sqrt{\pi}}(-2)^{(n+m-1)}\frac{((2(m+n)-3)!!}{\epsilon^{-2(m+n)-1}}, \quad m, n = 1, 2, ... \tag{4.18}$$

It is straightforward to show that the matrix B has non-zero determinant, i.e. the matrix C is invertible, and hence all the constraints in the chain are second class. One way to consider them all is using the Dirac bracket. To obtain Dirac bracket of any two arbitrary functions in the phase space, it is enough to calculate the Dirac brackets of (ϕ, ϕ) , (ϕ, Π) and (Π, Π)[2]. We have

[2] More detailed calculations can be found in the appendix

$$\{\phi(x),\phi(x')\}_{\text{D.B.}} = -\{\phi(x),\Phi^{(m)}\}C^{-1}_{mn}\{\Phi^{(n)},\phi(x')\} = 0. \quad (4.19)$$

$$\{\Pi(x),\Pi(x')\}_{\text{D.B.}} = -\{\Pi(x),\Phi^{(m)}\}C^{-1}_{mn}\{\Phi^{(n)},\Pi(x')\} = 0, \quad (4.20)$$

$$\begin{aligned}\{\phi(x),\Pi(x')\}_{\text{D.B.}} &= \delta(x-x') \\ &- \{\phi(x),\Phi^{(m)}\}C^{-1}_{mn}\{\Phi^{(n)},\Pi(x')\} \\ &= \delta(x-x') - R(x,x'). \end{aligned} \quad (4.21)$$

Without using the explicit form of C^{-1} one can show

$$R(x,x') = \kappa\epsilon\delta(x)\delta(x'), \quad (4.22)$$

where κ is a numeric factor. To find κ, let us obtain the Dirac bracket of the constraint Φ^0 with an arbitrary function f; using (2.10) we should have

$$\{\partial_x\phi(x)|_0, f(\phi,\Pi)\}_{\text{D.B.}} = \int\delta(x)\partial_x\{\phi(x),f\}_{\text{D.B.}} = 0. \quad (4.23)$$

Denoting $\partial f/\partial(\Pi(x')) \equiv g(x')$, we can write

$$\int\delta(x)\partial_x\{\phi(x),\Pi(x')\}_{\text{D.B.}}g(x') = 0. \quad (4.24)$$

Inserting (4.21) and (4.22) into (4.24) this reduces to

$$\int(\partial_x\delta(x) + \kappa\epsilon\delta(x)\partial_x\delta(x))g(x) = 0. \quad (4.25)$$

Remembering (4.15), we find

$$\kappa = -\sqrt{\pi}. \quad (4.26)$$

Hence

$$\{\phi(x),\Pi(x')\}_{\text{D.B.}} = \delta(x-x') + \kappa\epsilon\delta(x)\delta(x'). \quad (4.27)$$

The appearance of the regularization parameter ϵ in the Dirac bracket sounds bad, but since the second term has two delta functions, to be of the same order of the first term in fact an ϵ factor is necessary. We will clarify and discuss this point in the next section.

The Dirichlet boundary condition can be worked out similarly. In this case the constraint chain is obtained as

$$\Phi^{(n)} = \begin{cases}\partial_x^{(n)}\phi|_0, & n = 0,2,4,... \\ \partial_x^{(n-1)}\Pi|_0, & n = 1,3,5,...\end{cases} \quad (4.28)$$

Performing the calculations, one can show that the Dirac brackets are like the Neumann case, except for the κ factor, which is $+\pi^{1/2}$.

5 Mode expansion and reduced phase space

In the previous section we showed that a field theory subjected to the Neumann or Dirichlet boundary conditions is a system constrained to an infinite chain of *second class* constraints. As mentioned in Sect. 2, for a system with second class constraints, there is a subspace of phase space which is spanned by a set of unconstrained canonical variables, the reduced phase space. The important property of these variables is that the Poisson bracket in terms of them is equivalent to the Dirac bracket defined on the whole constrained phase space.

In this section we will explicitly find the reduced phase space and show that it is in fact equivalent to phase space determined by the Fourier modes.

Let us consider the Fourier transformed variables

$$\begin{aligned}\phi(x) &= \frac{1}{\sqrt{2\pi}}\int\phi(k)\mathrm{e}^{\mathrm{i}kx}\mathrm{d}k, \\ \phi(k) &= \frac{1}{\sqrt{2\pi}}\int\phi(x)\mathrm{e}^{-\mathrm{i}kx}\mathrm{d}x \end{aligned} \quad (5.1)$$

$$\begin{aligned}\Pi(x) &= \frac{1}{\sqrt{2\pi}}\int\Pi(k)\mathrm{e}^{-\mathrm{i}kx}\mathrm{d}k, \\ \Pi(k) &= \frac{1}{\sqrt{2\pi}}\int\Pi(x)\mathrm{e}^{\mathrm{i}kx}\mathrm{d}x. \end{aligned} \quad (5.2)$$

One can easily show that the above transformation is canonical:

$$\begin{aligned}\{\phi(k),\phi(k')\} &= 0, \\ \{\Pi(k),\Pi(k')\} &= 0, \\ \{\phi(k),\Pi(k')\} &= \delta(k-k'). \end{aligned} \quad (5.3)$$

The Neumann (Dirichlet) constraint chain, (4.12) and (4.28), in terms of the new variables are easily obtained. All the odd (even) moments of $\phi(k)$ and $\Pi(k)$ are zero. The most general solution to these conditions is that $\phi(k)$ and $\Pi(k)$ are even (odd) functions of k. Then (5.1) gives[3]

$$\begin{aligned}\phi(x) &= \frac{1}{\sqrt{\pi}}\int\phi(k)\cos kx\mathrm{d}k, \\ \Pi(x) &= \frac{1}{\sqrt{\pi}}\int\Pi(k)\cos kx\mathrm{d}k. \end{aligned} \quad (5.4)$$

The main advantage of the Fourier modes, $\phi(k)$ and $\Pi(k)$, is that although they are limited to even (odd) functions, they are still canonical variables, in contrast with the original fields $\phi(x)$ and $\Pi(x)$ which lose their usual canonical structure due to constraints.

To compare the Dirac bracket results with those of the reduced phase space, we work out the Poisson brackets of $\phi(x)$ and $\Pi(x)$. Using (5.2) and (5.3) we have

$$\begin{aligned}\{\phi(x),\phi(x')\} &= 0, \\ \{\Pi(x),\Pi(x')\} &= 0, \\ \{\phi(x),\Pi(x')\} &= \frac{1}{\pi}\int\cos kx\cos kx'\mathrm{d}k \\ &\equiv \delta_{\mathrm{N}}(x,x'), \end{aligned} \quad (5.5)$$

for the Neumann boundary conditions. For the Dirichlet case only $\{\phi,\Pi\}$ differs from the above:

[3] For the Dirichlet case cosine should be replaced by sine

$$\{\phi(x), \Pi(x')\} = \frac{1}{\pi}\int \sin kx \sin kx' \mathrm{d}k \equiv \delta_\mathrm{D}(x,x'). \quad (5.6)$$

Performing the integrations we have

$$\delta_\mathrm{N}(x,x') = \delta(x-x') + \delta(x+x'),$$
$$\delta_\mathrm{D}(x,x') = \delta(x-x') - \delta(x+x'). \quad (5.7)$$

If we consider only the positive x's, $x \geq 0$, δ_N and δ_D for $x, x' \neq 0$ are exactly $\delta(x-x')$. For $x, x' = 0$, using (4.15) the delta functions can be regularized to

$$\begin{cases} \delta(x-x') + \delta(x+x') = \dfrac{2}{\sqrt{\pi}\epsilon}, \\ \delta(x-x') - \delta(x+x') = 0, \end{cases} \quad \text{at } x = x' = 0. \quad (5.8)$$

Hence δ_N and δ_D for $x \geq 0$ are in exact agreement with the Dirac bracket results obtained in the previous section. The above argument clarifies why using the usual mode expansions to quantize a system with Neumann or Dirichlet boundary conditions, i.e. imposing the boundary conditions and *then* quantizing, works.

6 Mixed boundary conditions, another example

In this section we handle a more general family of boundary conditions, mixed boundary conditions, which are combinations of the Neumann and Dirichlet cases. It has been shown that these boundary conditions lead to unusual results in the context of string theory [2–7].

As a toy model for a field theory resulting in the mixed boundary conditions let us consider

$$S = \frac{1}{2}\int_0^l \mathrm{d}x \int_{t_1}^{t_2} \mathrm{d}t\big[(\partial_t\phi_i)^2 - (\partial_x\phi_i)^2 + F_{ij}\partial_t\phi_i\partial_x\phi_j\big], \quad (6.1)$$

where $i, j = 1, 2$ and F_{ij} is a constant antisymmetric background. Varying S with respect to ϕ_i leads to

$$\partial_t^2\phi_i - \partial_x^2\phi^i = 0, \quad (6.2)$$

$$\partial_x\phi_i + \mathcal{F}_{ij}\partial_t\phi_j = 0, \quad \text{at } x = 0, l. \quad (6.3)$$

Equations (6.3), as discussed in Sect. 3, give the Lagrangian constraints. In the discretized version, (6.3) are the equations of motion for the end points, and in the continuum limit the acceleration term disappears. It is worth noting that (6.3) reproduce the Neumann and Dirichlet boundary conditions for $F = 0$ and ∞, respectively.

Now to apply the Dirac method, we go to the Hamiltonian formulation:

$$\Pi_i = \partial_t\phi_i + \mathcal{F}_{ij}\partial_x\phi_j, \quad (6.4)$$

$$H = \frac{1}{2}\int_0^l (\Pi_i - F_{ij}\partial_x\phi_j)^2 + (\partial_x\phi_i)^2 \mathrm{d}x, \quad (6.5)$$

and the primary constraints

$$\Phi_i^{(0)} = \Phi_i(x)|_{x=0}, \quad (6.6)$$

with

$$\Phi_i(x) \equiv M_{ij}\partial_x\phi_j + \mathcal{F}_{ij}\Pi_j = 0, \quad M_{ij} = (\mathbf{1} - F^2)_{ij}. \quad (6.7)$$

Note that in this case the Lagrangian constraints, (6.3), depend on the velocities, and as mentioned before, the transformation (6.4), is non-singular and the Lagrangian constraints can be translated into Hamiltonian constraints, (6.7), without any difficulty. The consistency of the primary constraints should be verified:

$$\dot{\Phi}_i^{(0)} = \{\Phi_i^{(0)}, H_T\} = \{\Phi_i^{(0)}, H\} + \lambda_j\{\Phi_i^{(0)}, \Phi_j^{(0)}\} = 0. \quad (6.8)$$

The first term is easy to work out:

$$\Phi_i^{(1)} = \{\Phi_i^{(0)}, H\} = \partial_x\Pi_i|_{x=0}. \quad (6.9)$$

Similar to the arguments of Sect. 4, $\{\Phi_i^{(0)}, \Phi_j^{(0)}\}$ is infinitely large compared to the first term, and the only way for (6.8) to be satisfied is

$$\lambda_i = 0 \quad \text{and} \quad \Phi_i^{(1)} = 0. \quad (6.10)$$

Again, although the Lagrange multiplier, λ_i, is determined, there are secondary constraints, $\Phi_i^{(1)} = 0$. Moreover, we have the advantage that λ_i disappears in the remaining steps.

Direct calculations on the consistency conditions for the constraints leads to the chain

$$\Phi_i^{(n)} = \begin{cases} \partial_x^n\Phi_i|_0, & n = 0, 2, 4, ..., \\ \partial_x^{(n)}\Pi_i|_0, & n = 1, 3, 5, ... \end{cases} \quad (6.11)$$

To verify that these constraints are really second class, we study the matrix $C_{ij}^{mn} \equiv \{\Phi_i^{(m)}, \Phi_j^{(n)}\}$:

$$C_{ij}^{mn} = \begin{cases} 0, & m,n = 1,3,5,..., \\ -2(MF)_{ij}\int\delta(x)\delta(x')\partial_x^{m+1}\partial_{x'}^n\delta(x-x')\mathrm{d}x\mathrm{d}x', & m,n = 0,2,4,..., \\ M_{ij}\int\delta(x)\delta(x')\partial_x^{m+1}\partial_{x'}^n\delta(x-x')\mathrm{d}x\mathrm{d}x', & m = 0,2,4,..., n = 1,3,5,... \end{cases} \quad (6.12)$$

C can be written in the form of

$$C = F \otimes B, \quad (6.13)$$

where F is a 4×4 matrix:

$$F = \begin{pmatrix} -2(MF) & M \\ -M & 0 \end{pmatrix}, \quad (6.14)$$

and B is given by (4.18). In Sect. 4, we discussed that B is invertible. Since $\det F \neq 0$, C is invertible too; hence all the constraints in the chain (6.11) are second class.

One can show that the fundamental Dirac brackets are as follows:

$$\begin{aligned}
&\{\phi_i(x), \phi_j(x')\}_{\text{D.B.}} \\
&\quad = -\{\phi_i(x), \Phi_k^{(m)}\}(C^{-1})_{kl}^{mn}\{\Phi_l^{(n)}, \phi_j(x')\} \\
&\quad = (-2M^{-1}F)_{ij}(\epsilon^2\sqrt{\pi}\delta(x)\delta(x')), \qquad (6.15)\\
&\{\Pi_i(x), \Pi_j(x')\}_{\text{D.B.}} \\
&\quad = -\{\Pi_i(x), \Phi_k^{(m)}\}(C^{-1})_{kl}^{mn}\{\Phi_l^{(n)}, \Pi_j(x')\} = 0, \qquad (6.16)\\
&\{\phi_i(x), \Pi_j(x')\}_{\text{D.B.}} = \delta(x-x') \\
&\quad -\{\phi_i(x), \Phi_k^{(m)}\}(C^{-1})_{kl}^{mn}\{\Phi_l^{(n)}, \Pi_j(x')\} \\
&\quad = \delta(x-x') - R(x,x') = \delta_{\text{N}}(x,x'). \qquad (6.17)
\end{aligned}$$

The important result of the mixed case is (6.15); the Dirac bracket of two field components is non-zero. This means that in the quantized theory these field components are non-commuting. In the string theory, where the fields describe the space coordinates, (6.15) tells us that the space probed by open strings with mixed boundary conditions is a *non-commutative* space [2–4].

Using the canonical (or Fourier) transformations, (5.1) and (5.2), we can explicitly build up the reduced phase space for the mixed case. Let $\Phi_i(k)$ represent the Fourier modes of $\Phi_i(x)$ defined in (6.7),

$$\begin{aligned}
\Phi_i(x) &= \frac{1}{\sqrt{2\pi}}\int \Phi_i(k)\mathrm{e}^{\mathrm{i}kx}\mathrm{d}k, \\
\Phi_i(k) &= \frac{1}{\sqrt{2\pi}}\int \Phi_i(x)\mathrm{e}^{-\mathrm{i}kx}\mathrm{d}x, \qquad (6.18)
\end{aligned}$$

Using (5.2), the Poisson brackets of $\Phi_i(k)$ and $\Pi_i(k)$ can be worked out. Imposing the constraints (6.11), we find that $\Phi_i(k)$ and $\Pi_j(k)$, are odd and even functions of k, respectively:

$$\begin{aligned}
\Phi_i(x) &= \frac{1}{\sqrt{\pi}}\int \Phi_i(k)\sin kx\mathrm{d}k, \\
\Pi_i(x) &= \frac{1}{\sqrt{\pi}}\int \Pi_i(k)\cos kx\mathrm{d}k. \qquad (6.19)
\end{aligned}$$

Remembering (6.7), we can derive the field components:

$$\begin{aligned}
\phi_i(x) = \frac{M_{ij}^{-1}}{\sqrt{\pi}}\int \frac{-\mathrm{d}k}{k}(&\Phi_j(k)\cos kx \\
&+F_{jk}\Pi_k(k)\sin kx), \qquad (6.20)
\end{aligned}$$

which explicitly satisfy the mixed boundary conditions.

Having derived the mode expansions of the fields and their conjugate momenta, we can explicitly work out their Poisson brackets:

$$\begin{aligned}
&\{\phi_i(x), \phi_j(x')\} \\
&\quad = \frac{1}{\pi}\int \frac{\mathrm{d}k}{k}\frac{\mathrm{d}k'}{k'}[(M^{-1}F)_{ik}\{\Phi_k(k), \Pi_l(k')\}M_{lj}^{-1} \\
&\quad \times \cos kx \sin k'x' + (M^{-1}F)_{jk}\{\Pi_k(k), \Phi_l(k')\}M_{il}^{-1} \\
&\quad \times \cos k'x' \sin kx] \\
&\quad = \frac{-1}{\pi}\int \frac{\mathrm{d}k}{k}(M^{-1}F)_{ij}(\cos kx' \sin kx + \cos kx \sin kx') \\
&\quad = (M^{-1}F)_{ij}\int^x (\delta_{\text{N}}(y,x') - \delta_{\text{D}}(y,x'))\mathrm{d}y \\
&\quad = -2(M^{-1}F)_{ij}\int^x \delta(y+x')\mathrm{d}y. \qquad (6.21)
\end{aligned}$$

Since for $x, x' \geq 0$

$$\int^x \delta(y+x')\mathrm{d}y = \begin{cases} 1, & x = x' = 0, \\ 0, & \text{otherwise}, \end{cases} \qquad (6.22)$$

(6.21) is non-zero only for $x, x' = 0$:

$$\{\phi_i(0), \phi_j(0)\} = -2(M^{-1}F)_{ij}. \qquad (6.23)$$

Comparing (6.21) and (6.15), we find that they are exactly the same. In other words, (6.19) and (6.20) are functions defining the reduced phase space.

In the context of string theory, (6.21) implies that the end points of open strings subjected to mixed boundary conditions are living in a *non-commutative* space. The mixed open strings appear when we are studying D-branes in a NSNS two-form background. In this case, (6.21) tells us that the world-volume of such branes are non-commutative planes.

We can also calculate $\{\Pi_i(x), \Pi_j(x')\}$ and $\{\phi_i(x), \Pi_j(x')\}$. The results are in exact agreement with (6.16) and (6.17).

7 Concluding remarks

In this paper, we have studied the old and well-known problem of field theories with boundary conditions from a new point of view. We discussed that in the Lagrangian formulation boundary conditions are Lagrangian constraints which are not a consequence of a singular Lagrangian. For further study we built the Hamiltonian formulation, and considered boundary conditions as primary constraints. Asking for the constraints consistency conditions we found two new features in the context of constrained systems.

(1) Although the Lagrange multiplier in the total Hamiltonian is determined, the constraints chain is continued.
(2) Boundary conditions are equivalent to an *infinite* chain of *second class* constraints. This property was also observed in [6].

Constructing the Dirac brackets of the fields and their conjugate momenta for these second class constraints, we showed that the method based on a mode expansion is equivalent to working in the reduced phase space.

The relation between the Hamiltonian method we developed here and the usual method of imposing boundary conditions in the equations of motion can simply be understood. In the former, to ensure that boundary conditions are satisfied, we make the Taylor expansion of boundary conditions as a function of time, and put all the coefficients equal to zero. These coefficients are exactly our constraint chain. But in the latter, the Fourier mode expansion is used and boundary conditions are guaranteed by choosing all the Fourier components to satisfy the boundary conditions.

In the last section of the paper, we handled the mixed boundary conditions which is an exciting problem in the context of string theory [7]. Having non-commuting field components is the interesting feature appearing in this case. Besides the string theory, mixed boundary conditions can be encountered in the context of gauge theories when we also consider the θ term:

$$S = \frac{1}{4}\int(\mathcal{F}_{\mu\nu}^2 + \theta\epsilon_{\mu\nu\alpha\beta}\mathcal{F}_{\mu\nu}\mathcal{F}_{\alpha\beta}).$$

In the above action θ plays a role similar to F in our toy model. Varying the action gives a surface term, the vanishing of which leads to the mixed boundary conditions. Quantizing this theory is an interesting problem we postpone to future work.

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Appendix

In this appendix we present some of the calculation details. We have

$$\begin{aligned}
k^{(m)}(x) &\equiv \{\phi(x), \Phi^{(m)}\} \\
&= \begin{cases} 0, & m = 0, 2, 4, ..., \\ \{\phi(x), \partial_x^m \Pi^{(m)}|_0\} = k^m(x), & m = 1, 3, 5, ..., \end{cases} \\
l^{(m)}(x) &\equiv \{\Pi(x), \Phi^{(m)}\} \\
&= \begin{cases} \{\Pi(x), \partial_x^m \phi^{(m)}|_0\} = l^m(x), & m = 0, 2, 4, ..., \\ 0, & m = 1, 3, 5, ..., \end{cases} \\
k^m(x) &= \int \partial_{x'}^m \delta(x - x')\delta(x')\mathrm{d}x' \\
&= \frac{1}{\sqrt{\epsilon\pi}}\exp\left(\frac{-x^2}{\epsilon^2}\right)\frac{1}{\epsilon^m}H_m(0) \\
&\equiv \delta(x)k_m, \\
l^m(x) &= -\int \partial_{x'}^{m+1}\delta(x' - x)\delta(x')\mathrm{d}x' \\
&= \frac{1}{\sqrt{\epsilon\pi}}\exp\left(\frac{-x^2}{\epsilon^2}\right)\frac{1}{\epsilon^{m+1}}H_{m+1}(0) \\
&\equiv \delta(x)k_{m+1},
\end{aligned}$$

where $H_m(0)$ is the Hermite polynomial at zero. Then one can easily work out $\{\phi(x), \Pi(x')\}_{\text{D.B.}}$:

$$\{\phi(x), \Pi(x')\}_{\text{D.B.}} = \delta(x - x') + k_{m+1}k_n B_{mn}^{-1}\delta(x)\delta(x').$$

The power of ϵ in $k_{m+1}k_n B_{mn}^{-1}$, can be read off from the explicit form of k_m and B_{mn}, and the result is $k_{m+1}k_n B_{mn}^{-1} = \kappa\epsilon$. Calculations for the mixed boundary conditions can be performed similarly.

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