Boundary Poisson structure and quantization

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A new approach for treating boundary Poisson structures based on causality and locality analysis is proposed for a single scalar field with boundary interaction. For the case of linear boundary condition, it is shown that the usual canonical quantization can be applied systematically.

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Quantization of classical field in the presence of various boundary conditions is an old problem for which a systematical solution is still missing. This problem is important because it is related to a vast range of physical problems including, e.g., surface effect in condensed matter physics, cavity QED, Casimir energy, two-dimensional integrability, mass generation and especially conformal field theory and open string theory. Recently, there has been a renewed interests in this problem among string theorists since the discovery of D-branes, noncommutativity and other extended objects (like the so-called Horizontal branes) in string theory. In most recent papers on this subject, people are tempted to use the Dirac procedure for constrained systems to treat the inconsistency of Poisson structure with the boundary condition. However, for at least several reasons we think that this treatment of boundary condition is not quite appreciated. First, since the boundary condition is a constraint at a specific spatial point (or a spacial hypersurface if there are more than one spatial directions) which is of functional measure 0 in the space of field, the direct application of Dirac procedure necessarily fails because the standard definition of Dirac Poisson brackets in this case would involve the inverse of $\delta(0)$, which could hardly be given any practical sense. An alternative way is to put the spatial direction with the boundary into a lattice form and then implement the Dirac procedure. In this case the construction of Dirac brackets seems to make perfect sense, but, unfortunately, there seems to be no simple continuum limit for such lattice regularized theories for which the Dirac brackets remain consistent. More over, the appearance of an explicit length scale — the lattice spacing — is another drawback of this formalism, which is especially unfavorable in scale invariant theories.

In this article, we shall propose a new method to treat the inconsistency between the boundary condition and the canonical Poisson structure. Our treatment is in fact a modified definition of the canonical structure according to the analysis of the causality and locality of the theory in the presence of boundary condition. For simplicity we shall consider only the simplest case of a single scalar field in $(D+1)$-spacetime dimensions, where the time direction and the first $D-1$ spacial directions are boundaryless, and the only boundary condition appears in the direction of $x^D$, which extends over $[0, +\infty)$.

Before going into the concrete action level analysis, let us first analyze the causal structure of the scalar field theory in the presence of a boundary. Figure 1 depicts the $(x^0, x^D)$ slice of the lightcone of the theory. Noticing that the hypersurface $x^D = 0$ is a reflecting barrier for light signals, we have, in contrast to the case without boundaries, three different zones which are denoted as zone I, II and III respectively. Zone I and II are both lightlike, the difference is that zone I is a reflectionless zone which means that no signals of events happened in the causal past $y$ of the observer at $x$ can be reflected from the boundary to the observer, while events happened in zone II can be reflected without breaking the causality. Zone III of the lightcone is the usual spacelike zone. Therefore, without knowing any details of the action, we may conclude that the bare propagator of the scalar field theory with such a lightcone must behave like

$$\Delta_B(x, y) = \begin{cases} 
\Delta(x - y), & y \in \text{zone I} \\
\Delta(x - y) + B\Delta(x - \sigma(y)), & y \in \text{zone II} \\
0, & y \in \text{zone III}
\end{cases}$$

where $\Delta(x - y)$ is the standard propagator for the same theory in the bulk, $\sigma(y)$ is the reflection image of $y$ with respect to the boundary, i.e., if $y = (y^0, y^1, ..., y^{D-1}, y^D)$, then $\sigma(y) = (y^0, y^1, ..., y^{D-1}, -y^D)$, and $B$ is some operator which represents the effectiveness of the boundary reflection. For ideal reflection, we must have $||B|| = 1$ (of course the operator norm $||\cdot||$ must be assigned a proper sense — we shall come back to this point later).

Now let us write down the action of a single scalar field $\varphi$ with a bulk interaction $V(\varphi)$ and also a boundary
interaction $V_B(\varphi)$. It reads

$$S[\varphi] = \frac{1}{2} \int d^D x \int_0^\infty dx^D \left[ \partial_M \varphi \partial^M \varphi - m^2 \varphi^2 + 2g V(\varphi) \right] + \lambda_B \int d^D x V_B(\varphi) \Bigr|_{x^D = 0},$$

where throughout this article, $\int d^D x$ represents the integration over all the transverse spacetime directions to the direction of $x^D$, the Roman index $M$ runs from 0 to $D$, whereas the Greek index $\mu$ runs from 0 to $D - 1$. The constants $g, \lambda$ respectively represent the strength of the bulk and boundary couplings. As in the case of ordinary field theories without boundaries, the canonical conjugate momentum $\pi(x)$ is still defined via the bulk Lagrangian as

$$\pi(x) = \frac{\delta L}{\delta \partial \varphi(x)} = \partial_0 \varphi(x).$$

The variation of $S[\varphi]$ reads

$$\delta S[\varphi] = \int d^D x \int_0^\infty dx^D \left[ \partial_M (\delta \varphi \partial^M \varphi) - \delta \varphi \left( \partial_M \partial^M \varphi + m^2 \varphi - \frac{g}{\delta \varphi} \right) \right] + \lambda \int d^D x \delta \varphi \delta V_B(\varphi) \frac{\delta \varphi}{\delta \varphi} \Bigr|_{x^D = 0} = -\int d^D x \int_0^\infty dx^D \delta \varphi \left( \partial_M \partial^M \varphi + m^2 \varphi - \frac{g}{\delta \varphi} \right) + \int d^D x \delta \varphi \left( \partial_D \varphi + \lambda \frac{\delta V_B(\varphi)}{\delta \varphi} \right) \Bigr|_{x^D = 0}.$$

Therefore, the condition $\delta S[\varphi] = 0$ yields, for arbitrary $\delta \varphi$, the following equation of motion and boundary condition,

$$\partial_M \partial^M \varphi + m^2 \varphi - \frac{g}{\delta \varphi} = 0,$$

$$\partial_D \varphi + \lambda \frac{\delta V_B(\varphi)}{\delta \varphi} = 0 \Bigr|_{x^D = 0}. \quad (2)$$

The boundary condition (2) gives a constraint between $\partial_D \varphi$ and $\frac{\delta V_B(\varphi)}{\delta \varphi}$ on the spacetime hypersurface $x^D = 0$, and thus the naive canonical Poisson brackets

$$\{\varphi(x), \varphi(y)\} = \{\pi(x), \pi(y)\} = 0, \quad \{\varphi(x), \pi(y)\} = \delta(x - y) \quad (3)$$

(where $\delta(x - y)$ should be understood as $\delta(x^D) = \prod_{i=1}^D \delta(x_i - y_i)$) do not hold consistently.

As mentioned earlier, the usual Dirac procedure does not apply satisfactorily to the case of boundary constraints without discretizing the spacial coordinate with boundary condition. Fortunately, since now the inconsistency only occur at the hypersurface $x^D = 0$, we may expect, following the principle of locality, that the modification to the naive Poisson brackets should be non-trivial only on the same hypersurface. Moreover, since there is no dependence on the canonical momentum in the boundary condition, only $\{\varphi(x), \pi(y)\}$ needs to be modified. So, without loss of generality, we assume that the correct $\{\varphi(x), \pi(y)\}$ take the following form,

$$\{\varphi(x), \pi(y)\} = \delta(x - y) + B(y) \delta(x - \sigma(y)), \quad (4)$$

where one should notice that $\delta(x - \sigma(y))$ is nonzero only if both $x^D$ and $y^D$ are equal to 0, and $B(y)$ is an operator acting on the variable $y$ which represents the effect of boundary reflection. In this article, we adopt a slightly modified definition for the $\delta$-function. We assume that

$$\int_0^\infty dx^D \delta(x^D) = 1,$$

or, in terms of the standard definition for $\delta$-function, our $\delta(x^D)$ should be understood as $\lim_{\varepsilon \to 0^+} \delta(x^D + \epsilon)$.

Now let us check what form should the operator $B(y)$ take in order that the new Poisson bracket (3) be consistent. For this purpose we first write the boundary condition as a boundary constraint,

$$G = \int_0^\infty dx^D \delta(x^D) \left[ \partial_D \varphi + \lambda \frac{\delta V_B}{\delta \varphi} \right] \approx 0.$$

Examining the Poisson bracket $\{G, \pi(y)\}$ (we only need to do so because $G$ naively Poisson commutes with $\varphi(y)$), one gets

$$\{G, \pi(y)\} = \int_0^\infty dx^D \delta(x^D) \left[ \partial_D + \lambda \frac{\delta^2 V_B}{\delta \varphi^2} \right] \times \left( \delta(x - y) \delta(x - \sigma(y)) \right)$$

$$= -B(y) \left( \partial_{y^D} + \lambda \frac{\delta^2 V_B}{\delta \varphi^2} \right) - \left( \partial_{y^D} - \lambda \frac{\delta^2 V_B}{\delta \varphi^2} \right) \times \delta^{(D - 1)}(x - y) \delta(y^D).$$

In the last equality, $\frac{\delta^2 V_B}{\delta \varphi^2}$ is to be regarded as a function of $y$. The consistence condition $\{G, \pi(y)\} = 0$ yields

$$B(y) = \partial_{y^D} - \lambda \frac{\delta^2 V_B}{\delta \varphi^2} \frac{\delta \varphi}{\delta \varphi} \frac{\delta \varphi}{\delta \varphi} \quad (5)$$

The Poisson brackets (3) with the operator $B(y)$ given as (5) then form a consistent set of Poisson structure for our boundary scalar field theory. Noticing the fact that $B(y)$ always acts on $\delta(x - \sigma(y))$, one may just denote $\partial_{y^D}$ as $\partial_\sigma$.

The quantization of the above scalar field with boundary is still not an easy task because one still needs to assign proper meaning to the operator ordering and operator inverse appeared in the expression (5).
Fortunately, there is a simple illuminating case in which one does not need to worry about the above problem, i.e. the case of linear boundary conditions. In this special case, one simply take $V_B(\varphi) = -\frac{1}{2}\varphi^2$, and thus the boundary interaction becomes just a boundary mass term. The boundary condition (1) then becomes

$$ (\partial_D - \lambda)\varphi = 0|_{x^D = 0}, \quad (6) $$

and the operator $B(y)$ is now

$$ B(y) = \frac{\partial_D + \lambda}{\partial_D - \lambda}. \quad (7) $$

In the rest of this article, we shall be considering the scalar field theory with this last boundary condition.

To quantize the theory with the boundary condition (7), one only needs to quantize the corresponding free theory, i.e. the Klein-Gordon field with the boundary (1) and then apply the standard perturbation theory to introduce the effect of the quantized interaction term : $V(\varphi) :$ in the bulk.

Let us first write down the classical solution to the massive Klein-Gordon equation obeying the boundary condition (1):

$$ \varphi(x) = \int \frac{d^{D-1}k}{(2\pi)^{D-1}} \int_0^{+\infty} \frac{dk_D}{2\pi} \left[ a(k)f(k_D, x^D)e^{-ik_x x^D} 
+ a^*(k)f^*(k_D, x^D)e^{ik_x x^D} \right]|_{\omega_k = k_0}, \quad (8) $$

where $d^{D-1} = dk_1...dk_{D-1}$. $k_D$ runs over $[0, +\infty)$ because the function

$$ f(k_D, x^D) = e^{ik_D x^D} + B(-ik)e^{-ik_D x^D} $$

with $B(-ik)$ being the Fourier image of our boundary operator $B(y)$,

$$ B(-ik) = \frac{ik_D - \lambda}{ik_D + \lambda}, \quad (9) $$

is complete over the half $k_D$ line,

$$ \int_0^{+\infty} \frac{dk_D}{2\pi} f(k_D, x^D)f^*(k_D, y^D) = \delta(x^D - y^D) + B(y)\delta(x^D + y^D). \quad (10) $$

Notice that $f(k_D, x^D)$ solves the equation $(\partial_D - \lambda)f(k_D, x^D) = 0|_{x^D = 0}$. The $(D + 1)$-momentum $k$ naturally satisfies the standard mass shell condition

$$ k^2 - m^2 = 0. $$

The canonical quantization for the Klein-Gordon field is now accomplished by replacing the Poisson bracket \{ , \} by the equal-time commutator $-i[ [ , ] ]$,

$$ [\varphi(x), \varphi(y)] = [\pi(x), \pi(y)] = 0, $$

$$ [\varphi(x), \pi(y)] = i[\delta(x - y) + B(y)\delta(x - \sigma(y))]. \quad (11) $$

Let us remind that two special well-known cases are already contained in this simple illustration, namely, the Neumann boundary condition (which corresponds to $\lambda = 0$ or $B = 1$) and Dirichlet boundary condition (for which $\lambda = \infty$ or $B = -1$). Our result (10) agrees with the known result (2) on these two special cases. For generic value of $\lambda$, the relation $B(-ik)B^\dagger(-ik) = 1$ gives a simple explanation to the condition $||B|| = 1$ mentioned earlier.

Now, going to the momentum space representation, one simply replaces the momentum space coefficients $a(k), a^*(k)$ by their corresponding operators $\hat{a}(k)$ and $\hat{a}^\dagger(k)$,

$$ \varphi(x) = \int \frac{d^{D-1}k}{(2\pi)^{D-1}} \int_0^{+\infty} \frac{dk_D}{2\pi} \left[ \hat{a}(k)f(k_D, x^D)e^{-ik_x x^D} 
+ \hat{a}^\dagger(k)f^*(k_D, x^D)e^{ik_x x^D} \right]|_{\omega_k = k_0}. $$

Using this last expression and $\pi(x) = \partial_0 \varphi(x)$, one can get the commutation relation for the momentum space operators $\hat{a}(k), \hat{a}^\dagger(k)$,

$$ [\hat{a}(k), \hat{a}^\dagger(k')] = [\hat{a}^\dagger(k), \hat{a}(k')] = 0, $$

$$ [\hat{a}(k), \hat{a}(k')] = (2\pi)^D\delta(k - k'). $$

Following the standard argument in quantum field theory (see, e.g. (2)), we now can evaluate the propagator

$$ D^{(B)}(x, y) = \langle 0|T[\varphi(x)\varphi(y)]|0 \rangle $$

$$ = \theta(x^0 - y^0)\langle 0|\varphi(x)\varphi(y)|0 \rangle $$

$$ + \theta(y^0 - x^0)\langle 0|\varphi(y)\varphi(x)|0 \rangle, $$

which turns out to be

$$ D^{(B)}(x, y) = \int \frac{d^{D}k}{(2\pi)^D} \int_0^{+\infty} \frac{dk_D}{2\pi} \times \frac{i}{k^2 - m^2 + i\epsilon}f(k_D, x^D)f^*(k_D, y^D)e^{-ik_x(x - y)}, $$

where the integration with respect to $k_0$ is a contour integration over the complex $k_0$-plane which runs from $-\infty$ below the real axis to $k_0 = 0$, crossing the real axis and goes to $+\infty$ above the real axis. Substituting the definitions of $f(k, x^D), f^*(k, y^D)$ into the last equation and taking into account the relation (2), we get

$$ D^{(B)}(x, y) = D_F(x - y) + B(y)D_F(x - \sigma(y)), \quad (12) $$

where $D_F(x, y)$ is the $D$-dimensional Feynman propagator.
where
\[
D_F(x-y) = \int \frac{d^{D+1}k}{(2\pi)^{D+1}} \frac{i}{k^2 - m^2 + i\epsilon} e^{-ik_M(x-y)^M}
\]
is the standard Feynman propagator in \(D+1\) dimensions.

Notice that, following the standard discussion on the causality properties of the Feynman propagator \([1]\), we would find that the result \([10]\) agrees perfectly with our early postulation \([1]\). The propagator \([10]\) is then the very basic object in the Feynman rules of perturbation theory for the interacting boundary scalar field theory with generic interacting potential \(V(\phi)\) in the bulk.

We may also evaluate the retarded Green’s function for the boundary Klein-Gordon field as well. After some simple calculations, we have
\[
D_R(x-y) = \int \frac{d^{D+1}k}{(2\pi)^{D+1}} \frac{i}{k^2 - m^2 + i\epsilon} e^{-ik_M(x-y)^M},
\]
where the integration contour for \(k_0\) is taken to be running from \(-\infty\) to \(+\infty\) above the real axis. The fact that \(D_R^{(B)}(x, y)\) is a green’s function is now assured by the following equation,
\[
(\partial_M \delta^M + m^2)D_R^{(B)}(x, y) = \delta(x-y) + B(y)\delta(x - \sigma(y)).
\]

Before finishing this article, let us make some more comments on the commutation relation \([4]\). Though by definition we know that the quantities \(\varphi(x), \pi(x)\) live only on the half space \(x^D \geq 0\), we may, however, imagine to analytic continue them to the whole spacetime. In that case, writing
\[
\varphi(x) = \int \frac{d^Dk}{(2\pi)^D} A(k)e^{ikx}, \quad \pi(x) = \int \frac{d^Dk}{(2\pi)^D} A^\dagger(k)e^{-ikx},
\]
where \(d^Dk = dk_1...dk_D\) with \(k_D\) running from \(-\infty\) to \(+\infty\), we have, for the momentum space operators \(A(k)\) and \(A^\dagger(k)\), the following commutation relations,
\[
[A(k), A(k')] = [A^\dagger(k), A^\dagger(k')] = 0,
\]
\[
[A(k), A^\dagger(k')] = \delta(k-k') + \frac{i\lambda k_D + \lambda}{ik_D} \delta(k - \sigma(k')).
\]

These relations are the simplest case of the boundary exchange algebra introduced in \([7]\) and further explored in \([8]\).

So far, in this article, we considered the problem of boundary Poisson structure for the case of a single scalar field theory with boundary interaction \(V_B(\phi)\). The fact that the consistent Poisson bracket between \(\varphi(x)\) and \(\pi(y)\) depends on the second variation of \(V_B\) with respect to \(\varphi\) makes the problem of canonical quantization in the presence of boundary a difficult task for generic \(V_B\). For linear boundary conditions, i.e. for \(V_B\) at most quadratic in \(\varphi\), the canonical quantization can be pursued without difficulties. Though we have obtained the consistent Poisson structure for generic boundary interaction \(V_B\) depending only on the field \(\varphi\), we did not include more generalities, i.e. the cases in which \(V_B\) depends also on spacetime derivatives of the field \(\varphi\), and the cases in which there are more than one scalar fields and \(V_B\) couples different components of the fields etc. It is also tempting to study the case when the fundamental field is in group-valued, like the principal chiral model studied in \([10]\). The direct quantization for generic \(V_B\) is also a fascinating subject (some progress for the case of sine-Gordon field with integrable boundary condition has already been made in \([11, 12]\)).

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