

On the boundary conditions as Dirac constraints

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Received: 30 August 2004 / Revised version: 2 October 2004 /
Published online: 17 December 2004 – © Springer-Verlag / Società Italiana di Fisica 2004

Abstract. In this paper, the canonical quantization of singular Lagrangian defined in a finite volume is discussed by studying a 1+1 dimensional free Schrödinger field. We take the boundary conditions (BCs) as Dirac constraints, and show that those BCs as well as the intrinsic constraints (which are introduced by the singularities of Lagrangian) form the second class constraints. The quantization is performed canonically.

PACS. 11.25-W, 04.60.D, 11.10.E

1 Introduction

It is well known that to study a general field theory in a finite volume, one should take not only the equations of motion but also the boundary conditions (BCs) into consideration. BCs are usually the combinations of the field variables and their various derivatives (including the time derivatives, sometimes [1–4]) which are valid only on the boundaries and are expected to be held all the times. In the Hamiltonian formalism, those BCs are the combinations of the canonical variables in phase space, i.e., the fields and their conjugate momenta (or their spatial derivatives). In Dirac's language, these BCs are the constraints in the phase space. However, such constraints have the different origins compared to the traditional Dirac' context where the primary constraints are introduced by the singularities of Lagrangian and the secondary constraints are the requirements of the stability of the primary ones. Due to BCs, one can not quantize the system consistently in the whole space because on the boundaries those BCs are inconsistent with the usual canonical commutation relations generally [1–4].

This problem has been thoroughly studied in [1], there, the authors take the BCs as the Dirac's primary constraints and the Dirac procedure is applied to two models. However, their models are so simple that there are not intrinsic constraints. In this paper, we shall generalize the discussion in [1] to a more general case, in which both the intrinsic constraints and BCs are contained. We shall analyse a non-relativistic field, Schrödinger field (which is described by a singular Lagrangian) in a finite volume. So, from the point of view of origination, this model has two kinds of different constraints, one kind is due to the singularities of Lagrangian, the other kind is BCs. As a example, we study the Neumann BCs intensively, we show that those two kinds of constraints form second class constraint. The canonical quantization is performed.

The organization of this paper is as follows: in Sect. 2, we shall quantize the model canonically in an infinite volume. Then in Sect. 3, we analyse the model in a finite volume. The BCs are considered. Following the [1] we take the BCs as Dirac constraints, and the canonical quantization are given there. Sect. 4 are devoted some further discussions and remarks.

2 Schrödinger field in an infinite volume

We start from Schrödinger field in an infinite volume. For the sake of simplicity, we confine ourself to 1+1 dimension. The generalization to higher dimension is straightforward. The basic field variables are $\psi(x, t)$ and their Hermitian conjugate $\psi^\dagger(x, t)$. The action is (in order to have a Hermitian total Hamiltonian, we would like to write the action in a symmetry form)

$$\begin{aligned} S &= \int_{t_1}^{t_2} dt L \\ &= \frac{1}{2} \int_{t_1}^{t_2} dt \int_{-\infty}^{+\infty} dx \left(i\psi^\dagger(x, t)\partial_t\psi(x, t) \right. \\ &\quad \left. - i\partial_t\psi^\dagger(x, t)\psi(x, t) - \partial_x\psi^\dagger(x, t)\partial_x\psi(x, t) \right), \end{aligned} \quad (1)$$

where ∂_t and ∂_x denote $\frac{\partial}{\partial t}$ and $\frac{\partial}{\partial x}$ respectively, L is the Lagrangian

$$\begin{aligned} L &= \frac{1}{2} \int_{-\infty}^{+\infty} dx \left(i\psi^\dagger(x, t)\partial_t\psi(x, t) \right. \\ &\quad \left. - i\partial_t\psi^\dagger(x, t)\psi(x, t) - \partial_x\psi^\dagger(x, t)\partial_x\psi(x, t) \right), \end{aligned} \quad (2)$$

we set $m = \hbar = 1$. The variation of the action with respect to $\psi(x, t)$ and $\psi^\dagger(x, t)$ leads to

$$\delta S = \frac{1}{2} \int_{t_1}^{t_2} dt \int_{-\infty}^{+\infty} dx \delta\psi^\dagger(x, t)$$

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$$\begin{aligned}
& \times [2i\partial_t\psi(x,t) + \partial_x\partial_x\psi(x,t)] \\
& + [-2i\partial_t\psi^\dagger(x,t) + \partial_x\partial_x\psi^\dagger(x,t)]\delta\psi(x,t) \\
& - \frac{1}{2}\int_{t_1}^{t_2} dt \\
& \times [(\delta\psi^\dagger(x,t)\partial_x\psi(x,t)) + (\partial_x\psi^\dagger(x,t)\delta\psi(x,t))]_{-\infty}^{+\infty} \\
& + \frac{1}{2}\int_{-\infty}^{+\infty} dx [i\psi^\dagger(x,t)\delta\psi(x,t) - i\delta\psi^\dagger\psi(x,t)]_{t_1}^{t_2}.
\end{aligned} \tag{3}$$

For any arbitrary $\delta\psi$ and $\delta\psi^\dagger(x,t)$, the variation of the action vanishes if the four terms in the above equation vanish simultaneously. The vanishing of the first and the second terms gives the equations of motion, namely, the free Schrödinger equation and its Hermitian conjugation,

$$\begin{aligned}
i\partial_t\psi(x,t) + \frac{1}{2}\partial_x\partial_x\psi(x,t) &= 0, \\
-i\partial_t\psi^\dagger(x,t) + \frac{1}{2}\partial_x\partial_x\psi^\dagger(x,t) &= 0,
\end{aligned} \tag{4}$$

the last term leads to the initial conditions. For the third term in (3), it is zero because the variables $\psi(x,t)$, $\psi^\dagger(x,t)$ trend to vanish at spatial infinity.

This model can be quantized canonically. We can resort to Dirac's procedure to quantize it. In doing so, we should turn into phase space which is spanned by variables $\psi(x,t)$, $\psi^\dagger(x,t)$ and their canonical momenta $\Pi(x,t)$, $\Pi^\dagger(x,t)$, defined as

$$\begin{aligned}
\Pi(x,t) &= \frac{\delta S}{\delta\dot{\psi}(x,t)} = \frac{i}{2}\psi^\dagger(x,t), \\
\Pi^\dagger(x,t) &= \frac{\delta S}{\delta\dot{\psi}^\dagger(x,t)} = -\frac{i}{2}\psi(x,t),
\end{aligned} \tag{5}$$

where 'dot' means derivative with respect to time. The basic Poisson brackets among those canonical variables are

$$\begin{aligned}
\{\psi(x,t), \Pi(x',t)\} &= \delta(x-x'), \\
\{\psi^\dagger(x,t), \Pi^\dagger(x',t)\} &= \delta(x-x').
\end{aligned} \tag{6}$$

Others are vanishing. From the definition of canonical momenta, we can see that there are two primary constraints in Dirac's language appear,

$$\begin{aligned}
\phi_1^{(0)}(x,t) &= \Pi(x,t) - \frac{i}{2}\psi^\dagger(x,t) \approx 0, \\
\phi_2^{(0)}(x,t) &= \Pi^\dagger(x,t) + \frac{i}{2}\psi(x,t) \approx 0,
\end{aligned} \tag{7}$$

in which the symbol ' \approx ' means equivalence on the constraint hypersurface. The canonical Hamiltonian can be obtained by the Legendre transformation,

$$\begin{aligned}
H_C [\psi(x,t), \psi^\dagger(x,t), \Pi(x,t), \Pi^\dagger(x,t)] \\
= \int_{-\infty}^{+\infty} dx [H(x,t)\dot{\psi}(x,t) + \Pi^\dagger(x,t)\dot{\psi}^\dagger(x,t)]
\end{aligned}$$

$$- L [\psi(x,t), \psi^\dagger(x,t), \dot{\psi}(x,t), \dot{\psi}^\dagger(x,t)]. \tag{8}$$

Substitute (2) and (5) into the above equation, the canonical Hamiltonian can be obtained

$$\begin{aligned}
H_C [\psi(x,t), \psi^\dagger(x,t), \Pi(x,t), \Pi^\dagger(x,t)] \\
= \frac{1}{2}\int_{-\infty}^{+\infty} dx \partial_x\psi^\dagger(x,t)\partial_x\psi(x,t).
\end{aligned} \tag{9}$$

It can be shown that the dynamics of any functions F in phase space are determined by

$$\dot{F} \approx \{F, H_T\} \tag{10}$$

where H_T is the total Hamiltonian,

$$H_T = H_C + \int_{-\infty}^{+\infty} dx \lambda^i \phi_i^{(0)}(x,t), \quad i = 1, 2. \tag{11}$$

λ_i are the Lagrange multipliers. According to Dirac's procedure, one should further check the consistency conditions of the primary constraints to determine whether there are secondary constraints.

$$\dot{\phi}_i^{(0)}(x,t) \approx \{\phi_i^{(0)}(x,t), H_T\} \approx 0. \tag{12}$$

It is easy to find that there are no secondary constraints in this model, the consistency conditions only determined the Lagrangian multipliers λ^i . Also, it is easy to compute the matrix of mutual Poisson brackets of primary constraints (7), C_{ij} ,

$$C_{ij} = \{\phi_i^{(0)}(x,t), \phi_j^{(0)}(x',t)\}, \tag{13}$$

it is

$$C = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \delta(x-x'). \tag{14}$$

The inverse of matrix C , i.e., C^{-1} , is defined as

$$\int_{-\infty}^{+\infty} dy C_{ij'}(x,y,t) C_{j'j}^{-1}(x',y,t) = \delta_{ij} \delta(x-x'), \tag{15}$$

it is

$$C^{-1} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \delta(x-x'). \tag{16}$$

The dynamical properties of a system with second class constraints are determined by Dirac brackets

$$\begin{aligned}
& \{A(x,t), B(x',t)\}_{\text{IDB}} \\
& = \{A(x,t), B(x',t)\} \\
& - \int_{-\infty}^{+\infty} dy dz \\
& \times \{A(x,t), \theta_i(y,t)\} C_{ij}^{-1}(y,z) \{\theta_j(z,t), B(x',t)\}
\end{aligned} \tag{17}$$

(the reason why we label dirac brackets as IDB instead of DB will be explained in the next section) where $\theta_i(x,t)$

stand for all the second class constraints, in the present model, they are nothing but $\phi_1^{(0)}(x, t)$ and $\phi_2^{(0)}(x, t)$.

Now we are ready to calculate Dirac brackets among all the canonical variables, we only list the results:

$$\{\psi(x, t), \psi^\dagger(x', t)\}_{\text{IDB}} = -i\delta(x - x') \quad (18)$$

$$\{\psi(x, t), \Pi(x', t)\}_{\text{IDB}} = \frac{1}{2}\delta(x - x'). \quad (19)$$

Others are vanishing.

In fact, (18) can be directly read from the action according to Faddeev-Jackiw method [6]. Because the action (1) is in the first-order form, i.e.,

$$S \sim \int dt \int dx a_i(\xi) \dot{\xi}^i - H(\xi),$$

where ξ^i stand for all the symplectic variables $\xi^i = (\psi(x, t), \psi^\dagger(x, t))$, $a_i(\xi)$ are the corresponding canonical one-form $a_i(\xi) = (\frac{i}{2}\psi^\dagger(x, t), -\frac{i}{2}\psi(x, t))$. The canonical commutations can be read directly from the inverse of the matrix

$$f_{ij} = \frac{\partial a_j(\xi)}{\partial \xi^i} - \frac{\partial a_i(\xi)}{\partial \xi^j},$$

provided the inverse of f_{ij} exists. It is easy to compute

$f_{ij} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \delta(x - x')$, and the inverse of f do exist, $f_{ij}^{-1} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \delta(x - x')$. The commutation relation between $\psi(x, t)$ and $\psi^\dagger(x, t)$ can be read directly. They are in accordant with the results of (18).

The quantization procedure is complete once we take the following substitution:

$$\{ \quad , \quad \}_{\text{IDB}} \rightarrow \frac{1}{i} [\quad , \quad], \quad (20)$$

$$\psi \rightarrow \hat{\psi}, \quad \psi^\dagger \rightarrow \hat{\psi}^\dagger, \quad \Pi \rightarrow \hat{\Pi}, \quad \Pi^\dagger \rightarrow \hat{\Pi}^\dagger.$$

3 Schrödinger field in a finite volume

In this section, we shall study the model which has been studied in the previous section in a finite volume. The action is

$$\begin{aligned} S &= \int_{t_1}^{t_2} dt L \\ &= \frac{1}{2} \int_{t_1}^{t_2} dt \int_0^\pi dx i\psi^\dagger(x, t) \partial_t \psi(x, t) \\ &\quad - i\partial_t \psi^\dagger(x, t) \psi(x, t) - \partial_x \psi^\dagger(x, t) \partial_x \psi(x, t). \end{aligned} \quad (21)$$

Compared with the action (1), the spital integral is confined in a finite volume, i.e., $x \in [0, \pi]$. The variation of the action with respect to $\psi(x, t)$ and $\psi^\dagger(x, t)$ leads to

$$\delta S = \frac{1}{2} \int_{t_1}^{t_2} dt \int_0^\pi dx \delta\psi^\dagger(x, t) [2i\partial_t \psi(x, t) + \partial_x \partial_x \psi(x, t)]$$

$$\begin{aligned} &+ [-2i\partial_t \psi^\dagger(x, t) + \partial_x \partial_x \psi^\dagger(x, t)] \delta\psi(x, t) \\ &- \frac{1}{2} \int_{t_1}^{t_2} dt \\ &\quad \times [(\delta\psi^\dagger(x, t) \partial_x \psi(x, t)) + (\partial_x \psi^\dagger(x, t) \delta\psi(x, t))]_0^\pi \\ &+ \frac{1}{2} \int_{-\infty}^{+\infty} dx [i\psi^\dagger(x, t) \delta\psi(x, t) - i\delta\psi^\dagger \psi(x, t)] \Big|_{t_1}^{t_2}. \end{aligned} \quad (22)$$

For any arbitrary $\delta\psi$ and $\delta\psi^\dagger(x, t)$, the variation of the action vanishes if the four terms in the above equation vanish simultaneously. The vanishing of the first and the second terms gives the free Schrödinger equation and its Hermitian conjugation (4), and the last term leads to the initial conditions. For the third term in (22) to vanish, there are two choices which give two different boundary conditions, say, Neumann boundary conditions

$$\partial_x \psi(x, t)|_{x=0, \pi} = 0, \quad \partial_x \psi^\dagger(x, t)|_{x=0, \pi} = 0, \quad (23)$$

and Dirichlet ones

$$\delta\psi(x, t)|_{x=0, \pi} = 0, \quad \delta\psi^\dagger(x, t)|_{x=0, \pi} = 0. \quad (24)$$

Due to the BCs (23) and (24), one can not impose (18) on the whole space because they conflict with BCs on the boundaries. So, the commutators (18) need further modify, a careful treatment of BCs is needed. In the [1], BCs are treated as Dirac primary constraints, it has been proven that BCs form the second class constraints. and Dirac's procedure is applied there. In our model, things are more complicated because this model contains both intrinsic constraints (7) and BCS (23), (24). We shall follow the same idea suggested in [1], take the BCs (23), (24) as Dirac primary constraints. We only consider the Neumann BCs (23), the Dirichlet ones can be treated in a similar way.

Now besides the constraints (7), there are two additional constraints (23). It should be noted that although the BCs are only valid on the boundaries, we can safely extend them into the neighborhood of the boundaries, which means that we can rewrite them in the form as

$$\begin{aligned} \phi_3^{(0)} &= \int_0^\pi dx \partial_x \psi(x, t) \delta(x - B) \approx 0, \\ \phi_4^{(0)} &= \int_0^\pi dx \partial_x \psi^\dagger(x, t) \delta(x - B) \approx 0, \end{aligned} \quad (25)$$

where B stands for boundaries, $B = 0, \pi$.

Once we take BCs (25) as primary constraints, the total Hamiltonian is written as

$$H_T = H_C + \int dx \lambda^i \phi_i^{(0)}, \quad i = 1, 2, 3, 4. \quad (26)$$

It can be checked that the consistency conditions of the primary constraints give no secondary constraints¹. So the

¹ According to [5], if $\det\{\phi_i^{(0)}, \phi_j^{(0)}\} \neq 0$, no secondary constraints should be introduced, because the consistency requirements $\dot{\phi}_i^{(0)} \approx 0$ only determined the Lagrange multipliers.

constraints $\phi_i^{(0)}$, $i = 1, 2, 3, 4$ form second class constraints. The non-vanishing entries of the matrix of mutual Poisson brackets among primary constraints (7), (25) C'_{ij} are

$$\begin{aligned} C'_{12} &= -C'_{21} = -i\delta(x-x'), \\ C'_{13} &= -C'_{31} = \\ C'_{24} &= -C'_{42} = -\int dx' \delta(x'-B) \partial_{x'} \delta(x-x'). \end{aligned} \quad (27)$$

It is awkward to compute the inverse of C' directly. In order to simplify this problem, we prefer to do this in two steps: first, we construct intermediate Dirac brackets which correspond to the constraints $\phi_1^{(0)} \approx 0$, $\phi_2^{(0)} \approx 0$, and then construct the final Dirac brackets. Consistency of doing so is guaranteed by a known theorem [7]. In fact, the intermediate Dirac brackets is nothing but (17), this is the reason why we label Dirac brackets in the previous section as $\{ , \}_{\text{IDB}}$ instead of $\{ , \}_{\text{DB}}$. The intermediate Dirac brackets of remaining constraints $\phi_3^{(0)} \approx 0$, $\phi_4^{(0)} \approx 0$ are

$$\begin{aligned} &\{ \phi_3^{(0)}, \phi_4^{(0)} \}_{\text{IDB}} \\ &= -i \int dx dx' \delta(x-B) \delta(x'-B) \partial_x \partial_{x'} \delta(x-x'). \end{aligned} \quad (28)$$

Using the equality

$$\delta(x-x') = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon \sqrt{\pi}} e^{-(x-x')^2/\epsilon^2}, \quad (29)$$

the result of (28) can be obtained

$$\{ \phi_3^{(0)}, \phi_4^{(0)} \}_{\text{IDB}} = -\frac{2i}{\epsilon^3 \sqrt{\pi}}. \quad (30)$$

The matrix of intermediate Dirac brackets corresponding to $\phi_3^{(0)}$, $\phi_4^{(0)}$ is

$$\Delta = \begin{pmatrix} 0 & -\frac{2i}{\epsilon^3 \sqrt{\pi}} \\ \frac{2i}{\epsilon^3 \sqrt{\pi}} & 0 \end{pmatrix}. \quad (31)$$

This matrix can be easily inverted, and the final expression for the Dirac brackets is

$$\begin{aligned} &\{A(x, t), B(x', t)\}_{\text{DB}} \\ &= \{A(x, t), B(x', t)\}_{\text{IDB}} \\ &\quad - \{A(x, t), \theta_i\}_{\text{IDB}} \Delta_{ij}^{-1} \{\theta_j, B(x', t)\}_{\text{IDB}} \end{aligned} \quad (32)$$

in which θ_i are $\phi_3^{(0)}$ and $\phi_4^{(0)}$ now. The canonical commutators can be gotten from the above equation. We list our final results

$$\begin{aligned} \{ \psi(x, t), \psi^\dagger(x', t) \}_{\text{DB}} &= -i\delta(x-x') \\ &\quad + i \frac{\epsilon^3 \sqrt{\pi}}{2} \partial_x \delta(x-B) \partial_{x'} \delta(x'-B), \end{aligned} \quad (33)$$

$$\{ \psi(x, t), \Pi(x', t) \}_{\text{DB}} = \frac{1}{2} \delta(x-x') \quad (34)$$

$$- \frac{\epsilon^3 \sqrt{\pi}}{2} \partial_x \delta(x-B) \partial_{x'} \delta(x'-B).$$

Others are vanishing. As argued in [1], the appearance of the regularization parameter ϵ in the above equation seems uncomfortable, but it is necessary to keep the two terms on the right side to be of the same order.

Our final results (33,34) are equal to (18) and (19) if we only consider the bulk, i.e., $x, x' \in (0, \pi)$, however, on the boundaries, they are consistent with Newmann BCs. Using equality (29) one can verify that ²

$$\{ \partial_x \psi(x, t), \psi^\dagger(x', t) \}_{\text{DB}} \Big|_{x=B} = 0. \quad (35)$$

For this reason, we label the right hand side of (33), (34) as $-i\delta_N(x-x')$ and $\delta_N(x-x')$ respectively, i.e,

$$\begin{aligned} \{ \psi(x, t), \psi^\dagger(x', t) \}_{\text{DB}} &= -i\delta_N(x-x'), \\ \{ \psi(x, t), \Pi(x', t) \}_{\text{DB}} &= \frac{1}{2} \delta_N(x-x'). \end{aligned} \quad (36)$$

The canonical quantization procedure is straightforward, and the only modification to (20) is that the the subscript is DB instead of IDB.

4 Conclusions and remarks

In this paper, we show how to quantize a singular model defined in a finite volume canonically by studying free 1 + 1 dimensional Schrödinger field. Compared with the previous work [1], our model is more general because it contains both intrinsic constraints and BCs. Following [1], we take the BCs as Dirac primary constraints. It is shown that BCs entangle with the intrinsic constraints and they form the second class constraints. In order to quantize this model canonically, the calculation of Dirac brackets is inevitable. Based on a theorem [7], the calculation is greatly simplified. We construct the intermediate Dirac brackets $\{ , \}_{\text{IDB}}$ firstly, then the final Dirac brackets $\{ , \}_{\text{DB}}$ are calculated based on the intermediate ones. Although our model is only confined in 1 + 1 dimension, the generalization to higher space is quite straightforward.

Acknowledgements. The author thanks the referee's many valuable comments. This work is supported by the Youth Foundation of Beijing University of Chemical Technology (BUCT) with grand No. QN0413 and National Natural Science Foundation of China with grant No. 10247009.

Appendix

In this appendix, we shall give the explicit calculations of result (35). Consider equality (29), (35) is

$$\{ \partial_x \psi(x, t), \psi^\dagger(x', t) \}_{\text{DB}} \Big|_{x=B}$$

² The details of calculations will be given in the Appendix.

$$\begin{aligned}
&= -i\partial_x\delta(x-x')\Big|_{x=B} \\
&\quad + i\frac{\epsilon^3\sqrt{\pi}}{2}\partial_x^2\delta(x-B)\Big|_{x=B}\partial_{x'}\delta(x'-B) \\
&= -\frac{i}{\epsilon\sqrt{\pi}}\partial_x e^{-\frac{(x-x')^2}{\epsilon^2}}\Big|_{x=B} \\
&\quad + \frac{i\epsilon^2}{2}\partial_x^2 e^{-\frac{(x-x')^2}{\epsilon^2}}\partial_{x'}\delta(x'-B)\Big|_{x=B} \\
&= \frac{-2i}{\epsilon\sqrt{\pi}}(x'-B)e^{-\frac{(x-x')^2}{\epsilon^2}}\Big|_{x=B} \\
&\quad - i\partial_x\left[(x-B)e^{-\frac{(x-x')^2}{\epsilon^2}}\right]_{x=B}\partial_{x'}\delta(x'-B) \\
&= i\partial_{x'}\delta(x'-B) - i\partial_{x'}\delta(x'-B) \\
&= 0.
\end{aligned} \tag{37}$$

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