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THE SHORT-TIME PROPAGATOR AND THE BOUNDARY CONDITIONS IN THE QUANTUM MECHANICS *

P. Prešnajder and V. Pažma

1. Introduction

The retarded propagator $K(x,T;y,0)$ for $T>0$ is given in the Feynman formulation of the quantum mechanics as

$$K(x,T;y,0) = \lim_{N\to\infty} \int dx_{N-1}\dots dx_1 \; K_{T/N}(x,x_{N-1})\dots K_{T/N}(x_1,y) \qquad (1)$$

where $K_t(x,y)$ is a short-time propagator ($t = T/N$ is small). For the Lagrangeans of the type

$$L = \frac{1}{2}\dot{x}^2 - V(x)$$

Feynman put

$$K_t(x,y) = (2\pi it)^{-n/2} \exp\left[\frac{i}{2t}(x-y)^2 - itV\left(\frac{x+y}{2}\right) \right] \qquad (2)$$

(here n is the dimension of the configuration space).

The expression for the $K_t(x,y)$ is important, since it guarantees the formal equivalence of the Feynman and Schrödinger approaches: if $K_t(x,y)$ satisfies to the accuracy $o(t)$ the Schrödinger equation, then $K(x,t;y,0)$ given by the eq. (1) is formally its solution. The equivalence of both approaches is a formal one because the procedure based on the eqs. (1) and (2) does not guarantee the boundary conditions following from the physical requirements of the problem.

In Sect. 2 we shall therefore investigate the short-time propagator on a configuration Riemannian manifold (to the accuracy $o(t)$, because only those terms are essential for a formal proof of the Schrödinger equation from (1) and (2)) and propose a procedure how to include boundary conditions into the definition of the short-time propagator. In Sect. 3 we compare our method with more standard approaches. In Sect. 4 we study the boundary conditions

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* This paper is in final form and no version of it will be submitted for publication elsewhere.

in more detail and solve a simple non-trivial example as an illustration. Finally Sect. 5 is devoted to concluding remarks.

2. The short-time propagator

For $t>0$ we investigate on an n-dimensional Riemannian manifold M the solution $K = K(x,t;y,0)$ of the Schrödinger equation

$$i\,\partial_t K = -\frac{1}{2}\Delta K + VK \tag{3}$$

which satisfies the initial condition

$$K(x,0;y,0) = \delta(x,y) \tag{4}$$

and boundary conditions (which we shall specify later) on a boundary ∂M of the manifold M. Moreover K is a symmetric function of $x,y\in M$.

Let us seek the particular solution of the eq. (3) in the form of the following short-time expansion

$$K(x,t;y,0) =$$

$$= (2\pi it)^{-m/2}\, D(x,y)\, \exp\left[\frac{i}{2t}r^2(x,y) - itW(x,y) + o(t^2)\right] \tag{5}$$

where $r = r(x,y)$ satisfies the condition

$$(\nabla r, \nabla r) = 1 \tag{6}$$

The terms $o(t^2)$ in the bracket in (5) are of no interest for us. The condition (6) guarantees that

$$S(x,y,t) = \frac{1}{2t}\, r^2(x,y) \tag{7}$$

is the classical action for a free motion on the M, which is a solution of the Hamilton-Jacobi equation

$$-\partial_t S = \frac{1}{2}(\nabla S, \nabla S) \tag{8}$$

The factor in front of the exponent in (5) is necessary, because it guarantees the correct physical dimension of K.

Our procedure is similar to the proof of the Minakshisundaran -Pleijel theorem in (BERGER, GAUDUCHON, MAZET): we insert the expansion (5) into the Schrödinger equation (3) and by a comparison of expressions by lowest powers of t we obtain equations for the functions D and W

$$\frac{m-1}{2} = \frac{r}{D}\,(\nabla r, \nabla D) + r\Delta r \tag{9}$$

$$W + r(\nabla r, \nabla W) = V - \frac{1}{2D}\Delta D \tag{10}$$

Let us solve the eqs. (9) and (10). Consider a classical trajectory x(.) corresponding to a free motion from the point $y = x(0)$ to the point $x = x(t)$. We assume that we know the corresponding classical action $S(x,y,t)$ i.e. we assume that the function $r = r(x,y)$ is given. The vector field $e_1 = \nabla r$ has a unit lenght along x(.): $(e_1,e_1) = 1$. Further we shall assume along x(.) Jacobi fields $e_2,\dots,e_n$, which are linearly independent and perpendicular to e_1. In the basis $e_1,e_2,\dots,e_n$ the eq. (9) takes the form

$$\frac{m-1}{2} = \frac{r}{D} D' + \frac{e'}{2e} \tag{11}$$

where $e = (\det g)^{-1/2}$ (the metric tensor g should be calculated in the basis given above) and the prime denotes the differentiation with respect to r. The eq. (11) has a solution

$$D = a\, r^{(m-1)/2}\, e^{-1/2} \tag{12}$$

where a is an integration constant (i.e. a is such a function a(x,y), that $a'=0$). Similarly the eq. (10) could be rewritten as

$$(rW)' = V - \frac{1}{2D}\Delta D \tag{13}$$

It has a solution

$$W = \frac{1}{r}\int (V - \frac{1}{2D}\quad D)\, dr + \frac{b}{r} \tag{14}$$

where $b = b(x,y)$ is an integration constant.(i.e. $b'=0$) and one integrates in (14) along the assumed classical trajectory.

In principle we have to take into account every classical trajectory x(.) starting in the point $y = x(0)$ and ending in $x = x(t)$. Among these trajectories there is the shortest one corresponding to the "direct" motion from the point y to the point x (such a trajectory exists always, provided that the points x, y are enough close to each other). When the topology, or the boundary, of the manifold are non trivial, there could exist "indirect" trajectories winding around the manifold, or reflecting from its boundary (their number may be finite or infinite). The "direct" trajectory is not sufficient for the construction of the general solution K. We propose to search for the K in the form of the summ of all particular solutions (5)

$$K(x,t;y,0) = \sum (2\pi i t)^{-m/2}\, D(x,y)\, \exp\left[\frac{i}{2t} r^2(x,y) - itW(x,y) + o(t^2) \right] \tag{15}$$

As the short-time propagator $K_t(x,y)$ we denote any formula for K_t, which is identical to (15) in all terms explicitely written in the bracket in exponent.

For the direct path r is equal to the Riemannian distance d(x,y) on the M. For $t \longrightarrow 0+$ one has, (BERGER, GAUDUCHON, MAZET)

$$(2\pi it)^{-n/2}\ D(x,y)\ \exp \frac{i}{2t} d^2(x,y) \longrightarrow D(x,x)\ \delta(x,y)$$

The initial condition (4) thus fixes m = n and D(x,x) = 1. This fixes the multiplicative constant a in (13) for the direct trajectory. Moreover for this trajectory b = 0, because the term b/d(x,y) in (14) is undefined for x = y. The term in the eq. (15) corresponding to the direct trajectory is completely fixed.

For the indirect path it holds $r(x,y) > d(x,y)$ for arbitrary interior points x, y of M. For $m \leqslant n$ and $t \longrightarrow 0+$ one has

$$(2\pi it)^{-m/2}\ D(x,y)\ \exp \frac{i}{2t} r^2(x,y) \longrightarrow 0$$

Now we shall qualitatively investigate the short-time limit of (15). When x and y are interior points of M, then the term corresponding to the direct path dominates the (15) i.e.

$$K_t(x,y) = (2\pi it)^{-n/2}\ D(x,y)\ \exp \frac{i}{2t} d^2(x,y) + \dots \qquad (16)$$

and terms not explicitely indicated are inessential, since they contain much more oscillating factors $\exp \frac{i}{2t} r^2(x,y)$ with $r(x,y) > d(x,y)$.

The situation is different, when $x \in \partial M$ and $y \in M$. Then some of indirect path are reduced to the direct one and (15) is dominated by all the trajectories which for the x approaching ∂M are reduced to the direct trajectory. The $m \leqslant n$ and the integration constants a, b (and eventually the undetermined $o(t^2)$ contributions) in these terms should be chosen so that the short-time propagator

(i) is defined and symmetric on $M \times M$,

(ii) satisfies (to the accuracy o(t)) in dominant contributions the boundary conditions on ∂M.

We propose to use the short-time propagator determined in this way to calculate the Feynman integral (1). Of course this does not gaurantee the existence of the limit in (1) and its calculation remains generally extremely complicated. If the limit (1) exists we can intuitively expect that the propagator will satisfy the prescribed boundary conditions.

In what follows we compare the approximations (16) for the interior points x and y with the standard approaches. Then we present an explicite procedure how one can approximatively satisfy the boundary conditions $x \in \partial M$ with a suitable choice of dominant terms in (15) (in some simple cases the boundary conditions could be satisfied exatly taking into account all terms in (15), (PAŽMA, PREŠNAJDER; PREŠNAJDER, PAŽMA).

3. Other approaches to the construction of the short-time propagator

The Feynman's proposal (2) was extended by (DE WITT) to systems on Riemannian manifold; further generalisations could be found in (SCHULMAN). In these papers the boundaries and boundary conditions were not taken into account. The generalisations were based on a first WKB approximation to the propagator of the particle moving on a manifold i.e. the short-time propagator was defined instead of (2) as

$$\tilde{K}_t(x,y) = (2\pi it)^{-n/2}\, \tilde{D}^{1/2}(x,y,t) \exp i\tilde{S}(x,y,t) \tag{17}$$

where $\tilde{S}(x,y,t)$ is a classical action, which is a solution of the Hamilton-Jacobi equation describing the motion on the manifold M in the potential $V = V(x)$

$$-\partial_t\tilde{S} = \frac{1}{2}(\nabla\tilde{S},\nabla\tilde{S}) + V$$

and $\tilde{D}$ is the corresponding Van Vleck determinant. Usually one assumes the direct path only (in (SCHULMAN) there is a proposal to take into account homotopically inequivalent trajectories, but not in connection with the boundary conditions).

Let us investigate the connection between the proposal (17) and the short-time approximation (16) for the interior points x and y. In the short-time limit and for x close to y we have

$$\tilde{D}(x,y,t) = t^{-n}\, D^2(x,y) + o(t^2)$$

$$\tilde{S}(x,y,t) = \frac{1}{2t}\, d^2(x,y) - t\tilde{V}(x,y) + o(t^2)$$

where $\tilde{V}(x,y) = V(z)$ (and z is e.g. centre of the corresponding classical trajectory, roughly $z \approx (x+y)/2$).

By inserting these expressions into the formula (17) we shall not obtain the short-time propagator solving to the accuracy o(t) the Schrödinger equation (3). It turned out (DE WITT), that to the potential one should ad hoc add a term $-R(x)/12$ (where R is the scalar curvature of the manifold) i.e. one should use the potential

$$\tilde{W}(x) = V(x) - \frac{1}{12}\, R(x) \tag{18}$$

The formula (17) formula (17) for the short-time propagator is in this way chaged to (DE WITT)

$$\tilde{K}_t(x,y) = (2\pi it)^{-n/2}\, D(x,y)\, \exp[\, \tfrac{i}{2t} d^2(x,y) - it\tilde{W}(z)\,] \tag{19}$$

Let us compare this expression with our formula (16) for the short-time propagator K_t (the eq. (16) is valid in the case of the interior points x and y). Both expressions are identical up to terms $W(x,y)$ and $\tilde{W}(z)$. In our case $W(x,y)$ is given by (14) (with $b = 0$) and for x close y we have

$$W(x,y) \approx \tilde{W}(z) \tag{20}$$

Moreover one can show (BERGER, GAUDUCHON, MAZET), that

$$\frac{1}{6} R(x) = \frac{1}{D(x,y)} \Delta D(x,y)\Big|_{y=x} \tag{21}$$

We see that for the neighbouring interior points of the manifold the expression for the $K_t(x,y)$ is approaching the $\tilde{K}_t(x,y)$.

In the standard approach starting from the first WKB approximation the additional term in (18) is added "by hand". In fact it appears in the second WKB approximation (for the close points x and y).

One can simply show that for a free particle the individual WKB and short-time expansions are in one-to-one correspondence. In the short-time expansion one can include easily the potential (not as in WKB expansion): one solves first the Hamilton-Jacobi equation for the free particle and then one adds to W the mean value of the potential along the classical path of the free particle (see eq. (14)).

In our short-time expansion (corresponding to the second WKB approximation) there appears automatically the term $-\frac{1}{2r}\int \frac{1}{D}\Delta D\, dr$ in W, which for the infinitezimal paths reduces to the additional term in (18). Moreover the (modified) WKB approximation (19) is adequate only for infinitesimal trajectories, whereas short-time approximation is correct even for non-infinitesimal ones, which are important by taking the boundary conditions into account.

4. The boundary conditions

We shall take into account boundary conditions in one typical example. If the potential is not singular on the boundary ∂M, one takes usually the boundary condition in the form

$$\beta(x)\, K(x,t;y,0) + \partial_n K(x,t;y,0) = 0\ , \quad x \in \partial M,\ y \in M \tag{22}$$

where ∂_n denotes the differentiation in x along the normal direction on ∂M and $\beta(x)$ is a given function on ∂M.

When x is approaching the boundary, one from the indirect trajectories is reflecting from ∂M (in a point close to x) and for $x \in \partial M$ it is reduced to the direct trajectory. Then both equally contribute to the summ in (15) (see Fig. 1). For $x \in \partial M$ one should take the short-time propagator in the form

$$K_t(x,y) = (2\pi it)^{-n/2} \sum_{j=0}^{1} D_j(x,y) \exp[\frac{i}{2t} r_j^2(x,y) - itW_j(x,y)] \tag{23}$$

Here the index "0" corresponds to the direct trajectory and "1" to the reflected one (which of the indirect trajectories remains from (15) on the r.h.s. in (23) depends on the position of x on ∂M). We insert the expression (23) into the boundary condition (22). After cancelling the same factors in both sides, we obtain the equation, $(x \in \partial M)$

$$\sum_{j=0}^{1} [\beta D_j + D_j(\frac{i}{t} r_j \partial_n r_j - it\partial_n W_j) + \partial_n D_j] \exp(-itW_j) = 0 \tag{24}$$

We now expand the exponent in (24) into the power series and require that the expressions standing by the powers t^{-1} and t^{0} vanish. Using the formula (14) for the W_j, we obtain conditions

$$D_o \partial_n r_o + D_1 \partial_n r_1 = 0 \tag{25a}$$

$$(\beta + \partial_n)(D_o + D_1) = [b_1 + \frac{1}{2}\int (D_o^{-1}\Delta D_o - D_1^{-1}\Delta D_1)dr] D_o \partial_n r_o \tag{25b}$$

$$x \in \partial M$$

(here we have taken into account that for the direct path $b_o = 1$).

The eq. (25a) fixes the multiplicative constant a_1 in D_1, whereas (25b) determines the additive constant b_1 in W_1. Let us note that the conditions (25) do not depend on the potential V. For $\beta = \infty$ there remains only the condition

$$D_o + D_1 = 0 , \quad x \in \partial M \tag{25c}$$

which determines a_1 and we can consistently put $b_1 = 0$.

Generally the shape of the manifold and the boundary conditions could be such, that the corresponding conditions cannot be satisfied. This is an indication that there does not exist the propagator for the Schrödinger equation with the given boundary conditions i.e. that for the given problem does not exist the self-adjoint hamiltonian (in our approach we investigate this problem in the limit $t \longrightarrow 0+$).

As an illustration assume the free motion from the point $y = (v_1, v_2)$ to the point $x = (u_1, u_2)$ in quadrant of the plane $v_i > 0$, $u_i > 0$; $i = 1,2$. There are four classical trajectories with the actions (see Fig. 2)

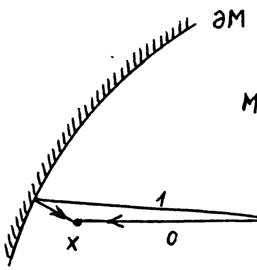

Fig. 1

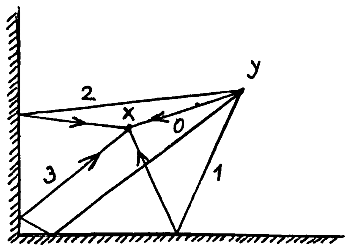

Fig. 2

$$S_j = \frac{1}{2t}(x-y_j)^2 , \qquad j = 0,1,2,3 \tag{26}$$

where $y_o = (v_1,v_2)$, $y_1 = (-v_1,v_2)$, $y_2 = (v_1,-v_2)$, $y_3 = (-v_1,-v_2)$. By dimensional arguments $m = 2$ in (15) for all these trajectories. The corresponding short-time propagator is

$$K_t(x,y) = \frac{1}{2\pi i t} \sum_{j=0}^{2} D_j \exp(iS_j - itW_j) \tag{27}$$

We shall not consider the doubly reflected path ($j = 3$) in (27), since it is unimportant for an approximative fulfilment of the boundary conditions.

It is instructive to solve the eqs. (9) and (10) directly. For every paths we change two variables u_1, u_2 to a new pair of variables r_j, ω_j ($j = 0,1,2$), where $r_j^2 = (x-y_j)^2$ and ω_j has the property $(\nabla r_j, \nabla\omega_j) = 0$. The eq. (9) is then reduced to

$$\partial_{r_j} D_j = 0 , \qquad j = 0,1,2 \tag{28}$$

and it follows that $D_j = D_j(\omega_j)$. Similarly the eq. (10) is reduced to

$$\partial_{r_j}(r_j W_j) = -\frac{1}{2} D_j^{-1} \Delta D_j , \qquad j = 0,1,2 \tag{29}$$

The initial condition for the direct path determines $D_o = 1$ and $W_o = 0$. Let us study the once reflected paths. We put

$$\omega_1 = (u_2-v_2)/(u_1+v_1), \qquad \omega_2 = (u_1-v_1)/(u_2+v_2) \tag{30}$$

Then

$$\frac{1}{2} D_j^{-1} \Delta D_j = r_j^{-2} c_j(\omega_j) , \qquad j = 1,2$$

where

$$c_j(\omega_j) = \frac{1}{2}(1+\omega_j^2) D_j^{-1} \partial_{\omega_j} [(1+\omega_j^2) \partial_{\omega_j} D_j]$$

The solution of the eq. (29) is

$$W_j = r_j^{-1}\, b_j(\omega_j) + r_j^{-2}\, c_j(\omega_j) \tag{31}$$

We take the boundary conditions in the form

$$\beta_1(u_2)\, K(0,u_2,t;v_1,v_2,0) + \partial_{u_1} K(0,u_2,t;v_1,v_2,0) = 0 \tag{32a}$$

$$\beta_2(u_1)\, K(u_1,0,t;v_1,v_2,0) + \partial_{u_2} K(u_1,0,t;v_1,v_2,0) = 0 \tag{32b}$$

Consider first the condition (32a). In this case we leave in (27) only the terms $j = 0,1$. Since for $u_1 = 0$ it holds

$$\partial_{u_1} r_1 = -\partial_{u_1} r_o = (1+\omega_1^2)^{-1/2}$$

the eq. (25a) gives $D_1 = D_o = 1$ (and consequently in (31) $c_1 = 0$). The eq. (25b) then reduces to

$$2\,\beta_1(u_2) = -\,(1+\omega_1^2)^{-1/2}\, b_1 \tag{33a}$$

In the same way one obtains from the condition (32b) $D_2 = D_o = 1$, $c_2 = 0$ and finally the condition

$$2\,\beta_2(u_1) = -\,(1+\omega_2^2)^{-1/2}\, b_2 . \tag{33b}$$

The conditions (33) will be satisfied for $u_1 = 0$ or $u_2 = 0$ respectively, if we put

$$b_j = -2(1+\omega_j^2)^{-1/2}\, \beta_j((u_1v_2+u_2v_1)/(u_j+v_j)) , \qquad j = 1,2 \tag{34}$$

The short-time propagator is then equal to

$$K_t = \frac{1}{2\pi it}[\, \exp(iS_o) + \exp(-itb_1/r_1)\exp(iS_1) + \\ + \exp(-itb_2/r_2)\exp(iS_2)\,] \tag{35}$$

where b_1, b_2 are given by (34).

If β_1, β_2 are constants, then (to the assumed accuracy) we can rewrite K_t as

$$K_t(u_1,u_2,v_1,v_2) = K_t^{(\beta_1)}(u_1,v_1)\, K_t^{(\beta_2)}(u_2,v_2) \tag{36}$$

where

$$K_t^{(\beta)}(u,v) = (2\pi it)^{-1/2}[\, \exp\frac{i(u-v)^2}{2t} + \\ + \exp\frac{it2\beta}{u+y}\, \exp\frac{i(u+v)^2}{2t}\,] \tag{37}$$

We have shown (PAŽMA, PREŠNAJDER) that the propagator of the particle freely moving on the half-line ($u > 0$), which satisfies the boundary condition

$$\beta K^{(\beta)}(0,t;v,0) + \partial_u K^{(\beta)}(0,t;v,0) = 0 \tag{38}$$

has precisely the short-time expansion (37). The decomposition (36) simply corresponds to the separation of variables. The factor in front of the last exponent in (37) has a natural interpretation: for small t we can write

$$\exp\frac{it2\beta}{u+v} = \frac{1 + it\beta/(u+v)}{1 - it\beta/(u+v)} = \frac{ik - \beta}{ik + \beta} \tag{39}$$

where $k = (u+v)/t$ is the classical momentum of the particle along the trajectory reflecting from the origin. The last expression in the eq. (39) corresponds precisely to the phase factor, which the incomming Schrödinger wave obtains after the reflection from the wall on which the boundary conditions. (38) should be satisfied (see e.g. (REED, SIMON)).

5. Concluding remarks

Postulating the form of K_t for a given classical system may be understood as a specification of a method of quantisation (more precisely as a determination of quantum dynamics). Starting from our (to some extend intuitive) results we can formulate the quantisation for the particle moving on the Riemannian manifold with the boundary in path integral approach as follows:

1. Find all classical trajectories x(.), starting in the point $y = x(0)$ and ending in the point $x = x(t)$.

2. The short-time propagator is given by the formula

$$K_t(x,y) = \sum (2\pi it)^{-m/2} D(x,y) \exp[\tfrac{i}{2t} r^2(x,y) - itW(x,y) + \ldots] \tag{40a}$$

where one makes a sum over all classical trajectories and

$$D(x,y) = a\, r^{(m-1)/2}\, e^{-1/2} \tag{40b}$$

$$W(x,y) = \frac{1}{r}\int_y^x (V - \frac{1}{2D}\Delta D)\, dr \tag{40c}$$

Here $r = r(x,y)$ is the lenght of the corresponding trajectory, $e = (\det g)^{-1/2}$ and one integrates along the trajectory.

3. The quantities a and b do not depend on r i.e. $(\nabla r, \nabla a) = 0$, $(\nabla r, \nabla b) = 0$. For the directtrajectory $b = 0$ and a is fixed by the condition $D(x,x) = 1$. For all other trajectories a and b should be chosen in such a way, that the $K_t(x,y)$ is symmetric in x, y and satisfies (to the accuracy o(t)) the boundary conditions.

When we succeed in constructing the short-time propagator, we intuitively expect, that the propagator given by eq. (1) will satisfy the boundary conditions. The non-existence of K_t indicates, that for given boundary conditions there does not exist self-adjoint Hamiltonian.

As we have pointed out in Sect. 3 the formula for the K_t is identical to the second WKB approximation for the free propagator

$$K_t^f = K_{WKB}^{(2)} = \exp \frac{i}{h}(S_o^f + hS_1^f + h^2S_2^f) \qquad (41)$$

(the index "f" means "free"). The term $S_2^f(x,y,t)$ has the interesting property, that

$$S_2^f(x,x,t) = \frac{t}{12} R(x)$$

where R(x) is the scalar curvature of the manifold. When we take

$$\tilde{K}_t^f = K_{WKB}^{(1)} = \exp \frac{i}{h}(S_o^f + hS_1^f) \qquad (42)$$

then in the Schrödinger equation for K appears the term -R(x)/12, which has not yet generally accepted interpretation. On the basis of our results, we think that the appearence of this term in Schrödinger equation reflects the uncompletness of the assumption (42), with respect to the correct one (41) (for a free particle). Let us note, that in our approach the potential is taken into account simply by adding the term $-t\overline{V}(x,y)$ to the $S_2^f(x,y,t)$ (here $\overline{V}(x,y)$ is the mean value of the potential along the classical trajectory; see eq. (40c)).

The proposed method of constructing K_f works satisfactorily in simple cases (the particle on a circle, on a finite interval, on a half-line, in a quadrant of a plane, ... (PREŠNAJDER, PAŽMA)). This indicates, that the proposed approach permits to construct the short-time propagators, which satisfy the boundary conditions following from the physical formulation of the problem.

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