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# The Jacobi principal function in quantum mechanics

Rafael Ferraro<sup>†</sup>

Instituto de Astronomía y Física del Espacio, Casilla de Correo 67, Sucursal 28, 1428 Buenos Aires, Argentina

and

Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, Pabellón I, 1428 Buenos Aires, Argentina

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**Abstract.** The canonical functional action in the path integral in phase space is discretized by linking each pair of consecutive vertebral points— $q_k$  and  $p_{k+1}$  or  $p_k$  and  $q_{k+1}$ —through the invariant complete solution of the Hamilton–Jacobi equation associated with the classical path defined by these extremes. When the measure is chosen to reflect the geometrical character of the propagator (it must behave as a density of weight  $\frac{1}{2}$  in both of its arguments), the resulting infinitesimal propagator is cast in the form of an expansion in a basis of short-time solutions of the wave equation, associated with the eigenfunctions of the initial momenta canonically conjugated to a set of normal coordinates. The operator ordering induced by this prescription is a combination of a symmetrization rule coming from the phase, and a derivative term coming from the measure.

## 1. Introduction

By taking Dirac’s ideas [1] into account, R P Feynman explained how non-relativistic quantum mechanics can be formulated from principles that make contact with the variational principles of Lagrangian mechanics [2]. Feynman showed that quantum mechanics can be based on the statement that the *propagator*, i.e. the probability amplitude of finding the system in the state  $q''$  at  $t''$ , given that it was found in  $q'$  at  $t'$ , can be obtained by means of the path integration:

$$K(q''t''|q't') = \int \mathcal{D}q(t) \exp \left[ \frac{i}{\hbar} S[q(t)] \right] \quad (1)$$

where  $S[q(t)]$  is the functional action of the system. Since the path integral is a functional integration, one gives a meaning to equation (1) by replacing each path by a *skeletonized* version where the path  $q(t)$  is represented by a set of interpolating points  $(q_k, t_k)$ ,  $k = 0, 1, \dots, N$ ,  $q_0 = q'$ ,  $q_N = q''$ ,  $q_k = q(t_k)$ . Then the functional action is replaced by a function  $S(\{q_k, t_k\})$ , and the functional integration reduces to integrate the variables  $q_k$ ,  $k = 1, \dots, N-1$ ‡. Finally, the limit  $\Delta t_k \equiv t_{k+1} - t_k \rightarrow 0$  (i.e.,  $N \rightarrow \infty$ ) is performed§.

The function  $S(\{q_k, t_k\})$  is chosen to be [2, 4]:

$$S(\{q_k, t_k\}) = \sum_{k=0}^{N-1} S(q_{k+1}t_{k+1}|q_k t_k) \quad (2)$$

<sup>†</sup> E-mail address: ferraro@iafe.uba.ar

<sup>‡</sup> The convergence is assured by endowing the time with an imaginary part of proper sign.

<sup>§</sup> The rigorous mathematical meaning of this limit can be consulted in [3] and references therein.

where  $S(\mathbf{q}_{k+1}t_{k+1}|\mathbf{q}_kt_k)$  is the Hamilton principal function, i.e.the complete solution (in each argument) of the Hamilton–Jacobi equation that is equal to the functional action evaluated on the classical path joining its arguments. Thus, the skeletonization (2) replaces each path  $\mathbf{q}(t)$  by a succession of pieces defined by the system itself, which join the interpolating points. The skeletonized action (2) retains the essential classical property of the functional action; namely it is stationary on the points interpolating the entire classical path between  $(\mathbf{q}', t')$  and  $(\mathbf{q}'', t'')$ . In fact,  $S(\{\mathbf{q}_k, t_k\})$  is stationary when

$$\frac{\partial}{\partial \mathbf{q}_k} S(\mathbf{q}_{k+1}t_{k+1}|\mathbf{q}_kt_k) + \frac{\partial}{\partial \mathbf{q}_k} S(\mathbf{q}_kt_k|\mathbf{q}_{k-1}t_{k-1}) = 0 \quad \forall k \tag{3}$$

meaning that the  $\mathbf{q}_k$  are such that the final momentum of the classical piece between  $(\mathbf{q}_{k-1}, t_{k-1})$  and  $(\mathbf{q}_k, t_k)$ , matches the initial momentum of the classical piece between  $(\mathbf{q}_k, t_k)$  and  $(\mathbf{q}_{k+1}, t_{k+1})$ . This continuity guarantees that the points  $\{\mathbf{q}_k, t_k\}$  are interpolating points of the entire classical path between  $(\mathbf{q}', t')$  and  $(\mathbf{q}'', t'')$ .

Although a proper skeletonization for the path integral exists in the configuration space, the measure in equation (1) remains ambiguous. For instance, the finite propagator for a quadratic Lagrangian is known to be [5, 6]

$$K(\mathbf{q}''t''|\mathbf{q}'t') = \left[ \det \left( \frac{i}{2\pi\hbar} \frac{\partial^2 S(\mathbf{q}''t''|\mathbf{q}'t')}{\partial \mathbf{q}'' \partial \mathbf{q}'} \right) \right]^{1/2} \exp \left[ \frac{i}{\hbar} S(\mathbf{q}''t''|\mathbf{q}'t') \right]. \tag{4}$$

This expression is also valid for the infinitesimal propagator of any classical system [7]. The prefactor in equation (4) is the Van Vleck determinant [8], which takes part in the measure, and is nontrivial even for the short-time pieces of the skeletonization.

A different kind of example is the (finite) Newton–Wigner propagator for the relativistic particle in flat space–time [9]:

$$K(\mathbf{q}''t''|\mathbf{q}'t') = -\frac{(t'' - t')m^2c^3}{\pi\hbar S(\mathbf{q}''t''|\mathbf{q}'t')} K_1 \left( \frac{i}{\hbar} S(\mathbf{q}''t''|\mathbf{q}'t') \right) \tag{5}$$

(in 1 + 1 dimensions), where  $S(\mathbf{q}''t''|\mathbf{q}'t') = -mc^2(t'' - t')^2 - (\mathbf{q}'' - \mathbf{q}')^2)^{1/2}$ , and  $K_1$  is a modified Bessel function. In this case, the exponential of the Hamilton principal function does not cleanly appear in the propagator, and neither does it in the short time version (actually the propagator (5) gets the form (4), not when  $t'' \rightarrow t'$  but in the classical limit when the Compton wavelength  $\hbar/(mc)$  goes to zero). Results of this sort could indicate a failure of (1) to give the quantum propagator for an arbitrary system [10]. Anyway, it lays bare our complete ignorance of the measure in the representation (1).

It was thought that a path integration in phase space could remedy this problem because there is a privileged measure in phase space: the Liouville measure  $d\mathbf{q} d\mathbf{p}/(2\pi\hbar)^n$  ( $n$  is the dimension of the configuration space), which is invariant under canonical transformations. In this case, one should find an appropriate recipe for the skeletonization of the canonical functional action

$$S[\mathbf{q}(t), \mathbf{p}(t)] = \int_{t'}^{t''} (\mathbf{p}(t) \cdot \dot{\mathbf{q}}(t) - H(\mathbf{q}, \mathbf{p})) dt \tag{6}$$

i.e., one should replace the functional in equation (6) by a function  $S(\{\mathbf{q}_k, \mathbf{p}_k, t_k\})$  of interpolating points for the path  $\mathbf{q}(t), \mathbf{p}(t)$ . The function  $S(\{\mathbf{q}_k, \mathbf{p}_k, t_k\})$  should be dictated by the system itself.

In [11] several recipes were essayed for a Newtonian system moving on a Riemannian manifold. Since the data  $(\mathbf{q}_k, \mathbf{p}_k; \mathbf{q}_{k+1}, \mathbf{p}_{k+1})$  overdetermine the classical path between  $t_k$  and  $t_{k+1}$ , the basic idea was to use the classical piece in the configuration space (just as in the previous case), together with the parallel transport of  $\mathbf{p}(t_k) = \mathbf{p}_k$  along that classical piece. Of

course, the parallel transport of  $\mathbf{p}_k$  does not end in  $\mathbf{p}_{k+1}$  (unless the points interpolate the entire classical path between  $t'$  and  $t''$ ). So the skeletonized path proves to be discontinuous in  $\mathbf{p}$  (an unavoidable fact in phase space). The different recipes for the skeletonization came from the possibility of replacing the metric by a bitensor with the right coincidence limit. After the momenta were integrated on, an infinitesimal propagator similar to the one of equation (4) was obtained. However, the different skeletonizations reflected in a measure differing from the Van Vleck determinant by corrections associated with the curvature of the manifold. As a consequence, the Hamiltonian operator in the Schrödinger equation had a term proportional to  $\hbar^2 R$ , where  $R$  is the curvature scalar (see also [4, 12] for Newtonian systems, and [9] for relativistic systems).

The skeletonization proposed in [11] successfully retains the covariance of the system, but it does not treat coordinates and momenta on an equal footing (a desirable feature in a canonical formalism).

In [13] the use of complete solutions of the Hamilton–Jacobi equation in the skeletonization has been suggested. A complete solution [14, 15]  $\phi(\mathbf{q}, \mathbf{P}, t)$  ( $\mathbf{P}'$  are  $n$  integration constants) can be regarded as the generator of a canonical transformation:  $\mathbf{p} = \partial\phi/\partial\mathbf{q}$ ,  $\mathbf{Q} = \partial\phi/\partial\mathbf{P}$ , where  $(\mathbf{Q}, \mathbf{P})$  is a set of classically conserved variables. Then  $d\phi = \mathbf{p} \cdot d\mathbf{q} + \mathbf{Q} \cdot d\mathbf{P} - H dt$ , and  $\Delta\phi_{\mathbf{P}} \equiv \phi(\mathbf{q}'', \mathbf{P}, t'') - \phi(\mathbf{q}', \mathbf{P}, t')$  coincides with the canonical functional action evaluated along a path such that  $\mathbf{P} = \text{const}$ . Besides,  $\Delta\phi_{\mathbf{P}}$  is stationary when  $\mathbf{P}$  has the value corresponding to the classical path joining  $(\mathbf{q}', t')$  and  $(\mathbf{q}'', t'')$ ; in that case  $\Delta\phi_{\mathbf{P}}$  turns out to be the Hamilton principal function [15]. These properties could make  $\Delta\phi_{\mathbf{P}}$  a candidate to take part in the skeletonization  $S(\{\mathbf{q}_k, \mathbf{p}_k, t_k\})$ .

But in order to obtain the propagator, some requirements concerned with the behaviour at short times and the character of the substitution  $\mathbf{p} \rightarrow \mathbf{P}$ —which must be well defined in all phase space—should be fulfilled by the complete solution to be chosen. In addition, the canonical coordinates and momenta should enter the skeletonization on an equal footing.

The rest of this paper is devoted to emphasizing the role played in phase-space path integration by two related complete solutions of the Hamilton–Jacobi equation, which will be called the Jacobi principal functions. In section 2 a scheme of skeletonization putting canonical coordinates and momenta on an equal footing suggests the initial condition that must be fulfilled by the complete solutions to be used. In section 3 the infinitesimal propagator induced by the path integration is obtained once the measure is worked up into a form that gives the same status to both arguments in the propagator. Section 4 explains how to treat a classical system with an arbitrary potential, in order to get the result (4) for the infinitesimal propagator. Section 5 shows the ordering for the Hamiltonian operator that is induced by the propagator of section 3. The conclusions are displayed in section 6.

## 2. Skeletonization in phase space: the Jacobi principal function

In order to introduce a skeletonization procedure treating coordinates and momenta on an equal footing, one should define a recipe joining classical pieces determined by mixed boundaries  $(\mathbf{q}_k, \mathbf{p}_{k+1})$  or  $(\mathbf{p}_k, \mathbf{q}_{k+1})$ . Then a path  $\mathbf{q}(t)$ ,  $\mathbf{p}(t)$  should be skeletonized by alternately giving the values of canonical coordinates and momenta at each  $t_k$ , and replacing the canonical functional action by something like

$$S(\{\mathbf{q}_k, \mathbf{p}_k, t_k\}) = \sum_{k=0}^{(N-2)/2} \{J(\mathbf{q}_{2k+2}t_{2k+2}|\mathbf{p}_{2k+1}t_{2k+1}) + J(\mathbf{p}_{2k+1}t_{2k+1}|\mathbf{q}_{2k}t_{2k})\}. \quad (7)$$

The building blocks  $J(\mathbf{q}t'|\mathbf{p}t)$  and  $J(\mathbf{p}t'|\mathbf{q}t)$  should be functions associated with the classical system, making the skeletonized action stationary on the classical path in phase space. A

comparison with equation (3) suggests that the stationary condition

$$\frac{\partial}{\partial \mathbf{p}_{2k+1}} J(\mathbf{q}_{2k+2} t_{2k+2} | \mathbf{p}_{2k+1} t_{2k+1}) + \frac{\partial}{\partial \mathbf{p}_{2k+1}} J(\mathbf{p}_{2k+1} t_{2k+1} | \mathbf{q}_{2k} t_{2k}) = 0 \quad \forall k \quad (8)$$

should mean that the final canonical coordinates of the classical piece between  $t_{2k}$  and  $t_{2k+1}$  coincides with the initial canonical coordinates of the classical piece between  $t_{2k+1}$  and  $t_{2k+2}$ . Once the stationary value for the momenta is replaced in equation (7), the skeletonization should go to the one of equation (2), so guaranteeing the continuity of both  $\mathbf{q}$  and  $\mathbf{p}$  at  $t_{2k+1}$ .

If the system exhibits invariance under a general coordinate change, then the skeletonization and the measure must preserve that invariance, in order that the quantization is independent of the chosen coordinates. Therefore both  $J$  in equation (7) should be invariant.

We are going to define  $\partial J / \partial \mathbf{p}$  to be the coordinate canonically conjugated to  $\mathbf{p}$ ; so we should look for coordinates transforming contravariantly to  $\mathbf{p}$ . We will assume that the configuration space is a Riemannian manifold  $\mathcal{M}$ ; thus, normal coordinates—which transform like the components of a vector at the origin of coordinates—could be introduced<sup>†</sup>. Let us choose a point  $O \in \mathcal{M}$  as the origin of normal coordinates. Let  $\{e_a\}$  be a basis for the tangent space  $T_O$  at  $O$ . To assign normal coordinates to a point  $P$ , consider the geodesic joining  $O$  and  $P$ <sup>‡</sup> and define  $\sigma = s\mathbf{u}$ , where  $s = \int \sqrt{g_{ij} dq^i dq^j}$  is the (invariant) length of the geodesic between  $O$  and  $P$ , and  $\mathbf{u} \in T_O$  is the unitary vector tangent to the geodesic at  $O$ . The components  $\sigma^a(q^j)$  of the vector  $\sigma \in T_O$  are normal coordinates for  $P$  [16]. By differentiating the invariant Hamilton principal function with respect to the normal coordinates of the (initial) final boundary, one gets the (initial) final momenta  $(-)$   $p_a = \partial S / \partial \sigma^a$ ; thus  $p_a$  are the components of a form  $\mathbf{p} = p_a e^a \in T_O^*$ . The set of canonically conjugated variables  $\{(\sigma^a, p_a)\}$  is invariant under changes  $q^j \rightarrow q^{j'}$ ;  $(\sigma^a, p_a)$  only change under changes of the basis  $\{e_a\}$  in  $T_O$  (and its dual basis  $\{e^a\}$  in  $T_O^*$ ).

Now we will introduce two invariant Legendre transforms of the Hamilton principal function  $S(\mathbf{q}'' t'' | \mathbf{q}' t')$ :

$$J(\mathbf{q}'' t'' | \mathbf{p}' t') \equiv \left( S - \frac{\partial S}{\partial \sigma'^a} \sigma'^a \right)_{p'_a = -\partial S / \partial \sigma'^a} \quad (9)$$

and

$$J(\mathbf{p}'' t'' | \mathbf{q}' t') \equiv \left( S - \frac{\partial S}{\partial \sigma''^a} \sigma''^a \right)_{p''_a = \partial S / \partial \sigma''^a} \quad (10)$$

that will be called *Jacobi principal functions*. They can be regarded as the evaluation on the classical trajectory of a functional action that has been added with surface terms to make it stationary under variations with mixed boundaries left fixed.

In spite of their definition in terms of the Legendre transform interchanging  $\sigma^a$  and  $p_a$ , the Jacobi principal functions can be written, if preferred, as functions of a different set of canonical coordinates connected with the normal ones by means of a canonical point transformation

$$q^j = q^j(\sigma^a) \quad p_j = \frac{\partial \sigma^a}{\partial q^j} p_a.$$

The  $p_j$  transform like the components of a form  $\mathbf{p} \in T_p^*$  on the coordinate basis.

From the properties of the Legendre transform, one easily gets that  $J(\mathbf{q}'' t'' | \mathbf{p}' t')$  and  $-J(\mathbf{p}'' t'' | \mathbf{q}' t')$  generate contact transformations:

$$p''_j = \frac{\partial J(\mathbf{q}'' t'' | \mathbf{p}' t')}{\partial q''^j} \quad \sigma'^a = \frac{\partial J(\mathbf{q}'' t'' | \mathbf{p}' t')}{\partial p'_a}. \quad (11)$$

<sup>†</sup> Actually, only a connection is needed to define normal coordinates.

<sup>‡</sup> We assume a global topology such that any pair of points is joined by a unique geodesic.

and

$$\sigma''^a = -\frac{\partial J(\mathbf{p}''t''|\mathbf{q}'t')}{\partial p''_a} \quad p'_j = -\frac{\partial J(\mathbf{p}''t''|\mathbf{q}'t')}{\partial q'^j}. \quad (12)$$

When  $t'' = t'$  they generate the identity

$$J(\mathbf{q}t|\mathbf{p}t) = p_a \sigma^a(q^j) \quad (13)$$

$$J(\mathbf{p}t|\mathbf{q}t) = -p_a \sigma^a(q^j). \quad (14)$$

$J(\mathbf{q}''t''|\mathbf{p}'t')$  and  $-J(\mathbf{p}''t''|\mathbf{q}'t')$  are complete solutions of the Hamilton–Jacobi equation in both arguments (take  $\partial/\partial t''$  and  $\partial/\partial t'$  in equations (9) and (10), and use equations (11) and (12)):

$$\frac{\partial J(\mathbf{q}''t''|\mathbf{p}'t')}{\partial t''} = -H\left(q^j, \frac{\partial J}{\partial q^j}, t''\right) \quad \frac{\partial J(\mathbf{q}''t''|\mathbf{p}'t')}{\partial t'} = H\left(\sigma^a = \frac{\partial J}{\partial p_a}, p_j, t'\right) \quad (15)$$

$$-\frac{\partial J(\mathbf{p}''t''|\mathbf{q}'t')}{\partial t''} = H\left(\sigma^a = -\frac{\partial J}{\partial p_a}, p_j, t''\right) \quad \frac{\partial J(\mathbf{p}''t''|\mathbf{q}'t')}{\partial t'} = H\left(q^j, -\frac{\partial J}{\partial q^j}, t'\right). \quad (16)$$

By changing  $t'' \longleftrightarrow t'$  in equations (15) and (16) one realizes that

$$J(\mathbf{p}''t''|\mathbf{q}'t') = -J(\mathbf{q}'t'|\mathbf{p}''t''). \quad (17)$$

If the system is conservative, then the Jacobi principal functions depend on  $t''$  and  $t'$  only through the difference  $t'' - t'$ . Therefore,  $J(\mathbf{q}'t'|\mathbf{p}''t'') = J(\mathbf{q}, \mathbf{p}, \tau \equiv \Delta t)$ , and the pieces of the skeletonized action (7) have the form

$$J(\mathbf{q}_{2k+2}t_{2k+2}|\mathbf{p}_{2k+1}t_{2k+1}) + J(\mathbf{p}_{2k+1}t_{2k+1}|\mathbf{q}_{2k}t_{2k}) = J(\mathbf{q}_{2k+2}, \mathbf{p}_{2k+1}, \tau_{2k+1}) - J(\mathbf{q}_{2k}, \mathbf{p}_{2k+1}, -\tau_{2k}). \quad (18)$$

Thus the skeletonization (7) gets the form  $\Delta\phi_{\mathcal{P}}$  proposed in [13], although a specific complete solution of the Hamilton–Jacobi equation is being used here.

Even for a nonconservative system, the short-time limit of the skeletonization (7) is

$$\begin{aligned} & J(\mathbf{q}_{2k+2}t_{2k+2}|\mathbf{p}_{2k+1}t_{2k+1}) + J(\mathbf{p}_{2k+1}t_{2k+1}|\mathbf{q}_{2k}t_{2k}) \\ & \simeq [p_{a2k+1}\sigma^a_{2k+2} - H(\sigma^a_{2k+2}, p_{j2k+1}, t_{2k+1})\Delta t_{2k+1}] \\ & - [p_{a2k+1}\sigma^a_{2k} + H(\sigma^a_{2k}, p_{j2k+1}, t_{2k+1})\Delta t_{2k}]. \end{aligned} \quad (19)$$

On any smooth path it is valid that  $\sigma^a_{2k+2} \rightarrow \sigma^a_{2k}$  when  $t_{2k+2} \rightarrow t_{2k}$ . Thus the skeletonized action goes to the canonical functional action:

$$\begin{aligned} & J(\mathbf{q}_{2k+2}t_{2k+2}|\mathbf{p}_{2k+1}t_{2k+1}) + J(\mathbf{p}_{2k+1}t_{2k+1}|\mathbf{q}_{2k}t_{2k}) \longrightarrow p_{a2k+1}(\sigma^a_{2k+2} - \sigma^a_{2k}) \\ & - H(\sigma^a_{2k}, p_{j2k+1}, t_{2k+1})(t_{2k+2} - t_{2k}). \end{aligned} \quad (20)$$

The skeletonization scheme proposed in this section is based on a pair of complete solutions of the Hamilton–Jacobi equation (in both arguments) that treat canonical coordinates  $\sigma^a$  and momenta  $p_a$  on an equal footing; this fact is evident in the initial conditions (13) and (14). The Jacobi principal functions do not depend on the chart  $\{q^j\}$  or on the basis of the tangent space at  $O$ . They do depend on the way the configuration space has been cut from the phase space (the quantum propagation is not invariant under arbitrary canonical transformations).

### 3. The propagator

In order to give sense to the functional integration in phase space

$$K(\mathbf{q}''t''|\mathbf{q}'t') = \int \mathcal{D}\mathbf{p}(t)\mathcal{D}\mathbf{q}(t) \exp\left[\frac{i}{\hbar}S[\mathbf{q}(t), \mathbf{p}(t)]\right] \quad (21)$$

our attention must now turn to the measure. Since the functional action is going to be replaced by an invariant skeletonized version, the ‘magical’ measure  $\mathcal{D}\mathbf{p}(t)\mathcal{D}\mathbf{q}(t)$  should also be consequently replaced by a measure in the space of the variables  $\{\mathbf{q}_{2k}, \mathbf{p}_{2k+1}\}$ . This measure must be able to retain the geometrical behaviour of the propagator, which is apparent in the manner of propagating the wavefunction:

$$\Psi(\mathbf{q}'', t'') = \int d\mathbf{q}' K(\mathbf{q}''t''|\mathbf{q}'t')\Psi(\mathbf{q}', t'). \quad (22)$$

If the wavefunction  $\Psi$  is regarded as scalar, then the propagator should be invariant in its final argument but a density in its initial argument. However, a scalar wavefunction would compel us to use an invariant measure  $\mu(\mathbf{q}) d\mathbf{q}$  in the inner product of the Hilbert space (the density  $\mu$  would be ultimately dictated by the result of the path integration [9]). So it may be more convenient to regard the wavefunction as a density of weight  $\frac{1}{2}$ . In this case the inner product of the Hilbert space is

$$(\Psi, \Phi) = \int d\mathbf{q}\Psi^*\Phi \quad (23)$$

whatever the generalized coordinates describing the system are. Thus the propagator in equation (22) must be a density of weight  $\frac{1}{2}$  in both arguments.

The issue of the measure can be studied at the level of an infinitesimal propagator. In fact, due to the composition law

$$K(\mathbf{q}''t''|\mathbf{q}'t') = \int d\mathbf{q}_{N-1} K(\mathbf{q}''t''|\mathbf{q}_{N-1}t_{N-1}) K(\mathbf{q}_{N-1}t_{N-1}|\mathbf{q}_{N-2}t_{N-2}) \dots \\ \dots d\mathbf{q}_2 K(\mathbf{q}_2t_2|\mathbf{q}_1t_1) d\mathbf{q}_1 K(\mathbf{q}_1t_1|\mathbf{q}'t') \quad (24)$$

—which holds whenever the added paths go forward in time—the finite propagator can be retrieved by composing infinitesimal propagators. If  $t'' - t' = \varepsilon$  is infinitesimal, then one should only integrate  $\mathbf{p}$  at some intermediate time  $t$ . However the measure  $d\mathbf{p}^{(t)}$  does not allow for a propagator behaving like a density in its arguments  $\mathbf{q}'$  and  $\mathbf{q}''$ . The use of  $d^n p'_j = \left| \det \frac{\partial p'_j}{\partial p_a^{(t)}} \right| d^n p_a^{(t)}$  instead of  $d\mathbf{p}^{(t)}$  is suitable when the wavefunction is regarded as a scalar, because the propagator will result a density in  $\mathbf{q}'$ . However, if the propagator has to be a density of weight  $\frac{1}{2}$  in both arguments, then the Jacobian in the previous measure must be split into two factors that will give an equal weight to  $\mathbf{p}'$  and  $\mathbf{p}''$ :

$$\left| \det \frac{\partial p''_j}{\partial p_a^{(t)}} \right|^{1/2} d^n p_a^{(t)} \left| \det \frac{\partial p'_j}{\partial p_a^{(t)}} \right|^{1/2} = \left| \det \left( \frac{\partial^2 J(\mathbf{q}''t''|\mathbf{p}t)}{\partial q''^j \partial p_a} \right) \right|^{1/2} \\ \times d^n p_a^{(t)} \left| \det \left( -\frac{\partial^2 J(\mathbf{p}t|\mathbf{q}'t')}{\partial q'^j \partial p_a} \right) \right|^{1/2}. \quad (25)$$

Concretely, the infinitesimal propagator has the form

$$K(\mathbf{q}''t'' = t' + \varepsilon|\mathbf{q}'t') = \int \frac{d^n p_a}{(2\pi\hbar)^n} \left| \det \frac{\partial^2 J(\mathbf{q}''t''|\mathbf{p}t)}{\partial q''^j \partial p_a} \right|^{1/2} \left| \det -\frac{\partial^2 J(\mathbf{p}t|\mathbf{q}'t')}{\partial p_a \partial q'^j} \right|^{1/2} \\ \times \exp\left[\frac{i}{\hbar}(J(\mathbf{q}''t''|\mathbf{p}t) + J(\mathbf{p}t|\mathbf{q}'t'))\right] \quad (26)$$

where  $t$  is prescribed to be the mid time:  $t \equiv t' + (\epsilon/2) = t'' - (\epsilon/2)$ . When  $\epsilon = 0$ , one gets the orthonormality relation between eigenstates of the operator  $\hat{q}$  (see equations (13) and (14)).

Since canonical coordinates and momenta were treated on an equal footing, one realizes that the propagator in the  $p_a$ -representation which is consistent with equation (26) is

$$\begin{aligned} \mathcal{K}(p''t'' = t' + \epsilon|p't') &= \int \frac{d^n q^j}{(2\pi\hbar)^n} \left| \det -\frac{\partial^2 J(p''t''|qt)}{\partial p''_a \partial q^j} \right|^{1/2} \left| \det \frac{\partial^2 J(qt|p't')}{\partial q^j \partial p'_a} \right|^{1/2} \\ &\times \exp \left[ \frac{i}{\hbar} (J(p''t''|qt) + J(qt|p't')) \right]. \end{aligned} \tag{27}$$

It will become clear in section 5 that the prescription of mid time in equations (26) and (27) together with the splitting of the Jacobian, guarantee the hermiticity of the Hamiltonian operator and the unitarity of the evolution.

#### 4. Classical systems

To illustrate the use of equation (26), let us consider a one-dimensional classical system governed by the Hamiltonian:

$$H = \frac{p^2}{2m} + V(q). \tag{28}$$

We will show how to manage the integration in equation (26) in order to get the infinitesimal propagator in the form of equation (4).

Since the metric in the Hamiltonian is a standard Euclidean metric ( $g^{ij} = \delta^{ij}$ ), the coordinate  $q$  is the normal coordinate. The Jacobi principal function  $J(q, p, \tau)$  can be guessed by writing

$$J(q, p, \tau) = pq - \frac{p^2}{2m} \tau + \sum_{l=1}^{\infty} J_l(q, p) \tau^l. \tag{29}$$

Then one solves the Hamilton–Jacobi equation order by order in  $\tau$ , and obtains

$$\begin{aligned} J_1 &= -V(q) \\ J_2 &= \frac{pV'(q)}{2m} \\ J_3 &= -\frac{p^2V''(q)}{6m^2} - \frac{V'(q)^2}{6m} \\ J_4 &= \frac{p^3V'''(q)}{24m^3} + \frac{5}{24} \frac{p}{m^2} V'(q)V''(q) \\ J_5 &= -\frac{1}{120} \frac{p^4}{m^4} V''''(q) - \frac{1}{15} \frac{p^2V''(q)^2}{m^3} - \frac{3}{40} \frac{p^2V'(q)V'''(q)}{m^3} - \frac{1}{15} \frac{V'(q)^2V''(q)}{m^2}. \end{aligned} \tag{30}$$

The recurrence formulae is

$$J_{l+1} = -\frac{1}{2(l+1)m} \sum_{k=0}^l \frac{\partial J_k}{\partial q} \frac{\partial J_{l-k}}{\partial q} \quad l \geq 1 \tag{31}$$

where  $J_0 \equiv pq$ . Each  $J_l$  is polynomial in  $p$ . Let us concentrate on the higher degree contributions; their addition is

$$-\sum_{l=1}^{\infty} \frac{1}{l!} \left(-\frac{p}{m}\right)^{l-1} V^{(l-1)}(q) \tau^l = \frac{m}{p} \int_q^{q-p\tau/m} V(q) dq. \tag{32}$$



We are going to replace this result, and  $\partial^2 J/\partial q \partial p = 1 + \mathcal{O}(\epsilon^2)$ , in the integrand of equation (26). After the substitution  $p \rightarrow P \equiv p\epsilon/(2m)$ , one gets

$$K(q''t'' = t' + \epsilon|q't') = \left(\frac{m}{\pi\hbar\epsilon}\right) \exp\left[\frac{im(\Delta q)^2}{2\hbar\epsilon}\right] \left\{ \int dP \exp\left[-\frac{i2m}{\hbar\epsilon}\left(P - \frac{\Delta q}{2}\right)^2 - \frac{i\epsilon}{2\hbar P} \left( \int_{q''-P}^{q''} V(q) dq + \int_{q'}^{q'+P} V(q) dq \right) + \dots \right] + \mathcal{O}(\epsilon^2) \right\}. \quad (33)$$

The contribution of the potential to the phase will be expanded about  $P = \Delta q/2$ :

$$\frac{1}{2P} \left( \int_{q''-P}^{q''} V(q) dq + \int_{q'}^{q'+P} V(q) dq \right) = \bar{V} - \frac{2}{\Delta q} \Delta \bar{V} \left( P - \frac{\Delta q}{2} \right) + \frac{4}{(\Delta q)^2} \Delta \bar{V} \left( P - \frac{\Delta q}{2} \right)^2 + \dots \quad (34)$$

where

$$\bar{V} \equiv \frac{1}{\Delta q} \int_{q'}^{q''} V(q) dq \quad \Delta \bar{V} \equiv \bar{V} - V\left(\frac{q' + q''}{2}\right). \quad (35)$$

Those contributions that were not explicitly written in equation (33) can be controlled by means of the result [17]

$$\int dx x^{2\gamma} \exp\left[-\frac{i2m}{\hbar\epsilon}x^2\right] \propto \left(\frac{\hbar\epsilon}{2m}\right)^{\gamma+\frac{1}{2}}. \quad (36)$$

Then the leading contribution to the integration (26) is

$$K(q''t'' = t' + \epsilon|q't') = \sqrt{\frac{m}{2i\pi\hbar\epsilon}} \exp\left[\frac{i}{\hbar} \left( \frac{m(\Delta q)^2}{2\epsilon} - \frac{\epsilon}{\Delta q} \int_{q'}^{q''} V(q) dq \right)\right]. \quad (37)$$

The infinitesimal propagator (37) has the form (4). In fact the phase in equation (37) solves the Hamilton–Jacobi equation in each argument at order  $\epsilon$  (for all values of  $q'$  and  $q''$ )<sup>†</sup>. The Schrödinger equation is satisfied at the lowest order in  $\hbar\epsilon/m$ .

## 5. Operator ordering

Each recipe to path integrate implies an operator ordering for the Hamiltonian in the wave equation. Our interest in this section is to find the operator ordering associated with the infinitesimal propagator (26). Let us derive equation (26) with respect to  $\epsilon$ , at  $\epsilon = 0$ :

$$i\hbar \frac{\partial}{\partial \epsilon} K(q''t'' + \epsilon|q't') \Big|_{\epsilon=0} = \int \frac{dp}{2\pi\hbar} \exp\left[\frac{i}{\hbar} p \Delta \sigma\right] \times \left\{ \frac{i\hbar}{4} \left( -\frac{\partial^2 H(q'', p)}{\partial q'' \partial p} + \frac{\partial^2 H(q', p)}{\partial q' \partial p} \right) + \frac{1}{2} (H(q'', p) + H(q', p)) \right\} \quad (38)$$

where the short-time approximation (19) has been used.

Equation (38) is linear in  $H$ . If  $H$  can be expanded in a power series, then it will be sufficient to handle the ordering for a Hamiltonian

$$H = q^m p^k. \quad (39)$$

<sup>†</sup> Although the phase in equation (37) has the merit of being a complete solution of the Hamilton–Jacobi equation at order  $\epsilon$ —it is the Hamilton principal function at that order—the integration on  $q$  in the composition of infinitesimal propagators (equation (24)) will be not sensitive to a replacement of  $\bar{V}$  by  $V((q'' + q')/2)$ , or  $(V(q') + V(q''))/2$ , etc. as a consequence of the result (36).

If  $q$  is a normal coordinate, then

$$i\hbar \frac{\partial}{\partial \epsilon} K(q''t' + \epsilon|q't') \Big|_{\epsilon=0} = \int \frac{dp}{2\pi\hbar} \exp \left[ \frac{i}{\hbar} p \Delta q \right] \times \left\{ \frac{i\hbar km}{4} p^{k-1} (-q''^{m-1} + q'^{m-1}) + \frac{p^k}{2} (q''^m + q'^m) \right\}. \quad (40)$$

Taking into account equation (22),

$$\begin{aligned} \hat{H}\Psi(q'', 0) &= \int \frac{dq' dp}{2\pi\hbar} \exp \left[ \frac{i}{\hbar} p \Delta q \right] \\ &\quad \times \left\{ \frac{i\hbar km}{4} p^{k-1} (-q''^{m-1} + q'^{m-1}) + \frac{p^k}{2} (q''^m + q'^m) \right\} \Psi(q', 0) \\ &= -q''^{m-1} \frac{i\hbar km}{4} \left( \frac{\hbar}{i} \frac{\partial}{\partial q''} \right)^{k-1} \int \frac{dq' dp}{2\pi\hbar} \exp \left[ \frac{i}{\hbar} p \Delta q \right] \Psi(q', 0) \\ &\quad + \frac{i\hbar km}{4} \left( \frac{\hbar}{i} \frac{\partial}{\partial q''} \right)^{k-1} \int \frac{dq' dp}{2\pi\hbar} q'^{m-1} \exp \left[ \frac{i}{\hbar} p \Delta q \right] \Psi(q', 0) \\ &\quad + \frac{1}{2} q''^m \left( \frac{\hbar}{i} \frac{\partial}{\partial q''} \right)^k \int \frac{dq' dp}{2\pi\hbar} \exp \left[ \frac{i}{\hbar} p \Delta q \right] \Psi(q', 0) \\ &\quad + \frac{1}{2} \left( \frac{\hbar}{i} \frac{\partial}{\partial q''} \right)^k \int \frac{dq' dp}{2\pi\hbar} q'^m \exp \left[ \frac{i}{\hbar} p \Delta q \right] \Psi(q', 0) \\ &= \frac{i\hbar km}{4} [\hat{p}^{k-1}, \hat{q}^{m-1}] \Psi(q'', 0) + \frac{1}{2} (\hat{p}^k \hat{q}^m + \hat{q}^m \hat{p}^k) \Psi(q'', 0). \end{aligned} \quad (41)$$

This means that the Hamiltonian operator is

$$\hat{H} = \frac{1}{2} (\hat{p}^k \hat{q}^m + \hat{q}^m \hat{p}^k) + \frac{i\hbar km}{4} [\hat{p}^{k-1}, \hat{q}^{m-1}]. \quad (42)$$

The operator  $\hat{H}$  is Hermitian thanks to the mid time prescription in section 3, which gave an equal weight to the terms depending on  $q'$  and  $q''$  in equation (38).

## 6. Conclusions

We have proposed a scheme to path integrate in phase space, which is applicable to Hamiltonian systems whose configuration space is a manifold where normal coordinates (i.e., coordinates behaving like the components of a vector in the tangent space at the origin) can be introduced. The skeletonization is based on the invariant Jacobi principal functions —those related with the variational principles of mechanics for mixed boundaries left fixed—and the measure gives to the propagator the character of a density of weight  $\frac{1}{2}$  in each argument. The so obtained infinitesimal propagators (26) and (27) naturally satisfy the Schrödinger equation, once the Hamiltonian operator is build in agreement with the operator ordering (42) induced by the path integral recipe.

The infinitesimal propagators (26) and (27) can be read in terms of the modes

$$\mathcal{F}_p(q^j, t) \equiv \left[ \det \left( \frac{1}{2\pi\hbar} \frac{\partial^2 J(\mathbf{q}, \mathbf{p}, t)}{\partial q^j \partial p_a} \right) \right]^{1/2} \exp \left[ \frac{i}{\hbar} J(\mathbf{q}, \mathbf{p}, t) \right] \quad (43)$$

which are well behaved on all phase space at short times (the matrix  $\partial^2 J / \partial q^j \partial p_a$  is not singular because the relation between initial and final momenta is bi-univoque at short times). At  $t = 0$  these modes are eigenfunctions of the momenta  $\hat{p}_a = -i\hbar \partial / \partial \sigma^a$  based at the

origin  $O$ , because of the boundary condition  $J(\mathbf{q}, \mathbf{p}, t = 0) = p_a \sigma^a$ . Therefore,  $\mathcal{F}_p(q^j, t)$  is a short-time approximation for  $\langle q^j | \hat{U}(t) | p_a \rangle$ , and  $\{\mathcal{F}_p\}$  is a basis of short-time solutions of the Schrödinger equation whatever the Hamiltonian system is. A change of the origin  $O$  implies a change of the basis  $\{\mathcal{F}_p\}$ ; of course, all bases  $\{\mathcal{F}_p\}$  are equally good for expanding the propagator.

For free systems it is  $J(\mathbf{q}, \mathbf{p}, t) = p_a \sigma^a - H(p_a)t$ , and the modes (43) are certainly exact solutions of the Schrödinger equation. They span the basis of eigenstates of the (conserved) momenta  $\hat{p}_a$ . In this case the propagator (26) is exact (i.e., it is the finite propagator). In particular, the Newton–Wigner propagator (5) for the relativistic particle— $H(p) = (p^2 + m^2)^{1/2}$ —can be obtained by integrating on the momenta in equation (26) [9].

In the case of the classical system of section 4, the modes  $\mathcal{F}_p$  satisfy the equation (use equation (15))

$$\left( i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} - V(q) \right) \mathcal{F}_p = \frac{\hbar^2}{2m} \left( \frac{\partial^2 J}{\partial q \partial p} \right)^{-1/2} \frac{\partial^2}{\partial q^2} \left[ \left( \frac{\partial^2 J}{\partial q \partial p} \right)^{1/2} \right] \mathcal{F}_p. \quad (44)$$

This equation is typical for any phase  $J$  being a solution of the Hamilton–Jacobi equation, and is commonly used to highlight the semiclassical character ( $\hbar \rightarrow 0$ ) of wavefunctions having the form (43). However, as was already stated, the Jacobi principal function  $J(\mathbf{q}, \mathbf{p}, t)$  confers an additional property to the modes (43)—which is the one exploited in this paper—and allows a different reading of equation (44): the modes  $\mathcal{F}_p$  are short-time solutions of the Schrödinger equation, for any value of  $\hbar$ . In fact, the results in section 4 show us that the rhs in equation (44) is zero for a quadratic potential<sup>†</sup> ( $\mathcal{F}_p$  is an exact solution),  $\hbar^2 t^4 / (8m^3) (V''')^2 \mathcal{F}_p + \mathcal{O}(t^5)$  for a cubic potential, and  $\hbar^2 t^2 / (8m^2) V'''' \mathcal{F}_p + \mathcal{O}(t^3)$  in a more general case.

The substitution of the functional action by a skeletonized version in the discrete-time approximation is one of the ways to give a meaning to the functional integration (1). A different approach to the same problem is the operator symbol method [18], where the path integral results from the product of the *symbols* associated with the short-time evolution operator. The product of symbols involves an integration containing the information about the operator ordering, which amounts to the prescription of the skeletonization in phase space. The different rules to generate the ordering for the quantum operator  $\hat{g}$  associated with a function  $g(q, p)$  in phase space, can be summarized as follows [19]:

$$\hat{g} \longleftrightarrow f \left( -i \frac{\partial}{\partial q}, -i \frac{\partial}{\partial p} \right) \exp \left( -\frac{i\hbar}{2} \frac{\partial^2}{\partial q \partial p} \right) g(q, p) \quad (45)$$

where  $\hat{g}$  in equation (45) is the normal form of the operator (the power series expansion where the  $q$  precede the  $p$ ), and  $f(u, v)$  contains the information about the ordering. Some well known rules of ordering are shown in table 1 [20].

The Weyl ordering is equivalent to a skeletonization where the Hamiltonian is evaluated in  $(q'' + q')/2$ . The symmetric ordering corresponds to replace the Hamiltonian by  $[H(q'', p) + H(q', p)]/2$  [21]. In this sense, the skeletonization prescribed in this paper seems to be related with the symmetrization rule (see equation (19)). Effectively, the ordering (42) for the normal coordinates and their conjugated momenta begins with a symmetrized contribution coming from the mean Hamiltonian in equation (38). However, our prescription includes a nontrivial measure (the Jacobians in equation (25)), which is needed in order that the wavefunction retains its condition of being a density of weight  $\frac{1}{2}$ . This measure is responsible for the second term

<sup>†</sup> If  $V(q) = m\omega^2 q^2/2$ , the Jacobi principal function is  $J(q, p, t) = -p^2 \tan(\omega t)/(2m\omega) + qp/\cos \omega t - m\omega q^2 \tan(\omega t)/2$ . Thus  $J(q, p, t)$  reflects the equivalent roles of  $q$  and  $p$  in both the initial condition and the Hamiltonian.

**Table 1.**

Name	$f(u, v)$	$g(q, p) = q^m p^k$
Standard	$\exp[\frac{1}{2}\hbar uv]$	$\hat{q}^m \hat{p}^k$
Anti-standard	$\exp[-\frac{1}{2}\hbar uv]$	$\hat{p}^k \hat{q}^m$
Symmetric	$\cos[\frac{1}{2}\hbar uv]$	$\frac{1}{2}(\hat{q}^m \hat{p}^k + \hat{p}^k \hat{q}^m)$
Weyl	1	$\frac{1}{2^m} \sum_{l=0}^m \binom{m}{l} \hat{q}^{m-l} \hat{p}^k \hat{q}^l$
Born–Jordan	$2(\hbar uv)^{-1} \sin[\frac{1}{2}\hbar uv]$	$\frac{1}{k+1} \sum_{l=0}^k \hat{p}^{k-l} \hat{q}^m \hat{p}^l$

in the ordering (42). Thus the function  $f(u, v)$  associated with the ordering (42) is

$$f(u, v) = \cos[\frac{1}{2}\hbar uv] + \frac{1}{2}\hbar uv \sin[\frac{1}{2}\hbar uv]. \tag{46}$$

Naturally  $f$  fulfills the requirements

$$\lim_{\hbar \rightarrow 0} f = 1 \quad \lim_{\hbar \rightarrow 0} \dot{f} = 0 \tag{47}$$

that guarantee the classical limit [19].

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