Notes on the phase space formulation of the propagator of Hamiltonians with spatially-dependent kinetic energy

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Abstract

These short notes present to the reader (students, in particular) a concise approach to the derivation of the propagator of Hamiltonians with position-dependent kinetic energy. The formalism is applied to the von Roos Hamiltonian with arbitrary ordering ambiguity parameters, and a simple scheme to convert the problem to a constant-mass motion is presented. The motion in curved spaces is treated along the same lines, where a phase space formulation is used to derive the propagator for arbitrary discretization choices.

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1 Introduction

The description of the dynamics of quantum systems is a central topic in modern physics which has attracted a great deal of interest soon after the foundations of the quantum theory have been established. In the non-relativistic domain, the basic tool that enables for a such description resides in the Schrödinger equation [1]. The latter has been extended to the relativistic domain yielding thus the Klein-Gordon and the Dirac equations [2]. Mathematically speaking, the above equations are second-order partial differential equations that may be solved exactly in some cases; this is in particular true for many potentials entering the Hamiltonian of the Schrödinger equation.

Feynman came out with another, but equivalent, formalism known as the path integral formulation of the quantum mechanics [3]. The latter concept has been successfully applied to many problems in physics, such as those in connection with field theory and condensed matter physics, to mention a few [1, 2, 6, 7]. The particular character of the path integral rests in the fact that there is no need to solve partial differential equations. Rather, one proceeds by evaluating the so-called propagator which makes it possible to link the wave function to its preceding history.

Both the operator and the path integral methods apply well to systems for which the kinetic energy part of the Hamiltonian is independent of the position. However, as soon as the dependence on the position is considered in the kinetic energy, the problem of the ordering and the discretization ambiguities immediately comes to play [3, 7]. Actually, these ambiguities are intimately related to each other since the discretization ambiguity is a mere translation of the operator ordering problem inherent to the Hamiltonian, which is a direct consequence of the non-commuting character of the operators in quantum mechanics. Among the most studied systems displaying spatial dependence in the kinetic energy, we mention the motion of particles with position dependent effective masses, and the motion in curved spaces. In particular, motivated by several applications in atomic and condensed matter physics [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 19, 20], a large number of works has been devoted to finding the solutions of the Schrödinger equation for position-dependent effective mass; in this case, one is usually interested in finding analytical results for the wave functions and the energy spectrum corresponding to different forms of the mass, the potential and the ordering ambiguity [24, 22, 23, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36]. The latter is often encoded in the general form of the Hamiltonian initially proposed by
von Roos[37].

On the other hand, some investigations have dealt with the application of the path integral formalism to the aforementioned problems[24, 22, 23, 38]. In the case of the von Roos Hamiltonian, one usually begins by adopting a particular choice of the ordering, then proceeds to derive the discretized version of the path integral. However, so far, there is no general approach that takes into account all the possible values of the ambiguity parameters in a concise and compact manner. The aim of this manuscript is to derive explicit expressions of the propagator for arbitrary values of these parameters, and to extend the investigation to the motion in curved space which turns out to be quite close to the problem of spatially-dependent mass.

The plan of the discussion is as follows: In section 2 we derive a compact formula for the action using a generalized definition of the symbol of the Hamiltonian in phase space. Section 3 is devoted to the application of the obtained result to the von Roos Hamiltonian, where we investigate different choices of the ordering parameters, and show how to reduce the propagator to that of a constant mass, generalizing thus the approach of Alhaidari. In section 4 we deal with the derivation of the propagator in curved spaces of arbitrary metrics. We end the manuscript with a brief conclusion.

2 Path integral formulation

Since our main concern is to formulate the propagator in terms of the phase space variables \( \vec{q} \) and \( \vec{p} \) corresponding to the particle in question, we associate with every operator \( A \), a symbol \( \mathcal{A}_\theta(\vec{q}, \vec{p}) \) that depends on \( \vec{q} \) and \( \vec{p} \) as follows:

\[
\langle \vec{q}_2 | A | \vec{q}_1 \rangle = \frac{1}{(2\pi \hbar)^{3/2}} \int \mathcal{A}_\theta \left( (1-\theta)\vec{q}_2 + \theta \vec{q}_1, \vec{p} \right) \langle \vec{q}_2 - \vec{q}_1 | \vec{p} \rangle d\vec{p},
\]

where \( \theta \) is a real parameter such that \( 0 \leq \theta \leq 1 \). As we shall see below, it is this parameter that enables one to account for the different discretization schemes in the (lattice) formulation of the path integral. Notice that when \( \theta = \frac{1}{2} \), we recover the Wigner transform of the operator \( A \)[39]. Moreover, it is a matter of direct calculation to show that the inverse transformation corresponding to (1) is given by

\[
\mathcal{A}_\theta(\vec{q}, \vec{p}) = (2\pi \hbar)^{3/2} \int \langle \vec{q} - \theta \vec{q}_1 | A | (1-\theta)\vec{q}_1 + \vec{q}_1 \rangle \langle \vec{q}_1 | \vec{p} \rangle d\vec{q}_1.
\]
The evolution of a non-relativistic quantum particle whose Hamiltonian is \( H \) and position is \( \mathbf{q} \), is described by its state vector \( \psi \) which satisfies the Schrödinger equation:

\[
\frac{i\hbar}{\partial t} \psi = H \psi. \tag{3}
\]

The solution of the latter equation can be formulated by means of the propagator \( K(\mathbf{q}_f, t_f; \mathbf{q}_i, t_i) \) as

\[
\psi(\mathbf{q}_f, t_f) = \int K(\mathbf{q}_f, t_f; \mathbf{q}_i, t_i)\psi(\mathbf{q}_i, t_i) d\mathbf{q}_i, \tag{4}
\]

where \( \psi(\mathbf{q}, t) = \langle \mathbf{q} | t | \psi \rangle \), and the kernel \( K(\mathbf{q}_f, t_f; \mathbf{q}_i, t_i) \) is given in terms of the time-evolution operator of the system by:

\[
K(\mathbf{q}_f, t_f; \mathbf{q}_i, t_i) = \langle \mathbf{q}_f | U(t_f, t_i) | \mathbf{q}_i \rangle. \tag{5}
\]

From here one, we assume that \( H \) does not depend explicitly on time. Then, by the Trotter formula one can write

\[
\langle \mathbf{q}_f | U(t_f, t_i) | \mathbf{q}_i \rangle = \lim_{N \to \infty} \langle q_f \rangle \left( 1 - \frac{iH}{\hbar N} (t_f - t_i) \right)^N | q_i \rangle
= \lim_{N \to \infty} \int d\mathbf{q}_{N-1} \int d\mathbf{q}_{N-2} \cdots \int d\mathbf{q}_1 T_{\mathbf{q}_f \mathbf{q}_{N-1}} T_{\mathbf{q}_{N-1} \mathbf{q}_{N-2}} \cdots T_{\mathbf{q}_1 \mathbf{q}_0}
\]

with

\[
T_{\mathbf{q}_k \mathbf{q}_{k-1}} = \langle \mathbf{q}_k | 1 - \frac{i\epsilon}{\hbar} | \mathbf{q}_{k-1} \rangle. \tag{7}
\]

In the above we have set \( \mathbf{q}_f = \mathbf{q}_N \), \( \mathbf{q}_i = \mathbf{q}_0 \), \( \epsilon = (t_f - t_i)/N \), and we have used the closure relation

\[
\int |\mathbf{q} \rangle \langle \mathbf{q}| d\mathbf{q} = 1. \tag{8}
\]

By using the transformation (1), together with the fact that

\[
\langle \mathbf{q}| \mathbf{p} \rangle = \frac{1}{(2\pi \hbar)^{3/2}} e^{\frac{i\mathbf{q} \cdot \mathbf{p}}{\hbar}}, \tag{9}
\]

we can rewrite equation (7) in the form

\[
T_{\mathbf{q}_k \mathbf{q}_{k-1}} = \frac{1}{(2\pi \hbar)^{3}} \int d\mathbf{p}_{k-1} e^{\frac{i}{\hbar}(\mathbf{q}_k - \mathbf{q}_{k-1}) \cdot \mathbf{p}_{k-1}} \left( 1 - \frac{i\epsilon}{\hbar} \mathcal{H}_0 ((1 - \theta) \mathbf{q}_k + \theta \mathbf{q}_{k-1}, \mathbf{p}_{k-1}) \right). \tag{10}
\]
Since $\epsilon$ is a very small quantity (in the end we shall take the limit $N \to \infty$) we can ascertain that

$$T_{\vec{q}_k \vec{q}_{k-1}} \approx \frac{1}{(2\pi \hbar)^3} \int d\vec{p}_{k-1} \exp\left\{\frac{i \epsilon}{\hbar} \left[\left(\frac{\vec{q}_k - \vec{q}_{k-1}}{\epsilon}\right)\vec{p}_{k-1} - \mathcal{H}_\theta\left((1-\theta)\vec{q}_k + \theta \vec{q}_{k-1}, \vec{p}_{k-1}\right)\right]\right\}. \quad (11)$$

It follows that the propagator can be expressed as

$$\langle \vec{q}_f | U(t_f, t_i) | \vec{q}_i \rangle = \lim_{N \to \infty} \int \int d\vec{q}_N d\vec{p}_N \int \int d\vec{q}_{N-2} d\vec{p}_{N-2} \cdots \int \int d\vec{q}_1 d\vec{p}_1 \left(2\pi \hbar\right)^3 \exp\left\{\frac{i \epsilon}{\hbar} \sum_{k=0}^{N-1} \left[\left(\frac{\vec{q}_{k+1} - \vec{q}_{k}}{\epsilon}\right)\vec{p}_k - \mathcal{H}_\theta\left((1-\theta)\vec{q}_k + \theta \vec{q}_{k-1} + \partial \vec{q}_{k+1}, \vec{p}_k\right)\right]\right\}. \quad (12)$$

One can clearly notice that the discretization is encoded in the value of the parameter $\theta$: When $\theta = 0$, we obtain a path integral with the postpoint discretization, whereas when $\theta = \frac{1}{2}$, we get a path integral with the midpoint discretization; the case $\theta = 1$ yields a prepoint discretization.

We can now put the propagator in a compact form as follows:

$$K(\vec{q}_f, t_f; \vec{q}_i, t_i) = \int \mathcal{D}\vec{q} \left(2\pi \hbar\right)^3 \exp\left\{\frac{i}{\hbar} \int_{t_i}^{t_f} dt (\vec{p} \dot{\vec{q}} - \mathcal{H}_\theta(\vec{q}, \vec{p}))\right\}. \quad (13)$$

The latter propagator describes the motion of a particle whose action in the phase space is given by

$$S = \int_{t_i}^{t_f} dt (\vec{p} \dot{\vec{q}} - \mathcal{H}_\theta(\vec{q}, \vec{p})). \quad (14)$$

Hence it suffices to determine the explicit form of the phase space function $\mathcal{H}_\theta$ in order to find the expression of the propagator $K$. In the following section, we shall apply the above approach to a special form of the Hamiltonian, namely the von Roos Hamiltonian.
3 Case of the von Roos Hamiltonian

3.1 General form of the propagator

The von Roos Hamiltonian was first introduced in order to account for the ordering ambiguities that arise when one tries to quantize the motion of a spatially-dependent mass, which we denote by \( m(\vec{q}) \), under the effect of a potential \( V(|\vec{q}|) \). It has the form \[ H = \frac{1}{4}(m(\vec{q})^\alpha \vec{p} \cdot \vec{p} m(\vec{q})^\beta \vec{p} m(\vec{q})^\gamma + m(\vec{q})^\gamma \vec{p} \cdot m(\vec{q})^\beta \vec{p} m(\vec{q})^\alpha) + V(|\vec{q}|), \] (15)

where the mass has to be dealt with as an operator that does not commute with the momentum operator \( \vec{p} \). The parameters \( \alpha, \beta \) and \( \gamma \) are real and satisfy the obvious condition \( \alpha + \beta + \gamma = -1 \), which ensures the correct form of the classical analog of \( H \).

By using the commutation relations satisfied by the position and momentum operators, the Hamiltonian can be recast as

\[ H = \frac{1}{2m} \vec{p}^2 + i\hbar \frac{\nabla m}{2 \frac{\bar{\nabla} m}{m^2}} \vec{p} - \frac{\hbar^2}{4m^3} \left[(\alpha + \gamma)m\Delta m - 2(\alpha\gamma + \alpha + \gamma)\bar{\nabla} m \cdot \bar{\nabla} m \right]. \] (16)

To construct the propagator, we first need to calculate the symbol \( \mathcal{H}_\theta \) corresponding to (16). For this reason we write \( H \) as the sum of three terms, namely,

\[ H = H^1 + H^2 + H^3, \] (17)

with

\[ H^1 = \frac{1}{2m} \vec{p}^2, \] (18)
\[ H^2 = i\hbar \frac{\nabla m}{2 \frac{\bar{\nabla} m}{m^2}} \vec{p}, \] (19)
\[ H^3 = -\frac{\hbar^2}{4m^3} \left[(\alpha + \gamma)m\Delta m - 2(\alpha\gamma + \alpha + \gamma)\bar{\nabla} m \cdot \bar{\nabla} m \right] + V(|\vec{q}|). \] (20)

Consequently it follows using equation (2) that

\[ \mathcal{H}_\theta^1(\vec{q}, \vec{p}) = \int d\vec{\xi} \ e^{i\vec{\xi} \cdot \vec{p}} (\vec{q} - \theta \vec{\xi}) \frac{1}{2m(\vec{q} - \theta \vec{\xi})} \vec{p}^2 |\vec{q} + (1 - \theta)\vec{\xi}\rangle \]
\[ = \int d\vec{\xi} \ e^{i\vec{\xi} \cdot \vec{p}} \frac{1}{2m(\vec{q} - \theta \vec{\xi})} (\vec{q} - \theta \vec{\xi}) \bar{\nabla} m \cdot \bar{\nabla} m |\vec{q} + (1 - \theta)\vec{\xi}\rangle. \] (21)
By inserting the completeness relation for the momentum variable:

\[ \int d\bar{p}\bar{p} |\bar{p}\rangle \langle \bar{p}| = 1, \quad (22) \]

we obtain

\[ \mathcal{H}_0^1(\vec{q}, \vec{p}) = \int\int \frac{d\vec{\xi}}{(2\pi\hbar)^3} \frac{d\xi}{2m(\vec{q} - \theta\vec{\xi})} \bar{p} e^{\frac{i}{\hbar} \vec{\xi}(\vec{p} - \bar{p})}. \quad (23) \]

This equation can be further simplified on account of the properties of the Dirac delta function; hence, we may write

\[ \mathcal{H}_0^1(\vec{q}, \vec{p}) = -\hbar^2 \int \frac{d\vec{\xi}}{2m(\vec{q} - \theta\vec{\xi})} e^{\frac{i}{\hbar} \vec{\xi}\vec{p}} \frac{\partial^2}{\partial \vec{\xi}^2} \delta(\vec{\xi}). \quad (24) \]

Afterwards, integrating by parts, we find that

\[ \mathcal{H}_0^1(\vec{q}, \vec{p}) = -\hbar^2 \lim_{\vec{\xi} \to 0} \frac{\partial^2}{\partial \vec{\xi}^2} \left( \frac{1}{2m(\vec{q} - \theta\vec{\xi})} e^{\frac{i}{\hbar} \vec{\xi}\vec{p}} \right). \quad (25) \]

It suffices now to carry on the partial derivation with respect to \( \vec{\xi} \) to end up with

\[ \mathcal{H}_0^1(\vec{q}, \vec{p}) = \frac{\vec{p}^2}{2m(\vec{q})} - 2i\hbar \theta \frac{\vec{\nabla} m}{m^2} \vec{p} + \frac{\hbar^2 \theta^2}{m^3} \left[ m\Delta m - 2\vec{\nabla} m \cdot \vec{\nabla} m \right]. \quad (26) \]

Similarly, we can calculate \( \mathcal{H}_0^2 \) as follows:

\[ \mathcal{H}_0^2(\vec{q}, \vec{p}) = \int d\vec{\xi} \ e^{\frac{i}{\hbar} \vec{\xi}\vec{p}} (\vec{q} - \theta\vec{\xi}) \frac{\vec{\nabla} m}{2m^2} |\bar{p}\rangle \langle \bar{p}| \vec{q} + (1 - \theta)\vec{\xi}) \]

\[ = \int d\vec{\xi} \ e^{\frac{i}{\hbar} \vec{\xi}\vec{p}} \frac{\vec{\nabla} m|_{\vec{q} - \theta\vec{\xi}}}{2m(\vec{q} - \theta\vec{\xi})^2} (\vec{q} - \theta\vec{\xi}) |\bar{p}\rangle \langle \bar{p}| \vec{q} + (1 - \theta)\vec{\xi}) \quad (27) \]

Inserting the closure relation \( (22) \), we obtain

\[ \mathcal{H}_0^2(\vec{q}, \vec{p}) = \int\int \frac{d\vec{\xi}}{(2\pi\hbar)^3} \frac{d\vec{\xi}}{2m(\vec{q} - \theta\vec{\xi})^2} \vec{\nabla} m|_{\vec{q} - \theta\vec{\xi}} \bar{p} e^{\frac{i}{\hbar} \vec{\xi}(\vec{p} - \bar{p})} \]

\[ = -\frac{\hbar}{i} \int d\vec{\xi} e^{\frac{i}{\hbar} \vec{\xi}\vec{p}} \frac{d\vec{\xi}}{2m(\vec{q} - \theta\vec{\xi})^2} \vec{\nabla} m|_{\vec{q} - \theta\vec{\xi}} \frac{\partial}{\partial \vec{\xi}} \delta(\vec{\xi}). \quad (28) \]
Then, integrating by parts yields:

\[
\mathcal{H}_\theta^2(\vec{q}, \vec{p}) = \frac{\hbar}{i} \lim_{\xi \to 0} \frac{\partial}{\partial \xi} \left( \frac{\vec{\nabla}m_{\vec{q} - \theta \vec{\xi}}}{2m(\vec{q} - \theta \vec{\xi})^2} e^{i \vec{\xi} \cdot \vec{p}} \right).
\]  

(29)

Carrying out partial derivation, one finds that

\[
\mathcal{H}_\theta^2(\vec{q}, \vec{p}) = \frac{\vec{p} \cdot \vec{\nabla}m}{2m} + \frac{i\hbar \theta}{2m^3} \left[ m \Delta m - 2 \vec{\nabla}m \vec{\nabla}m \right].
\]  

(30)

Regarding the operator \( \mathcal{H}^3 \), which depends only on the position, we simply have

\[
\mathcal{H}_\theta^3 = -\frac{\hbar^2}{4m^3} \left[ (\alpha + \gamma)m \Delta m - 2(\alpha \gamma + \alpha + \gamma)\vec{\nabla}m \cdot \vec{\nabla}m \right] + V(|\vec{q}|),
\]  

(31)

where now \( m \) is no longer an operator but a scalar that depends on the phase space variable \( \vec{q} \).

Summing up all the contributions we finally obtain

\[
\mathcal{H}_\theta(\vec{q}, \vec{p}) = \frac{\vec{p}^2}{2m} + \frac{i\hbar \vec{p} \cdot \vec{\nabla}m}{2m^2} (1 - 2\theta) + \frac{\hbar^2}{4m^3} \left\{ 2(\theta^2 - \theta) - \alpha - \gamma \right\} m \Delta m
\]  

\[
- 2 \left[ 2(\theta^2 - \theta) - \alpha \gamma - \alpha - \gamma \right] \vec{\nabla}m \cdot \vec{\nabla}m \right\} + V(|\vec{q}|).
\]  

(32)

The latter symbol, together with the expression (12), provide a unifying approach that takes into account both the ordering and the discretization ambiguities of the path integral.

Let us briefly discuss the general form of the propagator. Clearly, We can write the action as

\[
S = S_{\text{Cl}} + S_Q + iS_{\text{source}},
\]  

(33)

where \( S_{\text{Cl}} \) corresponds to the classical action, \( S_Q \) is the action of the quantum potential

\[
V_Q = \frac{\hbar^2}{4m^3} \left\{ 2(\theta^2 - \theta) - \alpha - \gamma \right\} m \Delta m - 2 \left[ 2(\theta^2 - \theta) - \alpha \gamma - \alpha - \gamma \right] \vec{\nabla}m \cdot \vec{\nabla}m \right\}.
\]  

(34)

and \( S_{\text{source}} \) is equivalent to the action of the source

\[
\vec{j} = \frac{\hbar}{2m^2} \vec{\nabla}m (1 - 2\theta).
\]  

(35)
that couples to the momentum $\vec{p}$. The above source vanishes for the midpoint discretization ($\theta = 1/2$), and is nonzero for both the prepoint and the postpoint discretization ($\theta = 0, 1$). Mathematically speaking, we may thus think of the motion as being equivalent to that of a particle under the effect of the potential $V + V_Q$ which is disturbed in some sense by an imaginary external source $\vec{j}$.

3.2 Reduction to a constant mass problem

3.2.1 Propagator in one dimension

From here on, in order to lighten the mathematical formulas, we restrict ourselves to the motion in one dimension. In this case we can write the full propagator as

$$K(q_f, t_f; q_i, t_i) = \lim_{N \to \infty} \prod_{k=0}^{N-1} \left( \frac{dp_k}{2\pi\hbar} \right) \exp \left\{ \frac{i}{\hbar} \sum_{k=0}^{N-1} \left( \frac{q_{k+1} - q_k}{\epsilon} \right) p_k - \frac{p_k^2}{2m(q_k)} + i\hbar \frac{p_k m'(\tilde{q}_k)}{2m(q_k)^2} (1 - 2\theta) \right\} \prod_{k=0}^{N-1} \left( \frac{dq_k}{2\pi\hbar} \right),$$

where $\tilde{q}_k = (1 - \theta)q_{k-1} + \theta q_k$, and the prime denotes the derivation with respect to the position coordinate. We also confine the upcoming discussion to Weyl ordering where $\theta = \frac{1}{2}$ which corresponds to the midpoint discretization of the path integral. The propagator becomes

$$K(q_f, t_f; q_i, t_i) = \int \mathcal{D}q \frac{Dp}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} \int_{t_i}^{t_f} \left( p\dot{q} - \frac{p^2}{2m(q)} - V_{\text{eff}}(q) \right) dt \right\}$$

where the effective potential is given explicitly by

$$V_{\text{eff}}(q) = -\frac{\hbar^2}{8m(q)} \left\{ \left[ 1 + 2\alpha + 2\gamma \right] \frac{m(q)''}{m(q)} - 2 \left[ 1 + 2\alpha \gamma + 2\alpha + 2\gamma \right] \left( \frac{m(q)'}{m(q)} \right)^2 \right\} + V(q).$$

(38)
Evidently, if we choose the von Roos parameters such that
\[ \alpha = \beta = -\frac{1}{2}, \quad \gamma = 0, \] (39)
or
\[ \gamma = \beta = -\frac{1}{2}, \quad \alpha = 0, \] (40)
the quantum potential (that is the term proportional to \( \hbar^2 \)) vanishes, and the effective potential reduces to
\[ V_{\text{eff}}(q) = V(q). \] (41)
This shows that when the midpoint discretization is combined with the Li and Kuhn ordering [40], the resulting effective Hamiltonian is identical to the classical one.

However, if we choose \( \alpha = \gamma = 0 \), which corresponds to the Ben Daniel and Duke ordering [41], we obtain
\[ V_{\text{eff}}(q) = \frac{\hbar^2}{8} \frac{d^2}{dq^2} \frac{1}{m(q)} + V(q). \] (42)
In the case of Zhu and Kroemer ordering [42], that is when \( \alpha = \gamma = -\frac{1}{2} \) and \( \beta = 0 \), one finds
\[ V_{\text{eff}}(q) = \frac{\hbar^2}{8m(q)} \left\{ \frac{m(q)''}{m(q)} - \left( \frac{m(q)'}{m(q)} \right)^2 \right\} + V(q). \] (43)

### 3.2.2 A simple scheme to convert the path integral to that of a constant mass

The path integral derived above contains the spatially-dependent mass in the kinetic energy term. One usually uses a time transformation together with regularizing functions [4, 5] to convert it to a path integral with constant mass.

We propose another simple method to accomplish this task which generalizes that proposed by Alhaidari [29] for any ordering, and avoids the use of the Green’s function. The essence of the proposed scheme may be summarized as follows. First consider the representation of the Kernel in the basis formed by the eigenfunctions of the operator \( H \), namely,
\[ K(q_f, t_f, q_i, t_i) = \sum_n e^{-\frac{i}{\hbar} E_n(t_f-t_i)} \psi_n(q_f, t_f) \psi_n^*(q_i, t_i). \] (44)
Suppose now that:

$$\psi(q, t) = \phi(q, t) F(q)^{1/4},$$

(45)

where $F(q)$ is a function of the position. Then we may write that

$$[F(q_f)F(q_i)]^{-1/4} K(q_f, t_f, q_i, t_i) = \tilde{K}(q_f, t_f, q_i, t_i)$$

(46)

where

$$\tilde{K}(q_f, t_f, q_i, t_i) = \sum_n e^{-\frac{i}{\hbar} E_n (t_f - t_i)} \phi_n(q_f, t_f) \phi_n^*(q_i, t_i).$$

(47)

Next let us consider the propagator in cartesian coordinate $x$:

$$\tilde{K}(x_f, t_f, x_i, t_i) = \int \int Dq \frac{Dp}{2\pi \hbar} \exp \left\{ \frac{i}{\hbar} \int_{t_i}^{t_f} \left( p \dot{x} - \frac{p^2}{2} - \tilde{V}(x) \right) \right\}$$

(48)

and make the transformation

$$x = F(q)$$

(49)

Then it can be shown by expanding about the midpoint that the propagator can be written as [4]

$$\tilde{K}(q_f, t_i, q_i, t_i) = [F(q_f)F(q_i)]^{-1/4} \int \int Dq \frac{Dp}{2\pi \hbar} \exp \left\{ \frac{i}{\hbar} \int_{t_i}^{t_f} \left( p \dot{q} - \frac{p^2}{2F'(q)^2} \right) \right\} - \tilde{V}(F(q)) - \frac{\hbar^2 F''(q)}{8 F^4(q)} \right\}.$$  

(50)

Thus comparing equations (50) and (37), it is sufficient on account of equation (46), to choose

$$F'(q)^2 = m(q)$$

(51)

which enables us to map the motion to that corresponding to a unit mass whose Hamiltonian is given by

$$H_{\text{red}} = \frac{p^2}{2} + V_{\text{eff}}(x) - \frac{\hbar^2 m'(x)^2}{32 m(x)^3} = \frac{p^2}{2} + V_{\text{red}}(x)$$

(52)

where

$$x = \int q \sqrt{m(q')} dq',$$

(53)
and

\[ V_{\text{red}}(x) = -\frac{\hbar^2}{8m(x)} \left\{ \left[ 1 + 2\alpha + 2\gamma \right] \frac{m(x)''}{m(x)} \right\} - 2\left[ \frac{7}{8} + 2\alpha_{\gamma} + 2\alpha + 2\gamma \right] \left( \frac{m(x)'}{m(x)} \right)^2 \right\} + V(x). \]  

(54)

The above formulas can easily be adapted to the case where the reduced mass is arbitrary (i.e. not necessarily a unit mass, see the illustrative examples given below). Notice also that when \( \alpha = \gamma = 0 \), that is for the Ben Daniel and Duke ordering, we recover the result of Alhaidari.

### 3.2.3 Illustrative examples

Let us illustrate the use of the above method by considering some particular forms of the mass. As a first example, we take

\[ m(q) = \frac{m_0}{(aq)^2}, \]
\[ V(q) = V_0, \]  

(55)

where \( m_0, a \) and \( V_0 \) are constants. Then from equation (54), one finds that for the Ben Daniel and Duke as well as for the Zhu and Kroemer orderings:

\[ V_{\text{red}} = \frac{\hbar^2 a^2}{8m_0} + V_0. \]  

(56)

In the case of the Li and Kuhn ordering, we obtain

\[ V_{\text{red}} = -\frac{\hbar^2 a^2}{8m_0} + V_0. \]  

(57)

All of the above orderings yield a constant potential, meaning that the wave function in the cartesian coordinate \( x \) are merely of the form

\[ \psi(x) = Ae^{-ikx} + Be^{ikx} \]  

(58)

where \( A \) and \( B \) are constants, and \( k = \sqrt{2m_0(E - V_{\text{red}})/\hbar} \), with \( E \) being the energy of the particle. But by virtue of equation (53):

\[ x = \frac{1}{a} \ln(aq), \]  

(59)
which leads to
\[
\psi(x) = A \exp\{-i \frac{k}{a} \ln(aq)} + B \exp\{i \frac{k}{a} \ln(aq)}.
\] (60)

A somewhat close form of this mass has been investigated by Schmidt in reference [32] in the context of the revival of the wave function. There, he also considered the form
\[
m(q) = \frac{x^\rho}{\tau^2}
\] (61)
with \(\rho \neq 2\). In this case, we obtain that for the Zhu and Kroemer ordering
\[
V_{\text{red}}(x) = -\frac{\hbar^2 \tau^2 \rho \rho}{8(\rho + 2)^2x^2}.
\] (62)

On the other hand for the Ben Daniel and Duke ordering, it turns out that
\[
V_{\text{red}}(x) = \frac{\hbar^2 \tau^2 \rho(3\rho + 4)}{8(\rho + 2)^2x^2}.
\] (63)

Similarly, we find that for the Li and Kuhn ordering,
\[
V_{\text{red}}(x) = -\frac{\hbar^2 \tau^2}{8(\rho + 2)^2x^2}.
\] (64)

All the above orderings yield a centrifugal potential; however, in contrast to the Ben Daniel and Duke ordering which leads to a repulsive barrier, those corresponding to Li and Kuhn, or Zhu and Kroemer produce an attractive barrier, leading thus to a completely different behavior of the motion of the particle. It is worthwhile mentioning that the wave function in this case is given by the Bessel function of the first kind, namely,
\[
\psi(x) = A \sqrt{x} J_{\nu}(\sqrt{2Ex}/2\hbar)
\] (65)

where \(E\) is the energy of the particle, and
\[
\nu = \begin{cases} 
\frac{1}{\rho + 2} & \text{for Zhu-Kroemer} \\
\frac{1}{2} \left[1 - \frac{1}{(\rho + 2)^2}\right]^{1/2} & \text{for Li-Kuhn} \\
\frac{\rho + 1}{\rho + 2} & \text{for Ben Daniel-Duke}
\end{cases}
\] (66)

To recover the \(q\)-dependence, we simply need to substitute
\[
x = \frac{2q^{1+\rho/2}}{\tau(\rho + 2)}.
\] (67)
in the expression of the wave function.
4 Propagator in curved space

In this section we intend to extend the investigation to curved spaces. Recall that the Hamiltonian of a particle moving in a curved space with metric tensor \( g_{\mu \nu} \) is given by [7]

\[
\hat{H} = \frac{1}{2} g^{-\frac{t}{2}} \hat{p}_\mu g^{\mu \nu} g^{\frac{t}{2}} \hat{p}_\nu g^{-\frac{t}{4}} + V(q)
\]

with \( g = \text{det} g_{\mu \nu} \). This problem (initiated by DeWitt [43]) has been investigated by Mizrahi [44] in the case of the Weyl ordering. There the metric tensor has been dealt with as an ordinary operator in rectangular coordinates. Because of the curvature of the space, it would be preferable to follow another path.

To begin we emphasize that to find the expression of the propagator describing the motion of the particle, we need to calculate the symbol \( \hat{H}_\theta \) associated with the above Hamiltonian. The direct use of equation (1) is not possible in this case since the points \( q - \theta q' \) and \( q + (1 - \theta) q' \) do not necessarily lie on a geodesic in the curved space of the particle. This problem does not come to play in the cartesian space since the geodesic is merely a straight line. Since our main aim is to deduce the correct transformation, it should be noted first of all that the eigenvectors of the operator \( \hat{p}_\mu \) may be calculated with the help of the expression

\[
\hat{p}_\mu |p\rangle = \bar{\hbar} \left( \frac{\partial}{\partial \mu} + \frac{1}{2} \Gamma^\nu_{\nu \mu} \right) |p\rangle
\]

where \( \Gamma^\nu_{\nu \mu} \) is the contracted affine connection. But since \( \Gamma^\nu_{\nu \mu} = \frac{1}{2} \partial_{\mu} \ln \sqrt{g} \), it follows that

\[
\langle q|p\rangle = \frac{e^{\frac{i}{\bar{\hbar}} q p}}{(2\pi \hbar)^{n/2} |g(q)|^{1/4}}
\]

where \( n \) is the dimension of the space. In this case the completeness relations in the position and the momentum spaces read:

\[
1 = \int dq \sqrt{g(q)} |q\rangle \langle q|,
\]

\[
1 = \int dp |p\rangle \langle p|.
\]

The symbol associated with the operator \( \hat{A} \) has the general form

\[
\mathcal{A}_\theta(q, p) = \int dq' Q_\theta(q, q') \langle q - \theta q'|\hat{A}|q + (1 - \theta) q'\rangle e^{\frac{i}{\bar{\hbar}} q p'}
\]
where the weighting function $Q_\theta(q, q')$ is to be determined. The inclusion of the latter quantity is necessary to ensure covariance \[45\]. Applying this to the operators $\hat{q}_\mu$ and $\hat{p}_\mu$ gives:

$$Q_\theta(q, 0) = \sqrt{g(q)},$$

$$\frac{\hbar}{i} \lim_{q' \to 0} \partial_\mu \left( e^{\frac{i p q'}{\hbar}} \frac{Q_\theta(q, q')}{\sqrt{g(q-q')g(q+(1-\theta)q')}} \right)^{1/4} = p_\mu. \quad (73)$$

where the partial derivative is with respect to $q'$. This immediately yields

$$Q_\theta(q, q') = \left[ g(q - \theta q')g(q + (1 - \theta)q') \right]^{1/4}, \quad (74)$$

which means that equation (72) becomes

$$A_\theta(q, p) = \int dq' [g(q - \theta q')g(q + (1 - \theta)q')]^{1/4} \langle q - \theta q' | A | q + (1 - \theta)q' \rangle e^{\frac{i p q'}{\hbar}}. \quad (75)$$

The latter formula enables us to calculate the symbol corresponding to the Hamiltonian of the particle as follows. First, one can see that the last two terms of $\hat{H}$ depend only on the position, meaning that the corresponding symbol is simply obtained by replacing the position operators by the corresponding phase space variables. We only need to find the expression of the symbol of the term $\hat{p}_\mu g^{\mu\nu} \hat{p}_\nu$, which is denoted in the subsequent discussion by $(\hat{p}_\mu g^{\mu\nu} \hat{p}_\nu)_\theta$. Explicitly we have that:

$$(\hat{p}_\mu g^{\mu\nu} \hat{p}_\nu)_\theta = \int dq' Q_\theta(q, q') \langle q - \theta q' | \hat{p}_\mu g^{\mu\nu} \hat{p}_\nu | q + (1 - \theta)q' \rangle e^{\frac{i p q'}{\hbar}}$$

$$= \int\int\int\int dq' dp' dp'' \sqrt{g(q'')} \frac{1}{(2\pi \hbar)^n} p_\mu p_\nu g^{\mu\nu} \langle q'' | p'' \rangle e^{\frac{i p q'}{\hbar}} \frac{1}{\sqrt{g(q-q')}} \frac{1}{\sqrt{g(q+(1-\theta)q')}}. \quad (76)$$

Using the completeness relation (70), we obtain

$$(\hat{p}_\mu g^{\mu\nu} \hat{p}_\nu)_\theta = \int\int\int\int dq' dp' dp'' dq'' \frac{1}{(2\pi \hbar)^n} p_\mu p_\nu g^{\mu\nu} \langle q'' | p'' \rangle e^{\frac{i p q'}{\hbar}} \frac{1}{\sqrt{g(q-q')}} \frac{1}{\sqrt{g(q+(1-\theta)q')}} + p q'. \quad (77)$$

Afterwards, on account of equation (69), we obtain after eliminating the variables $q''$, $p'$ and $p''$

$$\left(\hat{p}_\mu g^{\mu\nu} \hat{p}_\nu\right)_\theta = -\hbar^2 \int dq' e^{\frac{i p q'}{\hbar}} g^{\mu\nu} \langle q + (1 - \theta)q' | \partial_\mu \partial_\nu \delta(q') \rangle. \quad (78)$$
Whence,
\[
\left( \hat{p}_\mu g^{\mu \nu} \hat{p}_\nu \right)_\theta = -\hbar^2 \lim_{q' \to 0} \partial_\mu \partial_\nu \left( e^{iq'p} g^{\mu \nu} (q + (1 - \theta)q') \right),
\]
(79)
where the derivation is with respect to \( q' \). (Notice the similarity that exists between the latter equation and equation (25).) Now, performing the partial derivation, we find that
\[
\left( \hat{p}_\mu g^{\mu \nu} \hat{p}_\nu \right)_\theta = g^{\mu \nu} p_\mu p_\nu + i\hbar \left( \theta p_\mu \partial_\nu g^{\mu \nu} - (1 - \theta) p_\nu \partial_\mu g^{\mu \nu} \right) + \hbar^2 (1 - \theta) \partial_\mu \partial_\nu g^{\mu \nu}.
\]
(80)
Let us focus our attention on the term that is proportional to \( \bar{\hbar}^2 \). We need to calculate the derivative of the contravariant metric tensor \( g^{\mu \nu} \). To do so we make use of the fact that
\[
g^{\mu \nu} g^{\nu \rho} = \delta^\mu_\rho,
\]
to find that
\[
\partial_\nu g^{\mu \sigma} = \left( g^{\mu \rho} \Gamma^{\nu}_{\rho \sigma} + g^{\rho \sigma} \Gamma^{\mu}_{\rho \nu} \right).
\]
(81)
Then,
\[
\partial_\mu \partial_\nu g^{\mu \nu} = -\left[ \partial_\nu g^{\mu \rho} \Gamma^{\nu}_{\rho \sigma} + \partial_\nu g^{\rho \sigma} \Gamma^{\mu}_{\rho \nu} + g^{\rho \sigma} \Gamma^{\mu}_{\rho \nu, \sigma} - \partial_\nu g^{\rho \sigma} \Gamma^{\mu}_{\rho \nu, \sigma} - \partial_\nu g^{\rho \sigma} \Gamma^{\mu}_{\rho \nu} + g^{\rho \sigma} \Gamma^{\mu}_{\rho \nu} \Gamma^{\nu}_{\rho \sigma} \right].
\]
(82)
where \( \Gamma^{\nu}_{\rho \sigma} = \partial_\rho \Gamma^{\nu}_{\sigma \rho} \). Following the same method we can show that
\[
\frac{1}{4} g^{1/4} \Delta g^{-1/4} = \frac{1}{4} g^{-1/4} \partial_\mu \left( \frac{1}{4} g^{1/4} g^{\mu \nu} \Gamma^\rho_{\nu \mu} \right) = \frac{1}{4} g^{\mu \nu} \left[ \frac{1}{4} \Gamma^\rho_{\nu \mu} - \frac{1}{2} \frac{\Gamma^\rho_{\nu \sigma}}{\Gamma^\rho_{\sigma \nu}} - \frac{\Gamma^\rho_{\rho \sigma}}{\Gamma^\rho_{\sigma \rho}} \right].
\]
(83)
Summing up all the terms, we end up with following expression of the symbol associated with the Hamiltonian \( \mathcal{H}_\theta \):
\[
\mathcal{H}_\theta = \frac{1}{2} g^{\mu \nu} p_\mu p_\nu + \frac{i\hbar}{2} (1 - 2\theta) p_\nu \left( \theta p_\mu \Gamma^\nu_{\mu \rho} + g^{\rho \nu} \Gamma^{\mu}_{\mu \rho} \right) + V(q)
+ \frac{\hbar^2}{2} g^{\mu \nu} \left[ \left( \frac{1}{2} - \theta (1 - \theta) \right) \left( \Gamma^\sigma_{\mu \nu, \sigma} - \frac{1}{2} \Gamma^\sigma_{\mu \sigma, \nu} + \Gamma^\sigma_{\rho \sigma} \Gamma^\rho_{\mu \nu} \right) + \left( \theta (1 - \theta) - \frac{1}{4} \right) \Gamma^\sigma_{\rho \nu \sigma, \rho} \right].
\]

Introducing the curvature
\[ R = g^{\mu\nu} R_{\mu\nu} \]  
where \( R_{\mu\nu} \) denotes the Ricci tensor:
\[ R_{\mu\nu} = \Gamma^\sigma_{\mu\sigma,\nu} - \Gamma^\sigma_{\mu\nu,\sigma} - \Gamma^\rho_{\rho\sigma} \Gamma^\sigma_{\mu\nu} + \Gamma^\rho_{\mu\sigma} \Gamma^\sigma_{\rho\nu}, \]
we finally find
\[ H_\theta(q,p) = \frac{1}{2} g^{\mu\nu} p_\mu p_\nu + \frac{i\hbar}{2} (1 - 2\theta) p_\nu \left( g^{\mu\rho} \Gamma^\nu_{\mu\rho} + g^{\nu\gamma} \Gamma^\mu_{\nu\gamma} \right) + \frac{\hbar^2}{2} \left( \frac{1}{2} - \theta (1 - \theta) \right) R + \frac{\hbar^2}{8} \left( \Gamma^\rho_{\mu\sigma} \Gamma^\sigma_{\rho\nu} \right) \]
\[ + V(q). \]  
(87)
The propagator can thus be written for arbitrary values of the parameter \( \theta \) as:
\[ K(q', t'; q, t) = \left[ g(q)g(q') \right]^{-1/4} \lim_{N \to \infty} \int \frac{dp_{N-1}}{(2\pi\hbar)^n} \int \frac{dq_{N-1}}{(2\pi\hbar)^n} \ldots \]
\[ \times \int dq_1 \frac{dp_1}{(2\pi\hbar)^n} \int \frac{dp_0}{(2\pi\hbar)^n} \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{k=0}^{N-1} \left[ \frac{q_{k+1} - q_k}{\epsilon} \right] p_k \right\} \]
\[ - H_\theta(\theta q_k + (1 - \theta) q_{k+1}, p_k) \].  
(88)
Note finally that in the particular case of Weyl ordering, the symbol associated with the midpoint discretization reads
\[ H_{1/2} = \frac{1}{2} g^{\mu\nu} p_\mu p_\nu + V(q) + \frac{\hbar^2}{8} \left( R + g^{\mu\nu} \Gamma^\rho_{\mu\sigma} \Gamma^\sigma_{\rho\nu} \right) \]  
(89)
as should be \[ 7, 44 \].

5 Concluding remarks

We used a generalized definition of the phase space symbol to express the action in a concise manner, and to derive the propagator corresponding to
Hamiltonians with position-dependent kinetic energy for different choices the associated inherent ambiguities. It turns out that the lattice discretization ambiguity is encoded in the value of the parameter $\theta$. We have applied this formalism to the particular case of the von Roos Hamiltonian, with arbitrary values of the ordering ambiguity parameters. We find that in addition to the above quantities, the lattice parameter $\theta$ also determines the form of the quantum potential, providing thus a unifying approach to the ordering and the discretization ambiguities. Moreover, we proposed a simple scheme that enables one to map the position-dependent mass problem to that of a constant mass, and we have demonstrated how to use it by treating few simple examples. By extending the concept of the symbol to the case where the space is curved, we were able to express the propagator describing the motion in curved spaces.

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