

THE HAMILTON JACOBI EQUATION, THE FEYNMAN-KAC FORMULA AND THE CLASSICAL LIMIT

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ABSTRACT. We present a simplified approach to the problem of obtaining classical mechanics from a classical diffusion equation. It so happens that when the diffusion constant tends to 0 the diffusing particles move along the trajectory of a Newtonian particle. At the end we present a list of examples including particles in a static electro-magnetic field

1. INTRODUCTION AND PRELIMINARIES

Our goal in this review is to give some insight to what is now a well known theme: To obtain classical mechanics as the asymptotic limit $\hbar \rightarrow 0$ of non-relativistic quantum mechanics. We collected a series of results that were obtained by a large number of researchers over time. Perhaps we can say that the originality of this presentation lies on the simplification of proofs.

Let us begin with some introductory preliminaries. When the quantum mechanical description of microscopic phenomena based on Schrödinger's equation replaced the classical description based on the Newtonian-Hamiltonian formalism, the natural question to ask was: how is the later to be understood with regards to the former.

This was the birth of the $\hbar \rightarrow 0$ asymptotic procedures by means of which classical mechanics was to be recovered from quantum mechanics. A few exposés of techniques and interconnection with a variety of problems can be seen in [1], [6], [16], [17] and [24]. By the way, [17] contains an analytic approach to what we do here.

The simplest interesting Schrödinger's equation, that which describes the quantum behavior of a point particle of mass one in a potential $V(x)$, is

$$(1.1) \quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2} \Delta \psi + V\psi.$$

where Δ is the Laplace-Beltrami operator in the Euclidean metric in \mathbb{R}^n and $\hbar = \frac{h}{2\pi}$, with h being the Planck's constant. This equation can be transformed into a diffusion equation by means of the replacement of t by $\frac{t}{i}$, thus obtaining

$$(1.2) \quad \hbar \frac{\partial \rho}{\partial t} = \frac{\hbar^2}{2} \Delta \rho - V\rho,$$

where $\rho(\cdot, t) = \psi(\cdot, \frac{t}{i})$. This (formal) replacement is interesting for the simple reason that a well developed theory of functional integration exists, and which allows to represent solutions to (1.2) as path integrals, whereas path integration starting from

(1.1) is not a clear affair. How to relate both techniques? Different approaches have been tried and most listed in the references [1], [6], [16], [17] and [24], but we may single out a few, namely [5], [8], [11], [14] and [18].

A few of the references deal with the $\hbar \rightarrow 0$ limit from various related points of view are [3], [8], [9], [10], [12], [20] and we are not going to improve on the results presented there in various degrees of generality. What we are going to do instead is to play around the initial step, namely the representation of the solution of (1.2) as a path integral and take things to the point where the $\hbar \rightarrow 0$ limit becomes an obvious and clear fact, and the conditions under which it is valid become quite transparent.

The end product is similar but not identical to the approaches developed in [9] and [10], and we feel this makes a good preamble to that line of work. Let us now to prepare the stage.

We want to relate the solutions to the Hamilton-Jacobi equation, [2],

$$(1.3) \quad \frac{\partial S_0}{\partial t} + \frac{1}{2}(\nabla S_0)^2 + V(x) = 0, \quad S_0(x, P, 0) = \langle x, P \rangle,$$

to the asymptotic behavior of the solutions of (1.4) as $h \rightarrow 0$. Where h is a positive real number and ∇ is the gradient operator. It is important to remark above the sign of the function V , that $\langle \cdot, \cdot \rangle$ denotes the Euclidean scalar product in \mathbb{R}^n and as in physical literature we use $(x)^2 = \|x\|^2$ for $x \in \mathbb{R}^n$.

$$(1.4) \quad h \frac{\partial \psi_h}{\partial t} = \frac{h^2}{2} \Delta \psi_h + V(x) \psi_h \quad \psi_h(x, 0) = e^{-\frac{\langle x, P \rangle}{h}},$$

The connection between (1.3) and (1.4) being via the substitution

$$(1.5) \quad \psi_h(x, t) = e^{-\frac{S_h(x, P, t)}{h}},$$

which requires $S_h(x, P, t)$ to satisfy

$$(1.6) \quad \frac{\partial S_h}{\partial t} = \frac{1}{2}(\nabla S_h)^2 + V(x) = \frac{h}{2} \Delta S_h, \quad S_h(x, P, t) = \langle x, P \rangle.$$

Why (1.5)? In the trivially integrable case, this is that of a particle in a Hamiltonian $H(p)$. Below in section 2 we will study in more generality the movement of such a particle and in the particular case that we are considering we get the equation

$$\frac{\partial S_0}{\partial t} + H(\nabla S_0) = 0, \quad S_0(x, P, 0) = \langle x, P \rangle.$$

Which has $S_0(x, P, t) = \langle x, P \rangle - H(P)t$, as solution. Consider now the solution of

$$h \frac{\partial \psi_h}{\partial t} = H(-h\nabla) \psi_h, \quad \psi_h(x, 0) = e^{-\frac{\langle x, P \rangle}{h}},$$

which is by the theory of semigroups

$$\psi_h(x, t) = (e^{\frac{tH(-h\nabla)}{h}} \psi_h(\cdot, 0))(x) = e^{-\frac{S_0(x, P, t)}{h}}.$$

Then the function $S_0(x, P, t)$ can be recovered from the above solution by means of

$$S_0(x, P, t) = \lim_{h \rightarrow 0} -h \log \psi_h(x, t).$$

Another reason is that the solution of equation (1.4) admits a representation in terms of path integrals via the Feynman-Kac formula, see for example [21],

$$(1.7) \quad \psi_h(x, t) = \mathbb{E}_h^x [e^{-\frac{1}{h}(\langle P, B_h(t) \rangle - \int_0^t V(B_h(s)) ds)}].$$

This expression can be computed in a variety of simple cases and is a good starting point for theoretical analysis. Here, as usual, the symbol \mathbb{E}_h^x denotes the expectation with respect to the Brownian motion starting at the point $x \in \mathbb{R}^n$ and $B_h(t)$ denotes this process at time t with variance h .

2. SOME CLASSICAL MECHANICS

For completeness we are going to take a small digression into classical mechanics. The reason for the initial condition $S_0(x, P, 0) = \langle x, P \rangle$ is the following. For a mechanical system on \mathbb{R}^n , the function $S_0(x, P, t)$ generates a canonical transformation that brings the system to rest, that is, it maps the current state of the system (denoted by (x, p) to the initial state (denoted by (X, P)).

When $S_0(x, P, t)$ is known the state of the system at time t can be obtained from the state $t = 0$ by solving the transformation equations

$$(2.1) \quad X_i = \frac{\partial S_0}{\partial P_i}, \quad p_i = \frac{\partial S_0}{\partial x_i}.$$

We shall assume that there exists an appropriate time interval $[0, T]$ in which $S_0(x, P, t)$ is defined and the transformation (2.1) is well defined. It is plain to check that for a dynamical system with Hamiltonian $H(p)$ we have $S_0(x, P, t) = \langle x, P \rangle - H(P)t$ with $S_0(x, p, 0) = \langle x, P \rangle$, and (2.1) hold.

In general, see [2], a mechanical system on \mathbb{R}^{2n} is specified by giving the Hamiltonian $H(x, p)$, and the trajectories of the system are obtained by solving the Hamilton equations.

$$(2.2) \quad \dot{x}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}, \quad i = 1, \dots, n.$$

which is always possible, when the derivatives appearing in (2.2) are locally Lipschitz, bounded, in a local sense.

In general the problem of solving (2.2) can be translated into the problem of solving

$$(2.3) \quad \frac{\partial S_0}{\partial t} + H(x, \nabla S_0) = 0, \quad S_0(x, P, 0) = \langle x, P \rangle.$$

The connection and much more can be seen in [2].

The problem with (2.3) being the apparition of singularities which make the global existence of solutions a problem. Even though the curves $(x(t), y(t))$ may exist and be unique as curves in \mathbb{R}^{2n} , their projection $x(t)$ on \mathbb{R}^n may cross which makes it impossible in general to propagate an initial condition for (2.3) without the appearance of singularities.

Quite a lot on these matters can be found in [17].

What we do next is quite straight forward and is similar to, but shrouded in a less sophisticated jargon, the material in [10]. To begin with, suppose that $S_0(x, P, t)$ satisfies (1.3), and consider the curves defined for $0 \leq s \leq t$ as the solutions to:

$$(2.4) \quad \dot{\gamma}(s) = (\nabla S_0)(\gamma(s), P, s) \quad \gamma(t) = x,$$

which will always possible when there is a $T \leq \infty$, such a γ satisfying (2.4) exists if ∇S_0 is Lipschitz and bounded as function in x for $0 \leq t \leq T$. When we differentiate (2.4) once more and make use of (1.3) we obtain that

$$(2.5) \quad \ddot{\gamma}(s) = -\nabla V(\gamma(s)).$$

Consider for each t , the curve $x(s)$ defined on $[0, T]$ by $x(s) = \gamma(t - s)$. Then $x(0) = x$, $\dot{x}(t) = -\gamma(0) = -P$. Form $F(s) = S_0(x(s), P, t - s)$, differentiate with respect to s to obtain

$$\frac{dF}{ds} = -\left\{\frac{1}{2}(\nabla S_0)^2(x(s), P, t - s) - V(x(s))\right\},$$

and now integrate from 0 to t to obtain

$$(2.6) \quad S_0(x, P, t) = \langle x(t), P \rangle + \int_0^t \left(\frac{1}{2}\dot{x}^2(s) - V(x(s))\right) ds.$$

For some of the results in section 3 we need the following

Lemma 1. *Let $x(s)$ be as above and define*

$$U(x, P, t) = \langle x(t), P \rangle + \int_0^t \left(\frac{1}{2}\dot{x}^2(s) - V(x(s))\right) ds,$$

then we have $U(x, P, t) = S_0(x, P, t)$.

Remark 1. *This is implicit in (2.6), but the conceptual meaning is different, for in order to compute the right hand side of (2.6) one only has to solve $\ddot{x}(s) = -\nabla V(x(s))$, $x(0) = x$, $\dot{x}(t) = -P$, and then integrate to obtain the solution to (1.3).*

Proof. Notice to begin with that

$$\frac{\partial U}{\partial t} = \langle \dot{x}(t), P \rangle + \frac{1}{2}\dot{x}^2(t) - V(x(t)) = -\left\{\frac{1}{2}\dot{x}^2(t) + V(x(t))\right\},$$

since $\dot{x}(t) = -P$. Compute now

$$\begin{aligned} \frac{\partial U}{\partial x_i} &= \sum_{j=1}^n P_j \frac{\partial x_j(t)}{\partial x_i} + \int_0^t \sum_{j=1}^n \left\{ \dot{x}_j(t) \frac{\partial \dot{x}_j(s)}{\partial x_i} - \frac{\partial V}{\partial x_j}(x(s)) \frac{\partial x_j(s)}{\partial x_i} \right\} ds \\ &= \sum_{j=1}^n \left\{ P_j \frac{\partial x_j(t)}{\partial x_i} + \int_0^t \left\{ \frac{d}{ds} (\dot{x}_j(s)) \frac{\partial x_j(s)}{\partial x_i} \right\} ds \right\} \\ &= \sum_{j=1}^n \left\{ P_j \frac{\partial x_j(t)}{\partial x_i} + \dot{x}_j(t) \frac{\partial x_j(s)}{\partial x_i} - \dot{x}_j(0) \delta_{ij} \right\} = -\dot{x}_i(0), \end{aligned}$$

where in the second step we used $\ddot{x}_j(s) = -(\frac{\partial V}{\partial x_j}(x(s)))$ and in the third we again used $\dot{x}(t) = -P$.

Given that $x(0) = \gamma(t) = x$. Now a simple application of the law of the conservation of energy yields,

$$\begin{aligned} \frac{\partial U}{\partial t}(x, t) + \frac{1}{2}(\nabla U)^2(x, t) + V(x) \\ = -\left(\frac{1}{2}\dot{x}^2(t) + V(x(t))\right) + \left(\frac{1}{2}\dot{x}^2(0) + V(x(0))\right) = 0, \end{aligned}$$

which together with the fact that at $t = 0$, $U(x, P, 0) = \langle x, P \rangle$ yields the desired result.

3. THE CLASSICAL LIMIT

As we said above, what do here is similar in spirit to the methods in [8] and [10]. We shall proceed with formal manipulations to the very end, point at which we state the necessary qualifiers. We are interested in the behavior of (1.7) this is, of

$$\psi_h(x, t) = \mathbb{E}_h^x[e^{-\frac{1}{h}(\langle P, B_h(t) \rangle - \int_0^t V(B_h(s)) ds)},$$

as h becomes small.

Consider $S_0(B_h(s), P, t - s)$ for $0 \leq s \leq t$. From Itô formula

$$S_0(B_h(s), P, t - s)$$

$$= S_0(B_h(0), P, t) + \int_0^s \left(\frac{\partial S_0}{\partial t}(-) + \frac{h}{2} \Delta S_0(-) \right) du + \int_0^s \langle \nabla S_0(-), dB_h(u) \rangle,$$

where $(-)$ stands for $(B_h(u), P, t - u)$. Now set $s = t$, use $S_0(x, P, 0) = \langle x, P \rangle$ and (1.3) to rewrite (1.7) as

$$(3.1) \quad \psi_h(x, t) = e^{-\frac{1}{h} S_0(x, P, t)} \mathbb{E}_h^x[Z_h(t) e^{-\frac{1}{2} \int_0^t (\Delta S_0)(B_h(s), P, t-s) ds}]$$

where $Z_h(s)$ is the exponential martingale given by

$$(3.2) \quad Z_h(t) = e^{-\frac{1}{h} \left(\int_0^t \langle \nabla S_0 \rangle(B_h(s), P, t-s) ds + \frac{1}{2} \int_0^t (\nabla S_0)^2(B_h(s), P, t-s) ds \right)}.$$

A different way to reach (3.1) is to make $\psi_h(x, t) = \Lambda(x, t) e^{-\frac{1}{h} S_0(x, P, t)}$ and verify that $\Lambda(x, t)$ has to satisfy

$$(3.3) \quad \frac{\partial \Lambda}{\partial t} = \frac{h}{2} \Delta \Lambda - \langle \nabla S_0, \nabla \Lambda \rangle - \frac{\Delta S_0}{2} \Lambda, \quad \Lambda(x, 0) = 1$$

and we see that (3.1) expresses the solution to (3.3) as a path integral combining the Cameron-Martin-Girsanov and Feynman-Kac formula, see [21] for example.

Had we rigged things up so Schilder's conditions for his theorem A in [20] be satisfied we could at this point conclude that

$$(3.4) \quad \lim_{h \rightarrow 0} \mathbb{E}_h^x[Z_h(t) e^{-\frac{1}{2} \int_0^t \Delta S_0(B_h(s), P, t-s) ds}] = e^{-\frac{1}{2} \int_0^t \Delta S_0(x(s), P, t-s) ds}.$$

where $x(s)$ is the curve maximizing the following functional

$$(3.5) \quad \begin{aligned} \mathcal{L}(\xi) &= - \int_0^t \left(\langle \nabla S_0(\xi(s), P, t-s), \dot{\xi}(s) \rangle \right. \\ &\quad \left. + \frac{1}{2} (\nabla S_0)^2(\xi(s), P, t-s) + \frac{1}{2} \dot{\xi}^2(s) \right) ds \\ &= - \frac{1}{2} \int_0^t \left(\dot{\xi}(s) + \nabla S_0(\xi(s), P, t-s) \right)^2 ds \end{aligned}$$

which is obviously the curve $x(s)$ introduced in section 2, this is the curve solving

$$(3.6) \quad \dot{x}(s) = -(\nabla S_0)(x(s), P, t-s) \quad x(0) = x,$$

which makes (3.5) attain its maximum value.

We would thus obtain

$$\lim_{h \rightarrow 0} -h \log \psi_h(x, t) = S_0(x, P, t),$$

as well as the limit

$$\lim_{h \rightarrow 0} e^{\frac{1}{h} S_0(x, P, t)} \psi_h(x, t) = e^{-\int_0^t \Delta S_0(x(s), P, t-s) ds}.$$

But if we did not know about Schilder's result we could proceed as follows. Let $X_h(t)$ be the solution of the stochastic equation

$$(3.7) \quad dX_h(t)(s) = -(\nabla S_0)(X_h(s), P, t-s)ds + \sqrt{h}dB_1(s)$$

and now use the Cameron-Martin-Girsanov formula to rewrite $\psi_h(x, t)$ as

$$(3.8) \quad \psi_h(x, t) = e^{-\frac{1}{h}S_0(x, P, t)} \mathbb{E}_1^x \left[e^{-\frac{1}{2} \int_0^t (\Delta S_0)(X_h(s), P, t-s) ds} \right]$$

and we can now state the

Theorem 1. *Assume that $V(x)$ is such that for t in $[0, T]$, (1.7) is finite and that the solution to (1.3) exists, is smooth and ∇S_0 is Lipschitz or bounded and that ΔS_0 is smooth and bounded. Then X_h defined by (3.7) exists and*

$$\lim_{h \rightarrow 0} -h \log \psi_h(x, t) = S_0(x, P, t),$$

$$\lim_{h \rightarrow 0} e^{\frac{1}{h}S_0(x, P, t)} \psi_h(x, t) = e^{-\frac{1}{2} \int_0^t \Delta S_0(x(s), P, t-s) ds}.$$

Proof. The existence and uniqueness of $X_h(s)$ is standard and $X_h(s)$ tends uniformly in probability to $x(s)$ as h tends to zero. All this can be seen in [12]. The first limit is not a problem and for the second use the smoothness of ΔS_0 .

Remark 2. *In [12] we can also find the expansion of $X_h(s)$ in powers of \sqrt{h} and this combined with the smoothness of ΔS_0 allows us to obtain asymptotic expansions of $\psi_h(x, t)$. The whole point in doing things this way is to go around the heavy limiting procedures as appearing in [9], [10] and [20], since all that is involved are estimates in [12] that are typical of the theory of ordinary differential equations.*

What come next is a rehash of a standard theme, see [9] but we say it differently. As above let start from (1.7) and rewrite it by means of the Cameron-Martin-Girsanov translation formula as

$$(3.9) \quad e^{-\frac{1}{h}b(t)} \mathbb{E}_h^x \left[e^{-\frac{1}{h} \int_0^t \sum_{ij} B_h^i(s) B_h^j(s) H_{ij}(B_h(s)) ds} \right],$$

where

$$b(t) = \langle P, x(t) \rangle + \int_0^t \left(\frac{1}{2} \dot{x}^2(s) - V(x(s)) \right) ds.$$

We have seen in Lemma 2.6, equals $S_0(x, P, t)$, and where

$$H_{ij}(B_h(s)) = \int_0^1 (1-u) \frac{\partial^2 V}{\partial x_i \partial x_j} (u + B_h(s) + x(s)) du,$$

here $x(t)$ has been introduced in section 2. To arrive at (3.9) we use the fact that $x(s)$ maximizes the following functional

$$-\langle P, \xi(t) \rangle + \int_0^t \left(\frac{1}{2} \dot{\xi}^2(s) - V(\xi(s)) \right) ds,$$

over the set of trajectories that have square integrable velocity, $\xi(0) = 0$ and $\xi(t) = -P$ which can be seen in [10]. Then the first variation of this functional vanishes at $x(s)$ and we also make use of the fact that for a $f \in C^2(\mathbb{R}^n)$, and any $b \in \mathbb{R}^n$ we have

$$f(b+y) = f(y) + \sum_{i=1}^n b^i \frac{\partial f}{\partial x_i}(y) + \sum_{i,j} b^i b^j \int_0^1 (1-u) \frac{\partial^2 f}{\partial x_i \partial x_j} (u + b + y) du.$$

Now rescale the Brownian motion in (3.9) to obtain

$$(3.10) \quad \psi_h(x, t) = e^{-\frac{b(t)}{h}} \mathbb{E}_1^x [e^{-\int_0^t \sum_{i,j} B_1^i(s) B_1^j(s) H_{ij}(\sqrt{h} B_1(s)) ds}].$$

Then we see that any condition insuring integrability of (3.10) and smoothness of H_{ij} would yield what we want.

For example, when $H_{ij}(x)$ is a positive form for every x and is continuous we are in business. Also when $H_{ij}(x)$ has negative eigenvalues, we may pull things through by restricting t to an interval such that (3.10) is finite. It suffices to take

$$4 \inf_{ij} | \sum_{ij} \xi^i \xi^j H_{ij}(x) | < T.$$

The connection with the previous result being that

$$e^{-\frac{1}{2} \int_0^t \Delta S_0(x(s), P, t-s) ds} = \mathbb{E}_1^x [e^{-\frac{1}{2} \int_0^t B^i(s) B^j(s) \frac{\partial^2 V}{\partial x_i \partial x_j}(x(s)) ds}].$$

As can be seen in [15] pages 13-14.

4. MORE GENERAL CONDITIONS

We may want to consider (1.4) with the initial condition

$$(4.1) \quad \psi_h(x, 0) = f(x) e^{-\frac{1}{h} S(x)}.$$

as in [8] say. Proceeding as above, we would have to start studying

$$\frac{\partial S_0}{\partial t} + \frac{1}{2} (\nabla S_0)^2 + V(x) = 0, \quad S_0(x, 0) = S(x),$$

and we may assume the same hypothesis as in Theorem 1 to hold. As before, we can write the solution to (1.4) with initial condition (4.1) as

$$\psi_h(x, t) = \mathbb{E}_h^x [f(B_h(t)) e^{-\frac{1}{h} (S(B_h(t)) + \int_0^t \Delta S_0(B_h(s), P, t-s) ds)}],$$

which can, as in section 3, be transformed into

$$\psi_h(x, t) = e^{-\frac{1}{h} S_0(x, P, t)} \mathbb{E}_h^x [f(X_h(t)) e^{-\frac{1}{h} \int_0^t \Delta S_0(X_h(s), P, t-s) ds}],$$

where $X_h(s)$ was introduced in (3.7). At this point, with boundedness and continuity assumptions on f , the standard limit and asymptotic expansions can be obtained.

The alternative procedure described in section 3, goes along the same lines. The only difference is that now we have to maximize the functional

$$(4.2) \quad \int_0^t (V(\xi(s)) - \frac{1}{2} \dot{\xi}^2(s)) ds - S(\xi(t)),$$

over the curves with square integrable derivative in $[0, T]$, for a convenient T . Such curves would satisfy

$$\ddot{x}(s) = -\nabla V(x(s)), \quad x(0) = x, \quad \dot{x}(s) = -\nabla S(x(t)),$$

for $0 \leq s \leq t$. That they maximize (4.2) can be obtained by standard methods of calculus of variations.

Considering now

$$\psi_h(x, t) = \mathbb{E}_h^x [f(B_h(t)) e^{-\frac{1}{h} (S(B_h(t)) + \int_0^t V(B_h(s)) ds)}]$$

and applying the argument in section 3, it can be transformed into

$$\psi_h(x, t) = e^{\frac{1}{h} b(t)} \mathbb{E}_h^x [f(x(t) + B_h(t)) e^{-\frac{1}{h} \int_0^t \sum_{i,j} B_h^i(u) B_h^j(u) H_{ij}(B_h(u)) du}],$$

by means of the Cameron-Martin-Girsanov formula and a Taylor expansion about $x(u)$ up to second order. The term of first order in $B_h(\cdot)$ drop away due to the maximizing property of $x(s)$.

From this point on, the same comments as in the section 3 apply.

5. PARTICLE IN A STATIC ELECTRO MAGNETIC FIELD

The description of a particle moving through an electro-magnetic field is described by the Hamiltonian

$$(5.1) \quad H(x, p) = \frac{1}{2}(p - A(x))^2 + V(x),$$

with $A(x)$ being a smooth vector field on \mathbb{R}^3 and $V(x)$ being a smooth scalar function. We assume that $\nabla \times A(x)$ and $\nabla V(x)$ are either bounded or satisfy a growth condition such that either Newton's equations

$$(5.2) \quad \dot{x}(s) = \dot{x}(s) \times (\nabla \times A(x(s))) - \nabla V(x(s)),$$

or Hamilton's equations

$$(5.3) \quad \dot{x}_i = p_i - A_i(x), \quad \dot{p}_i = -\frac{\partial V}{\partial x_i} + (p_j - A_j) \frac{\partial A_j}{\partial x_i}$$

have a unique solution for every initial condition $(x(0), p(0))$. The Hamilton-Jacobi equation corresponding to (5.1) is

$$(5.4) \quad \frac{\partial S_0}{\partial t} = +\frac{1}{2}(\nabla S_0 - A(x))^2 + V(x) = 0, \quad S_0(x, 0) = S(x).$$

We assume that for all $t \in [0, T]$ it exists, has enough smoothness and ∇S_0 , ΔS_0 are smooth and bounded.

We shall furthermore make the simplifying assumption (usually called the transversality condition or gauge in the physical literature) that

$$(5.5) \quad \langle \nabla, A(x) \rangle = 0.$$

Consider now the diffusion satisfying

$$(5.6) \quad h \frac{\partial \psi_h}{\partial t} = \frac{1}{2}(h\nabla + A)^2 \psi_h + V \psi_h, \quad \psi(x, 0) = f(x) e^{-\frac{1}{h} S(x)},$$

for $x \in \mathbb{R}^3$ and $t > 0$. Under a variety of assumptions on $V(x)$ and $A(x)$, see [21] for example, the solution of (5.6) can be written as

$$(5.7) \quad \psi_h(x, t) = \mathbb{E}_h^x [f(B_h(t)) e^{\frac{1}{h} \int_0^t \langle A(B_h), dB_h(s) \rangle + \frac{1}{h} \int_0^t V(B_h(s)) ds - S_h(B_h(t))}]$$

by means of a combination of the Feynman-Kac and Cameron-Martin-Girsanov translation formula.

Remark 3. *Let us explain how one can obtain (5.7). For this, it suffice to compute the infinitesimal generator of the semigroup defined by :*

$$P_t(F)(x) = \mathbb{E}_h^x [F(B_h(t)) e^{\frac{1}{h} \int_0^t \langle A(B_h), dB_h(s) \rangle + \frac{1}{h} \int_0^t V(B_h(s)) ds}],$$

and $P_0(F)(x) = f(x) e^{-\frac{1}{h} S(x)}$. See (5.7) for more on this. From the definitions and rearranging the terms, we obtain

$$\begin{aligned}
& \frac{1}{t}[P_t(F)(x) - F(x)] \\
&= \frac{1}{t}\mathbb{E}_h^x[(e^{\frac{1}{2h}\int_0^t A^2(B_h(s))ds} + \frac{1}{h}\int_0^t V(B_h(s))ds \\
&\times (F(B_h(t))e^{\frac{1}{h}\int_0^t \langle A(B_h), dB_h(s) \rangle - \frac{1}{2h}\int_0^t A^2(B_h(s))ds} - F(x)) \\
&+ e^{\frac{1}{h}\int_0^t \langle A(B_h), dB_h(s) \rangle - \frac{1}{2h}\int_0^t A^2(B_h(s))ds}[F(x)e^{\frac{1}{2h}\int_0^t A^2(B_h(s))ds} + \frac{1}{h}\int_0^t V(B_h(s))ds - F(x)] \\
&\rightarrow_{t \rightarrow 0} \frac{h}{2}\Delta F(x) + A(x)\nabla F(x) + \frac{1}{2h}A^2(x)F(x) + \frac{1}{h}V(x)F(x) \\
&= \frac{1}{2h}(h\nabla + A(x))^2 F(x) + \frac{1}{h}V(x)F(x).
\end{aligned}$$

Recall that $\langle \nabla, A \rangle = 0$. Moreover, we have used above the following facts. Let A be a smooth vector field and consider the stochastic differential equation

$$dX_h(s) = A(X_h(s))ds + dB_h(t) \stackrel{\mathcal{L}}{=} A(X_h(s))ds + \sqrt{h}dB_1(t),$$

then

$$dY_h(s) := \frac{1}{\sqrt{h}}X_h(s) = \frac{1}{\sqrt{h}}A(\sqrt{h}Y_h(s)) + dB_1(t).$$

Now by using Girsanov's formula we get

$$\begin{aligned}
\mathbb{E}_h^x[G(X_h(\cdot))] &= \mathbb{E}_h^x[G(\sqrt{h}Y_h(\cdot))] \\
&= \mathbb{E}_1^x[G(\sqrt{h}B_1(\cdot))]e^{\frac{1}{\sqrt{h}}\int_0^t \langle A(\sqrt{h}B_1(s)), dB_1(s) \rangle - \frac{1}{2h}\int_0^t A^2(\sqrt{h}B_1(s))ds} \\
&= \mathbb{E}_h^x[G(B_h(\cdot))]e^{\frac{1}{h}\left(\int_0^t \langle A(B_h(s)), dB_h(s) \rangle - \frac{1}{2}\int_0^t A^2(B_h(s))ds\right)}.
\end{aligned}$$

We can now proceed as in section 3. That is, we compute $dS_0(B_h(s), t-s)$ as function of s for each $t \in [0, T]$ and then transform (5.7) into

$$(5.8) \quad \psi_h(x, t) = \mathbb{E}_h^x[f(B_h(t))Z_h(t)e^{-\frac{1}{2}\int_0^t \Delta S_0(B_h(s), t-s)ds}]e^{-\frac{1}{h}S_0(x, t)},$$

with $Z_h(t)$ being

$$Z_h(t) = e^{-\frac{1}{h}\left(\int_0^t \langle (\nabla S_0 + A)(B_h(s), t-s), dB_h(s) \rangle + \frac{1}{2}\int_0^t (\nabla S_0 + A)^2(B_h(s), t-s)ds\right)},$$

which is a martingale by the Novikov's criterion whenever

$$\mathbb{E}_h^x[e^{\frac{1}{2}\int_0^t (\nabla S_0 + A)^2(B_h(s), t-s)ds}] < \infty.$$

Rescale $B_h(t)$ as to have a fixed set of probability laws and consider the stochastic differential equation

$$(5.9) \quad dX_h(s) = -[\nabla S_0(X_h(s), t-s) + A(X_h(s))]ds + \sqrt{h}dB_1(s),$$

with initial condition $X_h(0) = x$. From our assumptions on A and ∇S_0 we obtain the uniqueness and existence of $X_h(s)$. Now rewrite (5.8) as

$$(5.10) \quad \psi_h(x, t) = e^{-\frac{1}{h}S_0(x, t)}\mathbb{E}_h^x[f(X_h(t))e^{-\frac{1}{2}\int_0^t \Delta S_0(X_h(s), t-s)ds}]$$

by making use of the Cameron-Martin-Girsanov theorem. Again, from the convergence of $X_h(s)$ as h tends to zero to the solution of

$$\dot{x}(s) = -(\nabla S_0(x(s), t-s) + A(x(s))), \quad x(0) = 0,$$

we obtain the desired limiting behavior of (5.8) and using the expansion of the solutions of $X_h(s)$ of (5.9) in terms of \sqrt{h} we can get asymptotic expansions of $\psi_h(x, t)$.

6. EXAMPLES

In this section we present a few examples, some of which are rather simple, so much seemingly nobody has cared to write them down. We do so never the less.

- (1) The case of the free particle with Hamiltonian $H(p) = \frac{p^2}{2}$ was mentioned in section (3). In this case

$$\psi_h(x, t) = E_h^x[e^{-\langle P, B_h(t) \rangle}] = e^{-\frac{1}{h}(\langle x, P \rangle - \frac{1}{2}tP^2)}.$$

Then we obtain that

$$-\lim_{h \rightarrow 0} h \log \psi_h(x, t) = \langle x, P \rangle - \frac{1}{2}tP^2 = S_0(x, P, t).$$

- (2) Consider now the case $V(x) = ax$ in \mathbb{R} . The general case $V(x) = \langle a, x \rangle$ in \mathbb{R}^n can be deduced from this by rotation. In this case the solution of (1.4) is given by

$$\psi_h(x, t) = e^{-\frac{1}{h}(xP + ax t + \frac{a^2 t^3}{6} + \frac{P^2 t}{2} + \frac{at^2 P}{2})},$$

from which it follows that

$$S_0(x, P, t) = xP - ax t - \frac{a^2 t^3}{6} - \frac{P^2 t}{2} - \frac{at^2 P}{2}.$$

To finish with this short list of well known cases consider now the model in \mathbb{R} when $V(x) = -\frac{x^2}{2}$. Thus

$$\psi_h(x, t) = e^{-\frac{1}{h}\left(\frac{x^2}{2} \coth t - \left(P - \frac{x}{\sinh t}\right)^2 \frac{\tanh t}{2} - h \log(\cosh t)^{\frac{1}{2}}\right)},$$

and we see as h tends to zero we get

$$-\lim_{h \rightarrow 0} h \log \psi_h(x, t) = S_0(x, P, t) = \frac{xP}{\cosh t} - \frac{P^2 - x^2}{2} \tanh t.$$

- (3) In this part we will consider the second order partial differential operator

$$\Delta = e^{2x} \frac{\partial^2}{\partial x^2} + e^{2x} \frac{\partial}{\partial x}.$$

Acting on the class of smooth real valued functions. That is the Laplace-Beltrami operator for the metric $g_{11} = e^{-2x}$. And it is associated to a geodesic flow on the line, with Hamiltonian $H(p, x) = e^{2x} \frac{p^2}{2}$ see [10] for diffusion on manifolds. The corresponding Hamilton-Jacobi equation is

$$(6.1) \quad \frac{\partial S_0}{\partial t} + \frac{e^{2x}}{2} \left(\frac{\partial S_0}{\partial x} \right)^2 = 0.$$

Being the associated diffusion equation

$$(6.2) \quad \frac{\partial \psi_h}{\partial t} = \frac{h}{2} \Delta \psi_h,$$

We shall take as initial condition for $S_0(x, t)$ the datum $s(x) = e^{-2x} p$ where p is a real number and put $\psi_h(x, 0) = \frac{s(x)}{h}$. A simple computation shows that the solution to (6.1) is given by

$$S_0(x, t) = e^{-2x} \frac{p}{1 + 2pt}.$$

Therefore the solution is defined when $p < 0$ only if $t < \frac{1}{2|p|}$. To find the diffusion with generator $\frac{h}{2}\Delta$ we have to solve

$$(6.3) \quad dX_h(t) = e^{X_h(t)} dB_h(t) + \frac{h}{2} e^{2X_h(t)} dt,$$

which for the law P^x is given by

$$X_h(t) = -\log(e^{-x} + x - B_h(t)).$$

The last assertion is readily verified by using the Itô's formula. Hence the solution is defined until an explosion time

$$T_h(e^{-x}) = \inf\{t \geq 0 : B_h(t) \geq e^{-x}\} = \frac{1}{h} T_1(e^{-x}),$$

the last equality holds by scaling and T_1 refers to the same object for standard Brownian motion.

From all this we see that

$$\begin{aligned} \psi_h(x, t) &= \mathbb{E}^x_h [e^{-\frac{p}{h} e^{-2X_h(t)}}] = \mathbb{E}^0 [e^{-\frac{p}{h} (e^{-x} - B_h(t))^2}; t < \frac{1}{h} T_1(e^{-x})] \\ &= \mathbb{E}^0 [e^{-\frac{p}{h} (e^{-x} - B_h(t))^2}] - \mathbb{E}^0 [e^{-\frac{p}{h} (e^{-x} - B_h(t))^2}; t \geq \frac{1}{h} T_1(e^{-x})] \\ &= \mathbb{E}^0 [e^{-\frac{p}{h} (e^{-x} - B_h(t))^2}] + o(1) = e^{-\frac{1}{h} S_0(x, t)} + o(1). \end{aligned}$$

For general conditions two problems arise: first there appear singularities in $S_0(x, t)$ besides the explosions in $X_h(t)$, and a general statement would have to take both of these facts into account.

7. FINAL COMMENTS

- Things seem so much easier than in [20] only because here the functionals involved are much simpler than those considered by Schilder.
- Apart from the important problem related to the limit $\log -h\psi_h(x, t)$, there is a class of problems related to the study of the eigenfunctions of $\frac{h}{2}\Delta + V$ as h tends to zero. See for instance [17] and [19].
- When a path integral representation for the solution of (1.1) exists see [3], a similar analysis can be performed.
- It is necessary to add that as far as asymptotic expansions goes, it is easier to start with an asymptotic expansion for A in (3.3) and solve the simple, linear, recursive set of equations that appears when an expansion in powers of h is considered.
- We want to observe that this exposition is a lengthening and an update of a previous article [13] written by the authors, that appeared in the already distant 1989.
- Last but not least. In statistics it is important to consider the transition density for a general diffusion when the step of discretization h tends to zero. This type of problem was considered for the first time by Dacunha-Castelle & Florens-Zmirou in [7] in the case of a general diffusion and $n = 1$. Recently this has become a subject of active research, because of its implications in approaching the likelihood in several applied problems. The difference with the approach developed here consists of, that instead of functionals

of Brownian motion, there it is necessary to study functionals of Brownian bridges.

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