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LETTER TO THE EDITOR

# Semiclassical approximation as a small-noise expansion

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**Abstract.** We discuss how the semiclassical approximation arises within the (classically improved) Langevin quantization. We derive a *new* representation of the semiclassical propagator (at imaginary time) in the form of a *white noise average*, which is valid over an *arbitrary* (imaginary) time interval. Although our result is ultimately equivalent to the standard representation of the semiclassical propagator, it nevertheless turns out to be more advantageous in dealing with certain problems that involve tunnelling and metastability.

Thanks to the analytic continuation to *imaginary time* $s = it$, quantum mechanics becomes a *classical* probabilistic theory, and so various mathematical techniques from the field of classical stochastic processes can be *directly* employed in the analysis of quantum systems [1]. It should be stressed that *stochastic differential equations* [2] play a central role in this programme. Unfortunately, the application of stochastic differential equations to (imaginary time) quantum mechanical problems is quite often doomed to failure from a practical point of view§, since the conventional stochastic treatment [4] demands the knowledge of an *exact* (nodeless) *solution* of the original Schrödinger equation.

A few years ago, a *different* stochastic formulation of quantum mechanics at $s = it$ (*Langevin quantization*) was proposed [5] and applied successfully to certain time-dependent problems [6]. This strategy is *free* of the above shortcoming, thereby permitting *a systematic application to quantum-dynamical systems of the analytic and numerical methods used in connection with stochastic differential equations*. Subsequently, a variant of that approach has been developed (*classically improved Langevin quantization*) [7], which exhibits a *manifest connection with classical mechanics* (at $s = it$).

Our aim is to discuss how the semiclassical approximation arises within the classically improved Langevin quantization. Comments about the relevance of our result will be offered toward the end of this letter. Given the illustrative character of the present analysis, we shall work throughout in the one-dimensional case, assuming that only a stationary scalar potential $\Phi(x)$ is operative.

Let us begin by cursorily summarizing the structure of the classically improved Langevin quantization (in the above-mentioned special case) [7]. The starting point is classical

§ A remarkable exception to this statement is represented by $N = 2$ supersymmetric quantum mechanics in the fermionic vacua, where the Langevin equation provides an explicit realization of the Nicolai mapping [3].

 

mechanics at $s = it$ as formulated *a là* Hamilton–Jacobi. Specifically, the Hamilton–Jacobi equation reads presently†

$$\frac{\partial}{\partial s}S(x,s)+\frac{1}{2m}S'(x,s)^2-\Phi(x)=0\,. \tag{1}$$

In connection with an *arbitrary* (particular) integral $S(x,s)$ of (1), consider the first-order equation that supplies the family of classical trajectories in configuration space as controlled by $S(x,s)$, namely,

$$\frac{\mathrm{d}}{\mathrm{d}s}q(s)=\frac{1}{m}S'(q(s),s) \tag{2}$$

whose solution with initial condition $q(s')=x'$ is denoted by $q(s;x',s';[S(\cdot)])$—this is just the classical trajectory selected by the initial data $q(s')=x'$, $p(s')=S'(x',s')$. *Quantization* is then accomplished by turning (2) into the *Langevin equation*‡

$$\frac{\mathrm{d}}{\mathrm{d}s}\xi(s)=\frac{1}{m}S'\big(\xi(s),s\big)+\left(\frac{\hbar}{m}\right)^{1/2}\eta(s) \tag{3}$$

where $\eta(s)$ is a *Gaussian white noise* defined by

$$\langle\eta(s)\rangle_\eta=0 \qquad \langle\eta(s'')\eta(s')\rangle_\eta=\delta(s''-s')\,. \tag{4}$$

We denote by $\xi(s;x',s';[S(\cdot),\eta(\cdot)])$ the solution of (3) with initial condition $\xi(s')=x'$ and controlled by $S(x,s)$—these solutions describe the *quantum random paths* (at imaginary time). Finally, the imaginary time quantum mechanical propagator—in terms of the quantum random paths§—is given by the following *noise average representation*:

$$\langle x'',s''|x',s'\rangle=\exp\{-[S(x'',s'')-S(x',s')]/\hbar\}$$
$$\times\left\langle\delta\big(x''-\xi(s'';x',s';[S(\cdot),\eta(\cdot)])\big)\Delta(s'';x',s';[S(\cdot),\eta(\cdot)])^{1/2}\right\rangle_\eta \tag{5}$$

where we have set‖

$$\Delta(s;x',s';[S(\cdot),\eta(\cdot)])\equiv\frac{\partial}{\partial x'}\xi(s;x',s';[S(\cdot),\eta(\cdot)])\,. \tag{6}$$

Two things about the random path representation (5) should be emphasized. First, $S(x,s)$ is an *arbitrary* solution of (1). Second, the considered procedure is actually valid under the additional assumption that $S(x,s)$ is a *single-valued* solution of (1). Barring fortuitous situations, this condition is satisfied by suitably restricting the (imaginary) time interval [8,9]. Yet, this is *not* a real limitation. Indeed, $\langle x'',s''|x',s'\rangle$ can first be computed within the above constraint by means of (5). Next, the result obtained in this manner can

† A prime denotes differentiation with respect to $x$.

‡ Observe that the drift is *classical* and *unaffected* by the quantization procedure (in sharp contrast to what happens in the conventional stochastic treatment [4]).

§ Notice that the propagator in question is presently denoted by $\langle x'',s''|x',s'\rangle$, while it was indicated by $P(x'',s''|x',s')$ in [7].

‖ Geometrically, $\Delta(\cdots)$ measures the change of an infinitesimal volume element in configuration space under the dynamical flow defined by (3).

be extended to *arbitrary* (imaginary) time intervals, thanks to the convolution property of the propagators.

A great advantage of the classically improved Langevin quantization is that classical mechanics (at $s = it$) *manifestly* emerges in the limit of vanishing $\hbar$†. Remarkably enough, this circumstance leads, in turn, to a very simple intuitive picture of the semiclassical approximation, as we are now going to see. We shall first outline the general scenario, which is next shown to lead to the semiclassical expression of the propagator at $s = it$.

The basic idea is quite simple. As is clear from the foregoing discussion, *all* quantum corrections to the classical behaviour are simulated by the Gaussian white noise fluctuations in the otherwise classical (3). This fact at once entails that the semiclassical approximation—small $\hbar$ regime—can be understood as the situation in which the noise term in the Langevin equation (3) is effectively 'much smaller' than the drift (since the former goes like $\sqrt{\hbar}$). As a result, the *semiclassical random paths* (at imaginary time)—controlled by a generic solution $S(x, s)$ of (1)—are provided by the Langevin equation (3) *as linearized about* $q(s; x', s'; [S(\cdot)])$. That is to say, we are implementing the semiclassical approximation through a *small-noise expansion* [2]—to lowest non-trivial order—as performed on the Langevin equation (3). As a preliminary step toward the realization of this strategy, we write

$$\xi_{SC}(s; x', s'; [S(\cdot), \eta(\cdot)]) = q(s; x', s'; [S(\cdot)]) + \zeta\left(s; x', s'; [S(\cdot), \eta(\cdot)]\right) \tag{7}$$

because then the function $\zeta(\cdots)$ obeys the *linear* Langevin equation

$$\frac{\mathrm{d}}{\mathrm{d}s}\zeta(s) = \frac{1}{m}S''(q(s; x', s'; [S(\cdot)]), s)\zeta(s) + \left(\frac{\hbar}{m}\right)^{1/2} \eta(s) \,. \tag{8}$$

On account of (7), equation (8) has to be solved with the initial condition $\zeta(s'; \ldots) = 0$. Finding the general integral of (8) is a simple job and ultimately we get‡

$$\zeta(s; x', s'; [S(\cdot), \eta(\cdot)]) = \left(\frac{\hbar}{m}\right)^{1/2} \Delta_0(s; x', s'; [S(\cdot)]) \int_{s'}^{s} \mathrm{d}u \, \eta(u) \; \Delta_0(u; x', s'; [S(\cdot)])^{-1} \tag{9}$$

with $\Delta_0(\cdots)$ denoting just $\Delta(\cdots)$—as defined by (6)—with, however, $\xi(\cdots)$ replaced by $q(\cdots)$. Observe that the semiclassical random paths controlled by $S(x, s)$ can be viewed as *fluctuations* $\zeta(\cdots)$ about the classical trajectory $q(\cdots)$ controlled by the *same* $S(x, s)$.

As in the standard small-noise expansion [2], we expect the imaginary time semiclassical propagator to arise by inserting the semiclassical random paths (7) into the general expression (5). However, we have to be very careful about two features of (5), which are *not* present in the usual Langevin representation of the transition probability for a diffusion process§:

(i) a smooth functional of $\xi(\cdots)$, namely $\Delta(\cdots)$, multiplies the delta function under the Gaussian noise average,

(ii) the quantum random paths $\xi(\cdots)$ obviously depend functionally on $S(x, s)$.

† Compare equation (3) with (2).

‡ In the derivation of (9) we used (12) of [7] with $\xi(\cdots)$ replaced by $q(\cdots)$.

§ We mean diffusion processes with *vanishing killing rate*, to which the small-noise expansion is commonly applied [2].

Therefore, some *additional* information is required in order to achieve our goal. As far as point (i) is concerned, it is *a priori* unclear how $\Delta(\cdots)$ (equation (5)) should be handled (since we might run the risk of *incorrectly* retaining terms that would produce higher-order corrections to the semiclassical approximation). As regard to point (ii), we do not know *a priori* which specific solution $S(x,s)$ of (1) should be used to control the semiclassical random paths (while the *exact* propagator is $S(x,s)$-*independent*, there is no reason why this circumstance should persist when an *approximation* is considered). Now, once the quantum random paths $\xi(\cdots)$ in (5) are replaced by the semiclassical ones $\xi_{SC}(\cdots)$, the quantity $\Delta(\cdots)$ in that equation becomes $\Delta_0(\cdots)$ plus $O(\sqrt{\hbar})$ corrections (owing to (7) and (9)). Because the semiclassical propagator can be regarded as the *leading term* in the asymptotic $\hbar$-expansion of the exact propagator, we are led to the *expectation*

$$\langle x'', s''|x', s'\rangle_{SC} = \exp\{-[S(x'', s'') - S(x', s')]/\hbar\}\cdot \\ \times \Delta_0(s''; x', s'; [S(\cdot)])^{1/2}\langle\delta\big(x'' - \xi_{SC}(s''; x', s'; [S(\cdot), \eta(\cdot)])\big)\rangle_\eta . \qquad (10)$$

In fact, while it should be clear that (10) is indeed the leading-order contribution (in $\hbar$) to the exact propagator, we still do not know what solution $S(x,s)$ has to be employed. Suppose first that $S(x,s)$ just happens to meet the *end-point constraint*

$$q(s''; x', s'; [S(\cdot)]) = x'' . \qquad (11)$$

Then it is more convenient to write $q(s; x', s'; x'', s'')$ and $\xi(s; x', s'; x'', s''; [\eta(\cdot)])$ instead of $q(s; x', s'; [S(\cdot)])$ and $\xi(s; x', s'; [S(\cdot), \eta(\cdot)])$, respectively†. Correspondingly, equation (10) can be worked out by standard manipulations‡ and the result is

$$\langle x'', s''|x', s'\rangle_{SC} = \exp\{-S(x'', s''; x', s')/\hbar\} \\ \Delta_0(s''; x', s'; x'', s'')^{1/2}\langle\delta\big(\zeta(s''; x', s'; x'', s''; [\eta(\cdot)])\big)\rangle_\eta \qquad (12)$$

where $S(x'', s''; x', s')$ is the time integral of the Lagrangian (at $s = it$) along $q(s; x', s'; x'', s'')$ for $s' \leqslant s \leqslant s''$§. At this point, it is a simple exercise to show‖ that

$$\Delta_0(s; x', s'; x'', s'')^{1/2}\langle\delta\big(\zeta(s; x', s'; x'', s''; [\eta(\cdot)])\big)\rangle_\eta \\ = (2\pi\hbar)^{-1/2}\left(-\frac{\partial^2 S(x, s; x', s')}{\partial x\partial x'}\right)^{1/2}\Bigg|_{x=q(s;x',s';x'',s'')} \qquad (13)$$

which turns (12) into the standard representation of the semiclassical propagator (at $s = it$). On the other hand, whenever $S(x,s)$ does *not* satisfy the end-point constraint (11), equation (10) *fails* to produce the semiclassical propagator¶.

Needless to say, equation (12) is obviously subject to the same limitation as (5), namely $|s'' - s'|$ should be small enough so as to ensure that the considered solutions $S(x,s)$ are *single-valued* for $s' \leqslant s \leqslant s''$. As a rule—at any given $s$—*focal points* [8,9] are the branch points of the Lagrangian manifold $p = S'(x,s)$ [8], and so it follows that *no* focal

† Analogously, we write $\Delta_0(s; x', s'; x'', s'')$ in place of $\Delta_0(s; x', s'; [S(\cdot)])$.

‡ Use the integral (Fourier) representation of the delta function and write the noise average as a functional integral. Then both integrals are Gaussian and can be done explicitly, leading to (12).

§ As $S(x,s)$ obeys the end-point constraint (11), we have $S(x'', s'') = S(x', s') + S(x'', s''; x', s')$ [9].

‖ Details will be reported elsewhere.

¶ This statement can be checked directly on the Schrödinger equation (at $s = it$).

points are encountered along $q(s;x',s';x'',s'')$ for $s' \leqslant s \leqslant s''$. This circumstance has two important implications. First, the trajectory $q(s;x',s';x'',s'')$ is *unique*, as long as $s' \leqslant s \leqslant s''$. Second, $\Delta_0(s;\ldots)$ is *strictly positive* for $s' \leqslant s \leqslant s''$ [8], thereby entailing that the semiclassical random paths in question are *well defined* (see equation (9)).

Clearly, a *naive* extension of (12) to an *arbitrary* (imaginary) time interval is impossible. Apart form the fact that we have no honest starting point, focal points are now expected to show up, since $(x',s')$ and $(x'',s'')$ will be joined by *several* classical trajectories $q^a(s;x',s';x'',s'')$ (which are labelled by the index $a$). As a consequence, $\Delta_0(s;\ldots)$ *vanishes* for certain $s$ values *within* the considered (imaginary) time interval [8], so that the relevant semiclassical random paths are hopelessly ill-defined (see equation (9)). Yet, it turns out that such an extension is nevertheless *possible* and can be derived by means of an intuitive physical argument†. Because the semiclassical motion can be understood as occurring 'near' the classical trajectory, the superposition principle entails that the desired semiclassical propagator should be given by a sum of terms like the right-hand side of (12), one for each $q^a(s;x',s';x'',s'')$. So, we get

$$\langle x'',s''|x',s'\rangle_{\mathrm{SC}} = \sum_a \exp\{-S^a(x'',s'';x',s')/\hbar\} \times \text{`}\Delta_0^a(s'';x',s';x'',s'')^{1/2}\langle\delta(\zeta^a(s'';x',s';x'',s'';[\eta(\cdot)]))\rangle_\eta\text{''} \qquad (14)$$

where $S^a(\cdots)$, $\Delta_0^a(\cdots)$ and $\zeta^a(\cdots)$ are just $S(\cdots)$, $\Delta_0(\cdots)$ and $\zeta(\cdots)$ with $q(\cdots)$ replaced by $q^a(\cdots)$. Moreover, the expression between quotes in (14) is the function

$$\Delta_0^a(s;x',s';x'',s'')^{1/2}\langle\delta(\zeta^a(s;x',s';x'',s'';[\eta(\cdot)]))\rangle_\eta \qquad (15)$$

which is *well defined* for $s' \leqslant s \leqslant s_*$‡ *as continued up to* $s = s''$ *after* the Gaussian noise average has been carried out. Basically, the correctness of (14) rests upon the relation

$$\Delta_0^a(s;x',s';x'',s'')^{1/2}\langle\delta(\zeta^a(s;x',s';x'',s'';[\eta(\cdot)]))\rangle_\eta = (2\pi\hbar)^{-1/2}\left(-\frac{\partial^2 S^a(x,s;x',s')}{\partial x\,\partial x'}\right)^{1/2}\Bigg|_{x=q^a(s;x',s';x'',s'')} \qquad (16)$$

whose proof is similar to that of (13). As it stands, equation (14) looks misleading and should be understood properly. Let us explain this point. Superficially, the leading contribution in the right-hand side of (14) comes from the term controlled by the *direct* classical trajectory joining $(x',s')$ with $(x'',s'')$, namely the one which minimizes the action, and so the exponential will be largest. Observe that *all* points of the direct trajectory are *non-focal* [8,9], hence the corresponding $\Delta_0(\cdots)$ is *strictly positive* [8]. As a consequence, the term in question is *real*. As long as the other terms—controlled by *non-direct* classical trajectories—are also real, they should be dropped from (14) because they are exponentially suppressed with respect to the previous one§‖¶. Still—depending on the form of the potential $\Phi(x)$—some of the terms in the right-hand side of (14) controlled by *non-direct* classical trajectories

† A more rigorous justification will be presented elsewhere.

‡ We define $s_*(s' \leqslant s_* \leqslant s'')$ in such a way that *no* focal points are encountered along *any* $q^a(s;x',s';x'',s'')$ for $s' \leqslant s \leqslant s_*$. Therefore *all* $\Delta_0^a(s;\ldots)$ are *strictly positive* for $s' \leqslant s \leqslant s_*$ and the fluctuations $\zeta^a(s;\cdots)$ are correspondingly *well defined.*

§ As already stated, the semiclassical propagator is the leading term in the asymptotic $\hbar$-expansion of the exact propagator. Therefore, all higher-order corrections have to be discarded.

‖ However, it can well happen that—because of a certain approximation—*infinitely-many* terms turn out to have an *identical* exponential prefactor [10]. In this case, all of them must be retained.

¶ Incidentally, here we have a dramatic simplification as compared to the semiclassical propagator at real time, where *all* terms controlled by *non-direct* classical trajectories *must be retained* (since there is no exponential suppression) [8].

can become complex as a result of the above-mentioned continuation of the function (15), thereby contributing an *imaginary* part to the semiclassical propagator (at $s = it$)†—this circumstance signals *quantum metastability* [12]. Generally speaking, then only the term with *largest* exponential prefactor should be kept in the imaginary part of (14)‡.

In conclusion, by working within the classically improved Langevin quantization [7], we have been able to derive a *new* representation of the semiclassical propagator—valid over an *arbitrary* (imaginary) time interval—which is in the form of a *white noise average*. Although such a representation is ultimately equivalent to the standard one, it nevertheless turns out to be more advantageous in dealing with certain problems which involve tunnelling and metastability. We will describe these applications in forthcoming letters [10, 11].

## References


[1] Glimm J and Jaffe A 1987 *Quantum Physics: a Functional Integral Point of View* (Berlin: Springer)
Parisi G 1988 *Statistical Field Theory* (New York: Addison-Wesley)

[2] Van Kampen N G 1981 *Stochastic Processes in Physics and Chemistry* (Amsterdam: North-Holland)
Risken H 1984 *The Fokker–Planck equation* (Berlin: Springer)
Gardiner C W 1985 *Handbook of Stochastic Methods* (Berlin: Springer)

[3] Parisi G and Sourlas N 1982 *Nucl. Phys.* B **206** 321
Cecotti S and Girardello L 1983 *Ann. Phys., NY* **145** 81

[4] Favella L F 1967 *Ann. Inst. H. Poincaré* **7** 77
Van Kampen N G 1977 *J. Stat. Phys.* **17** 71
Schneider T, Zannetti M and Badii R 1985 *Phys. Rev.* B **31** 2941
Graham R 1986 *Helv. Phys. Acta* **59** 241
Parisi G 1988 *Statistical Field Theory* (New York Addison-Wesley)

[5] Roncadelli M 1991 *Europhys. Lett.* **16** 609

[6] Defendi A and Roncadelli M 1993 *Europhys. Lett.* **21** 127
Defendi A and Roncadelli M 1993 *Europhys. Lett.* **23** 159

[7] Roncadelli M 1994 *Europhys. Lett.* **28** 379

[8] Littlejohn R G 1992 *J. Stat. Phys.* **68** 7

[9] Arnold V 1978 *Mathematical Methods of Classical Mechanics* (Berlin: Springer)

[10] Defendi A and Roncadelli M 1995 Langevin quantization and quantum tunnelling *Pavia preprint* FNT/T-95/08 to be published

[11] Defendi A and Roncadelli M 1995 in preparation

[12] Coleman S 1997 *Phys. Rev.* D**15** 2929
Callan C G and Coleman S 1977 *Phys. Rev.* D**16** 1762
Coleman S 1985 The uses of instantons *Aspects of Symmetry* (Cambridge: Cambridge University Press)


† An example of this phenomenon will be discussed within the present context in [11].

‡ Of course, the same statement made in the fourth footnote of the previous page should be repeated here, and this situation will be dealt with in [11].