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Maurice M. Mizrahi

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ABSTRACT

This paper presents a general expression for the WKB approximation to the propagator corresponding to an arbitrary Hamiltonian operator $\tilde{H}$. For example, if the correspondence rule used to pass from the classical Hamiltonian H_c to $\tilde{H}$ is such that it associates $a p_i Q_i^j + (1-a) Q_i^j p_i$ to $p_i q^j$, then the formula gives

$$K_{WKB} = K_{VV} \exp \left\{ (1/2 - a) \int_T (\partial^2 H_c / \partial q^i \partial p_i) (q_c(t), p_c(t), t) dt \right\},$$

where $K_{VV} = (2\pi i \hbar)^{-n/2} (\det M)^{1/2} \exp(i S_c / \hbar)$ is Van Vleck's well-known formula, S_c being the action functional evaluated at the classical path (q_c, p_c) and $M_{ij} = -\partial^2 S_c / \partial q_a^i \partial q_b^j$. More generally,

the formula presented here applies to any system described by a function $f(x, t)$ whose time evolution is given by

$$(\tilde{H}(x, \hbar \partial / \partial x, t) + \hbar \partial / \partial t) f(x, t) = 0, \text{ regardless of the form of } \tilde{H}.$$

The Schrödinger equation of quantum mechanics and the Fokker-Planck equation of diffusion are obvious examples. Many examples are discussed. This generalizes results obtained in a previous publication (J. Math. Phys. 18 (1977), 786-90).

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INTRODUCTION

The purpose of this paper is to obtain a general expression for the WKB approximation to the propagator corresponding to an arbitrary Hamiltonian operator. In an earlier publication¹ we determined a range of validity of Van Vleck's well-known formula², which was known not to be universally valid³. The approximation derived here, generalizing Van Vleck's formula, is also valid beyond quantum-mechanical applications, as it applies to any system described by a function $f(x, t)$ whose time evolution is dictated by

$$\left[\tilde{H}(x, k \partial / \partial x, t) + k \partial / \partial t \right] f(x, t) = 0, \quad (1)$$

such as the Fokker-Planck equation for diffusion processes.

THE GENERAL WKB APPROXIMATION FORMULAE

We operate in n dimensions and summation over repeated indices is implied. The following theorem summarizes our findings:

Theorem

Let

- $\tilde{H}(\tilde{Q}, \tilde{P}, t)$ be an arbitrary Hamiltonian operator (the lack of constraints imply that it could be non-Hermitian, time-dependent, non-quadratic in $\tilde{P}$, etc.)
- $H_c(q, p, t) = \tilde{H}(\tilde{Q} \rightarrow q, \tilde{P} \rightarrow p, \hbar = 0)$ be its classical counterpart.
- The correspondence rule used to pass from H_c to $\tilde{H}$ be such that it makes the following associations:

$$f(q) \leftrightarrow f(\tilde{Q}), \quad f(p) \leftrightarrow f(\tilde{P}), \quad (2)$$

$$p_i q^j \leftrightarrow a \tilde{p}_i \tilde{Q}^j + (1 - a) \tilde{Q}^j \tilde{p}_i \text{ for a given } a. \quad (3)$$

(Note that (2) and (3) do not imply Hermiticity of $\tilde{H}$, even if $a = \frac{1}{2}$).

- $(q_c(t), p_c(t))$ be the classical solution, solving Hamilton's equations for H_c such that $q_c(t_a) = q_a$ and $q_c(t_b) = q_b$,
- $S_c(q_b, t_b, q_a, t_a) \equiv \int_T [p_{ci}(t) \dot{q}_c^i(t) - H_c(q_c(t), p_c(t), t)] dt$ (4)
be the classical action ($T \equiv [t_a, t_b]$, also $T \equiv t_b - t_a$),
- $M_{ij}(q_b, t_b, q_a, t_a) \equiv -\partial^2 S_c / \partial q_a^i \partial q_b^j$ (5)

be the Van Vleck - Morette matrix, with determinant $\det M$,

- $K(q_b, t_b, q_a, t_a)$ be the propagator corresponding to $\tilde{H}$, defined by

$$\left[\tilde{H}(Q, P, t_b) - i\hbar \frac{\partial}{\partial t_b} \right] K = 0, \quad (6)$$

$$\lim_{t_b \rightarrow t_a} K = \delta(q_b - q_a), \quad (7)$$

where Q is represented by q_b and P by $-i\hbar \partial / \partial q_b$,

- $K_{WKB}(q_b, t_b, q_a, t_a)$ be the WKB approximation to the propagator, defined by:

$$K_{WKB}^{-1} \left[\tilde{H}(Q, P, t_b) - i\hbar \frac{\partial}{\partial t_b} \right] K_{WKB} = O(\hbar^2), \quad (8)$$

$$\lim_{t_b \rightarrow t_a} K_{WKB} = \delta(q_b - q_a). \quad (9)$$

Then the WKB approximation is given by

$$K_{WKB} = K_{VV} \exp \left[\left(\frac{1}{2} - a \right) \int_{t_a}^{t_b} \frac{\partial^2 H_c}{\partial q^i \partial p_i} (q_c(t), p_c(t), t) dt \right], \quad (10)$$

where K_{VV} is Van Vleck's formula:

$$K_{VV} = (2\pi i \hbar)^{-n/2} (\det M)^{1/2} \exp(i S_c / \hbar). \quad (11)$$

(The case where $\det M = 0$ is not examined here).

More generally, the WKB approximation is given by

$$K_{\text{WKB}} = A_0 \exp(iS_c/\hbar), \quad (12)$$

where

$$A_0 \equiv K_0(0, t_b, 0, t_a), \quad (13)$$

• $K_0(q_b', t_b, q_a', t_a)$ is the propagator corresponding to the Hamiltonian operator

$$H_0 \equiv \frac{1}{2} g^{ij}(t) \tilde{u}_{ij} + \frac{1}{2} f_{ij}(t) \tilde{v}^{ij} + k_i^j(t) \tilde{w}_j^i, \quad (14)$$

$$\bullet \quad g^{ij}(t) \equiv \left. \frac{\partial^2 H_c}{\partial p_i \partial p_j} \right|_{\substack{q=q_c(t) \\ p=p_c(t)}}, \quad f_{ij}(t) \equiv \left. \frac{\partial^2 H_c}{\partial q^i \partial q^j} \right|_{\substack{q=q_c(t) \\ p=p_c(t)}}, \quad k_i^j(t) \equiv \left. \frac{\partial^2 H_c}{\partial q^i \partial p_j} \right|_{\substack{q=q_c(t) \\ p=p_c(t)}}, \quad (15)$$

• The correspondence rule used to pass from H_c to H is such that it makes the following associations:

$$p_i p_j \leftrightarrow \tilde{u}_{ij}, \quad q^i q^j \leftrightarrow \tilde{v}^{ij}, \quad q^i p_j \leftrightarrow \tilde{w}_j^i. \quad (16)$$

PROOF OF THE GENERAL WKB APPROXIMATION FORMULAE

Let us begin by giving a simple example illustrating the fact that the Van Vleck formula K_{VV} in (11) is not always equal to the WKB approximation K_{WKB} . Let H be an operator such that $K_{\text{VV}} = K_{\text{WKB}}$.

The operator

$$\tilde{H}' \equiv F^{-1}(\underline{Q}) H F(\underline{Q}) \quad (17)$$

has the same H_c (and hence the same K_{VV}) as H . Yet its WKB approximation is not K_{WKB} but

$$K'_{\text{WKB}} = F(q_a) F^{-1}(q_b) K_{\text{VV}}, \quad (17a)$$

as can be verified by direct substitution.

We now prove the theorem. Formula (10) will be proved by generalizing the proof given in ref. 1. The more general formula (12) will be proved by generalizing the method used in ref. 4, which involves path integrals. It is presented separately because it is more on the heuristic side.

Proof of first formula

In ref. 1, where we investigated the range of validity of Van Vleck's formula, we assumed that the WKB approximation was of the form:

$$K_{\text{WKB}} = a(\hbar) C \exp(iB/\hbar), \quad (18)$$

where C and B are real functions of q_b , t_b , q_a , and t_a , independent of $\hbar$, and found that

$$\begin{aligned} K_{\text{WKB}}^{-1} \left(\frac{\hbar}{i} - \hbar \frac{\partial}{\partial t_b} \right) K_{\text{WKB}} &= \dot{B} + F(0) H_c(B', q_b, t_b) + \hbar \left[-i \frac{\dot{C}}{C} \right. \\ &\quad - \left(\frac{\partial^2}{\partial p_i \partial q_b^i} H_c(\rho, q_b, t_b) \right)_{\rho=B'} \left(F'(0) + \frac{i}{2} F(0) \right) \\ &\quad - \frac{i F(0) C_i}{C} \left(\frac{\partial H_c}{\partial p_i}(\rho, q_b, t_b) \right)_{\rho=B'} - i \frac{F(0)}{2} B''_{ij} \\ &\quad \times \left(\frac{\partial^2 H_c}{\partial p_i \partial p_j}(\rho, q_b, t_b) \right)_{\rho=B'} \left. \right] + \hbar^2 \left\{ \left[-\frac{1}{8} F(0) \frac{\partial^2}{\partial q_b^i \partial q_b^i} \right. \right. \\ &\quad - F(0) \frac{C'_i}{2C} \frac{\partial}{\partial q_b^i} - F(0) \frac{C''_{ij}}{2C} - \frac{1}{4} F(0) B''_{ij} \frac{\partial^2}{\partial p_k \partial q_b^k} \\ &\quad - F(0) \frac{C'_i}{2C} B''_{ij} \frac{\partial}{\partial p_k} - \frac{1}{8} F(0) B''_{ij} B''_{ks} \frac{\partial^2}{\partial p_k \partial p_s} \\ &\quad - \frac{1}{6} F(0) B''_{ijk} \frac{\partial}{\partial p_k} + \frac{i}{2} F'(0) \frac{\partial^2}{\partial q_b^i \partial q_b^i} + i F'(0) \frac{C'_i}{C} \frac{\partial}{\partial q_b^i} \\ &\quad \left. \left. + \frac{i}{2} F'(0) B''_{ij} \frac{\partial^2}{\partial p_k \partial q_b^k} + \frac{1}{2} F''(0) \frac{\partial^2}{\partial q_b^i \partial q_b^i} \right] \right\} \\ &\quad \times \frac{\partial^2}{\partial p_i \partial p_j} H_c(\rho, q_b, t_b) \Big|_{\rho=B'} + O(\hbar^3), \end{aligned} \quad (19)$$

where $B''_{ij} \equiv \partial^2 B / \partial q_b^i \partial q_b^j$, etc., and F is Cohen's F function,⁵

establishing the correspondence between $\tilde{H}$ and H_c by

$$\tilde{H} = (2\pi\hbar)^{-2n} \int_{\mathbb{R}^{2n}} dp \, dq \, du \, dv \, F(u, v) H_c(q, p, t) \exp \left\{ (i/\hbar) [(q-Q) \cdot u + (p-P) \cdot v] \right\}. \quad (20)$$

F effects the generating-function correspondence

$$F(u, v) \exp \left[(-i/\hbar) (Qu + Pv) \right] \leftrightarrow \exp \left[(-i/\hbar) (qu + pv) \right], \quad (21)$$

and a set of F s effecting a given correspondence $H_c \leftrightarrow \tilde{H}$ can be found by solving⁶

$$F(u, v) \int_{\mathbb{R}^{2n}} dp \, dq \, H_c(q, p, t) e^{i(qu + pv)/\hbar} = (2\pi\hbar)^n \text{tr} (e^{i(Qu + Pv)/\hbar} \tilde{H}). \quad (22)$$

This equation for F , to be understood in the sense of distribution theory, may or may not have a solution, and the solution may or may not be unique if it exists.

In ref. 1, F was assumed to be a function of $u \cdot v/\hbar$ only, and this requirement is maintained here, as $u \cdot v/\hbar$ is the only dimensionless quantity one can form with u , v , and $\hbar$, and it is assumed here that $\tilde{H}$ contains no constants (other than $\hbar$) that do not appear in H_c . It can be shown⁷ that the fact that F depends on the combination $u \cdot v/\hbar$ implies that the operator $\tilde{H}$ corresponding to $p^m q^n$ in 1 dimension is a linear combination of all the possible ordered arrangements of $\tilde{p}$ m times and $\tilde{q}$ n times (true "factor ordering"). Thus, no true divisors are allowed in Cohen's scheme⁸, an important restriction since the Laplacian in curved spaces contains true divisors. We shall return to this point later.

In ref. 1, F was also assumed to be real⁹ so as to insure the Hermiticity of $\tilde{H}$. This requirement is dropped here. Therefore, equating both the real and the imaginary part of the constant term and the term proportional to $\hbar$ to 0 in (19) yields the following 4 equations to be satisfied by B and C :

$$H_c(q_b, \frac{\partial B}{\partial q_b}, t_b) \operatorname{Re}[F(0)] + \frac{\partial B}{\partial t_b} = 0 \quad (23)$$

$$H_c(q_b, \frac{\partial B}{\partial q_b}, t_b) \operatorname{Im}[F(0)] = 0 \quad (24)$$

$$\begin{aligned} \operatorname{Re}[F(0)] \frac{\partial}{\partial q_j} \left[c^2 \frac{\partial H_c(q_b, p, t_b)}{\partial p_j} \right]_{p = \partial B / \partial q_b} \\ + \frac{\partial}{\partial t_b} (c^2) + 2c^2 \frac{\partial^2 H_c(q, p, t_b)}{\partial p_i \partial q_i} \Big|_{\substack{p = \partial B / \partial q_b \\ q = q_b}} \operatorname{Im}[F'(0)] = 0 \end{aligned} \quad (25)$$

$$\{ \operatorname{Re}[F'(0)] - \frac{1}{2} \operatorname{Im}[F(0)] \} \left[\frac{\partial^2}{\partial p_i \partial q_i} H_c(q, p, t_b) \right]_{\substack{p = \partial B / \partial q_b \\ q = q_b}} \quad (26)$$

$$+ \operatorname{Im}[F(0)] \left[\frac{C'_i}{C} \frac{\partial H_c(q_b, p, t_b)}{\partial p_i} + \frac{1}{2} B''_{ij} \frac{\partial^2 H_c}{\partial p_i \partial p_j} \right]_{p = \partial B / \partial q_b} = 0,$$

where the third equation was rewritten in a more compact form.

First, let us translate the conditions (2) and (3) on $\tilde{H}$ into conditions on F . These are:

$$F(0) = 1, \quad \operatorname{Re}[F'(0)] = 0, \quad \operatorname{Im}[F'(0)] = a - \frac{1}{2}. \quad (27)$$

Indeed, (2) readily results from (21) with $F(0) = 1$. If we differentiate (21) with respect to v , then set $v=0$, then do the same with u , we obtain

$$pq \leftrightarrow F(0) \frac{(QP+PQ)}{2} - \frac{1}{2} F'(0), \quad (28)$$

which yields the 2 conditions on $F'(0)$.

It is, in fact, possible to drop the requirement that the correspondence be given by an F function, so that the results are valid for any $\tilde{H}$ satisfying (2) and (3). This will be seen when we treat the more general formula (12).

Let us now solve (23)-(26) for B and C. Since $F(0) = 1$, (23) and (24) are recognized as being one of the Hamilton-Jacobi equations, yielding $B = S_c$. Note that since (23) and (24) stem from equating only the constant term to 0 in (19), an approximation to zeroth order in $\hbar$ yields $B = S_c$ and no information on C other than the fact that it must be such that the boundary condition (9) is satisfied (this is not sufficient to fix C).

To solve (25), we note that if $\text{Im}[F'(0)] = 0$ ($a = \frac{1}{2}$) then $C^2 = \det M$, since the (continuity) equation satisfied by the Van-Vleck - Morette determinant is precisely

$$\frac{\partial}{\partial q_b^i} [\dot{q}_c^j(t_b) \det M] + \frac{\partial}{\partial t_b} [\det M] = 0. \quad (29)$$

This leads us to write

$$C^2 = N \det M, \quad (30)$$

which, when substituted in (25) and using $\text{Im}[F'(0)] = a - \frac{1}{2}$ yields the equation for $N(q_b, t_b, q_a, t_a)$:

$$\frac{\partial N}{\partial t_b} + \dot{q}_c^j(t_b) \frac{\partial N}{\partial q_b^j} + N(2a-1) \frac{\partial^2 H_c(q, p, t_b)}{\partial q^i \partial p_i} \bigg|_{\substack{q=q_b \\ p=p_c(t_b)}} = 0, \quad (31)$$

with $N \rightarrow 1$ as $t_b \rightarrow t_a$ and $q_b \rightarrow q_a$ if $K_{VV} \rightarrow \delta(q_b - q_a)$ as $t_b \rightarrow t_a$.

The search for a solution of (31) is facilitated by the observation that the first two terms form the convective derivative of N with respect to the final endpoint. Knowing that the convective derivative of any function f of position, momentum, and time (at the classical path) with respect to either the initial or the final endpoint is 0, i.e.,

$$\left[\frac{\partial}{\partial t_b} + \dot{q}_c^j(t_b) \frac{\partial}{\partial q_b^j} \right] f(q_c(t), p_c(t), t) = 0 \quad (32)$$

(to be proved shortly), we are led to a trial solution of the form

$$N = \exp \left[(1-2a) \int_{t_a}^{t_b} \frac{\partial^2 H_c}{\partial p_i \partial q^i} (q_c(t), p_c(t), t) dt \right]. \quad (33)$$

By direct substitution in (31), (33) is seen to be the correct solution (use $f=q_c$ and $f=p_c$ in (32)).

To prove (32), we first observe that it is sufficient to prove it for $f=q_c$ and $f=p_c$: the chain rule will then extend its validity to any f . Now, derivatives of the classical solution with respect to any parameter introduced by the boundary conditions (here, t_a, t_b, q_a , or q_b) are known to be solutions of the equation of small disturbances, obtained from the second variation of the action functional¹⁰⁻¹³. Since this equation is linear, its general solution is a linear combination of $2n$ linearly independent solutions. Thus, the only solution vanishing at both t_a and t_b must be zero everywhere. Now, the left-hand-side of (32) with $f=q_c^i(t)$ is, by its very construction, a solution of the small-disturbance equation. It vanishes at t_a because $q_c(t_a) = q_a$ (a constant). It also vanishes at t_b because

$$\begin{aligned} \left. \frac{\partial q_c^i(t)}{\partial t_b} \right|_{t=t_b} &= \int_{t_a}^{t_b} dt \frac{\partial \dot{q}_c^i(t)}{\partial t_b} = -\dot{q}_c^i(t_b) + \frac{\partial}{\partial t_b} \int_{t_a}^{t_b} \dot{q}_c^i(t) dt \\ &= -\dot{q}_c^i(t_b) + \frac{\partial}{\partial t_b} (q_b^i - q_a^i) = -\dot{q}_c^i(t_b), \end{aligned} \quad (34)$$

(since $\partial/\partial t_b$ commutes with $\partial/\partial t$ when acting on $q_c(t, t_b, q_b)$). Thus, (32) is true for $f=q_c$. The case $f=p_c$ is proved by observing, by substitution in the equation of small disturbances in phase space ($\tilde{\sigma}h = 0$), that if u is a parameter introduced by the boundary conditions, then

$$\frac{\partial p_{c,i}(t)}{\partial u} = \tilde{D}_{ij}(t) \frac{\partial q_c^j(t)}{\partial u}, \quad (35)$$

where

$$\tilde{\sigma} = - \begin{pmatrix} f & k+d/dt \\ \tilde{k} - d/dt & g \end{pmatrix}, \quad h = \begin{pmatrix} \partial q_c(t)/\partial u \\ \partial p_c(t)/\partial u \end{pmatrix} \quad (36)$$

$$\tilde{D} \equiv g^{-1} \left(1 \frac{d}{dt} - \tilde{k} \right),$$

and f, g , and k are defined in (15). This completes the proof of the WKB approximation formula (10). ■

Note that (19) indicates that when H_c is quadratic in both p and q , the term proportional to $\hbar^2$ is 0 because C is independent of q_a and q_b (S_c being quadratic in q_a and q_b), and higher-order terms are 0 because they involve third and higher derivatives of H_c . Thus, the WKB approximation is exact in that case. This goes beyond the well-known result because $\tilde{H}$ does not have to be Hermitian, so that the extra exponential term in (10) supplementing the Van Vleck formula is not constant.

Proof of second formula

Formula (12) will be proved using the path-integral approach, generalizing a method presented in Ref. 4. More details on this method and its extension to a WKB expansion of the propagator for arbitrary Hamiltonians will be presented elsewhere.

The propagator K can be written as a phase space path integral as follows:

$$K(q_b, t_b, q_a, t_a) = \int_{\mathcal{P}} \left[\frac{dp dq}{h^n} \right] \exp(iS/\hbar), \quad (37)$$

where $S \equiv \int_T [p\dot{q} - H(q, p, t)] dt$ is the action functional and $\mathcal{P}$ is the space of paths (q, p) such that $q(t_a) = q_a$ and $q(t_b) = q_b$. If S is expanded around the classical path (q_c, p_c) , its first functional derivative vanishes by definition of the classical path and we obtain

$$K = e^{iS_c/\hbar} \int_{\mathcal{P}_0} \left[\frac{dx dy}{h^n} \right] e^{iS_c''(x, y)/\hbar} e^{-i\Omega_c(x, y)/\hbar}, \quad (38)$$

where $\mathcal{P}_0$ is the space of paths (x, y) such that $x(t_a) = x(t_b) = 0$, Ω_c contains the terms beyond the second functional

derivative, and the second functional derivative S''_c is:

$$S''_c(x, y) = \int_T dt \left[y_i(t) \dot{x}^i(t) - \frac{1}{2} g^{ij}(t) y_i(t) y_j(t) - \frac{1}{2} f_{ij}(t) x^i(t) x^j(t) - k^i_j(t) y_i(t) x^j(t) \right] \quad (39)$$

with f , g , and k in (15).

$\mathcal{P}_0$,

We can define a measure w_Λ normalized to 1 and absorbing the second variation of S by:

$$dw(x, y) \equiv A_0^{-1} \left[\frac{dx dy}{h^n} \right] \exp(i S''_c(x, y)/\hbar), \quad (40)$$

the normalization factor being

$$A_0 \equiv \int_{\mathcal{P}_0} \left[\frac{dx dy}{h^n} \right] \exp(i S''_c(x, y)/\hbar). \quad (41)$$

Now, it is observed that the S''_c term in (39) is in the form of an action functional corresponding to the fictitious Hamiltonian

$$H_0(x, y) \equiv \frac{1}{2} g^{ij}(t) y_i y_j + \frac{1}{2} f_{ij}(t) x^i x^j - k^i_j(t) y_i x^j. \quad (42)$$

Hence, (37) indicates that A_0 must be the propagator $K_0(q_b', t_b, q_a', t_a)$ corresponding to H_0 , evaluated at $q_a' = q_b' = 0$. But for which Hamiltonian operator H_0 ? It makes sense⁶ that it should be the operator derived from H_0 using the same correspondence rule linking H_c and H , i.e., (14) with (16). This leaves us with

$$K = A_0 e^{i S_c/\hbar} \int_{\mathcal{P}_0} e^{-i \Omega_c(x, y)/\hbar} dw(x, y). \quad (43)$$

It can be shown in this general case, as was done before for special cases¹¹⁻¹³, that the expansion of the Ω_c term followed by the evaluation of the path integrals (the correspondence rule being taken into account) yields a series in $\hbar$,

$$K = A_0 e^{i S_c/\hbar} (1 + \hbar K_1 + \hbar^2 K_2 + \dots), \quad (44)$$

which identifies the constant term as the WKB approximation. ■

Let us now retrieve formula (10) from this more general case. The operator H_0 in this case is

$$\tilde{H}_0 = \frac{1}{2} g^{ij}(t) \tilde{p}_i \tilde{p}_j + \frac{1}{2} f_{ij}(t) \tilde{Q}^i \tilde{Q}^j + k_j^i(t) [a \tilde{p}_i \tilde{Q}^j + (1-a) \tilde{Q}^j \tilde{p}_i], \quad (45)$$

which can be rewritten, using $[\tilde{Q}^i, \tilde{p}_j] = i\hbar \delta_j^i$, as

$$\tilde{H}_0 = \tilde{H}_{00} + i\hbar(\frac{1}{2}-a)k_i^i(t), \quad (46)$$

where

$$\tilde{H}_{00} = \frac{1}{2} g^{ij}(t) \tilde{p}_i \tilde{p}_j + \frac{1}{2} f_{ij}(t) \tilde{Q}^i \tilde{Q}^j + \frac{1}{2} k_j^i(t) (\tilde{p}_i \tilde{Q}^j + \tilde{Q}^j \tilde{p}_i). \quad (47)$$

Now, since $\tilde{H}_{00}$ is quadratic and Hermitian, its propagator K_{00} is given exactly by Van Vleck's formula, (11). In this case, however, the S_c in (11) is zero because $q_a' = q_b' = 0$. (In fact, in general $S_c = q_b'^i p_{co,i}(t_b) - q_a'^i p_{co,i}(t_a)$, where (q_{co}, p_{co}) is the classical solution for H_0). Further, the "det M" in (11) is the same as the "det M" for H_c because H_0 and H_c share the same equation of small disturbances and M_{ij} is a boundary value of a specific solution of that equation¹¹⁻¹³. Therefore, $K_{00} = (2\pi i\hbar)^{-n/2} (\det M)^{1/2}$. Now, if $\tilde{H}_1 = \tilde{H}_2 + f(t)$, the propagators K_1 and K_2 are related by $K_1 = K_2 \exp(-(i/\hbar) \int_T f(s) ds)$. $\tilde{H}_0$ and $\tilde{H}_{00}$ are related in this manner. Putting all these results together gives:

$$K_{WKB} = (2\pi i\hbar)^{-n/2} (\det M)^{1/2} \exp \left\{ \frac{i}{\hbar} S_c + (\frac{1}{2}-a) \int_T k_i^i(s) ds \right\}, \quad (48)$$

which is formula (10). Note that this suggests that the normalization factor $(2\pi i)^{-n/2}$ is universal and independent of H_c ¹⁴.

Note in passing that it is not always easy to find out what $p_i q^j$ corresponds to given the $H_c \leftrightarrow H$ correspondence. Scaling tricks (replacing Q by λQ in functions of Q , then differentiating with respect to λ and setting λ equal to 0) sometimes help.

SOME EXAMPLES

We begin with an example pointing out that formula (10) is not restricted to the correspondence rule being effected by an F-function. Consider the Hamiltonian

$$H = \frac{1}{2} g^{-1/2}(Q) \left[p_i - A_i(Q) \right] g^{1/2}(Q) g^{ij}(Q) \left[p_j - A_j(Q) \right] g^{-1/2}(Q) + V(Q) \quad (49)$$

corresponding to $H_c = \frac{1}{2} g^{ij}(q) [p_i - A_i(q)] [p_j - A_j(q)] + V(q)$, where (50)
 $g_{ik} g^{kj} \equiv \delta_i^j$ and $g \equiv \det(g_{ij})$. Since it is Hermitian, $a = \frac{1}{2}$. There is no F in general because of the divisors¹⁵. Nevertheless, a direct substitution shows that Van Vleck's formula applies, and we get:

$$\begin{aligned} K_{VV}^{-1} \left(H_b - i\hbar \frac{\partial}{\partial t_b} \right) K_{VV} &= \frac{\hbar^2}{4} g^{ij} \left(\Gamma_{mi}^m \frac{M_{,j}}{M} + \Gamma_{ij}^l \frac{M_{,l}}{M} + \frac{M_{,i} M_{,j}}{2M^2} \right. \\ &\quad \left. - \frac{M_{,ij}}{M} - \frac{1}{2} \Gamma_{mi}^m \Gamma_{lj}^l - \Gamma_{ij}^l \Gamma_{ml}^m + \Gamma_{lj,i}^l \right) (q_b) \\ &= O(\hbar^2), \end{aligned} \quad (51)$$

where the following properties and definitions were used:

$$\begin{aligned} M &\equiv \det M, \quad \Gamma_{jk}^i \equiv \frac{1}{2} g^{ia} (g_{ja,k} + g_{ka,j} - g_{jk,a}), \\ g^{ij}_{,k} &= - \Gamma_{mk}^i g^{mj} - \Gamma_{mk}^j g^{im}, \quad g^{\alpha}_{,i} = 2\alpha g^{\alpha} \Gamma_{li}^l, \\ \dot{q}_c^j(t_b) &= g^{ij}(t_b) [p_{ci}(t_b) - A_i(q_b)], \quad p_{ci}(t_b) = \partial S_c / \partial q_b^i, \\ \frac{\partial S_c}{\partial t_b} &= -H_c(q_b, \frac{\partial S_c}{\partial q_b}), \end{aligned} \quad (52)$$

as well as (29)¹⁶.

On the other hand, (19) gives the following expression for the miss term:

$$\begin{aligned} K_{VV}^{-1} (H_b - i\hbar \frac{\partial}{\partial t_b}) K_{VV} &= -\frac{\hbar^2}{4} \left[g^{ij}_{,ij} \left(\frac{1}{2} F(0) - iF'(0) - F''(0) \right) \right. \\ &\quad \left. + g^{ij}_{,j} (F(0) - 2iF'(0)) \frac{C'_{,i}}{C} + g^{ij} F(0) \frac{C''_{,ij}}{C} \right], \end{aligned} \quad (53)$$

an expression which cannot be matched with (51) for any F , for $C = M^{\frac{1}{2}}$.

Consider now the Fokker-Planck equation of diffusion processes:

$$\frac{\partial P}{\partial t} = \frac{1}{2} \frac{\partial^2}{\partial q^i \partial q^j} [D^{ij}(q, t) P] - \frac{\partial}{\partial q^i} [v^i(q, t) P], \quad (54)$$

where D is the diffusion matrix and v the drift vector¹⁷. It formally corresponds to a Hamiltonian $H \equiv \tilde{p}_i \tilde{p}_j D^{ij}(Q)/2i\hbar + \tilde{p}_i v^i(Q)$ with classical Hamiltonian $H_c = p_i p_j D^{ij}/2i\hbar + p_i v^i$. Since the $\tilde{p}$ factors precede the Q factors, α is simply equal to 1. Thus, formula (10) gives:

$$K_{WKB} = (2\pi i\hbar)^{-n/2} (\det M)^{1/2} \exp \left[\frac{i}{\hbar} S_c - (2i\hbar)^{-1} \int_{\tau} p_{ci}(t) D^{ij}_{,j}(q_c(t)) dt - \frac{1}{2} \int_{\tau} v^i_{,i}(q_c(t)) dt \right]. \quad (55)$$

Note that the dynamical equation gives $p_{ci}(t) = i\hbar \dot{q}_c^j(t) (D^{-1})_{ji}(q_c(t))$, so that in one dimension part of the integral can be performed, yielding

$$K_{WKB} = K_{VV} [D(q_b)/D(q_a)]^{-1/2} \exp \left(\frac{1}{2} \int_{\tau} ((vD' - v'D)/D) dt \right). \quad (56)$$

In the case of the backwards equation (Q precedes P , $\alpha=0$), the factors $1/2$ are replaced by $-1/2$ in (56) and inside the bracket of (55).

For constant diffusion parameter ($D=1$) and linear drift $v = -\gamma q$, one retrieves the well-known propagator¹⁸

$$K_{WKB} = \left[\frac{\gamma}{\pi (1 - 2e^{-2\gamma\tau})} \right]^{1/2} \exp \left[- \frac{\gamma (q_b - q_a e^{-\gamma\tau})^2}{1 - e^{-2\gamma\tau}} \right], \quad (57)$$

which, H being quadratic, is also exact (it satisfies (54) exactly).

It can be shown, by direct calculations, that the "miss factor" for (55) is exactly as given by (53) with $F(x) = \exp(ix/2)$.

Another interesting application is the "lognormal" process with Hamiltonian

$$H = \alpha \tilde{Q}^2 \tilde{P}^2 + \beta \tilde{Q} \tilde{P} \quad (58)$$

in one dimension, useful in modeling population growth¹⁹. Using formula (10) on $H_c = \alpha q^2 p^2 + \beta qp$ one gets:

$$K_{WKB} = (q_b/q_a)^{1-2a} K_{VV} \exp[\beta(a-\frac{1}{2})T], \quad (59)$$

where²⁰

$$K_{VV} = (2\pi i \hbar)^{-\frac{1}{2}} (2\alpha T q_a q_b)^{-\frac{1}{2}} \exp\left[\frac{i}{4\hbar\alpha T} \left(\text{Log} \frac{q_b}{q_a} - \beta T\right)^2\right]. \quad (60)$$

In our case, $a=0$. Note that for $a=0$ the exact propagator²¹ is

$$K = K_{WKB} \exp(-i\hbar\alpha T/4), \quad (61)$$

so that the expansion of the exponential gives the terms of a WKB expansion of K , useful for checking general formulas.

Let us also mention the elements of the WKB approximation for Hamiltonians in one dimension of the form

$$H_c = k p^m q^n \quad (62)$$

where k is a constant. The classical equation of motion is $\ddot{q}_c = (n/m) \dot{q}_c^2 / q_c$ and the Lagrangian is $L = (\dot{q}/q)^{\frac{m}{m-1}} (mk)^{\frac{1}{m-1}} (1-m^{-1})$. For $m \neq n$ these elements are:

$$\begin{aligned} q_c(t) &= A(t-t_0)^{\frac{m}{m-n}}, & p_c(t) &= [k(m-n)]^{\frac{1}{m-1}} (t-t_0)^{\frac{n}{n-m}} A^{\frac{1-n}{m-1}}, \\ A &\equiv q_a \left(\frac{1-\gamma}{\gamma T}\right)^{\frac{m}{m-n}}, & t_0 &\equiv \frac{t_a - \gamma t_b}{1-\gamma}, & \gamma &\equiv (q_a/q_b)^{\frac{m-n}{m}}, \\ S_c &= (m-1)(kT)^{\frac{1}{m-1}} (m-n)^{\frac{m}{m-n}} \left(q_b^{\frac{m-n}{m}} - q_a^{\frac{m-n}{m}}\right)^{\frac{m}{m-1}}, \\ M &= [Tk(m-n)]^{\frac{1}{m-1}} \frac{m-n}{m(m-1)} (q_a q_b)^{-n/m} \left(q_b^{\frac{m-n}{m}} - q_a^{\frac{m-n}{m}}\right)^{\frac{2-m}{m-1}}. \end{aligned} \quad (63)$$

For $m = n$, these elements are:

$$\begin{aligned}
 q_c(t) &= \exp(At+B), & q_c(t)p_c(t) &= (A/km)^{\frac{1}{m-1}}, \\
 A &\equiv T^{-1} \text{Log}(q_b/q_a), & B &\equiv \text{Log} [q_a (q_a/q_b)^{t_a/T}], \\
 S_c &= (mkT)^{-1/(m-1)} (1-m^{-1}) [\text{Log}(q_b/q_a)]^{m/(m-1)}, \\
 M &= (mkT)^{\frac{-1}{m-1}} [(m-1)q_a q_b]^{-1} [\text{Log}(q_a/q_b)]^{\frac{2-m}{m-1}}.
 \end{aligned} \tag{64}$$

In all cases,

$$K_{WKB} = K_{VV} (q_b/q_a)^{n(\frac{1}{2}-a)} \tag{65}$$

CONCLUSION

We have produced a formula to approximate the propagator corresponding to any system described by a function whose time evolution is given by a partial differential equation that is ^{of} first order in time. This approximation can be supplemented by correction terms that can be generated by path integrals, and this will be the subject of a follow-up study²².

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7. I. W. Mayes, Ph.D. Thesis, The University of Manchester, 1971.

8. "True" divisors are those that cannot be eliminated by use of the commutation relation $QP - PQ = i\hbar$. For example,

$$\tilde{H} \equiv \tilde{Q}^2 \tilde{P} \tilde{Q} \tilde{P} \tilde{Q}$$

does not contain true divisors because the commutation relation $Pf(Q) - f(Q)P = -i\hbar f'(Q)$ enables one to rewrite $\tilde{H}$ as $\tilde{P} \tilde{Q}^2 \tilde{P} - \frac{1}{4}\hbar^2$. We can then rewrite $-\hbar^2$ as $(QP - PQ)^2$ and conclude that $\tilde{H}$ is only an ordering of the factors of $\tilde{P}^2 \tilde{Q}^2$. However,

$$\tilde{H}' \equiv \tilde{Q}^{\frac{1}{2}} \tilde{P} \tilde{Q}^{\frac{1}{2}} \tilde{P} \tilde{Q}^{\frac{1}{2}}$$

does contain true divisors, because one can rewrite it as $\tilde{P} \tilde{Q} \tilde{P} + \hbar^2 \tilde{Q}^{-1}/16 = \tilde{P} \tilde{Q} \tilde{P} - (\tilde{Q} \tilde{P} - \tilde{P} \tilde{Q})^2 \tilde{Q}^{-1}/16$, which cannot be obtained simply by ordering the factors of $\tilde{P}^2 \tilde{Q}$. Thus, $\tilde{H}'$ is not covered by one of Cohen's F functions, but $\tilde{H}$ is (any $F(x)$ such that $F(0) = 1$, $F'(0) = 0$, $F''(0) = 1/8$ would do, for example $F(x) = \exp(x^2/16)$).

9. In fact, the "Conclusion" stated at the bottom of p. 788 in ref. 1 remains valid even if the requirement that F be real is dropped.

10. C. G. Jacobi, "On the theory of the calculus of variations and of differential equations", Crelle's Math. J. 17 (1837), 68-82, referred to in Oskar Bolza, Lectures on the Calculus of Variations (U. Chicago Press, Chicago, 1904; also Chelsea, New York, 1960, 1973).

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14. Unlike what was suggested in ref. 1.

15. In fact, direct use of (22) indicates that the correspondence $\frac{1}{2}g^{ij}(q)p_i p_j \leftrightarrow \frac{1}{2}g^{\alpha}(Q)p_i g^{-2\alpha}(Q)g^{ij}(Q)p_j g^{\alpha}(Q) + \hbar^2 \varphi(Q)$ is fulfilled by an F function iff $\varphi(q) + \eta(q) = k \xi(q)$, where k is a constant, $\xi(q) \equiv \frac{1}{2}g^{ij}_{,ij}$, and

$$\eta(q) \equiv \frac{1}{2}g^{ij} \left[\left(2\alpha + \frac{1}{2}\right)^2 \Gamma_{li}^l \Gamma_{mj}^m + \left(2\alpha + \frac{1}{4}\right) \Gamma_{ml}^m \Gamma_{ij}^l + \frac{1}{2} \Gamma_{is}^l \Gamma_{lj}^s - \frac{1}{4} \Gamma_{ij,l}^l - \left(2\alpha + \frac{1}{4}\right) \Gamma_{mi,j}^m \right].$$

If g^{ij} is such that the relation is satisfied, then any F such that $F(0) = 1$, $F'(0) = 0$, $F''(0) = k$ will do. Weyl's rule ($F=1$) is an example for $k=0$. In particular, there is no F in general for the case $\varphi=0$. In one dimension, $\eta = k\xi$ for all g^{ij} of the form $g^{11}(q) = (aq+b)^c$, a and b being arbitrary constants and $c \equiv (\alpha + \frac{1}{4} - k)/(\alpha^2 + \alpha + \frac{1}{4} - k)$.

16. The result in (51) matches that of DeWitt in ref. 3 for small T because, using the expansion of M in his equation (6.38) we readily get

$$K_{VV}^{-1}(H_b - i\hbar \partial/\partial t_b)K_{VV} = \hbar^2 \left[-R(q_b)/12 + o(t_b - t_a) + o(q_b - q_a) \right],$$

where $R \equiv g^{ij}(\Gamma_{lj,i}^l - \Gamma_{ij,l}^l + \Gamma_{mj}^l \Gamma_{li}^m - \Gamma_{ij}^l \Gamma_{ml}^m)$ is the Ricci scalar curvature tensor. In this case, a small-time approximation is the same as a WKB approximation.

17. See, e.g., Robert Graham, "Covariant formulation of non-equilibrium statistical thermodynamics", Z. Physik B 26 (1977), 397-405 and references listed there.

18. See, e.g., F. Reif, Fundamentals of Statistical and Thermal Physics, McGraw-Hill, 1965, p. 581.

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20. Note in passing that K_{VV} in (40) is the exact propagator for an ordering patterned after (49), i.e., $H = \alpha \tilde{Q}^{\frac{1}{2}} \tilde{P} \tilde{Q} \tilde{P} \tilde{Q}^{\frac{1}{2}} + \beta(QP+PQ)/2 \equiv \alpha(\tilde{P} \tilde{Q}^2 \tilde{P} - \frac{1}{4}) + \beta(QP+PQ)/2$, a rare case when the WKB approximation is exact for a non-quadratic H . Formula (53) for $F(0) = 1$, $F'(0) = 0$ and $F''(0) = 1/8$ will confirm this.

21. Exact propagators for Hamiltonians of the form $H = \sum_{i=1}^N a_i \tilde{Q}^i \tilde{P}^i$ in one dimension can sometimes be found using the identity

$$\left[\sum_{i=1}^N a_i x^i \left(\frac{d}{dx} \right)^i \right]^m x^n = \left[\sum_{i=1}^N a_i \frac{n!}{(n-i)!} \theta(n-i) \right]^m x^n,$$

where $\theta(x) = 0$ for $x < 0$ and 1 otherwise. Thus, for $T \equiv \sum_{i=1}^N a_i x^i (d/dx)^i$ one obtains

$$e^{Tf(x)} = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) \exp \left[\sum_{i=1}^N a_i \frac{n!}{(n-i)!} \theta(n-i) \right].$$

For $N=2$, use of the integral representation

$$e^{sn^2} = (4\pi s)^{-\frac{1}{2}} \int_{\mathbb{R}} e^{-x^2/4s + nx} dx \text{ gives}$$

$$e^{Tf(x)} = (4\pi a_2)^{-\frac{1}{2}} \int_{\mathbb{R}} dy e^{-y^2/4a_2} f(xe^{y+a_1-a_2}). \text{ Changing variables to } u = x \exp(y+a_1-a_2) \text{ gives}$$

$$e^T \delta(x-x') = (x')^{-1} (4\pi a_2)^{-\frac{1}{2}} \exp(-(\log(x'/x) + a_2 - a_1)^2 / 4a_2). \text{ Since, it will be recalled, the propagator } K \text{ is equal to}$$

$e^{-iTH/\hbar} \delta(q_b - q_a)$ when H is time-independent, the method can be applied here.

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