

Numerical mathematics of Feynman path integrals and the operator ordering problem

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Infinitesimal propagators have been used in quantum-mechanical problems to establish ordering rules for classical quantities. Ambiguities arise in operator ordering as a result of the freedom of choice in evaluating the classical action over a short-time interval. The primitive quadrature rule employed in a short-time propagator establishes the quantum system associated with the classical Hamiltonian. Normal propagators are constructed from products of infinitesimal propagators and represent a compound quadrature in which the path is broken into line segments and a separate quadrature rule is applied to each line segment. It is demonstrated for Hamiltonians involving the vector potential that higher-order quadratures of the infinitesimal propagator all give a unique and proper ordering. Similarly, Hamiltonians that are products of powers of position x and momentum p , i.e., $p^l x^m$, show some preference for Born-Jordan ordering as higher quadrature rules are applied. Unique orderings can be obtained in some cases by solving for the normal propagator. This is done for the Hamiltonian $p^l x^m$ by using a Fourier representation for the phase-space propagator. This formalism requires that both the momentum and position coordinates be represented by Fourier series. These results show that care must be taken when generating quantum-mechanical operators by using primitive quadrature rules in conjunction with a short-time propagator. These ambiguities are eliminated when the compound quadrature is performed to generate the normal propagator.

I. INTRODUCTION

Much of the original appeal of Feynman's path-integral formulation of quantum mechanics was its power in formal manipulations. In recent times it has been used as a computational tool as well (for a review see Ref. 1). For such applications it is useful to develop highly accurate short-time propagators (cf. Ref. 2). In the process of exploring more accurate representations of such propagators, a number of observations have been made with regard to the operator ordering problem. This is a long-standing quantum-mechanical problem (cf. Ref. 3) and briefly stated it is to define a unique correspondence between a classical quantity and its quantum-mechanical operator counterpart. This problem in a sense represents a gap between the Schrödinger equation and the operator formalism. The nonunique formulation of classical quantities is represented by a number of "ordering rules," the most prominent being the Born-Jordan, Weyl, and symmetrization rules. Initially it appeared that Feynman's path-integral formulation would resolve this problem and provide a unique ordering.^{4,5} However, subsequent work showed that the various ordering rules could be derived directly from path integrals.⁶⁻⁸ This is a direct result of the freedom of choice in calculating the classical action used in the short-time propagator. Thus a single classical Hamiltonian can be used to generate a number of quantum-mechanical operators. The correspondence with a particular quantum system is dictated by the method of evaluating the propagator.

In this work it is shown that the ordering problem is related to the numerical quadrature of path integrals. Most ordering problems have been formulated using a technique known as compound quadrature.⁹ The path in-

tegral is first divided into discrete segments. Usually the Schrödinger equation is derived from the infinitesimal behavior of the propagator. Thus the focus is on a single segment. However, additional rules are invoked (such as the midpoint rule) for evaluating the action in a line segment. The long-time behavior is then a compound quadrature. Operator ordering rules derived from a short-time propagator have an error associated with them as a result of the level of approximation of the quadrature. The correct ordering rule may be obscured by this quadrature error. Such problems do not exist for the normal, long-time propagator. However, these propagators are often difficult to evaluate. For Hamiltonians involving a vector potential term, it is well established that the "midpoint" rule must be used to generate the proper Schrödinger equation from the short-time propagators. In Sec. II it is demonstrated that the extra terms which appear in the Schrödinger equation when other quadrature rules are used are the same order of magnitude as the error of the quadrature. When higher-order quadrature rules are used the exact Schrödinger equation is always obtained. In Sec. III the "line segment" rule for one-dimensional Hamiltonians involving simple products of positions and momentum is examined. It is seen that Weyl's rule is a midpoint quadrature, and the rule of symmetrization is derived from a quadrature using the "trapezoid rule." The Born-Jordan rule is derived from an average classical Hamiltonian resulting from an integral over the line segment and is therefore an infinite-order quadrature. Surprisingly, when higher-order quadratures such as the Simpson and Newton-Cotes rules are used, close and sometimes exact approximations to the Born-Jordan rule are obtained. However, as even higher-order quadratures are considered, there is a small

but consistent deviation from the Born-Jordan rule. Thus from a purely computational perspective there would again appear to be some preference for a unique ordering but this ordering is difficult to justify solely on arguments of numerical accuracy. In Sec. III the order of error of the compound quadrature is compared with the error of the primitive rule. It is seen that the error in the compound quadrature is always much smaller than that of the individual quadrature of a given line segment, i.e., the normal propagator is much more accurate than the short-time or infinitesimal propagator. In Sec. IV a Fourier-series representation of the path is used to evaluate the normal propagator for a one-dimensional Hamiltonian of the form $p^l x^m$. The Schrödinger equation derived from these exact results show a small but significant correction to the Born-Jordan rule.

II. NUMERICAL QUADRATURE AND THE VECTOR POTENTIAL

The Lagrangian path integral $G(x, t; y)$ is given as

$$G(x, t; y) = \lim_{N \rightarrow \infty} \int d\mathbf{x}_1 \cdots d\mathbf{x}_N (m/2\pi i \hbar \epsilon)^{(N+1)/2} \exp \left\{ (i\epsilon/\hbar) \sum_j^N \left\{ (m/2)[(\mathbf{x}_{j+1} - \mathbf{x}_j)/\epsilon]^2 - V(\mathbf{x}_j) \right\} + (i\epsilon/\hbar c) \sum_j^N (\mathbf{x}_{j+1} - \mathbf{x}_j) \cdot \mathbf{A}(\mathbf{x}_j) \right\}, \quad (4)$$

with $\epsilon = t/(N+1)$. The Schrödinger equation is generated from the infinitesimal propagator employing "a small nightmare of Taylor expansions and Gaussian integrals".¹⁰ However, this approach is not without its ambiguities as the correctness of the final result depends on the choice of \mathbf{x} in the evaluation of $\mathbf{A}(\mathbf{x})$. A Riemann integral is of course independent of the choice of \mathbf{x} , provided an infinite sum is employed. The choice $\mathbf{A}((\mathbf{x}_{j+1} + \mathbf{x}_j)/2)$ or $1/2[\mathbf{A}(\mathbf{x}_{j+1}) + \mathbf{A}(\mathbf{x}_j)]$ gives the correct Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = (\mathbf{p} - e \mathbf{A}/c)^2 / 2m \psi + V \psi, \quad (5)$$

while the choice $\mathbf{A}(\mathbf{x}_{j+1})$ or $\mathbf{A}(\mathbf{x}_j)$ gives an additional factor $(i\hbar e/2mc)\psi \nabla \cdot \mathbf{A}$. Examination of the long-time propagator $G(x, t; y)$ shows that in these formulations it is approximated with a compound quadrature consisting of primary intervals represented by the infinitesimal propagator. However, the infinitesimal propagators are further divided to regain the proper form for the Schrödinger equation. Using a numerical mathematics parlance, forward or backward rectangle equations for the infinitesimal propagator do not yield the Schrödinger equation. The midpoint rule and the trapezoid rule give the proper equation. Higher-order rules such as the

$$G(x, t; y) = \int_{y,0}^{x,t} dx(\tau) \exp\{iS[x(\tau)]/\hbar\}, \quad (1)$$

where the action S in the presence of a vector potential \mathbf{A} is given by the integral of the Lagrangian L :

$$S[x(\tau)] = \int_0^t L \left[x, \frac{dx}{d\tau} \right] d\tau, \quad (2)$$

with

$$L = (m/2)(dx/d\tau)^2 + (e/c) \left[\frac{d\mathbf{x}}{d\tau} \right] \cdot \mathbf{A} - V(x), \quad (3)$$

where V is a potential and m , e , and c are the particle mass, charge, and the speed of light, respectively. Feynman verified this approach by demonstrating that the infinitesimal propagator generated the Schrödinger equation when propagating a wave function over an infinitesimal time step (cf. Ref. 10). This propagator corresponds to the quantity under the limit operation:

Simpson and Newton-Cotes quadrature also give the proper equation. In fact, all higher-order rules, except those that employ functional evaluations outside the interval of interest, appear to give the proper answer. The form of the vector potential term to be used in the infinitesimal propagator for some of the simpler rules is shown below along with the order of error of the quadrature (cf. Ref. 9).

For the rectangle rule,

$$h \cdot \mathbf{A}(\mathbf{x}_{j+1}) + O(h^2 A^{(1)}/2); \quad (6)$$

the trapezoidal rule,

$$h \cdot [\mathbf{A}(\mathbf{x}_{j+1})/2 + \mathbf{A}(\mathbf{x}_j)/2] + O(h^3 A^{(2)}/12); \quad (7)$$

the midpoint rule,

$$h \cdot \mathbf{A}(\mathbf{x}_{j+1}/2 + \mathbf{x}_j/2) + O(h^2 A^{(2)}/3); \quad (8)$$

the Simpson rule,

$$(h/2) \cdot [\mathbf{A}(\mathbf{x}_{j+1})/3 + 4\mathbf{A}(\mathbf{x}_{j+1}/2 + \mathbf{x}_j/2)/3 + \mathbf{A}(\mathbf{x}_j)/3] + O(h^5 A^{(4)}/90); \quad (9)$$

and the Newton-Cotes rule,

$$(h/4) \cdot [14\mathbf{A}(\mathbf{x}_{j+1})/45 + 64\mathbf{A}(3\mathbf{x}_{j+1}/4 + \mathbf{x}_j/4)/45 + 24\mathbf{A}(\mathbf{x}_{j+1}/2 + \mathbf{x}_j/2)/45$$

$$+ 64\mathbf{A}(\mathbf{x}_{j+1}/4 + 3\mathbf{x}_j/4)/45 + 14\mathbf{A}(\mathbf{x}_j)/45] + O(h^7 A^{(6)}/8/945), \quad (10)$$

where h is $x_{j+1} - x_j$ and the numerical superscripts represent derivatives. The expansion to derive the Schrödinger equation is to first order in ϵ and to second order in h . As can be seen from the above equations, the rectangle rule's error term is second order in h and therefore would not be expected to accurately reproduce the Schrödinger equation. All other methods are to greater order and they indeed give the appropriate final form. Thus the freedom of choice for evaluating the vector potential results in ambiguities only when the order of approximation of the quadrature rule is comparable to the order of expansion required to derive the Schrödinger equation. Note that this error only occurs in the infinitesimal propagator. The long-time propagator will always be independent of such choices when Riemannian sums are used. This point is discussed in greater detail in Sec. III.

III. NUMERICAL QUADRATURE AND OPERATOR ORDERING RULES

In this section the generation of ordering rules from a phase-space path integral is considered. The derivation of Kerner and Sutcliffe⁵ and of Cohen⁶ is followed. Connections between the phase-space integral and the Lagrangian approach have been discussed by Mayes and Dowker.⁷ In the phase-space approach the action is defined as

$$A = \int \left[p \frac{dx}{dt} - H \right] dt. \quad (11)$$

The infinitesimal phase-space propagator $K(x'', x', t'' - t')$ is given by $\sum_{\zeta} \exp[iA(\zeta)/h]$, where the sum is over all paths between x'' and x' . This function propagates the wave function as follows:

$$\psi(x'', t'') = \int K(x'', x', t'' - t') \psi(x', t') dx', \quad (12)$$

and it can be shown that

$$i\hbar \frac{\partial \psi(x'', t)}{\partial t} = \int k(x'', x') \psi(x') dx', \quad (13)$$

where the reduced propagator $k(x'', x')$ is defined as

$$k(x'', x') = (2\pi\hbar)^{-1} \int dp \bar{H} \exp[ip(x'' - x')/\hbar] \quad (14)$$

and the averaged Hamiltonian \bar{H} is given by

$$\bar{H} = (t'' - t')^{-1} \int H(x, p) dt. \quad (15)$$

The quantum-mechanical operator \hat{H} corresponding to the classical Hamiltonian \bar{H} is now given by

$$\hat{H}\psi = \int k(x'', x') \psi(x') dx'. \quad (16)$$

The form of \hat{H} is derived by using the infinitesimal operator (i.e., calculating the action for infinitesimal time difference) and by converting the sum over paths to an integral over p . For Hamiltonians of the form $f(x)p^k$ the well-known ordering rules are readily derived. The action over an infinitesimal time interval is given by

$$A = p(x'' - x') - (t'' - t') \sum_i^n w_i H[x' + \alpha_i(x'' - x')], \quad (17)$$

where w_i is a weighting factor for the evaluation of H at the point $x' + \alpha_i(x'' - x')$ and α_i is a factor less than 1. The specific values for w_i and α_i depend on the quadrature rule used in the evaluation of Eq. (15). The compound nature of the path integral quadrature is explicitly seen here since Eq. (17) represents one interval in the computation of the long-time propagator K . Following Cohen⁶ Eq. (16) can be brought to the form

$$\begin{aligned} \hat{H}\psi &= (-i\hbar)^k \int \delta^k(x'' - x') \\ &\times \sum_i^n w_i f(x' + \alpha_i(x'' - x')/n) \psi(x') dx', \end{aligned} \quad (18)$$

where the superscripts on δ represent the k th derivative with respect to the argument. Equation (18) gives

$$\hat{H} = \sum_i (-i\hbar)^k \binom{k}{l} \binom{m}{l} l! \left[\sum_i w_i \alpha_i^l \right] x^{m-1} p^{k-1}. \quad (19)$$

A midpoint rule, $\bar{H} = H(x''/2 + x'/2)$, gives the Weyl ordering rule; $\sum_i w_i \alpha_i^k = 1(1/2)^k$ and the trapezoidal rule, $\bar{H} = [H(x'' + H(x'))]/2$, gives the symmetrization rule, $\sum_i w_i \alpha_i^k = (1/2) \cdot 1^k$. The Born-Jordan rule holds when $\sum_i w_i \alpha_i^k = (k+1)^{-1}$. This rule was originally derived from the path integral (5) by defining \bar{H} to be the time average of H with p fixed:

$$\begin{aligned} \bar{H} &= (t'' - t')^{-1} \\ &\times \int_{t'}^{t''} H[x' + (x'' - x')(t - t')/(t'' - t'), p] dt \\ &= \int_0^1 H[x' + (x'' - x')u, p] du. \end{aligned} \quad (20)$$

Equation (20) is in a sense an infinite-order quadrature rule and therefore should be more accurate than all others. When other high-order quadrature rules are used, Born-Jordan behavior is seen for small k and is closely approximated for larger k . For instance, when the Simpson and Newton-Cotes rules [see Eqs. (9) and (10)] are applied to the Hamiltonian component of the action in Eq. (17), exact Born-Jordan results are obtained for $k < 5$ and good approximations for larger k . However, as even higher-order rules are used, the agreement does not improve but rather the approximations at lower k values actually get worse. Such behavior is not uncommon with high-order quadrature rules (cf. Ref. 9). The results of this section and those of Sec. II suggest that ambiguities in operator ordering are a result of the mathematical construct and do not reflect the underlying physics. As they stand, these results certainly are not a rigorous test for uniqueness of an ordering rule.

The infinitesimal propagator provides a convenient mathematical device for formal manipulations that does not require an explicit solution of the Hamiltonian. It is commonly used to check the validity of a propagator by demonstrating a correct expansion to the Schrödinger

equation. However, this propagator is not free from errors that may not appear in the long-time propagator. As was seen, the long-time propagator represents a compound quadrature and the general rule for the error for such a quadrature is⁹

$$E_{n \times R}(f) = \sum_i E_{i,R}(f) \\ = c(b-a)^{k+1} n^{-k} [f^{(k)}(b) - f^{(k)}(a)], \quad (21)$$

where a, b are the end points for integrating the function f , c is a constant, and the superscripts are derivatives. The compound rule has n intervals with k evaluations (subintervals) on the interval. The error in the i th interval with end points α and β is

$$E_{i,R} = c(\beta - \alpha)^{k+1} f^{(k)}(\xi) \quad (22)$$

with $\alpha < \xi < \beta$. It is readily seen that the quadrature of the action used to generate the symmetrization rule represents an $n \times 2$ compound quadrature. From Eq. (21) the quadrature is exact as $n \rightarrow \infty$, as is expected for the long-time propagator. Problems arise in the short-time propagators because they must remain finite in order to perform the expansions that recover the Schrödinger equation. Thus a term as that in Eq. (22) will always exist for these propagators. The operations that transform the infinitesimal propagator into the reduced propagator [Eqs. (13) and (14)] also carry along the error term in Eq. (22). The integral in Eq. (4) represents a Haar measure in the limit as $N \rightarrow \infty$.¹¹ The limiting form of the infinitesimal volume element is not a Haar measure. When additional operations are carried out on this form, an error is introduced into the resulting equation. This error has no counterpart in the long-time integral. As an alternative to using short-time propagators a Fourier representation of path integrals is used which is exactly solvable for Hamiltonians of the form $p^l x^m$.

IV. FOURIER REPRESENTATION OF PHASE-SPACE PATH INTEGRALS

In this section a Fourier expansion about a fixed path is used in the phase-space path integral. This method was originally used by Feynman to solve Lagrangian integrals for both quantum-mechanical¹² and statistical-mechanical¹³ problems. These methods have also found wide application in Monte Carlo calculations (cf. Ref. 14). In previous approaches the classical path for the problem of interest was found and the deviations from

this path were expanded in a Fourier series. The current application differs in two ways from these previous cases. First, because a phase-space integral is used a Fourier representation for both the momentum and position coordinate is required. Also, a given position coordinate path is assumed and the Fourier expansion corrects this path to make it appropriate for the given Hamiltonian. The mathematical consequence of this is that the function for the assumed path is not orthogonal to the Fourier series. This new path integral may be expanded with respect to time and a reduced propagator is associated with that expansion. For one-dimensional classical Hamiltonians of the form $p^l x^m$, the reduced propagator can be exactly solved to give a unique quantum Hamiltonian.

Following Garrod,¹⁵ the propagator is represented as

$$K(x'', x', t'' - t') = \int dx_1 \cdots dx_{N-1} dp_1 \cdots dp_{N-1} \\ \times \exp[iA(x)/\hbar], \quad (23)$$

where A is defined in Eq. (11). The discretized form of the action is a sum over $2N$ variable as opposed to N variables for the Lagrangian propagator. The discretized action requires alternate evaluations of momentum and position coordinates. This leaves one set of coordinates, momentum or position, unspecified during the "off" interval and prevents the quantum-mechanical problem from being overspecified (cf. Ref. 10). The Fourier representation for the coordinate path will be taken as

$$x(u) = x' + (x'' - x')u + \sum_{k=1}^{N-1} a_k \sin k \pi u, \quad (24)$$

where $u = (t - t') / (t'' - t')$. To generate the Fourier representation of the momentum variables a cosine series is used. This is because the momentum need only be evaluated every other interval and these evaluations must be out of phase with the coordinate evaluations. Thus the momentum variables are represented as

$$p(u) = b_0 + \sum_k^{N-1} b_k \cos k \pi u. \quad (25)$$

Using Eqs. (24), (25), and (11), the classical action is now

$$A = b_0(x'' - x') + \frac{1}{2} \sum_k k \pi b_k a_k - (t'' - t') \int_0^1 H(u) du. \quad (26)$$

The propagator is transformed from phase space to Fourier coefficient space, giving

$$K(x'', x', t'' - t') = J \int da_1 \cdots da_{N-1} db_0 \cdots db_{N-1} \exp \left[i/\hbar \left[b_0(x'' - x') + \left(\frac{1}{2} \right) \sum_k k \pi b_k a_k - (t'' - t') \int_0^1 H(u) du \right] \right], \quad (27)$$

where J is the Jacobian for the transformation. It can be determined from the normalization condition. As a check on the validity of the series representation in Eqs. (24) and (25), the free-particle Hamiltonian ($p^2/2m$) can be inserted into Eq. (27). The resulting integrals can be solved exactly and it is readily shown that the phase-space propagator reduces to the correct free-particle propagator. The propagator defined by Eq. (27) may be used to generate the Schrödinger equation in a manner analogous to the infinitesimal propagator [Eqs. (13)–(16)]. Thus the equivalent to Eq. (13) becomes

$$\hat{H}\psi = (1/2\pi\hbar) \int dx' da_1 \cdots da_{N-1} db_0 \cdots db_{N-1} \int_0^1 du H(u) \exp i/\hbar \left[b_0(x'' - x') + \left(\frac{1}{2}\right) \sum_k k\pi a_k b_k \right], \quad (28)$$

where the normalization condition is $J \prod_k (2\hbar/ik\pi) = 1$. Equation (28) is now solved for the classical Hamiltonian $H = p^l(u)x^m(u)$. Inserting Eqs. (24) and (25) into Eq. (28) and expanding in a binomial series gives

$$\int da_1 \cdots da_{N-1} db_0 \cdots db_{N-1} \exp(i/\hbar) \left[b_0(x'' - x') + \sum_k k\pi a_k b_k / 2 \right] \\ \times \int_0^1 du \left\{ \left[b_0^l + l b_0^{l-1} \left[\sum_k b_k \cos k\pi u + \cdots \right] \right] \left[\bar{x}^m + m \bar{x}^{m-1} \left[\sum_k a_k \sin k\pi u \right] + \cdots \right] \right\}, \quad (29)$$

where $\bar{x} = x' + (x'' - x')u$. By integrating with respect to either a_k or b_k (but not b_0) and using standard relationships such as $\delta'(a_k) = -\delta(a_k)/a_k$, it is possible to remove a large number of terms of Eq. (29). All terms involving $a_k^t b_k^s$ (with k and k' unspecified) are eliminated for $t < s$ by integrating over the a_k variable first. This gives expressions of the form

$$\delta^{(t)}(b_k) \Pi \delta(b_{k'}) b_k^s = [-\delta(b_k)]^t \Pi \delta(b_{k'}) b_k^{-t} b_{k'}^s, \quad (30)$$

where the superscript in parentheses represents the order of the derivative with respect to the argument. Similarly, for $t > s$ these terms are eliminated by first integrating over the b_k variables. After these operations the only terms which remain are those involving the product $b_0^l \bar{x}^m$ and products where $t = s$ and $k = k'$. Thus one obtains

$$\hat{H}\psi(x'') = (1/2\pi\hbar) \int dx' db_0 e^{(i/\hbar)b_0(x'' - x')} \\ \times \left[b_0^l \int_0^1 \bar{x}^m du + \sum_{n=1} \binom{m}{n} \binom{l}{n} b_0^{l-n} \int_0^1 du \bar{x}^{m-n} \sum_k^{N-1} (2\hbar/ik\pi)^n \cos^n(\pi k u) \sin^n(\pi k u) \right] \quad (31)$$

$$= (-i\hbar)^l \int dx' \left[\delta^{(l)}(x'' - x') \int_0^1 \bar{x}^m du \right. \\ \left. + \sum_{n=1} \binom{m}{n} \binom{l}{n} \delta^{(l-n)}(x'' - x') \int_0^1 du \bar{x}^{m-n} \sum_k^{N-1} (2\hbar/ih\pi)^n \cos^n \pi k u \sin^n \pi k u \right], \quad (32)$$

where the sum over n cannot exceed m or l . The first term in the right-hand side of Eqs. (31) and (32) is the form derived by Kerner and Sutcliffe⁵ for the Born-Jordan ordering rule. The second term represents a small but significant correction to this ordering. As a sample calculation the Hamiltonian $p^2 x^2$ is considered. The second term for this Hamiltonian is readily solved with the aid of the relationship

$$\sum_{k=1}^{\infty} k^{-2} = 2^{2n-1} \pi^{2n} |B_{2n}| / (2n!). \quad (33)$$

It is equal to $-\hbar^2/12$. The various ordering rules for this Hamiltonian are displayed below: For the Fourier series rule,

$$(x^2 p^2)_{\text{op}} = x^2 \hat{p}^2 - 2i\hbar x \hat{p} - (3/4)\hbar^2; \quad (34)$$

the Born-Jordan rule,

$$(x^2 p^2)_{\text{op}} = x^2 \hat{p}^2 - 2i\hbar x \hat{p} - (2/3)\hbar^2; \quad (35)$$

the Weyl-McCoy rule,

$$(x^2 p^2)_{\text{op}} = x^2 \hat{p}^2 - 2i\hbar x \hat{p} - (1/2)\hbar^2; \quad (36)$$

and the symmetrization rule,

$$(x^2 p^2)_{\text{op}} = x^2 \hat{p}^2 - 2i\hbar x \hat{p} - \hbar^2, \quad (37)$$

where $()_{\text{op}}$ represents an operator.

In the limit $N \rightarrow \infty$ the Fourier series will provide an exact representation of the path. Choosing different forms for the coordinate trajectory will result in different Fourier coefficients and different cross terms which ap-

pear in the expression for the action [Eq. (26)]. The resulting integration should again yield Eq. (31). It is tempting to try to recover the Weyl and symmetrization rules from this formalism. One choice of trajectories might be to replace the linear path in Eq. (24) by a midpoint constant (or zeroth-order Fourier coefficient). When this is done, the reduced propagator is indeterminate as a result of the integration over the b_0 variable.

V. SUMMARY

Short-time propagators are often used to establish a correspondence between a classical system and a quantum system. In many cases the choice of the primitive quadrature rule dictates the specific quantum system associated with a given classical Hamiltonian. When such primitive rules are used, the normal propagator may be viewed as a compound quadrature. Because of the error associated with the primitive quadrature, results obtained for short-time propagators may not represent the behavior of the normal propagator. Consequently, ordering rules derived from these short-time propagators may be incorrect. This is shown to be true for two simple cases: Hamiltonians involving the vector potential and the one-dimensional Hamiltonian $p^l x^m$. In the first case it is shown that all quadrature rules of higher order than the rectangle rules will generate the proper Schrödinger equation. In the second case a Fourier representation of the phase-space propagator is used to evaluate the normal propagator. This case also gives a unique ordering.

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